



Multifield aspects in the early Universe: Inflation and Reheating

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présentée par

Lucas Pinol

**Aspects multichamps dans l'Univers primordial :
Inflation et Réchauffement**

soutenue le 25 juin 2021 devant le jury composé de :

Mme. Ana Achúcarro	Examinatrice
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M. Nick Kaiser	Examineur
M. David Langlois	Examineur
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M. Sébastien Renaux-Petel	Directeur de thèse
M. Alexei A. Starobinsky	Membre invité
M. David Wands	Rapporteur

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Résumé

Cette thèse de doctorat traite des aspects théoriques et phénoménologiques de l'inflation cosmologique lorsqu'elle est provoquée par la présence de plusieurs champs scalaires. Bien que la théorie inflationnaire d'un Univers primordial en expansion quasi-exponentielle soit désormais largement acceptée comme la plus crédible, son mécanisme microphysique reste à déterminer. Les modèles les plus simples, dits à *un champ*, permettent d'expliquer les observations cosmologiques de manière satisfaisante. Pour autant, la plupart d'entre eux ne sont ni motivés par les théories physiques qui pourraient décrire l'Univers à ces échelles d'énergie très élevées, ni robustes face aux corrections quantiques qui semblent pourtant y jouer un rôle majeur. Ces fissures dans notre compréhension de l'Univers primordial amènent à se pencher sur des modèles plus complexes mais sans doute plus réalistes, car non seulement décrits dans le cadre de ces théories à hautes énergies, mais aussi peut-être moins sensibles à ces corrections quantiques. La large classe de modèles résultant de cette réflexion sont dits *multichamps*, car ils permettent d'avoir de multiples degrés de liberté en interaction dans l'Univers primordial.

Au-delà des motivations théoriques susmentionnées, l'inflation multichamps présente une phénoménologie extrêmement riche du fait des nouvelles dimensions qu'elle propose par rapport à l'inflation à un champ. Dans cette thèse, je me suis efforcé de diriger mes efforts théoriques vers la description de phénomènes physiques observés ou observables. Une partie importante de mes travaux s'est portée sur la prédiction des *non-Gaussianités primordiales*, ces non-linéarités initiales du cosmos qui ont pu se propager jusqu'à nous au travers du fond diffus cosmologique et de la toile cosmique de notre Univers local, et qui sont souvent particulièrement prononcées dans les modèles multichamps. Cette thèse a montré par exemple que les interactions cinétiques des divers champs scalaires, dont une élégante description géométrique est disponible, peuvent être responsables d'une dynamique inflationnaire non-triviale décrite par une trajectoire courbe dans l'espace interne des champs scalaires, et, ce faisant, produisent un signal non-Gaussien particulier qui permettrait facilement de discriminer ce type de modèles à l'aune des observations astronomiques à venir dans les prochaines années. Plus généralement, il est ici montré que même quand les perturbations des multiples champs scalaires se comportent *effectivement* comme celles d'une unique fluctuation, elles laissent une trace indélébile de leur caractère protéiforme dans la statistique de cette unique fluctuation.

Dans l'optique de dépasser le cadre conventionnel dans lequel les perturbations cosmologiques sont habituellement décrites, parfois dénommé *semi-classique* car il traite de la partie homogène de l'Univers comme d'une composante classique insensible aux phénomènes quantiques, cette thèse propose également une description stochastique des fluctuations primordiales aux échelles cosmologiques et dans l'inflation multichamps. Ces travaux, supposément techniques et peu conceptuels car l'*inflation stochastique* à un champ était déjà développée au début de ma thèse, ont finalement amené à une réflexion profonde sur les racines microphysiques de la théorie statistique et quantique des champs en cosmologie. En effet, cette thèse a révélé que la description stochastique souffrait d'un problème conceptuel lié à son absence de covariance sous reparamétrisation

des coordonnées dans l'espace des champs, et que cette *anomalie stochastique* était due à l'ambiguïté usuelle de l'interprétation discrète de l'intégrale de chemin en physique théorique. Dans le cadre de l'inflation multichamps, cette thèse montre que l'ambiguïté est résolue par la prise en compte des phénomènes physiques même que le cadre théorique est sensé dépeindre, et par une description discrète des phénomènes temporels lorsqu'elle s'avère nécessaire, le calcul dit *de Itô* y jouant un rôle important.

Par ailleurs, la présence de plusieurs degrés de liberté à la fin de l'inflation affecte crucialement les prédictions théoriques des observables astronomiques. En effet, les modèles multichamps deviennent sensibles aux détails physiques du *réchauffement cosmologique*, cette nécessaire période de transition durant laquelle l'énergie potentielle des champs scalaires doit être utilisée pour exciter les champs décrivant les particules du Modèle Standard et produire la matière noire observée dans l'Univers. Ce fait constitue à la fois une malédiction et une bénédiction, malédiction car le pouvoir de prédictivité de l'inflation multichamps semble grandement diminué, et bénédiction car en conséquence il paraît possible de discriminer divers modèles de réchauffement au vu des observations cosmologiques. Sur ce sujet, la présente thèse propose un formalisme général pour décrire les interactions des champs scalaires avec des fluides cosmologiques à la fin de l'inflation, ainsi qu'une méthode systématique assortie d'une résolution numérique pour suivre l'évolution des perturbations purement multichamps, appelées *isocourbes*, au travers du réchauffement. L'exemple de l'inflation double composée de deux champs scalaires libres et massifs, est exhaustivement traité, permettant d'affiner de manière conséquente notre compréhension de la physique des perturbations isocourbes après la fin de l'inflation, et donc de revisiter l'interprétation de leur absence d'observation en terme de modèles microphysiques de l'inflation. Dans le cas particulier de l'inflation à un champ, ce formalisme a aussi permis de suivre de manière continue l'instabilité génériquement présente aux petites échelles à la fin de l'inflation, un phénomène appelé *préchauffement*, tout en décrivant les interactions du champ scalaire avec un fluide cosmologique, c'est-à-dire le réchauffement à proprement parler, et qui permettent d'arrêter dynamiquement l'instabilité avant qu'elle ne transforme l'entièreté de l'Univers observable en un immense trou noir primordial.

La diversité des phénomènes physiques qui ont lieu dans l'Univers primordial rendent son étude à la fois difficile et passionnante. La grande quantité de données astronomiques d'excellente qualité, déjà disponibles et à venir dans les prochaines années, en font une science fondamentalement expérimentale et dans laquelle la théorie ne peut se contenter d'élucubrations mathématiques. Seules les observations futures nous permettront de dessiner avec précision les contours du scénario inflationnaire le plus crédible, grâce aux progrès combinés des méthodes expérimentales, des traitements de données, ainsi que des constructions théoriques.

Abstract

This PhD thesis aims at studying theoretical and phenomenological aspects of cosmic inflation when it is driven by the presence of several scalar fields. Although the inflationary theory of a quasi-exponential expansion of space is now widely accepted as being the current paradigm for the early Universe, its micro-physical origin remains to be determined. The simplest models, so-called *single-field* ones, are sufficient to explain cosmological observations in a satisfactory manner. However, most of them are neither motivated by physical theories that might describe the Universe as such high energy scales, nor are they robust against quantum corrections that nevertheless seem to play an important role. These glitches in our understanding of the early Universe lead to the consideration of more intricate models, but perhaps better motivated, not only because they are described in the context of high-energy theories, but also because they seem to be less sensitive to those quantum corrections. The large class of models that result from this reasoning are called *multifield*, because they leave open the possibility to have multiple interacting degrees of freedom in the early Universe.

On top of the aforementioned theoretical motivations, multifield inflation features an extremely rich phenomenology due to the new possibilities that it brings compared to single-field inflation. In this thesis, I tried to concentrate my theoretical efforts on the description of observed or observable physical phenomena. A consistent part of my work has been directed towards the prediction of *primordial non-Gaussianities*, those initial non-linearities in the cosmos that have reached us through the cosmic microwave background and the cosmic web in our local Universe, and that may be particularly pronounced in multifield setups. As an example, this thesis has enabled one to show that the kinetic interactions amongst the various scalar fields, which can be interpreted in an elegant geometrical way, possibly result in an inflationary dynamics featuring a bent trajectory in the internal space of the scalar fields, therefore producing a large and characteristic non-Gaussian signal that one may hope to detect with upcoming astronomical observations, which could thus help one to discriminate amongst those models of the early Universe. More generally, it is shown here that even when the perturbations of the full multifield system *effectively* behave as a single fluctuation, they still leave an imprint of their multifaceted properties in the statistics of this single fluctuation.

In order to circumvent the usual way to describe cosmological perturbations, often called *semi-classical* because it treats the homogeneous part of the Universe as a classical component insensitive to quantum phenomena, this thesis proposes a stochastic description of primordial fluctuations on large scales in the context of multifield inflation. These works, supposedly technical and poorly conceptual, because *stochastic inflation* was already developed when this thesis began, have eventually brought us to a deep reflection on the micro-physical origin of statistical and quantum field theory in cosmology. Indeed, this thesis uncovered that the stochastic description was suffering from a conceptual issue related to its absence of covariance under a reparameterisation of the fields' coordinates, and that this *stochastic anomaly* was due to the usual am-

biguity in the discrete interpretation of the path integral in theoretical physics. In the context of multifield inflation, this thesis shows that ambiguity is solved thanks to the consideration of the physical phenomena that the formalism is supposed to describe, by a discrete description of the temporal phenomena when it happens to be necessary, and where so-called *Itô calculus* plays an important role.

Moreover, the presence of multiple degrees of freedom at the end of inflation crucially affects the theoretical predictions of astronomical observables. Indeed, multifield models are sensitive to the physical details of *cosmic reheating*, a necessary epoch of transition during which the potential energy stored in the scalar fields must be transferred to the fields describing Standard Model particles and the dark matter that is observed in our Universe. This is both a curse and a blessing, a curse because the predictivity power of multifield inflation seems greatly diminished, and a blessing because it appears then possible to discriminate amongst the various reheating mechanisms given actual cosmological observations. On this topic, the current thesis proposes a general formalism to describe the interactions between scalar fields and cosmological fluids at the end of inflation, as well as a systematic method together with a numerical resolution to follow the evolution of the purely multifield perturbations, so-called *isocurvature* ones, through reheating. The example of double inflation, where two free massive scalar fields are responsible for inflation, is extensively studied, thus enabling to significantly sharpen our understanding of the physics of isocurvature perturbations after the end of inflation, and therefore to revisit how their absence of observation so far constrain the micro-physical details of inflation. In the particular case of single-field inflation, this formalism has also been used to follow continuously the generic small-scale instability developing at the end of inflation, a phenomenon called *preheating*, while still describing the interactions of the scalar field with a cosmological fluid, that enable one to stop the instability before it turns the entire Universe into a gigantic primordial black hole.

The diversity of the physical phenomena taking place in the early Universe render his study both challenging and fascinating. The huge amount of high-quality astronomical data, already available and to be collected in the upcoming years, make it a science grounded into experiments and where the theory cannot afford mathematical ramblings. Only future observations can help us to shape the details of the micro-physical origin of inflation, thanks to the combined progresses of experimental methods, data analysis techniques and theoretical constructions.

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Introduction

How is our Universe and what is it made of? Physical cosmology is the science that aims at describing the Universe as a dynamical system ruled by the laws of gravity that we otherwise experience, and filled with particles as we understand them in different contexts. Its modern interpretation makes use of the theory of General Relativity to follow the spacetime evolution, and of the Standard Model of Particle Physics for describing part of its matter content. Indeed, the current best model to describe it is called the Λ CDM one, and relies on the extra presence of two exotic components in the energy budget of the Universe, that are not correctly described by particle physicists yet: dark energy (in the form of a cosmological constant Λ), and cold dark matter (CDM). Despite the lack of micro-physical interpretation for its dark components, modern cosmology enables one to faithfully describe the cosmological evolution of our observable Universe, as we understand it from astronomical observations, for most of its 13.80 billion years of history. These experiments of ever-increasing complexity, ingenuity and accuracy have taught us that our Universe has always been expanding, even if sometimes at different paces that enable one to distinguish cosmological eras, from an extremely tiny and hot initial state to the gigantic, cold world that we now observe around us. This leading paradigm is called the Hot Big Bang model.

How far can we dig into the past of our own cosmic history? This is the obsession of Early Universe physicists, for the initial conditions of the subsequent known cosmological eras must be deeply rooted in a quantum theory of gravity, the current Holy Grail of theoretical physicists. Importantly, observations of the Cosmic Microwave Background (CMB) indicate that the standard Hot Big Bang model, according to which the early phase of cosmic history is made of a universe filled with relativistic species and therefore features a decelerated expansion, cannot be extrapolated too far in the past. Indeed, the study of this relic radiation carrying the picture of our baby Universe (approximately 380 000 years old, the equivalent of 1.006 day for a 100-years human life compared to the current 13.80 billion years of the Universe), teaches us puzzling facts. First, the Universe then was already very homogeneous, even on scales much larger than the particle horizon according to the Hot Big Bang model, meaning that they should never have been in causal contact in the past, and secondly it was consistent with a flat spatial geometry to a very high degree of fine-tuning [8–15]. These features (and other related puzzles, such as the absence of monopoles or other relics) are inconsistent with

the standard picture of a decelerated expansion, for reasons reviewed in this manuscript. These glitches in the understanding of cosmic history led physicists to revisit the possible expansion laws of spacetime, and to speculate about an accelerated expansion of the very early universe [16–23], before non-relativistic species set the stage of the radiation-domination era during which expansion is decelerating. For the expansion takes place at an ever-increasing speed, this cosmological epoch was dubbed cosmic inflation: it is the subject of this thesis. Although it was introduced as a necessity to solve the aforementioned puzzles of the standard Hot Big Bang model, the theory of cosmic inflation has proven extremely successful at predicting the statistics of the tiny anisotropies in the CMB [24–31], which had not been detected yet when this field of research was still developing. A huge success of the theory is that stating the initial conditions for the cosmological perturbations during inflation requires a careful semi-classical treatment involving the use of quantum field theory in curved spacetimes, a procedure that can be understood as a first step towards a quantum description of our Universe. Actually, inflation is the only known theory that necessitates both general relativity and quantum field theory to describe it, and that is also consistent so far with a large amount of high-precision experimental data.

What are the micro-physical details of inflation? If an initial epoch of quasi-exponential expansion of space as described by inflation is now the leading paradigm to describe the earliest phases of our cosmic history, one is not provided yet with a consistent theoretical framework in which to embed it. The simplest models of inflation feature an energy budget dominated by the presence of a scalar field, often denoted ϕ and called the inflaton, which must possess a potential energy described by a scalar potential $V(\phi)$, much larger than its kinetic energy. This peculiar matter content almost mimics the effect of a cosmological constant, which would correspond to a vacuum (potential) energy without a kinetic component at all, but provides a natural and dynamical way to terminate inflation when the scalar field reaches a steep part of its potential and therefore develops a large kinetic energy that terminates the acceleration of spacetime expansion. But what is this exotic scalar field that seems not to be described by the Standard Model of particle physics (at the notable exception of Higgs inflation)? How come that its scalar potential is so flat that its dynamical evolution corresponds to a slow roll in the direction of the potential gradient? Why is there only one fundamental degree of freedom and not many more interacting ones leading to a more intricate description? These conceptual questions can be phrased more rigorously in the language of theoretical physics. Indeed, attempts to describe gravity in a quantum framework, mainly including string theory, tend to generically predict that the early universe should be filled with a plethora of different particles, amongst which interacting scalar fields of various kinds (for a review in the context of string theory, see *e.g.* Ref. [32]). According to this so-called top-down approach (because it assumes a high-energy theory and extrapolates it to the lower energy scales relevant for inflation), the single-field models seem particularly fine-tuned: where have the other dynamical fields gone? Moreover, even without assuming a particular description of the high-energy physics, but simply considering inflation as

an Effective Field Theory at a given energy scale, it appears unnatural for a scalar field in the early universe to display a flat potential on a sufficiently long distance in the field space, as the estimated quantum corrections spoil this particular feature to the point of ruining inflation itself, an issue that is in many ways the cosmological counterpart of the hierarchy problem in particle physics (see [33, 34] for the historical papers and *e.g.* Refs. [35, 36] for pedagogical reviews of this so-called η -problem). With this bottom-up approach (because it begins with a description at the energy scale of interest, but estimates the order-of-magnitude effects of higher-dimensional operators that may eventually play a role), it seems evident that slow-roll single-field models alone cannot provide a consistent theoretical framework to describe inflation. But this so-called UV-sensitivity of inflation is both a curse and a blessing, and can be envisaged either in a pessimistic way or in an optimistic one. The pessimistic view would be that since theoretical physicists have not discovered a fully consistent theory of quantum gravity yet, it is hopeless to derive reliable predictions for early universe physics, while the optimistic one would be on the contrary to make assumptions about such possible theories and to test them with actual cosmological observations. Of course, I would rather like to embrace the second possibility, and consider inflation as a formidable opportunity to test theories of gravity and particle physics beyond the standard models.

How can we distinguish amongst different inflationary models? In order to test those Beyond Standard Model theories, one must first derive reliable observable predictions on the phenomenological side, and then compare them to the analysis of astrophysical and cosmological data. A substantial part of my thesis has been focused on phenomenological studies of multifield models of inflation, which can generically be described as a set of scalar fields ϕ^I where the index I labels coordinates in the multi-dimensional field space, that possess both potential interactions encrypted in the scalar potential $V(\phi)$ and kinetic interactions as encoded in the field-space metric $G(\phi)$ that mixes the individual kinetic terms of the scalar fields, resulting in a non-linear sigma model [37] of inflation:

$$\mathcal{L} = -\frac{1}{2}g^{\mu\nu}G_{IJ}(\phi)\partial_\mu\phi^I\partial_\nu\phi^J - V(\phi), \quad (1)$$

where g is the spacetime metric and greek indices μ, ν denote spacetime coordinates.

But first, one shall investigate upon what observations can actually tell us. So far, the most useful astronomical experiments for constraining the physics of inflation have been directed towards the analysis of the statistics of the anisotropies in the CMB. Indeed, they enable one to infer a few interesting properties of the initial conditions for the radiation-dominated era, as can be predicted by inflationary models. First, at the level of the background homogeneous spacetime, they are such that there must have been a sufficiently long accelerated expansion of space in order to solve the puzzles of the standard Hot Big Bang scenario, which puts a lower bound on the duration of a given inflationary model. Furthermore, although these initial conditions are highly homogeneous, they possess small anisotropies whose statistics are compatible with a Gaussian

distribution with a well-measured variance, called the power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ of adiabatic scalar fluctuations $\mathcal{R}_k$, where k is the wavenumber of the Fourier component of the corresponding adiabatic perturbation. CMB observations measure precisely the amplitude and the scale-dependence of this adiabatic scalar power spectrum at the largest available cosmological scales: writing $\mathcal{P}_{\mathcal{R}}(k) = A_s (k/k_*)^{n_s(k)-1}$ with k_* a scale of reference and $A_s = \mathcal{P}_{\mathcal{R}}(k_*)$, the Planck satellite [38] found the amplitude $A_s = 2.10 \times 10^{-9}$, and the spectral index $n_s(k_*) = 0.9649 \pm 0.0042$ at the reference scale, as well as a negligible running of the spectral index $\alpha_s = \partial_{\ln k} n_s(k)|_{k_*} \ll 1$. Deviations from a Gaussian distribution can be characterised by higher-order correlation functions than the power spectrum, the bispectrum for the three-point function and the trispectrum for the four-point function for example, respectively parameterised by the dimensionless numbers f_{NL} and g_{NL} , and are observably constrained: $f_{\text{NL}} \lesssim \mathcal{O}(10)$ and $g_{\text{NL}} \lesssim \mathcal{O}(10^4)$ [39], where the statement that non-Gaussianities are small corresponds to both $f_{\text{NL}} A_s^{1/2} < 1$ and $g_{\text{NL}} A_s < 1$, which is indeed well-verified.

During my thesis, I have directed my theoretical efforts towards the predictions of these observed or observable quantities in the CMB, when inflation is described according to a multifield Lagrangian of the kind displayed above. For many reasons that are developed in the manuscript, multifield inflation can display a much richer phenomenology than the simplest slow-roll single-field models, thanks to the diversity of the phenomena that can take place in higher-dimensional field spaces: imagine yourself and other humans as living on a line, in this context it is very unlikely that we would have developed complex enough social interactions to discuss one day of the origins of the Universe.¹ For example, it is well known that slow-roll, single-field inflation with canonical kinetic terms can only produce a negligible amount of non-Gaussianities, typically $f_{\text{NL}} \sim \mathcal{O}(0.01)$ for the bispectrum, thus leaving three empty orders of magnitude between this floor value and the observational constraints for richer physics to take place. And indeed, multifield inflationary dynamics present striking characteristic observational signatures, such as correlated adiabatic and isocurvature perturbations, features in the primordial power spectrum and order one non-Gaussianities with specific patterns (see, e.g., Refs. [2, 3, 40–76] for just a tiny sample of these works). More exotic features can also be found, such as a large flattened shape for the bispectrum and higher-order correlation functions [1, 77–79], a production of Primordial Black Holes (PBH) [80, 81] and of small-scale Primordial Gravitational Waves (PGW) [82–84]. Therefore, a detection of these primordial signals in the coming years, during which experiments of increasing sensitivity shall be launched in order to explore in further details CMB fluctuations, the clustering of visible and dark matter in our more recent Universe and primordial gravitational waves, could be interpreted as a detection of multifield physics.

¹I recommend the reading of the satirical novella *Flatland* by E. A. Abbott on a sexist society living in two dimensions, where males are regular polygons of increasing rank as they look more and more like circles and females are only segments. After mocking the king of a one-dimensional sub-world living on a line, a square understands that its own universe is embedded into a three-dimensional space as it encounters a sphere that drags it away from its plane to show it how constrained is its life. Then, the square tries to convince the sphere that it might also be embedded in a four-dimensional space, or of even higher dimension, a fabulous thought experiment a few decades before the advent of relativity.

How close can we get to genuine quantum effects during inflation? Even when exploring non-linear phenomena such as the ones probed by primordial non-Gaussianities, the standard treatment of the fluctuations during inflation is perturbative, in the sense that the effects of these quantum fluctuations are always supposed to be negligible compared to the classical dynamics. That is why the canonical treatment of inflation is only a first step towards quantum gravity. However, and even more particularly for the very flat potentials that seem to dictate the slow-roll dynamics of single-field inflation, there is a regime in which the quantum diffusion may overcome the classical drift along the potential gradient of the scalar field(s). In this corner of the theory where some of the relevant scalar fields are very light, the Universe may develop large quantum fluctuations that cannot be encapsulated in the regular perturbative analysis. These physical cases of interest clearly call for a new formalism, which happened to be called the stochastic formalism for inflation [85–94] because it treats the fluctuations that have been stretched to cosmological scales during inflation, as random variables subject to both the classical drift of a homogeneous background, and a continuous diffusion term originating from their small-scale quantum nature. This formalism is by nature non-perturbative, as it encapsulates large deviations from homogeneity on the largest cosmological scales that are treated in a stochastic but classical way, and therefore goes deeper in the effective description of a quantum phenomenon happening in a gravitational framework. And indeed, it has already enabled one to derive non-perturbative results of Quantum Field Theory in curved spacetimes that could not have been known otherwise, and that are matching existing computations in the perturbative limit [94–102]. But the theoretical foundations of stochastic inflation are shaky, and it is hard to extend it beyond the simplest massless, single-field case. Although an extension to the dynamics in the full phase space had already been proposed in the single-field case [103, 104], and multifield setups were investigated earlier [105–107] it is only in this thesis that it has been shown for the first time how to derive the Langevin equations of multifield stochastic inflation with kinetic interactions and in phase space, thanks to a quite rigorous path-integral approach borrowed from out-of-equilibrium field theory techniques. Many interesting phenomena remain to be explored with this promising formalism.

What is happening at the end of inflation? Inflation must also come to an end, and it is actually one of the successes of the theory that a scalar potential with a local minimum naturally results in oscillations with an average equipartition of the energy between the potential and the kinetic parts of the inflaton(s), therefore terminating the slow-roll regime and by the same time reaching a more usual decelerated expansion of space (an oscillating massive scalar field behaves on average as pressure-less matter, just like cold dark matter for example). But this cannot be the end of the story, because the Universe would then be cold and empty for ever, and the scalar fields must decay into other degrees of freedom, ultimately populating the number density levels of the quantum fields describing Standard Model particles and dark matter that we now observe around us in our local Universe. This physical phenomenon is called cosmic reheating,

for it results in such production of particles that then reach a thermal equilibrium, therefore enabling to define for the first time the temperature of the Universe [108–114]. But reheating can take various shapes, as it mixes both violent but transient particle production during the so-called preheating process involving quantum processes such as Bose enhancement, and less efficient perturbative couplings that are however necessary to terminate reheating (see Ref. [115] for a review). Both these aspects are explored in this thesis, for a particular subset of preheating, called metric preheating, is investigated (for once) in the single-field case, and perturbative reheating from multifield inflation to a multi-fluids system is also exhaustively studied. Indeed, although single-field models are only mildly sensitive to the details of reheating on large scales, this is neither the case for small scales in single-field inflation (that metric preheating is about), nor is it for multifield inflation at any scale. It is both intriguing and thrilling that such a crucial cosmological epoch, bridging the gap between the scalar fields’ description of inflation and the more usual cosmological fluids or particle description of the subsequent cosmological eras, is so poorly understood and studied.

What is the content of this thesis? This manuscript is divided into four parts displaying a total of nine chapters. The introductory Part I presents the current cosmological paradigm, from the birth of special and general relativity and the advent of physical cosmology during the 20th century in Chapter 1, to the description of cosmological perturbations, including discussions about gauges and definitions of useful gauge-invariant variables in Chapter 2.

Then, Part II proposes a detailed analysis of inflation, first at the level of the background and linear fluctuations but both in the single-field case in Chapter 3 where the horizon and flatness problems are exposed, and in the multifield one in Chapter 4 where their introduction is motivated by top-down and bottom-up approaches. Chapter 5 exposes the more advanced topics of primordial non-Gaussianities, by first reviewing how they are encoded in connected correlation functions (so-called cumulants in probability theory) of order strictly higher than two, and also explaining how to compute them either with the quantum in-in formalism or with the classical δN -formalism: interesting physical cases in both single-field and multifield setups are explored and their bispectra are computed, leading to the introduction of the shape functions used to observationally constrain the models of inflation. It then digs into the details of my research work with the presentation of my three research articles on the topic of primordial non-Gaussianities in multifield inflation with curved field space, both at the phenomenological and theoretical levels: a multifield instability and the resulting large, flattened non-Gaussianities are displayed, and the computation of the bispectrum in multifield inflation is revisited in the comoving gauge, leading to explicit results in terms of the observable curvature perturbation that encapsulate the richness of the multifield description such as geometrical effects coming from the curved field space.

Part III is about the stochastic formalism and how it has been extended to the multifield case during my thesis. First, Chapter 6 discusses the usual stochastic setup of single-field inflation and its extension in phase space, and then Chapter 7 proposes the

two research articles that I published on this topic in the multifield context, explaining how we unveiled the generic presence of inflationary stochastic anomalies at the conceptual level in the formalism, and also how to solve them by taking into account the very quantum nature of the inflationary perturbations. There, it is also shown how to properly derive the Langevin equations for multifield stochastic inflation with kinetic terms and in full phase space, taking advantage of the so-called Schwinger-Keldysh, or in-in formalism, in order to answer a few of the open questions left from the more usual approach at the level of the linear equations of motion.

The last, Part [IV](#), treats of (p)reheating in both single-field and multifield scenarios, by proposing a new formalism inspired from the literature but adapted to the physical situations of interest, to couple scalar fields with cosmological fluids. In [Chapter 8](#), the possible scenarios of reheating in the single-field case are reviewed in the introduction of my research article on this topic that is displayed there, and the effects of coupling the inflaton to a cosmological fluid in order to reheat the Universe at the end of inflation, in particular on the physical phenomenon called metric preheating, are discussed in details. Eventually, [Chapter 9](#) presents my research work containing the aforementioned generic formalism for any number of scalar fields and cosmological fluids, as well as a systematic method paired with an exact numerical resolution of the equations, in order to follow the evolution of all perturbations through the reheating process, including the relevant isocurvature fluctuations that do not have a single-field counterpart.

Then, the manuscript ends with some conclusions and prospects for future work.

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Part I

The cosmological paradigm

Chapter 1

The homogeneous and isotropic Universe

In this chapter, I review the modern foundations of physical cosmology – general relativity and the cosmological principle – as well as their theoretical implications.

1.1 Special Relativity and General Relativity: a description of spacetime

I propose in this section a modern interpretation of experiments taking place at the end of the 19th century and during the 20th one, that set the stage for our current understanding of spacetime.

1.1.1 Interferometer experiments and the constancy of the speed of light

It appears, from all that precedes, reasonably certain that if there be any relative motion between the earth and the luminiferous ether, it must be small.

Albert A. Michelson and Edward W. Morley

Although the exact role of the Michelson–Morley and subsequent interferometer experiments in the construction of special relativity is disputed, notably by Einstein himself (for an interesting discussion on this topic, see Ref. [116]), it undeniably provides an experimental validation of its fundamental principles. In this paragraph, I want to give credits to these pioneers in the exploration of spacetime, for these famously “most unsuccessful experiments ever” that prove the absence of ether, and display evidence for new symmetries of spacetime beyond the previously-known Galilean ones.

The Michelson–Morley experiment

At the end of the 19th century, it was believed that light was traveling through a particular medium, called ether, that would itself be in relative motion with the terrestrial frame with a velocity v . Given the Galilean transformation of velocities between two reference frames, and assuming that light propagates with the speed c in the ether frame, light should for example travel at a speed $c + v$ in the direction of the ether flow, in the terrestrial frame.¹

The 1887 Michelson–Morley experiment [117] was dedicated to the search for this hypothetical ether and to the potential measurement of the ether relative velocity v with respect to Earth. It relies on a now famous interferometer setup, with a light beam being split in two different, orthogonal paths, and then reconstructed. Positive and negative interferences build up depending on the exact orthogonality of the mirrors, the length difference between the two paths and the speed of light. Suppose the two arms of the interferometer are respectively parallel and orthogonal to the ether flow (and thus perfectly orthogonal to each other) and have the exact same length L , then two different pictures with similar conclusions arise, depending on the frame of reference, see Fig. 1.1. The most intuitive one might be the terrestrial frame, where every thing happens like for a swimmer in a flowing river: along the parallel direction light travels first downstream with a speed $c + v$ and then upstream with a speed $c - v$, while on the orthogonal one, light travels at a projected speed $\sqrt{c^2 - v^2}$ on both ways in order to compensate for the transverse flow. In the ether frame, light is always traveling at the speed c , but now it is the interferometric setup that is moving towards, away, or transversely to the light, leading to different effective lengths and times for light to travel on both ways: $t_{\parallel} = t_1 + t_2$ with $ct_1 = L - vt_1$ and $ct_2 = L + vt_2$, while $t_{\perp} = 2t_3$ with $ct_3 = \sqrt{L^2 + (vt_3)^2}$. Both pictures lead to estimating the time that light takes to travel on both ways to be respectively

$$t_{\parallel} = \frac{L}{c+v} + \frac{L}{c-v} \quad \text{and} \quad t_{\perp} = \frac{2L}{\sqrt{c^2 - v^2}},$$

leading to a mean path difference $\delta \simeq L \frac{v^2}{c^2}$ at first non-vanishing order in the correction v/c . Because the two arms of the interferometer can never be set to the exact same length L , this intrinsic path difference cannot be observed with just one configuration. However, this obstacle is easily overcome by switching the roles of the two arms and rotating the interferometer by an angle of $\pi/2$ radian: moving from one configuration to the other one should shift the positions of the fringes of interferences by a number of fringes $\Delta N = 2\delta/\lambda \simeq 2 \frac{L}{\lambda} \frac{v^2}{c^2}$ where λ is the wavelength of the supposedly monochromatic light source.

Surprisingly (for this epoch), this very precise setup was not able to measure any shift in the number of fringes when rotating the interferometer, indeed the upper limit on the

¹I am simplifying the historical discussion on ether since it was actually thought that due to the permeating medium possibly having a refractive index n , the correction to the velocity in the terrestrial frame could be corrected by a n -dependent factor in order to make the Snell-Descartes' laws of refraction work in any reference frame. This version of ether theory was called “partially dragging ether”.

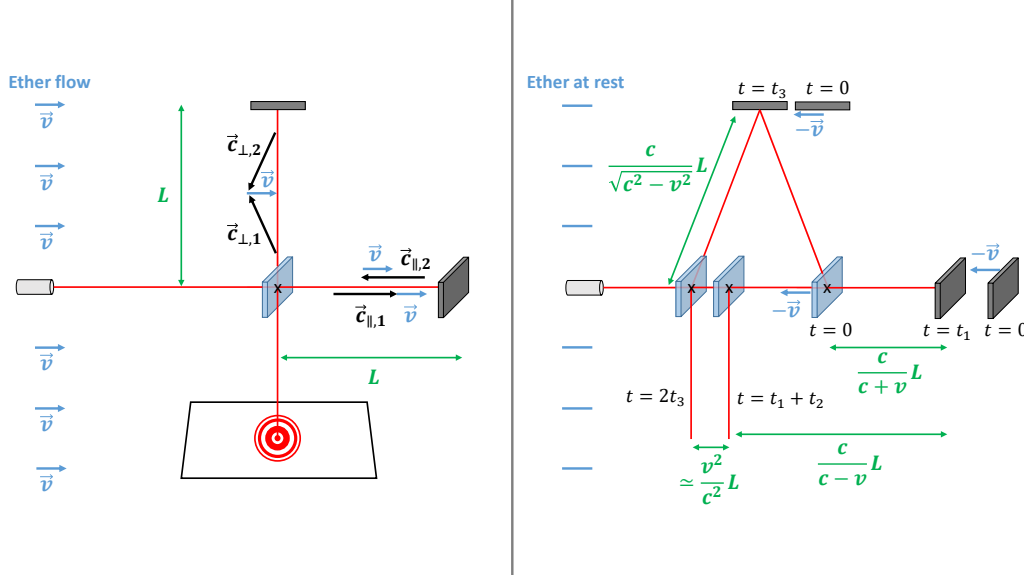


Figure 1.1: Michelson–Morley interferometer in the orthogonal configuration and interpretation with the ether theory. Left: frame of the experiment, the ether flow in which light propagates at speed c changes its relative velocity to $c+v$ or $c-v$ in the longitudinal direction, and to $\sqrt{c^2 - v^2}$ in the orthogonal one. Right: ether frame, the experiment is moving with a relative velocity $-\vec{v}$ which changes the distances light needs to travel, to $\frac{c}{c+v}L$ or $\frac{c}{c-v}L$ in the longitudinal direction, and to $\frac{c}{\sqrt{c^2 - v^2}}L$ in the orthogonal one.

shift of the number of fringes was found to be as low as $\Delta N \lesssim 0.01$. Even considering the ether at rest in the solar system's frame, just the orbital motion of the Earth around the Sun should give a relative velocity between the frame of the experiment and the ether frame, resulting in a shift of fringes of $\Delta N \simeq 0.4$. This means that if ether exists, its relative velocity with the experiment should be lower than $v \lesssim v_{\text{orbital}}/\sqrt{40} \simeq 5$ km/s (corresponding to $v/c \lesssim 2.10^{-5}$) because of the sensitivity of the experiment to the square of the velocity only. Michelson and Morley also pointed out the possibility that the ether is not at rest with respect to the solar system, and that this two relative velocities could precisely cancel. Of course, this was very unlikely and by repeating the experiment months later when the orbital motion of the Earth had changed of direction, it was possible to show that no such cancellation could occur. Strictly speaking, what the Michelson–Morley experiment was able to show, is that the speed of light is independent of the orientation of the experiment, providing the first subgroup of Lorentz symmetries: rotations. As one shall see in Sec. 1.1.2, this null result can be interpreted in the language of special relativity as an observation of length contraction for an observer at rest in a comoving frame with relative velocity v with respect to the experiment.

Subsequent interferometer experiments

The historical experiment of Michelson and Morley has been repeated with increasing sensitivity over time, always leading to the conclusion that ether was absent, or with smaller and smaller relative velocity with respect to the Earth, whatever the season.² Modern techniques using lasers and optical resonators enabled one to put an upper bound on the change of the speed of light under rotations as low as $v/c \lesssim 10^{-18}$ [118].

Even more importantly maybe, a different version of this initial interferometric setup was invented, in order to test the other Lorentz symmetries of spacetime present in the theory of special relativity. The Kennedy–Thorndike experiment of 1932 [119] indeed showed that the speed of light was also independent of the speed of the experiment with respect to an inertial frame. Besides technological improvements compared to the Michelson–Morley interferometer, the novelty in this experiment was to compare the fringes of interferences over months without changing the configuration of an apparatus with unequally long arms, $L_{\parallel}$ and $L_{\perp}$ (the existence of a monochromatic source of light with large coherence length, the mercury line at about 16cm, allows for the observation of interferences even with a sizeable difference in the lengths of the two paths). Due to the Earth rotating around the Sun, the relative velocity between the experiment and the ether changes, which should shift the fringes in an independent way from the Michelson and Morley experiment. By stabilising their experiment and taking regular photographs of the fringes, they found no shift in the fringes at all, even after months, and hence concluded that indeed the speed of light is independent of the speed of the experiment relative to a reference frame, implying the existence of a spacetime symmetry under Lorentz boosts. As one shall see in Sec. 1.1.2, this null result can be interpreted in the language of special relativity as an indirect observation of time dilation.

Long live the interferometers!

Notwithstanding the debate about the precise role of the Michelson–Morley experiment in the conceptual construction of special relativity by Einstein in 1905, interferometers undeniably played a crucial role in unveiling the mathematical Lorentz symmetries of spacetime, at the level of experiments. Ironically, interferometers will later play again a significant role in building up our understanding of spacetime, with the first direct observation by the LIGO experiment of gravitational waves the day of my 20th birthday [120], implying *en passant* the existence of binary black holes, as well as the many subsequent ones together with the Virgo collaboration, that in particular enabled one to measure a coincident speed of propagation for light and gravitational waves thanks to the newly born field of multi-messenger astronomy [121].

²With the notable exception of experiments conducted by Dayton Miller who was fiercely convinced by the existence of ether and regularly claimed that it had detected it. No one was ever able to reproduce his results, and both his data analysis and error estimations were judged incorrect by later checks. Apparently, there is still a community of “scientists” that believe in ether and think they detected it, and claim that mainstream science went the wrong way with relativity. Not to hurt the reader’s eyes, I will not provide links to such references.

1.1.2 Special Relativity: a consistent framework for particles, challenged by gravity

In the following, we promote this conjecture to a postulate (that one shall call “relativity principle” from now on) and introduce a second postulate – which is at first sight in contradiction with the former – stating that light propagates in empty space at a speed c independent of the state of motion of the emitting body.

Albert Einstein

Special relativity was only named like that after general relativity was proposed, when it was recognised as only a special case in the weak gravitational field limit. Despite this anachronism, I will use the denomination “special relativity” even for describing these early works.

Two-postulates formulation of special relativity and Lorentz covariance

In his historical paper [122], Einstein proposes two postulates on which to build a new theory aiming at describing “all” laws of physics (actually Newtonian mechanics together with electromagnetism):

- The principle of relativity: the laws of physics, expressed in a given system of coordinates, are not affected by a change from this system to another one, related to the former by a uniform rectilinear motion.
- The invariance of the speed of light: light propagates at a constant and universal speed c in vacuum, in any direction, irrespective of the motion of the light source.

Actually, it should be stressed that the principle of relativity dates back to Galileo’s thinking and is incorporated in the usual laws of Newtonian mechanics. However, the discovery of electric and magnetic fields later tested this principle, as it was thought that electromagnetic waves needed a medium in order to propagate, the aforementioned ether, which rather implied the existence of an absolute frame. Now, abandoning the law of composition of velocities for light, that is accepting the invariance of the speed of light, leads one to a different path: special relativity.

Indeed, Einstein showed that these two postulates implied the existence of symmetries under which the laws of physics should be covariant, and that these allowed transformations of space and time were nothing else than the Lorentz transformations (first rigorously described and called like that by Poincaré) that were already known from the study of how an electric field is converted into a magnetic one under a change of reference frame, and vice versa. Thus, special relativity unifies the description of electric and magnetic fields under electromagnetism. Most importantly, these Lorentz transformations mix time and space one with the other, making again an important step forward in the direction of relativity: what one calls a time interval can be a space interval for an observer in a different reference frame, and conversely. Of course, the lack of an absolute definition for time and space has wide philosophical implications, but it is not the aim of this manuscript to describe them. Rather, one shall here focus

on the physical implications of the Lorentz symmetries. Let us consider two systems $\mathcal{S}(t, x, y, z)$ and $\mathcal{S}'(t', x', y', z')$, each with its own set of coordinates, and suppose they are related one to the other by a uniform rectilinear motion at velocity v in the x direction (this is an arbitrary choice, but the spatial coordinates can always be chosen like that once the direction of the velocity between the two systems is specified). According to special relativity, the laws of physics should be the same for the two systems provided they are related by a Lorentz transformation (these transformations form a subgroup of the larger Poincaré group as shown by Poincaré himself, see *e.g.* [123]) which reads in this choice of coordinates:

$$t' = \gamma(t - vx/c^2), \quad x' = \gamma(x - vt), \quad y' = y, \quad z' = z, \quad (1.1)$$

where $\gamma = (1 - v^2/c^2)^{-1/2} > 1$ is called the Lorentz factor.

A first major outcome from these equations is that, as expected from the intuitive picture above, space and time are mixing one with the other: they are relative and not absolute. Actually, it is still possible to construct a spacetime invariant quantity, which can be called the event interval, defined as $\Delta s^2 = -c^2\Delta t^2 + \Delta \vec{x}^2$, where $\vec{x} = (x, y, z)$. It can indeed easily be checked that under a general Lorentz transformation, $\Delta s'^2 = \Delta s^2$. An absolute notion of event separation can then be defined with this quantity, with $(\Delta s^2 < 0)$ -separated events called timelike, $(\Delta s^2 > 0)$ -separated ones spacelike, and $(\Delta s^2 = 0)$ -separated ones lightlike. This can further lead to the definition of the past and future light cone of a given event A , see Fig. 1.2 for the simple spacetime diagram of special relativity, where it is clear that only events in the light cone of A ($s^2 - s_A^2 \leq 0$) are in causal contact with it. Note simply that the expression of the infinitesimal line element in special relativity defines a global spacetime metric, as $ds^2 = \sum_{\alpha\beta} \eta_{\alpha\beta} dx^\alpha dx^\beta$ in any inertial frame, where $\eta_{\alpha\beta} = \text{Diag}(-1, 1, 1, 1)_{\alpha\beta}$ is called the Minkowski metric with signature $(-, +, +, +)$, and is used to raise and lower spacetime indices α, β , etc.

Another simple implication of the Lorentz transformations is length contraction. Suppose there exists an object at rest in the frame without primes, $\mathcal{S}$, in which an observer measures it to be of length $\Delta x = L_0$. For an observer in the other, primed frame $\mathcal{S}'$, an instantaneous measure ($\Delta t' = 0$) of the object's length would give, according to Eq. (1.1) and the definition of the Lorentz factor γ ,

$$\Delta x' = \gamma \left(\Delta x - \frac{v^2}{c^2} \Delta x \right) = L_0 / \gamma < L_0.$$

The length measured in the moving frame $\mathcal{S}'$ relative to the object is thus smaller than the length of the object in the frame where it is at rest, hence the name contraction of length. Notice also that for the observer in the rest frame of the object, the measure done by the moving observer will have lasted some time $\Delta t = vL_0/c$, showing the relativity of the notion of simultaneity.

Let us finish this paragraph about the surprising implications of special relativity by explaining how time dilation takes place. Actually, this is merely the analog of length contraction, but for time and in the opposite way. Suppose an observer measures the

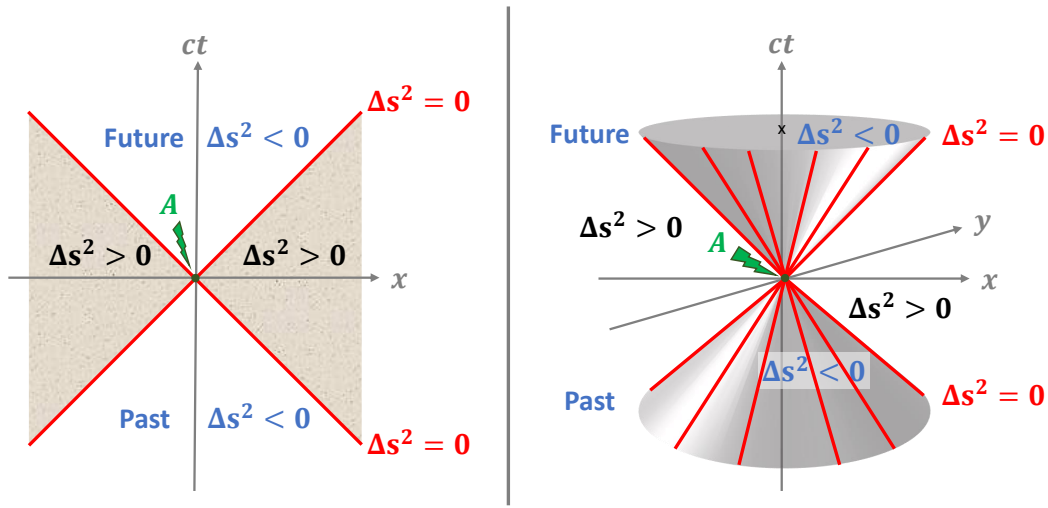


Figure 1.2: Minkowski spacetime diagram. Left: two-dimensional spacetime, the lightcone of A is just the two lines $\Delta s^2 = 0$. Right: three-dimensional spacetime, the lightcone of A is really a cone, generated by infinitely many lines $\Delta s^2 = 0$ (a few of them are represented in red). One should imagine (at least I cannot draw it) the lightcone for the four-dimensional spacetime of special relativity: each time slice of it corresponds to a three-dimensional sphere. Regions inside the lightcone, $\Delta s^2 < 0$, are in causal contact with A while those outside the lightcone, $\Delta s^2 > 0$, are not. With respect to A , the future corresponds to $t > 0$ and the past to $t < 0$.

regular ticking of a clock at rest in the frame $\mathcal{S}$ (hence $\Delta x = 0$) to be $\Delta t = T_0$. Now, another observer, but this time in the moving frame $\mathcal{S}'$ wants to measure the same ticking of the same clock. According to Eq. (1.1),

$$\Delta t' = \gamma T_0 > T_0.$$

The time interval measured in the moving frame relative to the clock is thus larger than the one in the clock's rest frame, hence the name time dilation. Notice of course that in everyday life in which things move at velocities much smaller than the speed of light, $v/c \ll 1$, these effects become negligible and one recovers one's much beloved non-relativistic regime.

An experimental validation of special relativity

Actually, the interferometer experiments of Michelson and Morley on one hand, and of Kennedy and Thorndike on the other hand, provide interesting tests of special relativity.

First, one should say that they are compatible with special relativity in the sense that length contraction and time dilation can be used to explain their null results. Actually, in the rest frame of the experiments, there is not even a question to ask any more: given the constancy of the speed of light independently of the relative motion with the emitting body, light travels at speed c on both arms of the interferometers, whatever is its orientation or its speed, and hence no shift in the fringes can be observed whatsoever. Now, in a comoving frame with a relative velocity v with respect to the experiment's rest frame, the quick calculation made in Sec. 1.1.1 for the Michelson–Morley experiment should be corrected by the fact that length contraction occurs in the direction longitudinal to the rectilinear uniform motion, leading to a time of travel along the parallel direction

$$t_{\parallel} = \frac{L/\gamma}{c+v} + \frac{L/\gamma}{c-v} = \frac{2L\gamma}{c} = t_{\perp},$$

and thus no shift in the fringes neither (time dilation does not change the picture here since the velocity is constant through the experiment and is thus equally experienced for both arms of the interferometer).

Using length contraction again, it is also possible to show that in the Kennedy–Thorndike experiment, the time difference between the two paths going through the arms of unequal length is actually given by $\Delta t = \frac{2(L_{\parallel} - L_{\perp})}{c} \gamma$ which should result in a shift of fringes $\Delta N = \frac{\Delta t_2 - \Delta t_1}{T} = \frac{2(L_{\parallel} - L_{\perp})}{c} (\gamma_2 - \gamma_1)$ when this relative velocity changes from v_1 to v_2 and thus the Lorentz factor from γ_1 to γ_2 , and where T is the period of oscillation of the light wave, assumed here to be constant through the experiment. Hence, length contraction alone fails to explain the null result of this experiment, but the twist comes from time dilation. Indeed, in the frame in relative motion with respect to the apparatus, the period of oscillation dilates according to special relativity, and the measured period is rather γT . Thus the expected number of shifts of fringes is actually

$$\Delta N = \frac{\Delta t_2}{\gamma_2 T} - \frac{\Delta t_1}{\gamma_1 T} = 0.$$

Strictly speaking, I showed that these two experiments are consistent with special relativity, but not that they implied special relativity. Actually, the Michelson–Morley experiment set the ratio between the coefficient of length contraction in the longitudinal direction β and the one in the transverse direction δ as $\beta/\delta = 1/\gamma$, while the Kennedy–Thorndike experiment set the ratio between β and the coefficient of time dilation α as $\beta/\alpha = 1/\gamma^2$, leaving still a one-parameter family of possible spacetime transformations. Fortunately, the Ives–Stilwell experiment of 1938 [124, 125] measured for the first time a relativistic contribution to the longitudinal Doppler shift of light frequency, an effect expected from time dilation, and provided a direct measure of the parameter α . The result, $\alpha = \gamma$ as expected in special relativity, further fixed uniquely the set of allowed coefficients to $\beta = 1/\gamma$ and $\delta = 1$,³ thus confirming the equivalence between these three experiments and the existence of special relativity as a theory to describe light propagation.

Of course, the successes of special relativity are not limited to interferometers of the 19th and 20th centuries, and to the measure of the relativistic contribution to the longitudinal Doppler shift. Indeed, other experiments went to confirm relativity as a guiding principle, including observations of the transverse Doppler effect (absent otherwise); of the relativistic version of the law of composition of velocities; of the relativistic aberration of light; of the increased lifetime of high-speed muons as measured by an observer at rest and compared to their rest-frame lifetime; as well as virtually all modern particle accelerators that are built to work in highly-relativistic regimes.

Incompleteness of special relativity: when gravity turns it all upside down

Special relativity relies on the principle that laws of physics are similar in any inertial frame, and from the previous paragraph one learnt that many experiments confirmed its validity. However, special relativity dismisses the effects of gravity and all these experiments work in a regime where gravity is negligible. Thus if not inconsistent, special relativity fails to describe gravitational effects which exist and are observed otherwise. Indeed, if inertial frames can be defined with respect to each other, there is no absolute inertial frame of reference to begin with (any way that would be against the relativity principle), and actually there seems to be no global inertial frame at all. Conceptually, gravity is always present for any particle, and always results in an acceleration of *a priori* inertial frames. Thus it seems that inertial frames can only be defined approximately, either locally in space and time by assuming that gravity has not yet resulted in a sizeable variation in velocity, or in a weak gravitational field regime where the effects of gravity are simply neglected. This conceptual issue faced by special relativity can be phrased as the absence of global inertial frames, and as one shall see in the next paragraph, Sec. 1.1.3, it leads, together with the equivalence principle, to consider the

³Here, I slightly modified the notations of the Robertson–Mansouri–Sexl test theory of special relativity [126, 127] in order not to introduce too many unnecessary formulae. I also simplified the discussion by not discussing the precise constraints that these experiments and subsequent ones put on the deviations of the parameters α , β and δ from their expected values according to special relativity, although this represents of course a huge literature.

possibility of a curved spacetime as described by general relativity.

On the experimental side, a few observations led to the conclusion that Newtonian gravity must be modified. Although they cannot really be attributed to a failure of special relativity, they render explicit the fact that special relativity does not solve the Newtonian ambiguities, and hence, must be extended. The first example concerns the light deflection of distant stars by the Sun, that Cavendish and then Soldner [128] calculated to be half that of the measured one, first by Eddington's team, much later in 1919. As a matter of fact, this missing factor of 2 is actually restored by taking into account general relativistic effects, the first correct calculation of it being made by Einstein in 1915 when releasing the implications of general relativity. The success of this prediction agreeing with the measurements of Eddington's expeditions during the solar eclipse of May 1919, is often considered as the birth of general relativity as a paradigm to describe gravity and the content of spacetime (although it seems that the first analyses were plagued with large uncertainties and a possible confirmation bias). Another example is the discrepancy between the measured perihelion precession of Mercury, and the one predicted by Newtonian dynamics taking into account the classical gravitational effects from all bodies in the solar system. Indeed, as early as 1859, Le Verrier [129] noted a $38''$ per century (cy) discrepancy between the two. Later calculations corrected this discrepancy to $43''/\text{cy}$ without changing its status: Newtonian dynamics alone fails to describe this precession, and special relativity alone does not help to bridge the gap (but rather amplifies it). Again, general relativity came to help, in particular with the clear understanding provided by the Schwarzschild's metric [130], and predicted a relativistic gravitational correction to the precession rate of exactly $43''/\text{cy}$, which indeed resolved the mystery.

1.1.3 General relativity and the bending of spacetime

Spacetime grips mass, telling it how to move... Mass grips spacetime, telling it how to curve.

John Archibald Wheeler

But Einstein realised quickly after he formulated special relativity that gravitation should be included in the description of spacetime. It is finally in November 1915, at the Prussian Academy of Science, that he presented his theory of general relativity which is quickly reviewed in this section.

The equivalence principle and the spaceship–ground laboratory picture

One of the building blocks of general relativity is the so-called equivalence principle. A crucial observation leading to this postulate is the universality of free fall, which can be stated as the equality between the inertial and the gravitational masses. Indeed, in the Newtonian description of the movement of a free-falling body in a gravitational field

$\vec{g}$, $m_i \vec{a} = m_g \vec{g}$, one observes experimentally that $m_i = m_g$.⁴ The conclusion is that gravity acts on all things independently of the constitution of their bodies. Therefore, two *a priori* very different situations seem to be indistinguishable: consider an isolated spaceship with running engines that accelerates at a uniform pace $-\vec{g}$, and a laboratory on the Earth surface. Because of the universality of free fall, an apple thrown in either of these frames will follow the exact same trajectory from the point of view of a local observer. This thought experiment leads to the following postulate,

- The equivalence principle: local laws of physics are independent on whether they take place in a gravitational field $\vec{g}$ or in a non-inertial frame with acceleration $-\vec{g}$.

Actually, this principle can be refined in the weak, respectively the strong, equivalence principle which states that the aforementioned local laws of physics concern only non-gravitational forces, respectively include also local gravitational effects such as self-gravitating objects. Therefore, the observational verification of the universality of free fall can be understood as a validation of the weak equivalence principle. The strong equivalence principle is more restrictive, as it requires the gravitational constant G be the same at every spacetime point in the Universe. Now, it should be clear that the equivalence principle is incompatible with the picture of spacetime drawn by special relativity, and that the Minkowski metric is only valid when gravity is negligible. Imagine the observer in the accelerating spaceship is sending light in a horizontal direction, because his frame is accelerated in the upper vertical direction, the light will hit the opposite wall at a lower altitude compared to the spaceship's ground, see Fig. 1.3. It means that the actual trajectory of light in the accelerated spaceship bends, and according to the equivalence principle, the trajectory of light in the ground-based laboratory should also bend due to the gravitational field of Earth. Similarly, suppose an observer O_1 in the spaceship sends light at the same frequency as the ticking of his clock to an other observer O_2 placed in his upper vertical direction, and that this second observer also has a clock, of similar fashion, and a light source. Because the spaceship is accelerating, a given wavepacket of light sent from O_1 will take more time to reach O_2 than if the experience was happening in an inertial frame, so O_2 will notice that the frequency of the light he receives is smaller than the one of his ticking clock: it is redshifted. Conversely, the light that O_1 will receive from O_2 who set the light frequency with his own clock, will appear blueshifted. Using the equivalence principle, it means that two similar clocks placed at different altitudes on Earth cannot be synchronized and that lower clocks are slower when observed from the upper one, and vice versa. These two effects, light deflection by massive bodies and gravitational redshift, are key predictions of the equivalence principle, and thus of general relativity.

⁴Newton found this equality to be correct at 10^{-3} relative accuracy using pendulums of different masses, the Eötvös balance comparing the weight $\propto m_g$ and the centrifugal pseudo-force due to Earth rotation $\propto m_i$ enabled one to go down to 10^{-9} in 1922 [131] and the recent MICROSCOPE mission composed of free-floating test masses in a satellite gave the current best accuracy of 10^{-15} [132].

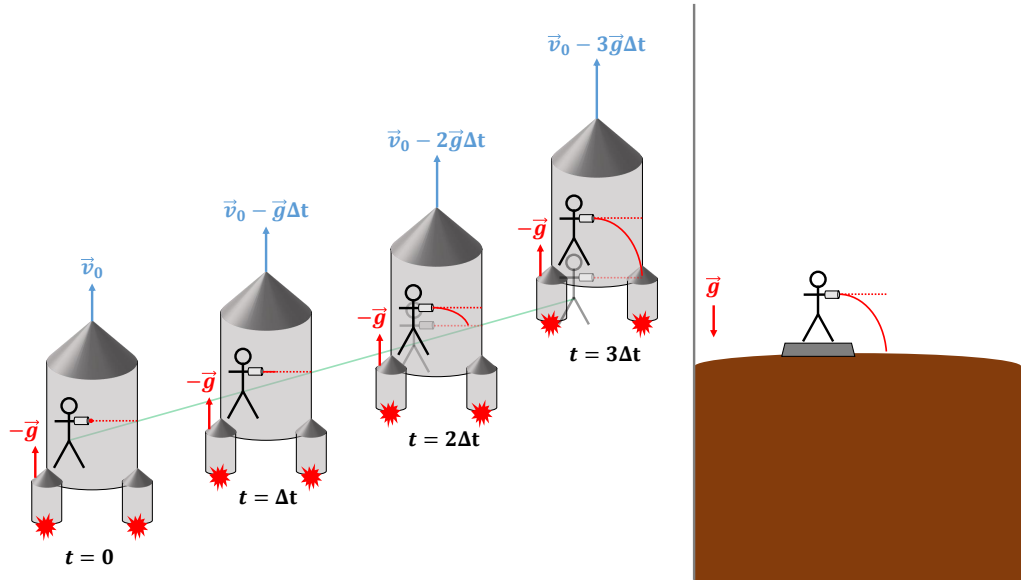


Figure 1.3: Bending of light due to the presence of a massive body creating a gravitational field $\vec{g}$, according to the equivalence principle. Left: the non-inertial frame of a spaceship is accelerated at a uniform pace $-\vec{g}$, the initial inertial frame in which light is emitted and has a straight trajectory, follows the green line, and hence light bends in the non-inertial frame of the spaceship. Right: according to the equivalence principle, light emitted in a gravitational field $\vec{g}$ follows the same path as in the spaceship with acceleration $-\vec{g}$, and hence light bends due to gravity.

Geodesics structure spacetime, and the Einstein equations

It appears thus, if global inertial frames cannot be defined and if gravitational fields act as non-inertial effects in an accelerated frame, that straight trajectories cannot be defined in an absolute way. The closest notion to a straight trajectory seems to be the free-falling motion, but as one understood with the example of light bending on Earth, free fall is actually bent by the presence of mass. A possible conclusion is that spacetime itself is curved, which affects the free-falling trajectories (that one shall call geodesics), that spacetime curvature is due to the presence of mass, and that gravity has no other effect than these geometric ones. With this picture, bearing in mind that, locally, inertial frames can be defined and special relativity should apply, one has all the fundamental pillars of general relativity.

Locally, near an event A , it is possible to describe spacetime with inertial coordinates $X_A^\alpha = (T_A, \vec{X}_A)$, and with the Minkowski metric as in special relativity, $ds^2 = \sum_{\alpha,\beta} \eta_{\alpha\beta} X_A^\alpha X_A^\beta$. Now in any other frame, described by coordinates x^μ , the same invariant event interval reads

$$ds^2 = \underbrace{\sum_{\alpha,\beta} \frac{\partial X_A^\alpha}{\partial x^\mu} \frac{\partial X_A^\beta}{\partial x^\nu} \eta_{\alpha\beta}}_{g_{\mu\nu}(x)} dx^\mu dx^\nu, \quad (1.2)$$

in which one identifies a generic local metric $g_{\mu\nu}(x)$. Thus one can use the tools of Riemannian geometry to describe spacetime and gravitational effects. This geometric interpretation of gravity is perhaps the most impressive feature of general relativity.

Conventions

From now on, one adopts the following conventions:

- the summation convention on repeated indices (unless otherwise stated);
- the use of natural units whereby $\hbar = c = G = k_B = 1$ and hence the only remaining dimension is mass (or equivalently energy), often expressed in units of the reduced Planck mass $M_{\text{Pl}} = \sqrt{\hbar c / 8\pi G}$, and where usual units can be restored by noting that $M_{\text{Pl}} = 2.435 \times 10^{18} \text{ GeV}/c^2$;
- the spacetime metric g has the $(-, +, +, +)$ signature, and spacetimes indices (labelled by Greek letters) are lowered and raised using the metric $g_{\mu\nu}$ and its inverse $g^{\mu\nu}$.

Rather than a historical approach of the derivation of the Einstein equations, one shall adopt a modern point of view and assume that the description of spacetime alone by general relativity can be encoded in the following Einstein-Hilbert action:

$$S_{\text{EH}} = \frac{1}{2} \int \sqrt{-g} d^4x M_{\text{Pl}}^2 R, \quad (1.3)$$

where R is nothing but the four-dimensional scalar Ricci curvature of spacetime, and $\sqrt{-g}d^4x$ is the invariant four-dimensional volume element in curved spacetime, g being the determinant of the spacetime metric. Now suppose that matter is composed of fields φ^i with any kinds of masses, spins and interactions (they do not necessarily need be bosonic spin-0 scalars), that can be described by a given matter Lagrangian $\mathcal{L}_m$ resulting in

$$S_m = \int \sqrt{-g}d^4x \mathcal{L}_m(\varphi^i, \nabla_\mu \varphi^i, g_{\mu\nu}), \quad (1.4)$$

and from which a stress-energy tensor can be defined as

$$T_{\mu\nu} = g_{\mu\nu} \mathcal{L}_m - 2 \frac{\partial \mathcal{L}_m}{\partial g^{\mu\nu}}. \quad (1.5)$$

Then, writing the Euler-Lagrange equations for the total Lagrangian density $\mathcal{L} = \mathcal{L}_{\text{EH}} + \mathcal{L}_m$, yields the famous Einstein equations:

$$\frac{\partial(\sqrt{-g}\mathcal{L})}{\partial g^{\mu\nu}} - \partial_\rho \frac{\partial(\sqrt{-g}\mathcal{L})}{\partial(\partial_\rho g^{\mu\nu})} = 0 \implies \underbrace{R_{\mu\nu} - g_{\mu\nu} \frac{R}{2}}_{G_{\mu\nu}} = \frac{1}{M_{\text{Pl}}^2} T_{\mu\nu}, \quad (1.6)$$

where $G_{\mu\nu}$ is the Einstein tensor of spacetime ($R_{\mu\nu}$ being itself the rank-2 Ricci tensor of the four-dimensional spacetime). From the Einstein equations, it is clear that not only the geometry of spacetime (encoded in $G_{\mu\nu}$) affects the dynamics of matter (encoded in $T_{\mu\nu}$), but also that the presence of matters modifies the geometry of spacetime, a key feature of general relativity.

The Lagrangian describing gravity may be supplemented by a cosmological constant Λ , a procedure that does not lead to a violation of the equivalence principle and is hence perfectly valid to represent general relativity (any operator allowed by the symmetries of the problem, including a constant here, should indeed be expected from Effective Field Theory arguments), $S_{\text{EH}} = \frac{1}{2M_{\text{Pl}}^2} \int \sqrt{-g}d^4x M_{\text{Pl}}^2 (R - 2\Lambda)$. Then, the Einstein equations read

$$\boxed{R_{\mu\nu} - g_{\mu\nu} \frac{R}{2} + \Lambda g_{\mu\nu} = \frac{1}{M_{\text{Pl}}^2} T_{\mu\nu}}, \quad (1.7)$$

while for consistency with the contracted Bianchi identities, $\nabla_\mu R^{\mu\nu} = \frac{1}{2} \nabla^\nu R$, the stress-energy tensor should verify the following continuity equation:

$$\boxed{\nabla_\mu T^{\mu\nu} = 0}. \quad (1.8)$$

1.2 Cosmology: the Universe has a history

This part is devoted to the introduction of cosmology, with a brief discussion of early philosophical works, but mostly presents the modern conception of how the Universe evolves according to general relativity and the cosmological principle.

1.2.1 Expansion of the Universe, from philosophy to modern science

Le rayon de l'Univers croît sans cesse. L'éloignement des nébuleuses extra-galactiques est un effet cosmique dû à l'expansion de l'espace. ⁵

Georges Lemaître

Discussing the evolution of the philosophical, religious and scientific thinking on cosmology through human times could be the topic of an entire thesis. I will thus only present in a very subjective way a few steps that led to the current understanding of our Universe as a physical system which evolves under the laws of nature. As primitive civilisations as the Mesopotamian one considered around 2000 BC that one's daily life is part of a bigger world, created by divinities with some organisation around a privileged center: Babylon. Although this thinking is linked to religious beliefs and mythological politics (the creation of Babylon), it clearly represents an attempt to understand the Universe as a whole, and hence, is part of cosmology. Actually, this kind of conception of the Universe as being built around one's every day experience survived for a very long time, for example through so-called geocentrism which is often exemplified by the Ptolemaic system. According to Ptolemaeus in the 2nd century, the Earth is at the center of the Universe around which celestial objects (including the Moon, the Sun, other planets of the solar system as well as stars) revolve following circular orbits (epicycles) whose centers themselves are revolving around the Earth (following so-called deferents). It is interesting to notice in Ptolemaeus's work a mix between ancient Greek philosophy, in particular from Aristotle, and a will to reconcile his cosmological model with early astronomical observations.⁶ Impressively, Ptolemaeus's system has been used for more than a thousand years, first by philosophers but also by astronomers to predict quite accurately the orbits of planets and stars in the visible sky, although it was challenged by specific observations.

The Scientific Revolution beginning in the 16th, arguably with Copernican heliocentrism, upset our understanding of the Universe. According to it, it is not the Earth but rather the Sun which is at the center of the Universe, and the Earth, just like other planets of the solar system, revolves around it. The apparent motion of celestial bodies in the sky is due to a combination of the orbits of the planets around the Sun, and of the Earth rotation on itself, while stars are located much further away. However,

⁵Translation: *The radius of the Universe is ever increasing. The distancing of extra-galactic nebulae is a cosmic effect due to the expansion of space.*

⁶Actually, placing the Earth close to the center of the Universe is motivated by the fact that almost exactly half of the stars are visible at a time from the ground: indeed otherwise, due to the finiteness of the Universe, there would be more stars on one side than on the other. Also, because of the apparent motion of planets viewed from the Earth, deviating from the projection of circles, Ptolemaeus introduced the notion of equant, a point displaced from the exact position of the Earth from which an observer would observe the epicycle's center to move with a constant velocity. In a similar spirit, the Earth is slightly displaced from the center of the Universe around which it revolves, in order to explain the difference in the duration of seasons. These provide clear examples of compromises between philosophical thinking (Aristotle's idea of purity could only be compatible with circular orbits) and astronomical constraints. Of course, we now understand these effects as due to the orbits of solar system's bodies being elliptic rather than circular, and the Earth revolving around the Sun rather than the opposite.

Copernicus's system kept elements from Ptolemaeus's cosmology, such as the circularity of orbits (though he did not use equants but rather a combination of epicycles), and did not prove to be scientifically more accurate than the latter. It was moreover contradicting many religious beliefs, including the Bible, and hence was not widely accepted by his contemporaries. The paradigm shifted with the 17th century and a new generation of scientists, including astronomers Kepler and Galileo who respectively introduced elliptical orbits and observed four moons of Jupiter with his newly invented telescope, providing the first proof that some bodies were not orbiting the Earth, and culminating in 1687 with the works of Isaac Newton on the universal law of gravitational attraction for massive bodies, and thus explaining Kepler's elliptical orbits. Astronomy and cosmology had then entered the field of natural sciences, with both theoretical predictions from the Newton's laws of gravity, and precise astronomical observations with telescopes. Although our understanding gradually got more and more accurate, one had to wait for general relativity to see another major shift in paradigm.

Indeed, although the Universe was less and less believed to be centered on our human experience (from Babylon to the Sun), it was mostly thought finite and static. But with general relativity accepted as an accurate theory to describe the motion of bodies in gravitational fields, it became evident in the 20th century that the Universe had to evolve. Actually, Einstein himself noted that a consequence of his field equations (1.6) was that the Universe itself could be evolving. Assuming this was impossible, and that the distribution of matter in the Universe should be (quasi-)static, he famously introduced the cosmological constant in general relativity in order to counter-balance this effect [133]. However the Einstein universe was unstable to perturbations, and Lemaître noticed in 1927 that depending on the value of the cosmological constant, the Universe could be expanding, leading to the now-called Friedmann-Lemaître-Robertson-Walker class of universes, and to the birth of the Big Bang theory [134]. Decisively, Hubble observed in 1929 [135] that distant galaxies were all receding from Earth. Calibrating their physical distance using Cepheid stars, and measuring the redshifting of their electromagnetic spectra, he was able to draw the first distance-redshift relation, see Fig. 1.4, a plot now called Hubble diagram. Assuming our solar system and our galaxy do not rest at a privileged place in the Universe, it implies that all galaxies are receding from each other, and the further they are the faster they recede. Only an expanding Universe as the one proposed by Lemaître can explain such an uniform and isotropic expansion of space. From then, cosmology is not merely the description of the Universe as a static and absolute recipient in which events take place, but an attempt to describe the past and future evolution of the Universe as a physical system governed by the laws of nature.

1.2.2 Modern approach to cosmology

The cosmological principle and the Friedmann–Lemaître–Robertson–Walker metric

The modern, paradigmatic approach to cosmology, relies on the assumption that general relativity is a valid description of spacetime and gravitational effects, and on the validity

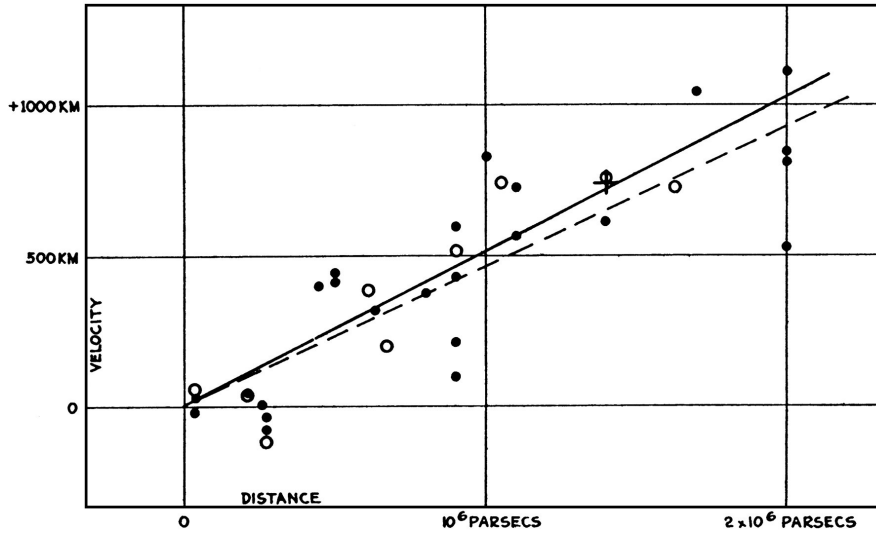


Figure 1.4: The first Hubble diagram, drawn by Hubble himself and taken from [135]. On the vertical axis is the velocity (in km/s) at which a given galaxy is receding from Earth as inferred with the redshifting of their electromagnetic spectra. On the horizontal axis is the distance to the galaxy (in parsecs, where $1 \text{ pc} \simeq 3.26 \text{ light-years} \simeq 3.09 \times 10^{19} \text{ m}$; for example the closest star to the Sun, Proxima Centauri, is located at 1.32 pc from the Sun), which could be computed using Cepheid stars as standard candles. The expansion is found to be happening at a constant rate $H_0 \simeq 500 \text{ (km/s)/Mpc}$, with a too large value by a factor of roughly seven compared to modern observations, mostly due to a lack of knowledge about Cepheid stars and thus errors in the distance calibration.

of

- The cosmological principle: on large enough scales, the Universe is homogeneous and isotropic.

The cosmological principle roughly states that the Universe is statistically equivalent for observers, wherever they are (homogeneity) and in whatever direction they are looking to (isotropy), once the small-scale structures have been averaged out. Hence it does not prevent from having local structures such as solar systems and galaxies, or even clusters of galaxies, filaments and walls in the galaxy distribution, etc., but simply states that when viewed from far enough away, homogeneity and isotropy should be recovered in a statistical way. Although simple, this statement has important consequences for the theoretical modelling of cosmology. In particular, it strongly constrains the possible forms of the spacetime metric on large scales, leading to the Friedmann–Lemaître–Robertson–Walker (FLRW) class of universes which can be described on large scales by the eponymous metric:

$$ds^2 = -dt^2 + a^2(t) \left[\frac{dr^2}{1 - kr^2} + r^2 (d\theta^2 + \sin(\theta)^2 d\varphi^2) \right], \quad (1.9)$$

where spherical coordinates (r, θ, φ) instead of Cartesian ones (x, y, z) were used to describe the spatial part of the metric. The parameter k can be understood as the Gaussian curvature of the three-dimensional space and is only constrained to be constant by the cosmological principle. In particular, it can be positive and corresponding to a spherical space, negative and corresponding to a hyperbolic space, or vanishing and corresponding to a flat space, and only astronomical observations can tell us about the value of this spatial curvature. The function $a(t)$ is called the scale factor and describes the expansion of space as time passes, that is the expansion of the Universe as observed first by Hubble. Note that the scale factor is well-defined up to an irrelevant factor which is often chosen such that the current scale factor is unity, $a_0 = 1$.

Fluid description of the matter content, and Friedmann equations

Now suppose that the matter content of the Universe can be described by a collection of perfect fluids labelled by (α) , where parentheses explicit that these are not spacetime indices (and thus their upper or lower position has no physical meaning and changes only for convenience), then the total stress-energy tensor can be written as

$$T_{\mu\nu} = \sum_{(\alpha)} (\rho_{(\alpha)} + P_{(\alpha)}) u_{\mu}^{(\alpha)} u_{\nu}^{(\alpha)} + P_{(\alpha)} g_{\mu\nu}. \quad (1.10)$$

Bearing in mind a large-scale description of the Universe, which should be homogeneous, the energy densities $\rho_{(\alpha)}$, pressures $P_{(\alpha)}$ and individual velocities $u_{\mu}^{(\alpha)}$ should be considered functions of time only. Isotropy has also been already taken into account by not

allowing an anisotropic stress tensor $\Pi_{\mu\nu}^{(\alpha)}$ in Eq. (1.10).⁷ The total stress-energy tensor can be written as the one of a single fluid, $T_{\mu\nu} = (\rho + P)u_\mu u_\nu + Pg_{\mu\nu}$ where

$$\rho = \sum_{(\alpha)} \rho_{(\alpha)}, \quad P = \sum_{(\alpha)} P_{(\alpha)}, \quad \text{and} \quad u_\mu u_\nu = \sum_{(\alpha)} \frac{\rho_{(\alpha)} + P_{(\alpha)}}{\rho + P} u_\mu^{(\alpha)} u_\nu^{(\alpha)}.$$

Here, u_μ represents the total 4-velocity of the fluid and is very constrained on large scales by homogeneity, isotropy, the conservation of stress-energy tensor and the normalisation $u_\mu u^\mu = -1$: it can only read $u_\mu = (1, 0, 0, 0)$ in the basis (t, x, y, z) . Writing the 0–0 and i – j components of the Einstein equations (1.6) for this system (the 0– i component is trivially vanishing for a homogeneous and isotropic universe on large scales), yields the famous Friedmann equations of cosmology:

$$\boxed{H^2 + \frac{k}{a^2} = \frac{\rho}{3M_{\text{Pl}}^2} + \frac{\Lambda}{3} \quad \text{and} \quad \left(2\frac{\ddot{a}}{a} + H^2 + \frac{k}{a^2}\right) = -\frac{P}{M_{\text{Pl}}^2} + \Lambda,} \quad (1.11)$$

where $H(t) = \dot{a}/a$ is the instantaneous rate of growth⁸ of the scale factor in cosmic time units t (a dot represents a derivative with respect to t), called the Hubble parameter. The current value of the Hubble parameter, H_0 , is called the Hubble factor and describes the expansion of the local universe, it was first computed by Hubble using his diagram as explained in the caption of Fig. 1.4.

In order to understand the expansion of the Universe depending on its matter content, it will prove useful to define the equation-of-state parameter of a fluid as the ratio between its pressure and its energy density, $w_{(\alpha)} = P_{(\alpha)}/\rho_{(\alpha)}$. One can also define an equation of state for the effective fluid filling the Universe, as $w = P/\rho = \sum_{(\alpha)} w_{(\alpha)} \frac{\rho_{(\alpha)}}{\rho}$. Note also that the cosmological constant, which was introduced as a possible operator in the Lagrangian describing the gravitational sector of the theory, can be understood phenomenologically in (1.11) as a perfect fluid with $\rho_\Lambda = -P_\Lambda = \Lambda M_{\text{Pl}}^2$ corresponding to a constant equation of state $w_\Lambda = -1$. From now on, one will thus treat the cosmological constant as such perfect fluid and assume that it was taken into account when defining the total effective fluid, which concretely will amount to forgetting Λ in the Friedmann equations (1.11). One shall also define the critical energy density of the Universe at a given time as $\rho_c = 3H^2 M_{\text{Pl}}^2$, and the energy density parameter of the Universe as $\Omega = \rho/\rho_c$. The first Friedmann equation can thus be rewritten as:

$$\Omega = 1 + \frac{k}{a^2 H^2}, \quad (1.12)$$

⁷However note that isotropy only requires that the sum of all the anisotropic stress tensors, $\Pi_{\mu\nu} = \sum_{(\alpha)} \Pi_{\mu\nu}^{(\alpha)}$ is vanishing. Individual ones can be non-vanishing but compensating each other, providing an interesting cosmological scenario.

⁸Mathematically speaking, one has no clue on whether H is positive or negative since it only appears squared in the Friedmann equations. However, observations tell us that the Universe is expanding rather than contracting, at least from the beginning of inflation which is expected to happen around the first 10^{-35} s after the Big Bang. For a review on bouncing cosmologies inspired by a quantum gravity framework, where a contracting phase takes place before inflation, see, *e.g.*, Ref. [136].

where it is evident that a deviation of the energy density parameter Ω from unity should be interpreted as a sign of spatial curvature. Another way to describe spatial curvature would be to notice that it behaves as a perfect fluid with equation of state $w_k = -1/3$, and incorporate it in ρ as explained for the cosmological constant. Note that by combining the two Friedmann equations, one can get the second derivative of the scale factor, $\ddot{a}$, as

$$\frac{\ddot{a}}{a} = -\frac{\rho}{6M_{\text{Pl}}^2} (1 + 3w) , \quad (1.13)$$

where one can already note that the expansion is accelerated if and only if $w < -1/3$. The Friedmann equations explain how the Universe evolves depending on its matter content, but not how the matter content evolves in an expanding Universe. As one shall see now, this information is rather encoded in the continuity equations, and explains the various possible expansion histories depending on which species dominate the energy budget in the Universe.

Continuity equation in cosmology, and the dilution of species

Assuming that the different species in the Universe do not interact otherwise than gravitationally, the continuity equation for the total stress-energy tensor, Eq. (1.8), which should always hold because of the Bianchi identities of general relativity, can hold true for every individual stress-energy tensor: $\nabla_\mu T_{(\alpha)}^{\mu\nu} = 0$. Conversely, the non-conservation of the individual stress-energy tensors can be understood as inter-species interactions $Q_{(\alpha)\leftrightarrow(\beta)}^\nu$, a formalism that is explained at length and used to treat novel scenarios of reheating in Part IV of this manuscript. The individual continuity equations yield:

$$\dot{\rho}_{(\alpha)} = -3H\rho_{(\alpha)} (1 + w_{(\alpha)}) , \quad (1.14)$$

which can be solved exactly using that $d\rho_{(\alpha)}/\rho_{(\alpha)} = 3(1 + w_{(\alpha)}) da/a$ and assuming the equation of state $w_{(\alpha)}$ is constant, giving:

$$\rho_{(\alpha)} = \rho_{(\alpha),0} \left(\frac{a}{a_0} \right)^{-3(1+w_{(\alpha)})} . \quad (1.15)$$

Thus any fluid satisfying $w_{(\alpha)} > -1$ is diluting as the Universe expands and a grows bigger. But crucially, the exponent of the power law depends on the exact value of the equation-of-state parameter and thus different species dilute at different paces. Some examples of perfect fluids are:

- a potential fluid (such as the cosmological constant, or a scalar field sitting at the minimum of its classical potential, or the quantum 0-mode of such scalar field) with $w_V = -1$;
- a fluid with $w_k = -1/3$ such as the fictitious fluid describing the spatial curvature of the Universe;

- a pressureless matter fluid (describing non-relativistic particles such as baryonic matter and cold dark matter) with $w_{\text{m}} = 0$;
- a radiation fluid (describing relativistic particles, photons) with $w_{\text{r}} = 1/3$;
- a kinetic fluid (known as a fluid with a stiff equation of state, it can describe the kinetic part of a scalar field) with $w_{\text{K}} = 1$.

Table 1.2.2 summarizes the power-law dilution of species depending on their equations of states (eos), as well as the subsequent time evolution of the scale factor $a(t)$ if the Universe is dominated by only of them (meaning that $\exists(\alpha)$, $\rho \simeq \rho_{(\alpha)}$ and thus $w \simeq w_{(\alpha)}$) as can be found using the Friedmann equations which then give $a(t) \propto t^{\frac{2}{3(1+w)}}$ for $w \neq -1$ and $a(t) \propto e^{Ht}$ if $w = -1$.

eos $w_{(\alpha)}$	power-law dilution	expansion law if (α) dominates
-1	$\rho_{\text{V}} = \rho_{\text{V},0}$	$a(t) \propto \exp\left(\sqrt{\frac{\rho_{\text{V}}}{3M_{\text{Pl}}^2}}t\right)$
-1/3	$\rho_{\text{k}} = \rho_{\text{k},0} (a/a_0)^{-2}$	$a(t) \propto t$
0	$\rho_{\text{m}} = \rho_{\text{m},0} (a/a_0)^{-3}$	$a(t) \propto t^{2/3}$
1/3	$\rho_{\text{r}} = \rho_{\text{r},0} (a/a_0)^{-4}$	$a(t) \propto t^{1/2}$
1	$\rho_{\text{K}} = \rho_{\text{K},0} (a/a_0)^{-6}$	$a(t) \propto t^{1/3}$

Table 1.1: For each species described by a perfect fluid with constant equation of state (eos) $w_{(\alpha)}$, the power-law dilution due to the expansion of space is shown together with the scaling law of evolution of the scale factor if this species comes to dominate the energy budget of the Universe.

Λ CDM concordance model of cosmology

Knowing this, one can rewrite the first Friedmann equation in an even other way:

$$\begin{aligned} \frac{H^2(a)}{H_0^2} = & \Omega_{V,0} + \Omega_{k,0} \left(\frac{a}{a_0}\right)^{-2} + \Omega_{m,0} \left(\frac{a}{a_0}\right)^{-3} + \Omega_{r,0} \left(\frac{a}{a_0}\right)^{-4} + \Omega_{K,0} \left(\frac{a}{a_0}\right)^{-6} \\ & + \sum_{(\alpha), \text{ others}} \Omega_{(\alpha),0} \left(\frac{a}{a_0}\right)^{-3(1+w_{(\alpha)})}, \end{aligned} \quad (1.16)$$

where $\Omega_{(\alpha),0}$ is the current value of the partial density parameter $\Omega_{(\alpha)} = \rho_{(\alpha)}/\rho_c$. Note that Ω_k can either be defined as ρ_k/ρ_c with $\rho_k = -3kM_{\text{Pl}}^2/a^2$ if spatial curvature is understood in the total energy density ρ , or as $1 - \Omega$ where Ω is the total energy density parameter deviating from unity due to spatial curvature, see Eq. (1.12). Either way, $\Omega_k = -k/(a^2 H^2)$ deviates from 0 only if there is some spatial curvature. Of course, taking into account $\Omega_{k,0}$, the sum of all partial density parameters are constrained to equal one. The cosmological redshift z can be introduced as another possible time parameter, with $1 + z = a_0/a$, and Eq. (1.16) can be rewritten as $H^2(z)/H_0^2$.

In the so-called Λ CDM (Λ , Cold Dark Matter) model of cosmology, the matter content of the Universe is supposed to be composed of only baryons and cold dark matter ($w_m = 0$), and a cosmological constant Λ ($w_V = -1$). Radiation is neglected, as the current photon density parameter was computed to be $\Omega_{\gamma,0} \simeq 5.38 \times 10^{-5}$ thanks to measurements of the current CMB black-body temperature, $T = (2.72548 \pm 0.00057)$ K for the most recent computation [137] using combined results from several experiments. A complication arises when taking into account neutrinos which first contribute effectively as radiation when they are relativistic, typically at the time of CMB emission and before that, and then reach a non-relativistic regime because of their non-vanishing masses (at a redshift z_{NR} that depends on the exact value of these masses m_ν) from when they should be treated as pressureless matter. Hence the above quoted result for $\Omega_{\gamma,0}$ is actually equivalent to the radiation density parameter $\Omega_{r,0}$ only nowadays, but it cannot be used to represent all radiation for redshifts $z > z_{\text{NR}}$, where it should be effectively supplemented by the neutrino contribution: $\Omega_{r,0}^{\text{eff}} = \left(1 + N_{\text{eff}} \frac{7}{8} \left(\frac{4}{11}\right)^{4/3}\right) \Omega_{\gamma,0}$ with N_{eff} the effective number of relativistic neutrino species. Spatial curvature is allowed and results in a possibly non-zero partial density parameter Ω_k .

By measuring the $H^2(z)/H_0^2$ law in our local universe (*i.e.* at relatively low redshifts where visible matter is already organised in galaxies which cluster and form filaments, walls, etc.), and by studying the statistics of the Cosmic Microwave Background (CMB) and Baryons Acoustic Oscillations (BAO) in the early universe, one can find the best-fit parameters for the current energy budget in the Universe. Using CMB data (temperature, polarization and lensing maps) combined with BAO measurements, the Planck

collaboration in 2018 [138] found the following cosmological parameters:⁹

$$\begin{aligned}
 \Omega_{V,0} &= 0.6889 \pm 0.0056, \\
 \Omega_{k,0} &= 0.001 \pm 0.002 \implies \rho_0 = \rho_{c,0} (1 - 0.001 \pm 0.002), \\
 \Omega_{m,0} &= 0.3111 \pm 0.0056 \text{ where } \Omega_{m,0} = \Omega_{b,0} + \Omega_{cdm,0} \text{ with} \\
 \Omega_{b,0} &= 0.0492 \pm 0.0006 \text{ and } \Omega_{cdm,0} = 0.2619 \pm 0.0051, \\
 100\theta_* &= 1.04101 \pm 0.00029, \sigma_8 = 0.8102 \pm 0.0060 \text{ and } \tau = 0.0561 \pm 0.0071, \\
 N_{\text{eff}} &= 2.99 \pm 0.17 \text{ and } \sum_{\nu} m_{\nu} < 0.12 \text{ eV}, \\
 A_s &= (2.105 \pm 0.029) \times 10^{-9}, n_s = 0.9665 \pm 0.0038 \text{ and } r < 0.07. \\
 H_0 &= (67.66 \pm 0.42) \text{ (km/s)/Mpc}
 \end{aligned} \tag{1.17}$$

where the distinction between baryons ($\Omega_{b,0}$) and cold dark matter ($\Omega_{cdm,0}$) was made in the pressureless matter sector. The angular acoustic scale of BAO θ_* , the optical depth τ of reionisation and the amplitude of matter fluctuations σ_8 were also introduced, together with the parameters describing the dimensionless primordial spectra: the amplitude A_s and spectral index n_s of the scalar sector, as well as the tensor-to-scalar ratio r measuring the amount of power in tensor modes compared to scalar ones. Note that interestingly, there seems to be no spatial curvature to day, corresponding thus to flat space. As will be reviewed in Chapter 3, the fact that the current energy density of the Universe is so close to the critical energy density can be understood as a necessary fine-tuning of the initial conditions to the usual radiation and matter-dominated epochs (for which $\Omega = 1$ constitutes a repulsive point in the language of dynamical attractors), which motivates the introduction of inflation as taking place in the very early phases of the cosmological history. Also, the current energy budget of the Universe is dominated by a cosmological constant (but not since a long time), and most of the matter contribution comes from cold dark matter rather than baryonic one. Indeed, the observable baryonic matter that composes galaxies, stars and the gas in between, only represent 4.9% of the total current energy density. About neutrinos, the displayed central value for N_{eff} is in agreement with latest Standard Model calculations of neutrino flavour oscillations and primordial nucleosynthesis, giving a value of 3.044 [139], and the upper limit on the sum of their masses, is one of the most stringent ever found. Primordial scalar perturbations are small on CMB scales, with a root mean square of roughly 4.6×10^{-4} , and the scalar power spectrum is close to being scale invariant (which would correspond to $n_s = 1$), but with scale invariance excluded at almost 9σ . Primordial tensor modes are not observed, but their dimensionless power spectrum is constrained to be smaller than the scalar one by a factor of 7% at least.

A great success of modern cosmology is that observations of very different kinds, probing the Universe at multiple redshifts, are compatible with the same values of the

⁹I roughly estimated myself the central value and uncertainties for $\Omega_{b,0}$ and $\Omega_{cdm,0}$ given their values in h^{-2} units, where $h = H_0 / (100 \text{ km/s)/Mpc}$, and the central values and uncertainties for H_0 and $\Omega_{m,0}$, hence the displayed values might deviate slightly from more rigorous analyses. Uncertainties are given at a 68% confidence level while upper bounds are given at a 95% one.

cosmological parameters, hence the name “concordance model of cosmology”. In the following paragraph, I briefly mention a few notable exceptions which trigger intensive research works contemporary to the work presented in this thesis.

A few clouds on the horizon

The Hubble tension is likely to be the biggest trouble for the Λ CDM model. Indeed, the value of the Hubble factor H_0 differs depending on if it is probed in the early universe with CMB and BAO observations, $H_0 = (67.66 \pm 0.42)$ (km/s)/Mpc from Planck 2018, or in the local universe with, *e.g.* Cepheid stars, $H_0 = (74.03 \pm 1.42)$ (km/s)/Mpc from the most recent result of the SH0ES collaboration [140], which corresponds to a statistical tension of 4.4σ . Importantly, this discrepancy is generic to probes in the early and late universe, independently of CMB maps and Cepheid stars: it also exists between the values for H_0 found with BAO combined with Big Bang Nucleosynthesis (BBN) constraints on one side [141] (early), and with lensing time delays by the H0LiCOW collaboration [142] (late). This indicates that the Hubble tension could be due to a physical effect taking place in the Universe rather than systematic errors in the data analysis of CMB or Cepheid stars. If this tension is confirmed in the coming years to be a clear-cut incompatibility between the two values, new physics beyond the Λ CDM model would be required to explain it, which constitutes in itself a very exciting prospect.

In the same spirit, one should also note the slight tension between the σ_8 value from Planck and early universe physics on one side, $\sigma_8 = 0.8102 \pm 0.0060$, and the one inferred from the local universe on the other side, for example $\sigma_8 = 0.78 \pm 0.01$ from Sunyaev–Zeldovich cluster counts [143] and $\sigma_8 = 0.783 \pm 0.023$ from the DES weak-lensing survey [144]. This tension of more than 2σ is another topic of research currently receiving attention. Several ideas have already been proposed to explain this variation of the best-fit values for H_0 and σ_8 , including modifications of early and late universe physics compared to the current cosmological paradigm, but it is not the aim of the current manuscript to review them.

One shall also mention the current debate amongst cosmologists about the spatial curvature of the Universe. It was pointed out that, although the CMB data combined with BAO is compatible with a spatially flat universe to a high level of accuracy, the CMB temperature and polarisation data alone prefer a negative $\Omega_{k,0}$ parameter with a vanishing value excluded at roughly 2.5σ , corresponding to a positively curved space (see, *e.g.* Refs. [145,146]). If the trustworthiness of the CMB data alone to probe spatial curvature is debated (the Planck team itself seems to believe this slight preference for a closed universe is a result of systematic errors), it is at least fair to say that there is a statistical tension between the result from CMB maps of temperature and polarisation on one side, and the one from CMB lensing, BAO and other probes on the other side, which all indicate a spatially flat Universe.

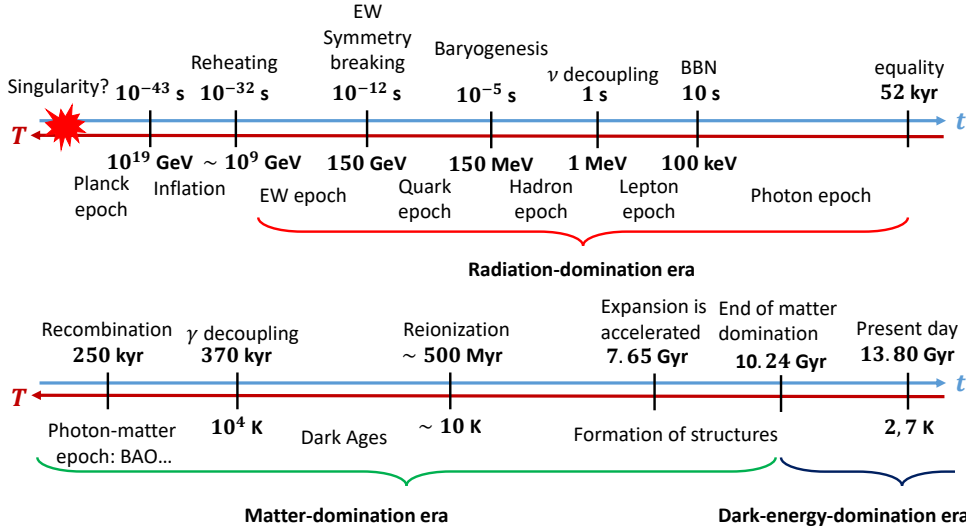


Figure 1.5: Schematic timeline of the universe as depicted in this section.

1.2.3 A brief reverse history of 13.8 billion years

Or in other words, why does disorder increase in the same direction of time as that in which the universe expands?

Stephen Hawking

This section is devoted to a brief review of the major cosmological eras and important dates in the history of the universe, from very early phases when inflation is likely to take place, up to the current dark-energy dominated epoch. A schematic timeline of the important steps in the cosmic evolution, is represented in Fig. 1.5. However, in the spirit of cosmologists being archaeologists of the cosmos, I chose to present the cosmic history following a reverse arrow of time (but increasing redshift and temperature), mainly for Hawking to turn over in his grave as the entropy of the (told) Universe will be decreasing while you read this paragraph.

The current, glacial cosmic era: a dark-energy-dominated universe

Since the observations of Hubble, humans know that they live in an expanding Universe. However it seems that the expansion of the Universe does not happen at a constant pace, and the famous Hubble-Lemaître law of the receding of galaxies depending on their distances, $v = H_0 d$, is only valid at a fixed redshift, *i.e.* for a short range of distances. This should not come as a surprise, as any law is locally linear. Actually, a major outcome of modern cosmology, is the simultaneous discovery of the acceleration of the expansion of the Universe by two independent teams, the Supernova Cosmology Project [147] led by Perlmutter and the High-Z Supernova Search Team led by Riess and Schmidt [148].

The two teams used Type-Ia Supernovae: white dwarfs are expected to explode when they reach a fixed critical mass, which results in a known absolute luminosity and thus distance, once calibrated with Supernovae at known distances. Knowing both the distance luminosity D_L and the redshift of their electromagnetic spectra z , one can draw a Hubble diagram $D_L(z)$ which is determined theoretically by the Friedmann equation in the form $H(z)$, depending on the values of the cosmological parameters. What both teams found is that the best-fit values correspond to a flat space, $\Omega_{k,0} = 0$, with a cosmological constant dominating the energy budget: $\Omega_{V,0} = 0.68$ and $\Omega_{m,0} = 0.32$. Even though recent experiments came up with more precise measurements of the cosmological parameters, the conclusion that the Universe is expanding in an accelerated way, and that this expansion is due to a form of “dark energy” (because it corresponds neither to matter nor it is visible) consistent with a cosmological constant, has not changed ever since.

Assuming that the Universe is spatially flat, that radiation is negligible, and that the cosmological parameters take the values found by Planck 2018,¹⁰ one can infer the redshift at which the expansion stops being accelerated, and the Universe becomes dominated by matter rather than dark energy. Indeed, then (we choose $a_0 = 1$ here) $H(a) = H_0 \sqrt{\Omega_{m,0} a^{-3} + \Omega_{V,0}}$ has a non-trivial solution

$$a(t) = (\Omega_{m,0}/\Omega_{V,0})^{1/3} \sinh^{2/3}(t/t_V) \simeq \begin{cases} (\Omega_{m,0}/\Omega_{V,0})^{1/3} (t/t_V)^{2/3} & \text{if } t \ll t_V, \\ (\Omega_{m,0}/4\Omega_{V,0})^{1/3} \exp\left(\frac{2t}{3t_V}\right) & \text{if } t \gg t_V, \end{cases}$$

that interpolates between the two regimes (see Table 1.2.2, and note that $2/(3t_V) = \sqrt{\rho_V/3M_{Pl}^2}$), where $t_V = 2/(3H_0\sqrt{\Omega_{V,0}}) = 2/\sqrt{3\Lambda}$, the second equality being valid only if dark energy is due to a cosmological constant Λ .

The transition between matter-domination and vacuum-energy-domination thus proceeds at a time t_Λ such that $a(t_\Lambda) = a_\Lambda = (\Omega_{m,0}/\Omega_{V,0})^{1/3} = 0.77$, corresponding to a redshift $z_\Lambda = 0.30$ and a time $t_\Lambda = 10.24$ Gyr. Note however that this transition is far from being instantaneous. In particular, it is possible to compute the time at which the expansion of the universe begins to be accelerating, t_{acc} , by solving $\ddot{a}(t_{acc}) = 0$. One finds that $\sinh^2(t_{acc}/t_V) = 1/2$, so that $a_{acc} = (\Omega_{m,0}/2\Omega_{V,0})^{1/3} = 0.61$, $z_{acc} = 0.65$ and $t_{acc} = 7.65$ Gyr. We also find *en passant* the current age of the Universe t_0 by solving the equation $a(t_0) = a_0 = 1$ which gives $t_0 = t_V \times \operatorname{argsinh}(\sqrt{\Omega_{V,0}/\Omega_{m,0}}) = 13.80$ Gyr. Thus, the expansion has been accelerated for the last 6.15 Gyr even though there has been more dark energy than matter in the energy budget of the Universe for “only” 3.56 Gyr. Note that all these estimates neglected the time spent before matter domination, but as one shall see in the next paragraph, this assumption is well motivated.

¹⁰This choice is made in order to keep a consistent set of cosmological parameters, even though the correct value of the Hubble constant H_0 is likely to be more precise when inferred from more direct, local Universe measurements. If one uses the value of H_0 which is larger according to other experiments like SH0ES, one would find all transition times to be (sometimes significantly) smaller than the ones quoted in this paragraph.

During dark-energy-domination, the cosmic web made of galaxies and dark matter clusters has evolved under the competing effects of gravity and the expansion of space, new galaxies were born and others have stopped producing stars, but the Universe has roughly been the same for these long billion years, hence justifying the name of glacial cosmological era.

The birth of stars and galaxies: a matter-dominated universe

The diversity of physical phenomena taking place in the matter-dominated universe, is much richer. But first it should be said that matter domination is not the earliest cosmological era, contrary to what would suggest the Λ CDM model. Indeed, although the relative quantity of radiation is nowadays negligible, it is mainly because it redshifts much faster (a^{-4}) than pressureless matter (a^{-3}), hence the ratio ρ_r/ρ_m grows as $1/a = 1+z$ as we dig down in the past of our Universe. At some point, radiation should come to dominate the energy budget, just like matter was dominating before its energy density decreased lower than the cosmological constant's one at $t_\Lambda \leftrightarrow a_\Lambda \leftrightarrow z_\Lambda$. The time of transition between radiation and matter domination is called the equality and it can be found by solving the equation $a(t_{\text{eq}}) = a_{\text{eq}}$ where $a_{\text{eq}} = \Omega_{r,0}^{\text{eff}}/\Omega_{m,0} = 2.93 \times 10^{-4}$ giving $z_{\text{eq}} = 3412$ (note that the much more precise analysis of Planck 2018 quotes the value $z_{\text{eq}} = 3387 \pm 21$ which is very close to the simple estimate I made, and that taking into account neutrinos in $\Omega_{r,0}^{\text{eff}} \simeq 9.10 \times 10^{-5}$ is crucial in order to get a correct value), which corresponds to a time $t_{\text{eq}} = 51.7$ kyr.¹¹

So, after roughly 50 thousand years, the Universe begins to be dominated by matter, which we know is now composed at 84.2% of dark matter and only at 15.8% of baryonic matter. But still for hundreds of thousands of years, radiation perturbations play a crucial role as they keep interacting with the baryonic nuclei. Photons keep ionizing unstable atoms made of protons and electrons and being produced by electron capture: $H + \gamma = p^+ + e^-$. These pressure interactions, counterbalanced by gravity, lead to oscillations in the primordial plasma made of photons, baryons and leptons, the so-called Baryon Acoustic Oscillations (BAO). Although photons do not interact directly with dark matter, these oscillations create gravitational potential wells in which the dark matter particles eventually collapse diffusely, following in the steps of the baryon-photon fluid. But this dance stops with recombination, when the temperature of the Universe has decreased to a point that the photons in the bath are not energetic enough to ionize atoms that inevitably form. But those newly stable atoms are often formed in a higher energy configuration than the ground state to which they must relax by emitting new photons which are now free from interactions. This process is nothing but decoupling, the physical source of the Cosmic Microwave Background. Importantly, after decoupling the

¹¹For this estimate of the age of the Universe at equality and following ones, I used the cosmology calculator of the International Center of for Radioastronomy Research (ICRAR) available online at the following link: <https://cosmocalc.icrar.org/>, consistently using the cosmological parameters displayed above and used in previous calculations of this manuscript. Indeed only few of the freely available calculators take into account the radiation energy density and provide cosmic time for a given redshift at the kyr precision needed for this computation.

photons of the CMB are free-streaming, and they carry with them information about the Universe at the time of decoupling: temperature but also statistics of the perturbations. In particular, the acoustic peaks of the pressure waves in the primordial plasma, are clearly visible in the power spectrum of the CMB. In standard textbooks, it is shown that recombination and decoupling should happen around $z_{\text{rec}} \simeq 1370$ corresponding to $t_{\text{rec}} \simeq 250$ kyr and $z_{\text{dec}} \simeq 1090$ corresponding to $t_{\text{dec}} \simeq 370$ kyr, although realistically those processes should not be considered instantaneous.

Except the freely streaming photons of the CMB, very few light is present in the subsequent cosmological epoch, often called “Dark Ages”. Indeed, there is still no light source from gravitationally bound structures like stars, and only neutral hydrogen atoms occasionally release low-energy photons because of the spin-flip transition between the two hyperfine levels of energy of the hydrogen 1s ground state, leading to the so-called 21cm-hydrogen line. But matter structures begin to form. Indeed, because the Universe has become pressureless, matter perturbations that were feeling competing effects from gravity and pressure forces, now collapse at a much faster pace at locations where the density was only slightly higher than others. These seeds for large-scale overdensities and underdensities can already be seen in the CMB cold and hot spots. And because cold dark matter is not interacting otherwise than gravitationally, dark matter structures form earlier than the baryonic ones, forming halos in which baryons are then trapped, imprinting in particular the BAO scale on the large-scale structures. But those halos are diffuse, indeed because dark matter does not interact it does not thermalize, and only baryons are able to bind and form gas clouds from which the first stars emerge, in a local environment that becomes primitive galaxies. These first stars are believed to be born a few hundreds of millions of years after the Big Bang, and they eventually illuminate the Universe, bringing the Dark Ages to an end, and forming for the first time the heavy elements of the Periodic Table of Mendeleiev. Moreover, the ultraviolet photons released by the first, hydrogen-burning stars, are energetic enough to ionize the primitive, dense hydrogen clouds, a physical process known as reionization that can be probed by studying the Lyman series of energy transitions for neutral hydrogen atoms, absent in ionized ones. But due to the expansion of space, the Universe gradually cools and matter spreads out, and the ionized hydrogen mostly becomes neutral again.

By the end of matter domination and the beginning of the dark-energy-dominated epoch, the Universe looked a lot like the one we observe nowadays, with stars in galaxies and galaxies organized in clusters, filaments and walls in the great cosmic web.

The formation of elementary particles: a radiation-dominated universe

Except the tiny fraction of a second in the very early Universe, the first 52,000 thousand years of the cosmic history happen in the regime of radiation domination. At the onset of this cosmological epoch, particles are remains of the cosmological reheating taking place at the end of cosmic inflation.

Around 10^{-22} s after the Big Bang, the Universe is filled by a hot plasma at thermal equilibrium due to very efficient interactions, at an initial temperature of roughly 10^{14} GeV (or roughly 10^{27} K). At that time, the electroweak symmetry breaking is believed

not to have taken place yet, meaning that the masses of elementary particles have not yet been created by the Brout–Englert–Higgs mechanism, and that electromagnetic and weak forces are still unified and mediated by massless bosons. The electroweak symmetry breaking happens when the temperature of the Universe drops below roughly 10^{15} K, and from that time the well-known particles and forces of the Standard Model of particle physics are relevant. The quark epoch begins, with all the energy of the Universe stored in a plasma made of gluons, quarks, leptons and their antiparticles which interact very efficiently with each others, until the temperature dropped enough to allow the stability of the hadrons, made of quarks, leading to the so-called hadron epoch. In particular, the creation of baryons taking place at that time is a phenomenon called baryogenesis, and a big mystery of this epoch is the observed baryon–anti-baryon asymmetry. Indeed, baryons and anti-baryons initially annihilate each others but are also created in pairs by high-energy photons, until the point when photons were not energetic enough to produce these pairs of particles. Then, if baryons and anti-baryons were initially present in the same proportions, they should all annihilate to produce photons, and no baryons should be observed nowadays. However one does observe baryons (and not their antiparticles that were called anti-baryons), leading to an estimation of the relative baryon asymmetry of $\sim 10^{-10}$.

When almost all hadrons have annihilated with their antiparticles, they have created a huge amount of photons which now can only create lighter pairs: leptons and anti-leptons, leading to the lepton epoch. At that time, around 1 s after the Big Bang when the temperature of the Universe is of the order of the MeV (10^{10} K), neutrinos decouple from the rest of the particles, in a very similar fashion to the photon decoupling at 370 kyr. Indeed, neutrinos were coupled to the rest of the particles through weak interactions, whose strengths relative to the expansion rate of space are decreasing. When those interactions become negligible, nothing stops the neutrinos from free-streaming, leaving a relic radiation in the Universe called Cosmic Neutrino Background ($C\nu B$) that is yet to detect directly. The lepton epoch ends when the temperature has decreased so much that photons are not energetic enough to produce pairs of leptons and anti-leptons. Similarly to the end of the hadron epoch, almost all leptons annihilate with their anti-particles, leaving only photons and a small residue of leptons because of a slight lepton–anti-lepton asymmetry (that may be required to ensure the electric neutrality of the Universe). Then, the photon epoch begins with almost all the radiation-like energy in the form of photons which keep interacting strongly with the remaining relativistic particles until photon decoupling.

A crucial step in the cosmic history is Big Bang Nucleosynthesis (BBN), happening in the photon epoch when $T \sim 0.1$ MeV and around 2 min after the Big Bang, and during which light nuclei are created. Indeed, the Universe is still hot enough for the processes of nuclear fusion to take place, but has cooled enough to form stable nuclei: protons fuse with neutrons and form deuterium isotopes, which themselves fuse to form helium-4, and other nuclei are also formed in much smaller proportions (helium-3, lithium-7, etc.). Strikingly, the observed abundance of light elements in the Universe coincides very precisely with the predictions of BBN, making it likely the most robust probe of

the radiation-domination epoch.¹² BBN theory also enables one to compute the effective number of relativistic neutrino species, giving the value $N_{\text{eff}} = 3.044$ quoted above and in agreement with, *e.g.*, Planck 2018 observations. After a few minutes, almost all baryons are in bound nuclei and primordial nucleosynthesis is over.

The formed nuclei keep interacting with the overwhelming number of photons in the Universe for the next few hundreds of thousands of years, forming the Baryon Acoustic Oscillations that will later freeze at the time of photon decoupling during the matter-domination epoch. For completeness, one shall mention the possibility of Primordial Black Holes (PBH) formation during radiation domination, if huge overdensities exist on large scales, when they re-enter the growing comoving cosmic horizon and eventually collapse. Such black holes are expected to be much lighter than the ones formed by the collapse of heavy stars (and thus some of them should have evaporated by Hawking radiation much before our contemporary epoch), but the theoretical range of possible masses is extremely large and model-dependent, from a fraction of grams to dozens of solar masses. However, there is a growing number of astronomical observations that put tighter and tighter bounds on the maximum amount of PBH in the Universe and their allowed range of masses, and their detection is still to be confirmed.

The first fraction of seconds: a universe full of exotic particles during inflation and reheating

What happens before radiation domination can be understood as being at the frontier between knowledge and exploration. The elementary particles of the Standard Model might not be present at all, and the laws of physics were likely to be very different. That is why this epoch of the very early Universe is such an exciting topic of research: physicists need to build on the knowledge that is well known in other areas of physics (general relativity, quantum field theory, statistical physics, etc.), but also to explore new paths in order to understand better the building blocks of the laws of Nature in situations as extreme as the one of the baby Universe. Indeed, physical phenomena at that time happen at energies much higher than will ever be reached by terrestrial experiments, and there is no hope to reproduce them in a laboratory. Also, the initial conditions for this very early phase should probably be set by a quantum theory of gravity, when the typical energy was bigger than the Planck mass M_{Pl} .

Although one has no direct observation of the pre-radiation-domination epoch, the study of the CMB implies very important conclusions. In particular, one knows that the Universe has probably gone through a phase of accelerated expansion in its very early phases, similar to the dark-energy acceleration happening in our contemporary era. This epoch is known as cosmic inflation. Many more details about inflation are

¹²One exception to this is the so-called Lithium-7 anomaly, see *e.g.* Ref. [149], where it is reviewed that BBN predicts a primordial relative abundance compared to hydrogen that is ${}^7\text{Li}/\text{H} = (4.68 \pm 0.67) \times 10^{-10}$ while the observed primordial relative abundance is rather ${}^7\text{Li}/\text{H} = (1.58 \pm 0.31) \times 10^{-10}$, corresponding to an inconsistency larger than 5σ and therefore possibly more than a statistical error. Physicists are currently working on trying to explain the anomaly with new physics or independent astronomical observations.

given in Chap. 3, including the motivation for its introduction, its simplest incarnation by single-field chaotic models, and precise CMB constraints on the allowed models of single-field inflation. The limitations (mostly theoretical) of this simple picture are presented, and motivation is given for considering more complicated but perhaps more realistic, multifield models of inflation. These models and their phenomenological consequences constitute the main topic of research of the present thesis and are further explored in Chap. 4–6.

Most often, cosmic inflation must be completed by a transition epoch, called cosmological reheating, during which the scalar field(s) responsible for inflation, or at least the exotic particles of the very early Universe and their alleged forces, must decay and let the stage to the quark-gluon plasma and the strong and electroweak interactions of the Standard Model of particle physics. The usual single-field paradigm of cosmological reheating is reviewed in Chap. 7 and extended to the case of several interacting species in Chap. 8.

The arrow of time and the initial singularity

What happens before the Planck era, say in the first $1/M_{\text{Pl}} \sim 10^{-43}$ s, is purely speculative as one would expect general relativity to fail to describe gravity at those energy scales. A quantum theory of gravity would be required to describe phenomena happening at that time, and as is well known there is still no satisfactory such theory at the time of writing this thesis. A motivation for considering the quantum nature of spacetime at this epoch is the so-called initial singularity problem. Indeed, extrapolating the GR prediction, the scale factor must initially vanish, leading to an infinitely large energy density that one thinks of as unphysical, therefore showing as expected that GR should not be trusted in this regime but should rather be completed by a quantum theory. And indeed this problem could be overcome by a quantum theory of gravity, in a similar fashion than a quantum theory of electrodynamics enabled one to solve the issue of the infinitely large electric field at the boundary of the proton in the hydrogen atom. Some people would also wonder about what happens even before that, what happens before the Big Bang and our Universe is created. However this question probably does not make sense as before spacetime begins, there is no time, and hence no notion of “before”. That would be when the arrow of time ends, and according to Hawking’s thoughts, when the Universe was the least disordered, in a perfect organisation, for whatever this means: maybe just vacuum?

Chapter 2

Cosmological perturbation theory

After the long and general Chap. 1, this chapter is rather short and technical. Its aim is to present the tools and define the quantities, relevant for cosmological perturbation theory, that are used in the remaining of this manuscript. Since this topic is now well established in the cosmological community, the discussion presented here is simple and focused on what matters for early universe physics that is the subject of this thesis. For a comprehensive review of cosmological perturbation theory, I can only recommend reading Ref. [150].

The cosmological principle states that the Universe is homogeneous and isotropic *on very large scales*, but it does not prevent it from being inhomogeneous or anisotropic on smaller scales. Actually, observations of the local universe show that it is not homogeneous at all on small or intermediate scales: stars and planets are very dense objects surrounded by extremely diffuse gas, and so are individual galaxies. However when going to larger and larger scales, one observes the appearance of a regular pattern: the cosmic web of galaxies, made of filaments, walls and clusters, which is compatible with the cosmological principle. Thanks to observations of the CMB, one also knows that the early universe was not perfectly homogeneous. Indeed, even though the monopole radiation is dominant and corresponds to a black body radiation at a high level of precision, higher multipoles are clearly populated, indicating tiny but non-vanishing anisotropies in the primordial plasma. Cosmological perturbation theory is a tool to take into account the fact that the Universe is of the FLRW kind on large scales, but not on smaller ones. It however assumes that inhomogeneities are small and can be treated perturbatively, a description that breaks down when gravitational interactions eventually enter the so-called *non-linear regime* on small scales. Since this issue is more relevant for late-time cosmology than primordial cosmology, no more precise statement concerning the breakdown of the validity of cosmological perturbation will be made in this chapter, and one will only keep this limitation in mind in the following.¹

¹Note however that there can be mechanisms in the early universe that cosmological perturbation theory fails to describe comprehensively. Such violent, non-linear events, can happen *e.g.* in the context of preheating or of another inflationary instability, and is often transcribed as a production of particles. Examples of instabilities can actually be found in this manuscript, with a transient multifield inflationary

2.1 Perturbing spacetime

The spacetime metric of the Universe, $g_{\mu\nu}(x)$, is expanded around a spatially flat FLRW background described in units of conformal time τ (defined by $a d\tau = dt$), by $\bar{g}_{\mu\nu}(\tau)$ with $\bar{g}_{\mu\nu} dx^\mu dx^\nu = a^2(\tau) (-d\tau^2 + \delta_{ij} dx^i dx^j)$. One thus writes:

$$g_{\mu\nu}(x) = \bar{g}_{\mu\nu}(\tau) + \underbrace{\delta g_{\mu\nu}^{(1)}(x) + \frac{1}{2!} \delta g_{\mu\nu}^{(2)}(x) + \dots + \frac{1}{n!} \delta g_{\mu\nu}^{(n)}(x) + \dots}_{\delta g_{\mu\nu}(x)}, \quad (2.1)$$

where $\delta g_{\mu\nu}^{(n)}(x)$ is the perturbation at n^{th} order of the spacetime metric. Because $g_{\mu\nu}$ is symmetric and spacetime is four-dimensional, the spacetime metric of GR generically contains 10 degrees of freedom. With the cosmological principle that assumes homogeneity and isotropy, only one degree of freedom (and depending only on time) remains for the background FLRW metric $\bar{g}_{\mu\nu}(\tau)$ with no spatial curvature: the scale factor $a(\tau)$. However perturbations are not constrained by the cosmological principle, and thus one should naively expect 10 degrees of freedom (dof) in $\delta g_{\mu\nu}(x)$,² which can be decomposed into (1+3+6 dof):

$$\delta g_{00} = -2a^2 \phi, \quad \delta g_{0i} = a^2 B_i, \quad \delta g_{ij} = 2a^2 C_{ij}, \quad (2.2)$$

where C_{ij} is symmetric, and latin indices like $i \in \{1, 2, 3\}$, are used to denote spatial coordinates.

SVT decomposition

But those degrees of freedom are of different kinds: they can be further decomposed into scalar, transverse vector and transverse traceless tensor degrees of freedom. Even though the aim of this section is not to enter into geometrical details or describe the active and passive spacetime transformations, one shall recall here that scalars, vectors and tensors are not simply defined by their number of indices, but rather by how they transform under spacetime diffeomorphisms. This is described by the so-called Scalar-Vector-Tensor (SVT) decomposition generalizing the longitudinal-transverse decomposition of electromagnetic fields. According to it, a seemingly vectorial quantity with one index like B_i in δg_{0i} and containing three degrees of freedom, can be decomposed into one scalar B (1 dof) and one vector $\hat{B}_i$ (2 dof):

$$B_i = \hat{B}_i + \partial_i B, \quad \text{where } \partial^i \hat{B}_i = 0, \quad (2.3)$$

instability presented in Sec. 5.2 but where it is shown that perturbation theory still holds, and in Sec. 8.1 with the single-field preheating instability that is stopped by continuous decays of the scalar field to a cosmological fluid (reheating) before entering the non-linear regime.

²This statement is rigorously wrong in GR since perturbations are subject to so-called constraint equations that relate δg_{00} and δg_{0i} on one side to the perturbations of the matter content on the other side. This is better understood using the Arnowitt-Deser-Misner (ADM) formalism [151] as reviewed in Sec. 2.4. Moreover, 4 degrees of freedom are present only due to spurious gauge dependence as explained later, and should be removed. At the end, linearised GR in vacuum contains only 2 degrees of freedom: the two polarisations of gravitational waves γ_+ and $\gamma_\times$.

where $\hat{B}_i$ is now a true vector under spacetime diffeomorphisms, that is a transverse vector. Similarly for a seemingly tensorial quantity with two indices like C_{ij} in δg_{ij} and containing six degrees of freedom, which can be decomposed into two scalars ψ and E (1 dof each so 2 dof in total), one vector $\hat{E}_i$ (2 dof) and one tensor γ_{ij} (2 dof):

$$C_{ij} = -\psi\delta_{ij} + \partial_i\partial_j E + \partial_{(i}\hat{E}_{j)} + \frac{1}{2}\gamma_{ij}, \text{ where } \partial^i\hat{E}_i = 0 \text{ and } \partial^i\gamma_{ij} = 0 = \gamma_i^i, \quad (2.4)$$

where $\hat{E}_i$ is a transverse vector and γ_{ij} is a symmetric, transverse, traceless, rank-two tensor. Here, indices inside parentheses are understood as symmetrised: $\partial_{(i}\hat{E}_{j)} = \frac{1}{2}(\partial_i\hat{E}_j + \partial_j\hat{E}_i)$.

Note that until here it was possible to use perturbations including every order in perturbation theory. But in order to derive a closed set of equations, one should work consistently at a given fixed order in perturbation theory. The SVT decomposition that was shortly reviewed here, can actually be done at any order n in perturbation theory, both for $B_i^{(n)}$ and $C_{ij}^{(n)}$ as well as for other perturbed quantities in the matter sector. In the remaining of this chapter, one shall only derive expressions at linear order (but forgetting the upper index ⁽¹⁾ every where in order to avoid cluttered notations) that is most relevant for primordial universe physics. Higher-order terms might be needed to compute non-Gaussianities, but this is done specifically in Chap. 5 where it is necessary to do so. For example, keeping only linear terms and using the identity $g_{\mu\nu}g^{\nu\rho} = \delta_\mu^\rho$, the perturbed contravariant inverse metric can be written:

$$g^{00} = -a^{-2}(1 - 2\phi), \quad g^{0i} = a^{-2}\delta^{ij}B_j, \quad g^{ij} = a^{-2}(\delta^{ij} - 2\delta^{ik}\delta^{jl}C_{kl}), \quad (2.5)$$

The SVT decomposition is not only conceptually clearer because it enables one to manipulate only quantities whose geometrical properties are transparent, but it is also technically simpler: at the linear order, perturbations of different kinds are decoupled and *cannot* interact. Indeed, the linear EoM are found from the Lagrangian that is quadratic in those linear perturbations, and must be a scalar quantity. Therefore the only possible contractions are of the forms ϕ^2 , $\hat{B}^i\hat{B}_i$, $\gamma^{ij}\gamma_{ij}$, and mixings are not possible at all even when using spatial derivatives to contract, *e.g.*, a scalar and a vector (but a similar argument holds for the scalar-tensor and vector-tensor contractions with spatial derivatives): $\partial^i\phi\hat{B}_i = -\phi\partial^i\hat{B}_i + \partial^i(\phi\hat{B}_i) = 0$, where one has used the possibility to make integrations by parts in the Lagrangian and to dismiss total spatial derivatives, and used the transverse condition for true vectors: $\partial^i\hat{B}_i = 0$. Of course, this holds only true at the linear order of perturbation theory and perturbations of different kinds crucially mix at the non-linear order, thus enabling for example to have a matter source (beyond the ever-present vacuum contribution) of gravitational waves in the early universe even if it is solely filled with scalar fields, although beginning at second order in perturbation theory only.

2.2 Perturbing the matter content

The stress-energy tensor representing the matter content of the Universe, or equivalently the matter Lagrangian in the total action, can also be expanded perturbatively in small inhomogeneous quantities. In this section, one encounters the usual linear perturbations of a perfect fluid at the level of its stress-energy tensor, as well as the treatment of scalar fields with non-canonical kinetic terms at second order in covariant perturbations, as a warm-up for the subsequent topic of multifield inflation.

2.2.1 Perturbations of perfect fluids

The stress-energy tensor of a perfect fluid without anisotropic stress can be written non-perturbatively as $T_{\mu\nu} = (\rho + P) u_\mu u_\nu + P g_{\mu\nu}$, where ρ is the energy density, P is the pressure and u^μ is the timelike 4-velocity of the fluid. This covariant equation can now be perturbed, and the background value is:

$$\bar{T}_{\mu\nu} = a^2 (\bar{\rho} + \bar{P}) \delta_{\mu 0} \delta_{\nu 0} + \bar{P} \bar{g}_{\mu\nu} = a^2 \text{Diag} (\bar{\rho}, \bar{P}, \bar{P}, \bar{P})_{\mu\nu} , \quad (2.6)$$

where one used the fact that $\bar{u}_\mu = f(\tau) \delta_{\mu 0}$ for homogeneity and isotropy at the background level, and that $u_\mu u^\mu = -1$ non-perturbatively, which gives $\bar{u}_\mu = -a \delta_{\mu 0}$ (the minus sign is only a convention meaning that this 4-vector is oriented towards the future and not the past).

Moreover at the linear level one can define $\delta\rho$, δP , δu^μ as:

$$\delta T_{\mu\nu} = a^2 (\delta\rho + \delta P) \delta_{\mu 0} \delta_{\nu 0} - 2a (\bar{\rho} + \bar{P}) \delta_{0(\mu} \delta u_{\nu)} + \delta P \bar{g}_{\mu\nu} + \bar{P} \delta g_{\mu\nu} , \quad (2.7)$$

where one used the fact that the perturbed stress-energy tensor should be symmetric and thus that $\delta(u_\mu u_\nu) = 2\bar{u}_{(\mu} \delta u_{\nu)}$ at the linear level. But note that δu_μ is further constrained by $u_\mu u^\mu = -1$ which fixes $\delta u_0 = -\frac{a^3}{2} \delta g^{00} = -a\phi$. However the spatial part δu_i of the perturbed 4-velocity is not constrained and can be decomposed into a scalar v and a transverse vector $\hat{v}_i$ according to the SVT decomposition:

$$\delta u^\mu = \frac{1}{a} (-\phi, \delta^{ij} v_j) , \text{ with } v_i = \partial_i v + \hat{v}_i \text{ and where } \partial^i \hat{v}_i = 0 . \quad (2.8)$$

Note that then $\delta u_\mu = \bar{g}_{\mu\nu} \delta u^\nu + \delta g_{\mu\nu} \bar{u}^\nu = a (-\phi, v_i + B_i)$, and that the perturbation of the stress-energy tensor with one index up and one down simply reads:

$$\delta T^0_0 = -\delta\rho , \delta T^i_0 = -(\bar{\rho} + \bar{P}) \delta^{ij} v_j , \delta T^0_i = (\bar{\rho} + \bar{P}) (v_i + B_i) \text{ and } \delta T^i_j = \delta P \delta^i_j . \quad (2.9)$$

At the end, a perfect fluid without anisotropic stress contains two background dof, $\bar{\rho}$ and $\bar{P}$, as well as three scalar perturbative dof, $\delta\rho$, δP and v and one vector dof $\hat{v}_i$. An anisotropic stress π_{ij} could be added in the perturbed stress-energy tensor (at the level of the background, it should vanish, or at least the sum of all the anisotropic stresses of the fluids in the universe should vanish), resulting in more scalar, vector and tensor dof in the perturbations, according to the SVT decomposition. Neutrinos in

cosmology constitute an example of species that can sometimes be treated as a perfect fluid whose perturbations contain an anisotropic stress. Moreover, in some cases it is relevant to study perfect fluids which have a constant equation of state $w = P/\rho$ at the non-perturbative level. Then the fluid has only one background dof ρ and two scalar perturbative dof $\delta\rho$ and v , as well as one vector $\hat{v}_i$. But the constancy of the equation of state can also hold true only at the background level. Then the background equation of state $\bar{w} = \bar{P}/\bar{\rho}$ is different from the speed of sound of the fluids' fluctuations $c_s^2 = \bar{P}'/\bar{\rho}'$, where a prime denotes a derivative with respect to conformal time τ .

This description of the perturbations of perfect fluids should be completed by the description of the interactions amongst those fluids. Indeed, although the sum of all the individual stress-energy tensors should be conserved, $\nabla_\mu T^{\mu\nu} = 0$, each individual fluid (α) can exchange energy and momentum if $\nabla_\mu T^{\mu\nu}_{(\alpha)} = Q^\nu_{(\alpha)} \neq 0$. Of course, a requirement is that $\sum_{(\alpha)} Q^\nu_{(\alpha)} = 0$. But this topic is presented at length in Part IV that treats the cosmological reheating and more particularly in Sec. 9.1, and thus no more detail will be given here and the interested reader is referred to this part of the manuscript.

Of course, another interesting extension is the study of perturbations of perfect fluids beyond the linear order, but since there is no application of this formalism in the present thesis, one will avoid unnecessary definitions, notations and equations.

2.2.2 Covariant perturbations of scalar fields

For the first time in this manuscript, one writes the covariant Lagrangian of non-linear sigma models in cosmology, which are composed of a certain number N_{field} of scalar fields $\phi^I(x)$ that interact both through potential terms in $V(\phi)$ and through kinetic terms due to the *a priori* non-trivial field-space metric $G_{IJ}(\phi)$:

$$\mathcal{L}_{\text{NLMS}} = - \left[\frac{1}{2} g^{\mu\nu} G_{IJ}(\phi) \partial_\mu \phi^I \partial_\nu \phi^J + V(\phi) \right]. \quad (2.10)$$

Note that the metric G_{IJ} can be used to define distances in field space, as $d\sigma^2 = G_{IJ} d\phi^I d\phi^J$. If G_{IJ} is non-trivial, then the field-space manifold can be understood as being curved, in a very similar fashion to the fact that spacetime is curved when its metric $g_{\mu\nu}$ is non-trivial. Thus any relevant geometrical quantity to describe the field space can be constructed out of G_{IJ} , such as the Riemann curvature tensor, the Ricci scalar curvature, the Weyl tensor, the Kretschmann scalar, etc. A notion of field-space covariance also exists, and a general effort of this thesis has been to use final expressions that are always explicitly covariant under field-space redefinitions. This includes but is not limited to, the use of field-space, and sometimes phase-space, covariant derivatives (with respect to time or to the scalar fields themselves), efforts to combine derivatives of G_{IJ} as Riemann terms and their covariant derivatives, and the introduction of covariant perturbations of the scalar fields (and momenta), see below. A particular emphasis on field-space covariance is given in my works about multifield stochastic inflation in Chap. 7.

This issue of field-space covariance can be understood by noting the similarity with spacetime covariance. Just like x^μ are coordinates in spacetime (and not a vector, the

letter μ is only a label for several scalar quantities $x^1, x^2, \dots$), ϕ^I are coordinates in field space (and not a vector, the letter I is only a label for several scalar quantities $\phi^1, \phi^2, \dots$). Then, quantities $\propto dx^\mu$ like the 4-velocity $u^\mu = dx^\mu/|ds|$ are spacetime vectors, and quantities $\propto d\phi^I$ like $\dot{\phi}^I = d\phi^I/dt$ are vectors of the field space. However in a curved manifold, simple derivatives of covariant vectors are not covariant quantities themselves. For example, $du^\mu/|ds| = -\Gamma^\mu_{\nu\rho} u^\nu u^\rho$ from the geodesic equations of GR, involves the product of the covariant vectors u^ν and u^ρ with the non-covariant Christoffel symbols $\Gamma^\mu_{\nu\rho}$ and thus is not covariant. Similarly, $\ddot{\phi}^I = d\dot{\phi}^I/dt$ is not covariant and a notion of field-space covariant, time derivative can be defined as

$$D_t \dot{\phi}^I = \ddot{\phi}^I + \Gamma^I_{JK} \dot{\phi}^J \dot{\phi}^K. \quad (2.11)$$

At the level of the background, the scalar fields $\bar{\phi}^I(t)$ should be homogeneous, hence the background action simply reads

$$\bar{\mathcal{L}}_{\text{NLSM}} = \left(\bar{G}_{IJ} \dot{\bar{\phi}}^I \dot{\bar{\phi}}^J / 2 - \bar{V} \right), \quad (2.12)$$

where $\bar{G}_{IJ} = G_{IJ}(\bar{\phi})$ and $\bar{V} = V(\bar{\phi})$ are functions of the background fields only.

To go further one needs to expand the action, and thus the scalar fields, in small perturbations:

$$\phi^I(x) = \bar{\phi}^I(t) + \underbrace{\delta\phi^I_{(1)}(x) + \frac{1}{2!}\delta\phi^I_{(2)}(x) + \dots + \frac{1}{n!}\delta\phi^I_{(n)}(x) + \dots}_{\delta\phi^I(x)} \quad (2.13)$$

However, as already mentioned, extra care should be given to the covariance of these perturbative quantities, more particularly in the case of such scalar fields living on a non-trivial field-space manifold described by the metric G_{IJ} . And actually, beyond the linear order $\delta\phi^I_{(1)}(x)$ which is indeed a covariant vector in field space, the higher-order perturbations $\delta\phi^I_{(n)}(x)$ for $n > 1$ are not covariant quantities alone. To see this, the argument of Ref. [57] is quickly reviewed here, and an extension to covariant perturbations in phase space is presented in Sec. 7.2 with our article [5]. The problem of defining covariant perturbations stems from the fact that $\bar{\phi}^I(t)$ and $\phi^I(x)$ are different points in field space and thus that their difference truncated at a given order in perturbation theory is not necessarily a true vector. Because these two points are infinitesimally close, there is a unique geodesic $\phi^I_{\text{geo}}(\lambda)$ parameterised by a dimensionless number λ that connects them, and where $\phi^I_{\text{geo}}(\lambda = 0) = \bar{\phi}^I(t)$ and $\phi^I_{\text{geo}}(\lambda = \epsilon) = \phi^I(x)$ with $\epsilon \ll 1$ a small number. One can then expand $\phi^I_{\text{geo}}(\lambda)$ in $\lambda \leq \epsilon \ll 1$ as:

$$\phi^I_{\text{geo}}(\lambda) = \bar{\phi}^I(t) + \underbrace{\lambda \frac{d\phi^I_{\text{geo}}}{d\lambda} \Big|_{\lambda=0}}_{\tilde{Q}^I} + \frac{1}{2!} \lambda^2 \frac{d^2\phi^I_{\text{geo}}}{d\lambda^2} \Big|_{\lambda=0} + \dots, \quad (2.14)$$

where one identified $\tilde{Q}^I$, a vector of the tangent field space at the point $\bar{\phi}^I(t)$, which must by definition be a field-space covariant vector. Now, since $\phi^I_{\text{geo}}(\lambda)$ follows a geodesic of

the field space, it must verify the geodesic equation, that is $D_\lambda (d\phi_{\text{geo}}^I/d\lambda) = 0$ where D_λ is the field-space covariant derivative with respect to λ defined in the same way than the time derivative above. Hence $d^2\phi_{\text{geo}}^I/d\lambda^2 = -\Gamma^I_{JK} (d\phi_{\text{geo}}^J/d\lambda) (d\phi_{\text{geo}}^K/d\lambda)$, and evaluating Eq. (2.14) at $\lambda = \epsilon \ll 1$, one eventually finds:

$$\delta\phi^I(x) = \bar{\phi}^I(t) + Q^I - \frac{1}{2}\Gamma^I_{JK}Q^JQ^K + \dots, \quad (2.15)$$

where the tangent vectors $\tilde{Q}^I$ were rescaled by incorporating consistently factors of ϵ in the covariant perturbations $Q^I = \epsilon\tilde{Q}^I$. From this expression, it is clear that although $\delta\phi_{(1)}^I(x) = Q^I$ is a covariant perturbation, $\delta\phi_{(2)}^I(x) = -\Gamma^I_{JK}Q^JQ^K$ is not, and that one should rather use directly the covariant field perturbations Q^I in order to manipulate only equations that are explicitly covariant. This argument can be extended to any order n in perturbation theory, for which $\delta\phi_{(n)}^I(x)$ can always be obtained as a sum of products of the covariant field perturbations Q^I .

Although the linear and quadratic Lagrangians in the covariant field perturbations Q^I could already be straightforwardly derived, they are better understood when simplified after the use of the background equations of motion verified by the homogeneous fields $\bar{\phi}^I(t)$, a subject that is left for Chap. 4 and more particularly Sec. 4.2 about the dynamics of multifield inflation. One shall now move to the subject of gauge freedom and the definitions of gauge-invariant quantities.

2.3 Gauge freedom and gauge-invariant quantities

2.3.1 Generalities

Gauge freedom can be understood as the result of the introduction of spurious degrees of freedom due to an arbitrary identification between spacetime points, on the background manifold $\bar{\mathcal{M}}$ described by the background metric $\bar{g}_{\mu\nu}$ on one hand, and on the true, perturbed manifold $\mathcal{M}$ described by the full metric $g_{\mu\nu}$ on the other hand. Technically, perturbed quantities like $\rho(x)$ (or equivalently $\delta\rho(x)$) are defined at a spacetime point $x \in \mathcal{M}$ that needs not coincide with the spacetime point $\bar{x} \in \bar{\mathcal{M}}$ at which the background energy density $\bar{\rho}(\bar{x})$ is defined.³ The bijection $i : \bar{\mathcal{M}} \rightarrow \mathcal{M}$ that identifies $\bar{x}$ to $x = i(\bar{x})$ is called a gauge choice and is not unique, indeed any other bijection i' defining $x' = i'(\bar{x})$ from $\bar{x}$ would be equally valid. Going from a gauge i to another gauge i' is called a gauge transformation, and perturbed quantities must not have the same numerical value in different gauges. This ambiguity is problematic since one would like to identify uniquely the value of a physical quantity such as the energy density of a fluid, and therefore the gauge should be fixed once for all, or equivalently only quantities that are invariant under a gauge transformation should be used. Those quantities are called *gauge invariant* and play a major role in our understanding of modern cosmology.

³Here one voluntarily confuses a spacetime point p with its coordinates $x(p)$ in order to simplify the introduction of the gauge freedom, see a few lines below for a more rigorous approach.

Without entering into the details of active and passive gauge transformations (see Ref. [152] for a comprehensive and rigorous approach), it is worth knowing the basics of their properties in order to understand the laws of transformation of physical quantities defined in the previous sections of this chapter. Consider a gauge transformation generated by the vector field $\xi^\mu = (T, \delta^{ij} \partial_j L)$, where $L_i = \partial_i L + \hat{L}_i$ is split in a scalar L and a vector $\hat{L}_i$ which verifies $\partial^i \hat{L}_i = 0$. The 4-vector $\xi^\mu = \sum_{(n)} \xi_{(n)}^\mu / (n!)$ thus contains at every order in perturbation theory 4 dof, 2 of which being independent scalar modes $T_{(n)}$ and $L_{(n)}$ and 2 others in a vector mode $\hat{L}_{i,(n)}$. In the so-called active approach, any spacetime covariant, tensorial quantity X with any number of indices, is transformed under the effect of the vector field ξ^μ that displaces a point p to another point q , as [152, 153]

$$X \longrightarrow \tilde{X} = e^{\mathcal{L}_\xi} X, \text{ where } \mathcal{L}_\xi \text{ is the Lie derivative with respect to } \xi^\mu. \quad (2.16)$$

When applied to the (scalar) spacetime coordinates x^μ , one finds the law of transformation from $x^\mu = x^\mu(p)$ the coordinates of p , to $\tilde{x}^\mu = x^\mu(q)$ the coordinates of q :

$$\tilde{x}^\mu = x^\mu + \xi_{(1)}^\mu \Big|_{x(p)} + \frac{1}{2!} \left(\xi_{(1),\nu}^\mu \xi_{(1)}^\nu + \xi_{(2)}^\mu \right) \Big|_{x(p)} + \dots \quad (2.17)$$

Now a different question could be, what are the new coordinates x'^μ such that the description with coordinates x' after the gauge transformation is equivalent to the one with coordinates x before the gauge transformation. Technically, one is looking for a chart x' such that $\forall p \in \mathcal{M}, x'^\mu(q) = x^\mu(p)$ where q is the image of p under the active gauge transformation. Reverting the above expression of $x^\mu(q)$ as a function of $x^\mu(p)$, and expressing every quantity at the new point q , one finds the following relation between the two sets of coordinates:

$$x'^\mu(q) = x^\mu(q) - \xi_{(1)}^\mu \Big|_{x(q)} + \frac{1}{2!} \left(\xi_{(1),\nu}^\mu \xi_{(1)}^\nu - \xi_{(2)}^\mu \right) \Big|_{x(q)} + \dots \quad (2.18)$$

This equation is the basis of the passive approach, that enables one to compute how tensorial quantities are transforming under a change of coordinates from x^μ to x'^μ . Although the passive approach might seem more intuitive, the active approach is more efficient to compute the effect of gauge transformations beyond linear order. One can now compute how scalars, vectors and tensors change under the gauge transformation ξ^μ , at any order in perturbation theory.

2.3.2 Spacetime

To keep the discussion simple, one focuses here only on the linear order and finds from the Lie derivative of the metric that reads $\mathcal{L}_\xi g_{\mu\nu} = g_{\mu\nu,\rho} \xi^\rho + g_{\mu\rho} \xi^\rho_{,\nu} + g_{\rho\nu} \xi^\rho_{,\mu}$, the

transformation of spacetime perturbations as

$$\begin{aligned}
\tilde{\phi} &= \phi + \mathcal{H}T + T', \\
\tilde{\psi} &= \psi - \mathcal{H}T, \\
\tilde{B} &= B - T + L', \\
\tilde{E} &= E + L, \\
\tilde{B}_i &= \hat{B}_i + \hat{L}'_i, \\
\tilde{E}_i &= \hat{E}_i + \hat{L}_i, \\
\tilde{\gamma}_{ij} &= \gamma_{ij},
\end{aligned} \tag{2.19}$$

where $\mathcal{H} = a'/a = aH$ is the conformal Hubble parameter.

It is clear from these formulae that naive metric perturbations are not gauge-invariant quantities, except the symmetric, transverse traceless tensor γ_{ij} . However, it is possible to construct combinations of those metric perturbations that are invariant under gauge transformations. In particular, it is straightforward to see that the following quantities are gauge invariant:

$$\begin{aligned}
\tilde{\Phi} &= \phi - \mathcal{H}\sigma - \sigma', \\
\tilde{\Psi} &= \psi + \mathcal{H}\sigma, \\
\hat{\sigma}_i &= \hat{E}'_i - \hat{B}_i,
\end{aligned} \tag{2.20}$$

where $\sigma = (E' - B)$ is the shear potential (and transforms as $\tilde{\sigma} = \sigma + T$) and $\hat{\sigma}_i$ is the shear vector, and that together with γ_{ij} they form a family of six perturbative degrees of freedom. Ψ and Φ are two gauge-invariant scalar dof, sometimes called the Bardeen potentials to refer to the early work [154], and note that any combination of them should also be a gauge-invariant quantity. $\hat{\sigma}_i$ is a gauge-invariant vector composed of two dof and γ_{ij} is still a transverse traceless tensor composed of two dof. Note that requiring the use of gauge-invariant quantities effectively reduced the number of degrees of freedom from 10 to 6, in particular two scalar dof and one vector with two dof were suppressed. This should not come as a surprise, since the arbitrary vector field ξ^μ exactly carries those degrees of freedom.

2.3.3 Matter content

Although this is best understood using the ADM formalism (see Sec. 2.4 below), the scalar and vector gauge-invariant perturbations defined in Eq. (2.20) are actually constrained to be proportional to perturbations of the matter content in the Universe. Thus in vacuum, they should vanish, and only the tensorial degrees of freedom γ_+ and $\gamma_\times$ of the two polarisations of gravitational waves, can propagate. But in cosmology spacetime is assumed to be filled with cosmological fluids, scalar fields or any other medium which is responsible for the expansion of the Universe, and this matter content must have inhomogeneous components that mix with spacetime perturbations. Here one shall see how

the most used matter perturbations transform at linear order under a gauge transformation, and how they can be used with metric perturbations to define gauge-invariant quantities.

First, it can be shown that the four-scalars $\delta\rho$ and δP of perfect fluids transform under ξ^μ as:

$$\begin{aligned}\widetilde{\delta\rho} &= \delta\rho + \bar{\rho}'T, \\ \widetilde{\delta P} &= \delta P + \bar{P}'T.\end{aligned}\tag{2.21}$$

Writing the active gauge transformation of the four-velocity $u_\mu = a[-(1+\phi), v_i + B_i]$, and using the law of transformation of B and $\hat{B}_i$ that was found above, one finds:

$$\begin{aligned}\tilde{v} &= v - L', \\ \tilde{\hat{v}}_i &= \hat{v}_i - \hat{L}'_i.\end{aligned}\tag{2.22}$$

The only gauge-invariant quantity (and combinations thereof) that one can construct only from matter perturbations is the so-called non-adiabatic pressure perturbation:

$$\delta P_{\text{nad}} = \delta P - c_s^2 \delta\rho, \quad \text{where } c_s^2 = \bar{P}'/\bar{\rho}'.\tag{2.23}$$

The remaining of matter perturbations can only be gauge invariant once combined with spacetime perturbations. Scalar quantities like $\delta\rho$ and δP can be combined for example with the shear σ , or the spatial perturbation ψ , or the combination $V = v + B$ (that transforms as $\tilde{V} = V - T$) which allows us to define the following gauge-invariant quantities:

$$\begin{aligned}\delta\rho^{(\text{gi})} &= \delta\rho - \bar{\rho}'\sigma, \\ \delta\rho^{\text{flat}} &= \delta\rho + \bar{\rho}'\frac{\psi}{\mathcal{H}}, \\ \delta\rho^{\text{com}} &= \delta\rho + \bar{\rho}'V,\end{aligned}\tag{2.24}$$

where the subscript “gi” stands for gauge-invariant, and other ones shall become clear soon, and similarly for the pressure perturbation δP . For the velocity potential v and vector $\hat{v}_i$, one finds the following gauge-invariant variables:

$$\begin{aligned}v^{(\text{gi})} &= V + \sigma = v + E', \\ \hat{V}_i &= \hat{v}_i + \hat{B}_i.\end{aligned}\tag{2.25}$$

One can also define

$$\begin{aligned}v^\Psi &= V - \psi/\mathcal{H} = v^{(\text{gi})} - \Psi/\mathcal{H}, \\ \hat{v}_i^{(\text{gi})} &= \hat{V}_i + \hat{\sigma}_i = \hat{v}_i + \hat{E}'_i,\end{aligned}\tag{2.26}$$

as useful combinations of previously defined gauge-invariant perturbations.

The covariant perturbations of scalar fields Q^I transform under a change of gauge like other spacetime, scalar quantities:

$$\tilde{Q}^I = Q^I + \bar{\phi}'^I T, \quad (2.27)$$

and thus can be used to define gauge-invariant quantities only when mixing with space-time perturbations, just like $\delta\rho$:

$$\begin{aligned} Q_{(\text{gi})}^I &= Q^I - \bar{\phi}'^I \sigma, \\ Q_{\text{flat}}^I &= Q^I + \bar{\phi}'^I \frac{\psi}{\mathcal{H}}, \\ Q_{\text{com}}^I &= Q^I + \bar{\phi}'^I V. \end{aligned} \quad (2.28)$$

2.3.4 Popular gauges and relations with gauge-invariant variables

Although it is possible to perform calculations without picking a particular choice of gauge $(T, L, \hat{L}_i)$, simply by identifying and using only gauge-invariant perturbations as the ones presented in the previous subsection, it is often more convenient to first fix a gauge and then identify perturbations in this gauge with the usual gauge-invariant quantities. A few examples of gauges and such relations are presented below, where one recalls that two scalars and one vector can be arbitrarily fixed to zero for simplicity.

Longitudinal gauge

The longitudinal gauge (in which quantities are denoted with a label ℓ) is defined by a vanishing shear $\sigma_\ell = 0$ and spatial perturbation $E_\ell = 0$ (which further fixes $B_\ell = 0$). It can be obtained from an initially arbitrary definition of the perturbations $(E, B, \sigma \text{ etc.})$ by the choice $T_\ell = -\sigma$ and $L_\ell = -E$. In this gauge, scalar quantities like $\delta\rho$, Q^I and v now read:

$$\begin{aligned} \delta\rho_\ell &= \delta\rho - \bar{\rho}' \sigma = \delta\rho^{(\text{gi})}, \\ Q_\ell^I &= Q^I - \bar{\phi}'^I \sigma = Q_{(\text{gi})}^I, \\ v_\ell &= v + E' = v^{(\text{gi})}, \end{aligned} \quad (2.29)$$

where one clearly sees that scalar perturbations in this gauge coincide with the gauge-invariant scalar perturbations with the label (gi) that were defined above. The longitudinal gauge can be completed by choosing the vector part $\hat{L}_i^\ell$ such that either $\hat{B}_i^\ell = 0$ or $\hat{E}_i^\ell = 0$.

In the first case where $\hat{B}_i^{\ell-\text{Poisson}} = 0$, called the Poisson gauge, one finds $\hat{L}_i^{\ell-\text{Poisson}} = -\int \hat{B}_i d\tau + \hat{C}_i(x^j)$ where $\hat{C}_i$ is an arbitrary constant (in conformal time) vector of integration that can depend on the spatial position x^j . In this longitudinal-Poisson gauge, vectors like the fluid velocity $\hat{v}_i$ read:

$$\hat{v}_i^{\ell-\text{Poisson}} = \hat{v}_i + \hat{B}_i = \hat{V}_i, \quad (2.30)$$

where one recognizes the gauge-invariant velocity vector perturbation $\hat{V}_i$ defined above. Note that rigorously, to completely fix the gauge ambiguity, one should choose once and for all the value of the constant $\hat{C}_i$.

In the second case where $\hat{E}_i^{\ell-\text{mixed}} = 0$ (I must confess I do not know the name of such a gauge, let it be called longitudinal-mixed gauge), one finds $\hat{L}_i^{\ell-\text{mixed}} = -\hat{E}_i$ and thus in this gauge the fluid velocity reads:

$$\hat{v}_i^{\ell-\text{mixed}} = \hat{v}_i + E'_i = \hat{v}_i^{(\text{gi})}, \quad (2.31)$$

where in the second equality one has identified the gauge-invariant velocity $\hat{v}_i^{(\text{gi})}$.

Moreover in these longitudinal gauges the remaining spacetime perturbations

$$\begin{aligned} \phi_\ell &= \phi - \mathcal{H}\sigma + \sigma' = \Phi, \\ \psi_\ell &= \psi + \mathcal{H}\sigma = \Psi, \end{aligned} \quad (2.32)$$

coincide with the two Bardeen potentials, and $\hat{B}_i^{\ell-\text{mixed}} = \hat{B}_i - \hat{E}'_i = -\hat{\sigma}_i$ is the opposite of the shear vector that was defined above, while $\hat{E}_i^{\ell-\text{Poisson}} = \hat{E}_i - \int \hat{B}_i d\tau + \hat{C}_i = \int \hat{\sigma}_i d\tau$ corresponds to its integrated value over conformal time.

Flat gauge

The flat gauge corresponds to flat spatial hypersurfaces, that means $\psi_{\text{flat}} = 0 = E_{\text{flat}}$ and $\hat{E}_i^{\text{flat}} = 0$. This gauge is obtained from an initially arbitrary set of perturbations by the following gauge transformations: $T_{\text{flat}} = \psi/\mathcal{H}$, $L_{\text{flat}} = -E$ and $\hat{L}_i^{\text{flat}} = -\hat{E}_i$. Scalar quantities like $\delta\rho$ and Q^I in this gauge indeed coincide with the gauge-invariant variables defined as $\delta\rho^{\text{flat}}$ and Q_{flat}^I in Eqs. (2.24) and (2.28), and one notices *en passant* that scalar quantities in the flat and longitudinal gauges are related by formulae similar to $\delta\rho^{\text{flat}} = \delta\rho^{(\text{gi})} + (\bar{\rho}'/\mathcal{H})\Psi$. Moreover, the velocity perturbations of a fluid read

$$\begin{aligned} v_{\text{flat}} &= v + E' = v^{(\text{gi})}, \\ \hat{v}_i^{\text{flat}} &= \hat{v}_i + \hat{E}'_i = \hat{v}_i^{(\text{gi})}. \end{aligned} \quad (2.33)$$

One already sees the redundancy of some gauges, as for example the velocity potential v reads the same in the longitudinal and flat gauges, or the velocity transverse vector $\hat{v}_i$ in the longitudinal-mixed and flat gauges. To be complete, one quotes the values of the remaining spacetime perturbations in the flat gauge as

$$\begin{aligned} \phi_{\text{flat}} &= \phi + \psi + \left(\frac{\psi}{\mathcal{H}}\right)' = \Phi + \Psi + \left(\frac{\Psi}{\mathcal{H}}\right)', \\ B_{\text{flat}} &= -\psi/\mathcal{H} - \sigma = -\Psi/\mathcal{H}, \\ \hat{B}_i^{\text{flat}} &= -\hat{\sigma}_i. \end{aligned} \quad (2.34)$$

Comoving orthogonal gauge

The comoving orthogonal gauge is the one in which the scalar and vector velocity of matter vanishes, $v_{\text{com}} = 0 = \hat{v}_i^{\text{com}}$, and the scalar part of the momentum of matter $v_i + B_i$ vanishes too: $v_{\text{com}} + B_{\text{com}} = 0$.⁴ It is obtained from an arbitrary initial set of perturbations by the following transformation: $T_{\text{com}} = v + B$, $L_{\text{com}} = \int v d\tau + C$ and $\hat{L}_i^{\text{com}} = \int \hat{v}_i d\tau + \hat{C}_i$, where C and $\hat{C}_i$ are scalar and vector constants of integration.

Scalar quantities like $\delta\rho$ and Q^I in this gauge indeed coincide with the gauge-invariant variables defined as $\delta\rho^{\text{com}}$ and Q_{com}^I in Eqs. (2.24) and (2.28), and one notices *en passant* that scalar quantities in the comoving gauge can be related to their values in the longitudinal and flat gauges by formulae similar to $\delta\rho^{\text{com}} = \delta\rho^{(\text{gi})} + \bar{\rho}' v^{(\text{gi})} = \delta\rho^{\text{flat}} + \bar{\rho}' v^\Psi$, where $v^{(\text{gi})}$ and v^Ψ were defined in Eqs. (2.25) and (2.26).

The scalar spacetime perturbations read in the comoving orthogonal gauge:

$$\begin{aligned}\phi_{\text{com}} &= \phi + \mathcal{H}V + V' = \Phi + \mathcal{H}v^{(\text{gi})} + v^{(\text{gi})'}, \\ \psi_{\text{com}} &= \psi - \mathcal{H}V = \Psi - \mathcal{H}v^{(\text{gi})}, \\ \sigma_{\text{com}} &= E' + v = v^{(\text{gi})} \implies E_{\text{com}} = \int d\tau v^{(\text{gi})} + C,\end{aligned}\tag{2.35}$$

where

$$\boxed{\psi_{\text{com}} = -\mathcal{H}v^\Psi \equiv \mathcal{R}}\tag{2.36}$$

is often called the comoving curvature perturbation and is widely used in modern cosmology. For completeness, the vector perturbation in this gauge is $\hat{B}_i^{\text{com}} = \hat{B}_i + \hat{v}_i = \hat{V}_i$.

Uniform density gauge

In the uniform density gauge, the perturbations of the matter energy density vanish, meaning that $\delta\rho_{\text{uni}} = 0$ and corresponding to $T_{\text{uni}} = -\delta\rho/\bar{\rho}'$ for an arbitrary initial set of perturbations. This uniquely fixes the truly scalar perturbations such as ψ which reads in this gauge:

$$\boxed{\psi_{\text{uni}} = \psi + \mathcal{H}\frac{\delta\rho}{\bar{\rho}'} = \mathcal{H}\frac{\delta\rho_{\text{flat}}}{\bar{\rho}'} \equiv -\zeta},\tag{2.37}$$

and where ζ is called the curvature perturbation on uniform energy density hypersurfaces, and is also widely used in modern cosmology. Note that the two curvature perturbations ζ and $\mathcal{R}$ are related at linear order by the simple relation:

$$\zeta = -\mathcal{R} - \mathcal{H}\frac{\delta\rho_{\text{com}}}{\bar{\rho}'},\tag{2.38}$$

and it can be shown from the linearized Einstein equations that $\delta\rho_{\text{com}}$ vanishes in the long-wavelength (super-Hubble) limit, hence $\zeta \underset{k \ll aH}{\sim} -\mathcal{R}$ for these scales.

⁴Actually, if the matter content of the universe is a single scalar field $\phi = \bar{\phi} + Q$, then the velocity of matter (which starts at linear order in perturbations) is proportional to the field perturbation Q , $v = -Q/\bar{\phi}'$. Therefore in that case, the comoving gauge in which $v_{\text{com}} = 0$ corresponds to the gauge in which one has $Q_{\text{com}} = 0$.

The uniform density gauge only fixes T , one of the two scalar gauge dof, but there remains both L and $\hat{L}_i$ the scalar and vector dof of the spatial part of the gauge transformation, that can be fixed arbitrarily. Other perturbations in these gauges can be found, but since they are not so much used, they are not quoted here.

Other gauges such as the synchronous gauge, the total matter gauge, the Newtonian gauge, and others, can also be useful, but they are not reviewed here since they were not used during my thesis. I hope the material presented in this section is comprehensive enough that any one can now use their preferred gauges and gauge-invariant quantities without misunderstanding the notion of gauge invariance: $\Phi, \Psi, \mathcal{R}, \zeta$, etc. can always be defined, but they coincide with different spacetime and matter perturbations in different gauges.

2.4 ADM formalism and constraint equations

Another possible parameterisation of the spacetime metric of GR with a matter content beyond the homogeneous case, corresponds to the Arnowitt-Deser-Misner (ADM) formalism. It is best suited for a perturbation theory defined at the level of the action rather than the Einstein equations, and does not require a fluid description of the matter content. It rather relies on a foliation of spacetime in spatial hypersurfaces as described in the early works [151, 155]. Because it is used at several instances in this thesis, more or less in an exhaustive way, it is introduced in a rather short manner in the following, only in order to understand how the constraint equations reduce the effective number of propagating degrees of freedom.

Generalities

Instead of the naive parameterisation of spacetime perturbations of Eq. (2.2), the invariant 4-dimensional length element is written non-perturbatively as

$$ds^2 = -N^2 d\tilde{t}^2 + h_{ij}(dx^i + N^i d\tilde{t})(dx^j + N^j d\tilde{t}), \quad (2.39)$$

where $\tilde{t}$ is an arbitrary time parameter and h_{ij} is the three-dimensional metric of spatial hypersurfaces. The inverse (symmetric) metric $g^{\mu\nu}$ can be found exactly and reads:

$$g^{00} = -\frac{1}{N^2}, \quad g^{0i} = g^{i0} = \frac{N^i}{N^2} \quad \text{and} \quad g^{ij} = h^{ij} - \frac{N^i N^j}{N^2}, \quad (2.40)$$

with h^{ij} the inverse of the spatial metric. The lapse N and the shift N^i are at the heart of the ADM formalism as they tell how to move forward in time from one spatial hypersurface to the next one, while the spatial metric h_{ij} contains all the dynamical degrees of freedom. And indeed the constraint equations will show that neither N nor N^i are dynamical, and that they must be proportional to quantities derived from the matter Lagrangian $\mathcal{L}_m$. In order to see this at the level of the action, which is expressed as

$$S = \int \sqrt{-g} d^4x \left(M_{\text{Pl}}^2 \frac{R}{2} + \mathcal{L}_m \right), \quad (2.41)$$

one first needs to use the so-called Gauss-Codazzi relations that enable one to express the 4-dimensional scalar curvature R as a function of the intrinsic curvature $R^{(3)}$ and the extrinsic curvature K_{ij} and its trace $K = h^{ij}K_{ij}$, of the spatial hypersurfaces (see, *e.g.*, Ref. [156]). These relations give:

$$R = R^{(3)} + K_{ij}K^{ij} - K^2 + \text{boundary terms}, \quad (2.42)$$

with $K_{ij} = \frac{1}{N} \left(\nabla_{(i} N_{j)} - \frac{1}{2} \frac{\partial h_{ij}}{\partial t} \right),$

and where ∇_i is the spatial covariant derivative consistently defined with the metric on spatial hypersurfaces h_{ij} . Here, boundary terms in the form of total derivatives were forgotten, and the interested reader is either referred to Sec. 5.3.2 or my article [5] for a few more details on the role of boundary terms in cosmology. With the ADM parameterisation, $\sqrt{-g} = N\sqrt{h}$, so the total action can be rewritten

$$S = \frac{1}{2} \int d\tilde{t} d^3\tilde{x} N \sqrt{h} M_{\text{Pl}}^2 \left[R^{(3)} + K_{ij}K^{ij} - K^2 + \frac{2}{M_{\text{Pl}}^2} \mathcal{L}_{\text{m}} \right], \quad (2.43)$$

where it is clear that time derivatives of the lapse N and of the shift N^i never appear. Therefore, these variables can be understood as Lagrange multipliers in constrained systems, and by writing the extremisation of the action with respect to them, one finds:

$$\frac{\delta S}{\delta N} = 0 \implies R^{(3)} - K_{ij}K^{ij} + K^2 = -\frac{2}{M_{\text{Pl}}^2} \mathcal{L}_{\text{m}} - \frac{2N}{M_{\text{Pl}}^2} \frac{\partial \mathcal{L}_{\text{m}}}{\partial N} \text{ (energy constraint)}, \quad (2.44)$$

$$\frac{\delta S}{\delta N^i} = 0 \implies \nabla_j \left(K \delta_i^j - K_i^j \right) = \frac{N}{M_{\text{Pl}}^2} \frac{\partial \mathcal{L}_{\text{m}}}{\partial N^i} \text{ (momentum constraint)}. \quad (2.45)$$

Those constraint equations relate the geometry of spatial hypersurfaces to the matter content of the universe, and therefore express a redundancy of the description in general relativity.

Use in perturbation theory

Now, in a perturbative setup, the lapse $N = \bar{N} + \alpha$ is expanded around a homogeneous value $\bar{N}$ that sets the value of the time variable $\tilde{t}$ compared to cosmic time t as $dt = \bar{N}d\tilde{t}$, and the shift, written as $N^i = \delta^{ij}\beta_j/a^2$, must vanish at the level of the background to respect the isotropy as stated by the cosmological principle. In the following, the time variable $\tilde{t}$ is chosen to coincide with cosmic time t so that $\bar{N} = 1$, although other choices are possible: conformal time τ (for $\bar{N} = a$), e -folding number N (not to confuse with the lapse N , for $\bar{N} = H$), or any other time variable of interest. α and β_i are perturbative quantities that can be expanded at any order in perturbation theory: $\alpha = \sum_{(n)} \alpha_{(n)} / (n!)$ and $\beta_i = \sum_{(n)} \beta_i^{(n)} / (n!)$.

First, one shall look at the solutions of the constraint equations (2.44) at the linear order (therefore one forgets the indices (1) every where in the following), after using

the SVT decomposition, in particular $\beta_i = \partial_i \beta + \hat{\beta}_i$ with β a scalar and $\hat{\beta}_i$ a vector, and reminding that perturbations of the scalar, vector, and tensor types do not mix at linear order. For definiteness, and for what matters in this thesis, one shall also assume here that the matter Lagrangian is the one of Eq. (2.10) consisting in a certain number N_{field} of scalar fields with both kinetic and potential interactions described by the field-space metric G_{IJ} and the potential V . The computation can be done in any gauge, and here for simplicity it will be done in the flat gauge in which the spatial metric $h_{ij}^{\text{flat}} = a^2 (\delta_{ij} + \gamma_{ij})$ does not contain any scalar degree of freedom. Then by definition, $R_{\text{flat}}^{(3)} = 0$ and covariant derivatives ∇_i coincide with usual partial derivatives ∂_i . In this gauge, one recalls that the covariant perturbations of the scalar fields are denoted by Q_{flat}^I . With this setup in mind (but of course the ADM formalism and in particular the constraint equations can be more generally used), the energy constraint gives at the level of the background and at the linear level:

$$3M_{\text{Pl}}^2 H^2 = \frac{1}{2} \bar{G}_{IJ} \dot{\phi}^I \dot{\phi}^J + \bar{V}, \quad (2.46)$$

$$-2M_{\text{Pl}}^2 H \frac{\partial^2 \beta_{\text{flat}}}{a^2} = \bar{G}_{IJ} \dot{\phi}^I D_t Q_{\text{flat}}^J + \bar{V}_{,I} Q_{\text{flat}}^I + 2\bar{V} \alpha_{\text{flat}}, \quad (2.47)$$

where one recalls that D_t are field-space covariant, time derivatives (here understood in terms of the background scalar fields, *i.e.* explicitly $D_t Q_{\text{flat}}^I = \dot{Q}_{\text{flat}}^I + \bar{\Gamma}^I_{JK} \dot{\phi}^J Q_{\text{flat}}^K$). The first of these two equations is nothing but the first Friedmann equation (1.11) when the matter content of the universe is represented by a non-linear sigma model (2.10), while the second one relates the linear perturbations of the lapse and the shift to linear perturbations of the scalar fields, in the flat gauge. The momentum constraint is only non-trivial at the linear level in perturbations and reads:

$$\alpha_{\text{flat}} = \frac{1}{2M_{\text{Pl}}^2 H} G_{IJ} \dot{\phi}^I Q_{\text{flat}}^J, \quad (2.48)$$

$$\partial^2 \hat{\beta}_i^{\text{flat}} = 0 \quad (2.49)$$

which enables one to uniquely determine α_{flat} and β_{flat} in terms of perturbations of the scalar fields in the flat gauge, and from which it is clear that vector perturbations cannot develop at linear order in a FLRW universe filled by scalar fields.

To summarize, the perturbations of the lapse and the shift are constrained to be proportional to matter perturbations, such as Q_{flat}^I and $D_t Q_{\text{flat}}^I$ in the case of non-linear sigma models and in the flat gauge. Then, it is possible to expand the total action (2.43) at a given order of perturbation theory, and replace the perturbations $\alpha_{(n)}$, $\beta_{(n)}$ and $\hat{\beta}_{(n)}$ by their expressions in terms of the matter perturbations. However one will see that, to expand consistently the action up to cubic order, a procedure that is relevant to compute cosmological three-point functions also known as bispectrum shapes, it is sufficient to know the lapse and the shift at the linear order as given by Eqs. (2.46)–(2.48).

Part II

Canonical inflation: a classical background and quantum perturbations

Chapter 3

Single-field inflation, the minimal working example

This chapter is devoted to the introduction of cosmic inflation as a physical theory for the very early universe, before the onset of the radiation-domination era. In sec. 3.1, it is reviewed how a few puzzles of the standard Hot Big Bang scenario (with only matter and radiation in the early universe) led to the consideration of an initially accelerated expansion of space. This accelerated expansion, in many ways similar to the current dark-energy-dominated era, is most often explained by the presence of a single scalar field, called the *inflaton*, in the matter sector. If the scalar field is dominated by its kinetic energy rather than its potential energy, the Friedmann equations show that the expansion of space is indeed quasi-exponential, leading to an almost de Sitter spacetime. This rather simple, but tremendously successful model is called *single-field, slow-roll inflation*.

Indeed, as is shown in Sec. 3.2, not only does it solve the aforementioned puzzles of cosmology without inflation on very large scales, but it also provides one with predictions for the statistics of primordial perturbations, which can be compared to temperature and polarisation anisotropies of the CMB for a wide range of scales. One of the greatest successes of inflation is that it predicts with a high level of accuracy the statistics of CMB fluctuations, in particular the small but non-zero departure from scale invariance as measured by the parameter n_s . What is impressive is that this procedure requires the use of quantum field theory in curved spacetime in order to set initial conditions for cosmological perturbations, thus making a first step towards a quantum theory of gravity.

However inflation is plagued by an unusual issue: many different models, even in the single-field context, have very similar predictions. It is therefore of high importance to study in detail how CMB observations constrain single-field models, and this is reviewed shortly in Sec. 3.3.

In the recent years, it has been shown that inflation could be formulated without the *ad hoc* introduction of an unknown scalar field in the matter sector. Rather, a scalar degree of freedom can be understood as emerging from a spontaneous breaking

of symmetry of de Sitter spacetime, a so-called Goldstone boson of broken time diffeomorphisms. This propagating degree of freedom can be related to the usual curvature perturbations, and by studying the decoupling limit of such effective field theory, one encounters a model-independent theory of fluctuations around a quasi-de Sitter spacetime, which is called *Effective Field Theory of Inflation* and that is reviewed in Sec. 3.4.

3.1 Why inflation? The puzzles of the standard Hot Big Bang scenario

The Hot Big Bang scenario can be understood as a logical implication of the observed expansion of space. It states that the current inhomogeneous Universe made of stars, galaxies and large-scale structures, is the deterministic result of the forward evolution of a dense and homogeneous initial state, under the combined effects of Standard Model forces and gravity. Pushing the reasoning, there must be a time before which the Universe was so dense that it must have been opaque. And indeed, before photon decoupling, the Thomson scattering of photons off electrons was so efficient that light could only travel on very short distances, and an observer in the primordial Universe could only see its immediate surroundings, in a very analog way to what happens in fog. When the Universe cooled enough, photons were able to free-stream, forming the Cosmic Microwave Background (CMB) that one can observe nowadays and which carries an impressive amount of information about the photon–baryon–dark-matter primordial plasma. A few interesting properties of this relic radiation are listed here:

- The CMB is almost isotropic over the whole sky, and its spectrum corresponds to a black-body radiation (see, *e.g.*, the historical though accidental discovery [8] and subsequent interpretation in the Big Bang scenario [9], the COBE measurement by the instrument FIRAS [157] and latest calculations [137] of the current CMB temperature yielding $T = (2.72548 \pm 0.00057)$ K). See Fig. 3.1 for the CMB black-body spectrum as measured by COBE-FIRAS;
- Although their amplitude is small, the CMB contains temperature anisotropies that are distributed according to Gaussian statistics, and that have been more and more precisely measured on smaller and smaller scales, and over the whole sky, first by the COBE (see [10] for the first detection), then WMAP (see [14] for the conclusions after the 9-year release) and eventually Planck (see [15] for a summary of the Planck legacy) satellites. See upper panel of Fig. 3.2 for the CMB temperature anisotropies as measured by Planck;
- CMB photons are polarized in E- and B-modes, but currently detected B-modes are understood as produced only by secondary effects after the emission of CMB, such as weak lensing (represented by the local potential ϕ). The temperature and E-modes are cross-correlated. See the lower panels of Fig. 3.2 for the power spectra of E- and ϕ -modes, and the middle panel for the cross-power spectrum of temperature and E-modes. Given perturbative quantities $X(\hat{n})$, $Y(\hat{n})$, etc. defined

on the celestial sphere, where $\hat{n}$ is a unit vector denoting the direction in the sky, the rotationally invariant angular power spectra are

$$C_\ell^{XY} = \sum_{m=-\ell}^{\ell} a_{\ell m}^X a_{\ell m}^Y / (2\ell + 1),$$

where one used the decomposition in spherical harmonics $Y_{\ell,m}(\hat{n})$, $\ell \in \mathbb{N}$ and $m \in \{-\ell, \dots, \ell\}$, as

$$X(\hat{n}) = \sum_{\ell,m} a_{\ell,m}^X Y_{\ell m}(\hat{n}) \quad \text{with} \quad a_{\ell m}^X = \int d\Omega Y_{\ell m}^*(\hat{n}) X(\hat{n});$$

- The positions and heights of the acoustic peaks and troughs in these power spectra contain even more information (see Ref. [12] for an analytical and physical interpretation of these). The position of the first peak in the temperature power spectrum tells us about the angular scale of the Baryon Acoustic Oscillations (BAO), which depends on the cosmological parameters. In particular, the best-fit value for the spatial curvature contained in Ω_k is compatible with zero, meaning that the Universe is spatially flat [11]. The positions of the following peaks, and the presence of peaks in the TE and EE power spectra, are compatible with initial perturbations with coherent phases only, even on very large scales [13]. These perturbations are also measured to be adiabatic at more than 98% [38], meaning that the relative overdensities at any given point $\vec{x}$ of each species are equal: $\delta\rho_{(\alpha)}(\vec{x})/\bar{\rho}_{(\alpha)} = \delta\rho_{(\beta)}(\vec{x})/\bar{\rho}_{(\beta)}, \forall \alpha, \beta$.

Although these properties are fairly well understood, they call into question the standard cosmological picture of an early Universe made only of matter and radiation. Here are summarized the two major issues of the Hot Big Bang scenario without cosmic inflation, the so-called horizon and flatness problems.

The horizon problem

The horizon problem is tightly connected to the notion of *causality*. Whether it is in a flat, Minkowskian spacetime, or in a curved spacetime as described by General Relativity, information is believed to propagate always at a speed lower than or equal to the speed of light. Therefore by drawing spacetime diagrams and null geodesics, as was done in Chap. 1 in the simple example of special relativity, one can understand the causality structure of a given spacetime. To put it in a nutshell, the causality structure of FLRW spacetimes filled by radiation and matter, is such that two points in the CMB sphere spaced by an angular distance larger than roughly 2° , are not causally connected in the past, and therefore their physical properties cannot be correlated. This fact should prevent from having a signal in the CMB featuring a large homogeneous monopole with very small anisotropies, as well as (anti-)correlations for these anisotropies with multipoles smaller than roughly $\ell = 200$ (I shall not entertain the possibility of a God-given correlated initial state of the Universe). This being in contradiction with the

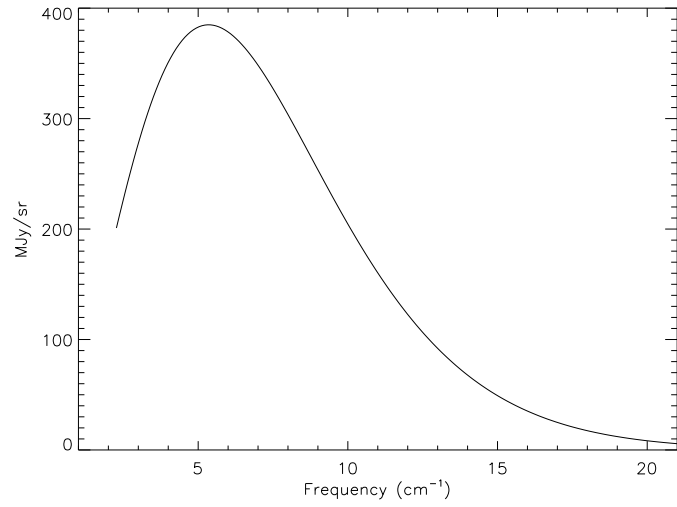


Figure 3.1: Black-body spectrum of the CMB. The flux represented on the vertical axis is in units of Jansky (Jy) per steradian (sr) where $1 \text{ Jy} = 10^{-26} \text{ W m}^{-2} \text{ Hz}^{-1}$. The visible black curve is the theoretical prediction of a black-body spectrum for the best-fit temperature, while measurements by COBE-FIRAS are not visible by eye because they perfectly overlap with the prediction (the uncertainties are smaller than the thickness of the black line). Figure taken from [157].

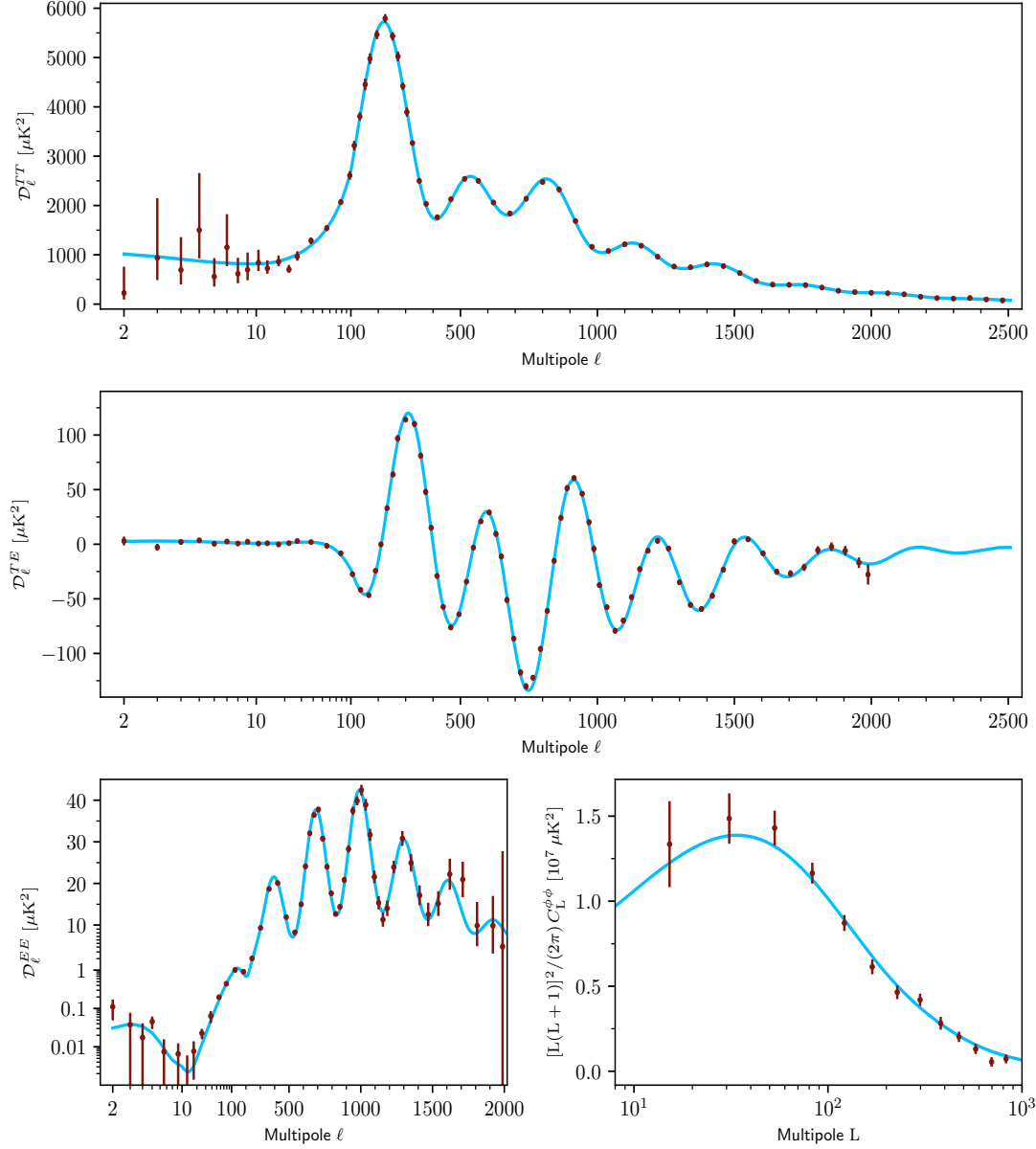


Figure 3.2: Rescaled power spectra $\mathcal{D}_\ell = \ell(\ell + 1)C_\ell/(2\pi)$ of the CMB anisotropies of temperature (upper panel), E-modes (lower left panel), weak lensing potential (lower right panel), and cross-power-spectrum of temperature and E-modes (middle panel). Red dots with uncertainties are measurements by Planck and blue curves correspond to theoretical predictions for the best-fit cosmological parameters. Figure taken from [15].

aforementioned observations of the CMB, one concludes that the early Universe cannot only be described by a FLRW spacetime mostly filled with matter and radiation. These statements are made more precise and quantitative in the following.

Using the conformal time τ as a time variable (one recalls that it is defined as $a d\tau = dt$), and assuming that the Universe is spatially flat, $k = 0$, one can see that null geodesics ($ds^2 = 0$) must verify the simple relation:

$$r_{\text{null}}(\tau) = \pm\tau + \text{constant} . \quad (3.1)$$

Therefore the geodesic distance that light travels between an initial time (formally understood as 0 here, even though for very early times, comparable to or smaller than the Planck time, quantum gravity effects must kick in and distort the classical picture of the FLRW spacetime) and an arbitrary time t , which is interpreted as the maximal distance over which two spatial points at the time t are causally connected in the past, reads

$$\Delta r_{\text{max}}(t) = \tau(t) - \tau(0) = \int_0^t \frac{dt'}{a(t')} , \quad (3.2)$$

and is called the *comoving particle horizon* for the reasons mentioned just above. Note that since the behaviour of $a(t)$ is known when the Universe is filled by a cosmological fluid with constant equation of state w , see Table 1.2.2, one can easily estimate the behaviour of the integral and finds $\Delta r_{\text{max}}(t) \propto a(t)^{\frac{1+3w}{2}}$, where a necessary condition to yield a finite result was to assume that matter verifies the so-called *strong energy condition*,

$$(\text{SEC}): \quad 1 + 3w > 0 . \quad (3.3)$$

This condition also ensured that the major contribution to the integral was coming from times t' close to the upper bound t . Since matter and radiation both verify the SEC, it appears clearly that information can only propagate a finite distance from the initial time to the time of decoupling at which CMB photons are emitted, in a FLRW universe with only matter and radiation. On the contrary, if the SEC is violated and $w < -1/3$, then the integral in Eq. (3.2) diverges due to dominant contributions from times t' close to the lower bound 0, and any two points seem to be causally connected in the past.

A key quantity is the comoving Hubble parameter, $\mathcal{H} = aH$, since the conformal time τ can be rewritten

$$\tau = \int \frac{1}{\mathcal{H}} d \ln a \propto \frac{2}{1+3w} \times a^{\frac{1+3w}{2}} + \text{constant} \quad (3.4)$$

where one used that

$$\mathcal{H}^{-1} \propto a^{\frac{1+3w}{2}} . \quad (3.5)$$

Therefore, there is a strong connection between causality, the evolution of the comoving Hubble radius $\mathcal{H}^{-1}$, and the strong energy condition. When the SEC is verified, the comoving Hubble radius is increasing, and the comoving particle horizon is finite. Note also that in that case the initial conformal time corresponding to a cosmic $t \rightarrow 0$, or equivalently $a \rightarrow 0$, is vanishing: $\lim_{t \rightarrow 0} \tau(t) = 0$ (taking the constant in Eq. (3.4) to be

0 for definiteness). However when the SEC is violated, the comoving Hubble radius is decreasing, and the comoving particle horizon is divergent. This is because in that case the initial conformal time itself is divergent: $\lim_{t \rightarrow 0} \tau(t) = -\infty$.

In the standard Hot Big Bang scenario without inflation, the early universe is either filled with radiation or matter, which both verify the SEC, and therefore there is a maximum angular separation in the sky between two causally connected points. Computing this angular separation $\theta_{\text{connected}}$ requires the computation of two distances: the angular diameter distance between the decoupling surface at t_{dec} and us at t_0 , $d_A(t_{\text{dec}})$, and the comoving particle horizon at the time of decoupling, $\Delta r_{\text{max}}(t_{\text{dec}})$. In terms of them, it reads

$$\theta_{\text{connected}} = 2 \frac{\Delta r_{\text{max}}(t_{\text{dec}})}{d_A(t_{\text{dec}})} = 2 \frac{\int_{z_{\text{dec}}}^{\infty} \frac{dz}{H(z)}}{\int_0^{z_{\text{dec}}} \frac{dz}{H(z)}}, \quad (3.6)$$

where the variable of integration has been changed from cosmic time t to redshift z with $a(t) = (1+z)^{-1}$ and hence $dt/a(t) = -dz/H(z)$, where

$$H(z) = H_0 \sqrt{\Omega_{\text{r},0}^{\text{eff}}(1+z)^4 + \Omega_{\text{m},0}(1+z)^3 + \Omega_{\text{V},0}},$$

assuming that the Universe is spatially flat. Numerically evaluating the integrals with the cosmological parameters presented in Chap. 1, I find $\theta_{\text{connected}} = 2.3^\circ$, corresponding roughly to $\ell \sim 80$.¹

To conclude, the standard Hot Big Bang scenario fails to explain correlations in the CMB for angles larger than 2.3° , since any two points separated by more than this scale are not causally connected in a FLRW early universe filled by matter and radiation. Before explicating the solution to the horizon problem, that clearly necessitates a violation of the SEC, one shall investigate another key puzzle of cosmological scenarios without inflation.

The flatness problem

The first acoustic peak in the CMB (and its overall structure) is (are) compatible with a spatially flat universe. Actually, it was shown in Chap. 1 that, when combined with other probes such as BAO, one derives relatively tight constraints on the spatial curvature: $\Omega_{\text{k},0} = 0.001 \pm 0.002$. But remember the temporal evolution of spatial curvature, $\Omega_{\text{k}} = -k\mathcal{H}^{-2}$, and the fact that the comoving Hubble radius $\mathcal{H}^{-1}$ is usually increasing. Therefore Ω_{k} is also increasing with time,

$$\Omega_{\text{k}} = \Omega_{\text{k},0} \left(\frac{a}{a_0} \right)^{1+3w}, \quad (3.7)$$

when the Universe is filled by a cosmological fluid with eos w and satisfying the SEC. Therefore the value of the spatial curvature in the past was even smaller, by many

¹Note that the effect of neutrinos, taken into account in $\Omega_{\text{r},0}^{\text{eff}}$, is to increase $H(z)$ at high redshifts and therefore to diminish this angle, numerically by 0.3° . A refined treatment would require to separate the integrals before and after the redshift at which neutrinos become non-relativistic, z_{NR} , and to take into account the neutrino contribution accordingly.

orders of magnitude. For example, one can find a simple estimate of Ω_k at the time of photon decoupling: ignoring the contribution from the late-time, dark-energy-dominated epoch at $z \lesssim 1$ (during which by definition the scale factor has only evolved by a factor of two) as well as the remaining radiation which is negligible after decoupling, gives $w \simeq 0$ and $\Omega_k(z_{\text{dec}}) \simeq \Omega_{k,0}/z_{\text{dec}} \lesssim 10^{-6}$. Therefore the spatial curvature at the time of the CMB emission must have been very small in order to produce the spectrum that is measured nowadays. Estimating the effect of the radiation-dominated era before the emission of the CMB is more difficult, for the reheating temperature T_{reh} at the onset of this cosmological epoch is largely unknown so far (and therefore so is the duration of the radiation era itself). Without giving a value for the initial temperature of the radiation-dominated era, during which $T \propto a^{-1}$ up to roughly decoupling ($T_{\text{dec}} \sim 10^3$ K), one further pushes the initial value of the spatial curvature component at the time of reheating to $\Omega_k(z_{\text{reh}}) \simeq \Omega_k(z_{\text{dec}}) (T_{\text{dec}}/T_{\text{reh}})^2 \lesssim 10^{-54} \times (10^{27} \text{ K}/T_{\text{reh}})^2$, where the contribution from matter around z_{eq} was neglected, and the numerical value 10^{-54} corresponds to the case of a reheating temperature $T_{\text{reh}} \sim 10^{27}$ K. The flatness problem is actually a fine-tuning issue: how comes that a free dimensionless parameter of our cosmological model must assume such a small initial value to match current observations? This therefore calls into question the Hot Big Bang scenario too.

Other problems are sometimes mentioned, such as the absence of observation of magnetic monopoles, remnants from the era before electro-weak symmetry breaking, but just like the horizon and the flatness problems, they are all related to the fact that the comoving Hubble radius is increasing if the SEC is verified.

Problems solved!

Indeed, one can consider an epoch before radiation domination, during which the Universe is dominated by an exotic form of matter violating the SEC, $w < -1/3$, and that one shall call cosmic inflation. Then, during that phase, the comoving Hubble radius is decreasing, which enables one to evade both the horizon and the flatness problems. Actually, a decreasing comoving Hubble radius, $(\mathcal{H}^{-1}) = d(1/\dot{a})/dt < 0$ is equivalent to an accelerated expansion, $\ddot{a} > 0$. Therefore one has the following equivalences:

$$\begin{array}{ll}
 w < -1/3 & \text{(violation of SEC)} \\
 \iff (\mathcal{H}^{-1}) < 0 & \text{(shrinking comoving Hubble radius)} \\
 \iff \ddot{a} > 0 & \text{(accelerated expansion)}.
 \end{array} \tag{3.8}$$

Regarding causality, this pushes the initial singularity at large and negative conformal times, $\tau \rightarrow -\infty$, leaving plenty of time for particles to interact in the primordial Universe and reach thermal equilibrium on comoving scales that will then leave the comoving Hubble radius (since it is shrinking), called comoving horizon, and seem causally disconnected on the CMB sphere. A sketch of a few relevant comoving scales is presented in Fig. 3.3, together with a geometric interpretation of why the comoving particle horizon is greatly enhanced by such an initial phase of accelerated expansion.

As for the spatial curvature, it is simply evident that when the comoving Hubble radius is shrinking, Ω_k is also decreasing. Therefore, whatever is the initial value of Ω_k at the beginning of inflation, it will decrease until reaching a small value, potentially as small as 10^{-54} if inflation provides enough expansion. It is easy to estimate this minimal amount of expansion: assuming that Ω_k at the onset of inflation is not smaller than 1% for definiteness, solving the flatness problem requires the scale factor $a \propto e^N$, where N is called the e -folding number, to decrease as much as $\Delta N > -52/(1+3w) \times \ln(10)$ for a constant eos w . For values of $w \simeq -1$ (which is the case for most inflationary models, see Sec. 3.2), one finds that inflation needs to last roughly 60 e -folds, a value that coincides with the amount of expansion needed for the largest scales observed in the CMB to have been once under the horizon and therefore for solving the horizon problem too.

3.2 Dynamics of single-field inflation

Although the exact dynamics of inflation are still to be determined, a large class of minimalist models now constitute our paradigm for the very early universe. Historically denoted as “chaotic inflation” models (see Ref. [158] for a historical review of early works in inflationary cosmology), they feature a single scalar field ϕ in the matter sector, evolving under the force derived from its potential $V(\phi)$ and the expansion of space as described by general relativity. Importantly, the initial conditions can be quite generic (hence the name “chaotic”), and the scalar potential can be in principle of any type, as long as it is sufficiently flat as one shall see soon. In the remaining of this section, the dynamics of these single-field, slow-roll, models of inflation at the level of the background and linear perturbations, are shortly reviewed.

3.2.1 Background

Generalities

Consider the setup where the matter sector is described by the Lagrangian

$$\mathcal{L}_\phi = - \left[\frac{1}{2} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi + V(\phi) \right]. \quad (3.9)$$

The stress-energy tensor then reads

$$T_{\mu\nu} = \partial_\mu \phi \partial_\nu \phi - g_{\mu\nu} \left(\frac{1}{2} g^{\rho\sigma} \partial_\rho \phi \partial_\sigma \phi + V(\phi) \right), \quad (3.10)$$

whence on cosmological scales (at the background level), one finds the expressions for the energy density and pressure of matter (for simplicity in the following, one omits the bars on background quantities like $\bar{\rho}$, $\bar{\phi}$, etc.):

$$\rho = \frac{1}{2} \dot{\phi}^2 + V(\phi) \quad \text{and} \quad P = \frac{1}{2} \dot{\phi}^2 - V(\phi). \quad (3.11)$$

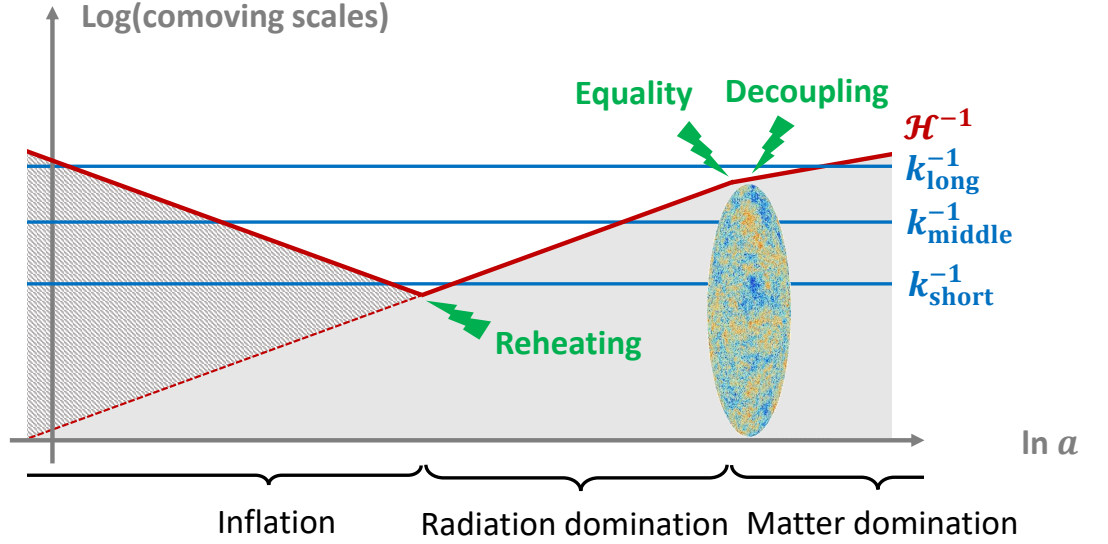


Figure 3.3: Sketch of the evolution of the comoving Hubble radius (solide red curve) during inflation, an era during which the Universe is dominated by an exotic matter violating the SEC, then radiation domination and finally matter domination. Three comoving scales are represented (blue horizontal lines), they all exited the shrinking comoving Hubble radius during inflation and then re-entered this “horizon” at different times. In particular, the mode k_{long} was outside the horizon at the time of decoupling and therefore no correlation on comoving scales k_{long}^{-1} should be observed in the CMB if inflation had not occurred (see the evolution of the comoving Hubble radius without inflation in dashed red line). With inflation though, this mode was first inside the horizon and causal interactions could happen on these scales, explaining why apparently causally disconnected points can be correlated. The grey shaded area corresponds to the integral $\int \mathcal{H}^{-1} d \ln a$ and therefore corresponds to the comoving particle horizon. Its subset which is striped on the left is the amount of comoving particle horizon, or equivalently conformal time, that is added by considering inflation as happening before radiation domination. This amount can be enormously larger than the remaining, note the logarithmic vertical scale and the fact that inflation can last for many e -folds, *i.e.* for a large range of $\ln a$, before reheating.

It follows that the instantaneous equation of state of the Universe, if this scalar field is the only dominant contribution to the total energy density in the very early universe, reads

$$w = \frac{\frac{1}{2}\dot{\phi}^2 - V(\phi)}{\frac{1}{2}\dot{\phi}^2 + V(\phi)} = \frac{(\text{kinetic energy} - \text{potential energy})}{(\text{kinetic energy} + \text{potential energy})}, \quad (3.12)$$

and violates the SEC, $w < -1/3$, provided the kinetic energy is sufficiently smaller than the potential energy: $\dot{\phi}^2 < V(\phi)$. Therefore, a period of inflation, *i.e.* an accelerated expansion of space, *i.e.* a shrinking comoving Hubble radius, is possible if the rolling of the scalar field on the slope of its potential, is not too fast. The velocity of the scalar field can be parameterised by the first Hubble slow-roll parameter, ϵ , which is actually defined as

$$\epsilon = -\frac{\dot{H}}{H^2} = \frac{\dot{\phi}^2}{2H^2 M_{\text{Pl}}^2}, \quad (3.13)$$

where for the second equality one used the Friedmann equations (1.11) in a spatially flat Universe and without a cosmological constant, which read

$$3H^2 M_{\text{Pl}}^2 = \frac{1}{2}\dot{\phi}^2 + V(\phi) \quad \text{and} \quad \dot{H} = -\frac{1}{2} \frac{\dot{\phi}^2}{M_{\text{Pl}}^2} \quad (3.14)$$

in the inflationary context after replacing the above expressions for ρ and P . Another rewriting of this first slow-roll parameter is $\epsilon = 3 \left(1 + 2V/\dot{\phi}^2\right)^{-1}$ from which it is clear that the necessary condition for violating the SEC and having inflation is $\epsilon < 1$. Note that ϵ measures the deviation of the FLRW inflationary spacetime from a perfect de Sitter space which corresponds to $H = \text{constant} \iff \epsilon = 0 \iff \dot{\phi} = 0$ and therefore to an exactly exponential expansion of space, $a(t) = e^{Ht}$, as happens during a cosmological era dominated by a vacuum contribution such as the cosmological constant Λ .

Moreover, in order for inflation to last long enough to solve the horizon and flatness problems (remember the typical minimal amount of 60 e -folds of expansion), ϵ should remain smaller than unity for such a duration. The logarithmic rate of evolution of ϵ in Hubble units is called the second slow-roll parameter and reads:

$$\eta = \frac{\dot{\epsilon}}{\epsilon H} = 2(\epsilon - \delta) \quad \text{where} \quad \delta = -\frac{\ddot{\phi}}{H\dot{\phi}}. \quad (3.15)$$

For slowly evolving values of η ,² ϵ behaves as $\epsilon \propto e^{\eta N}$ and therefore in order to sustain inflation, $\epsilon < 1$, for long enough, one typically has in mind $|\eta| \ll 1$.³

²This quantity can be parameterised by $\dot{\eta}/(\eta H)$, and actually an infinite series of slow-roll parameters can be defined as $\epsilon_{n+1} = \dot{\epsilon}_n/(\epsilon_n H)$ with $\epsilon_1 = \epsilon$ as an initial condition, and where one recognizes η as ϵ_2 .

³Note that η can *a priori* be either negative or positive. If it is positive, clearly $\eta \ll 1$ for ϵ to remain small long enough, but if it is negative then ϵ is actually decreasing. This scenario can lead to a different phase called *ultra-slow-roll* [159–161] and proven to be a dynamical attractor [162], during which $\eta \sim -6$, but even though it features an interesting phenomenology, it shall not be considered further in the following, simply because it does not provide a natural end to inflation, and is necessarily followed by a more mainstream period of inflation during which η is positive and drives ϵ towards unity.

Background equations of motion and slow-roll approximation

Writing the Euler-Lagrange equations related to the Lagrangian (3.9) supplemented by the Einstein-Hilbert term of general relativity, at the level of the background spacetime described by a spatially flat FLRW metric, yields

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi}(\phi) = 0, \quad (3.16)$$

where a coma denotes a field-derivative, whence $V_{,\phi} = dV/d\phi$. Then, one needs either to solve this equation numerically once initial conditions for ϕ and $\dot{\phi}$ have been set, together with a model for the scalar potential $V(\phi)$, or to make assumptions to push the analytical treatment further. The simplest and most natural assumption is the so-called *slow-roll* (SR) approximation, according to which both the velocity and the acceleration of the scalar field, are small:

$$\boxed{\text{(Single field, slow roll):} \quad \{\epsilon, |\delta|\} \ll 1 \iff \{\epsilon, |\eta|\} \ll 1.} \quad (3.17)$$

In that case, the background Equations of Motion (EoM) (3.16) simplify to give

$$\dot{\phi} \approx -\frac{V_{,\phi}(\phi)}{3H}, \quad (3.18)$$

where the symbol “ $\approx$ ” is used here and in the following to denote that only the first non-vanishing order in slow-roll is considered. This equation can be integrated, at least formally and implicitly, to give:

$$-\int \frac{d\phi/M_{\text{Pl}}}{\sqrt{2\epsilon_V(\phi)}} \approx \int dN, \quad (3.19)$$

where one used the number of e -folds as a time variable in the RHS, $dN = Hdt$, as well as the first potential slow-roll parameter, ϵ_V , which can be defined together with the second potential slow-roll parameter, η_V , as

$$\boxed{\epsilon_V = \frac{M_{\text{Pl}}^2}{2} \left(\frac{V_{,\phi}}{V} \right)^2 \approx \epsilon \quad \text{and} \quad \eta_V = M_{\text{Pl}}^2 \frac{V_{,\phi\phi}}{V} \approx \epsilon + \delta = 2\epsilon - \frac{\eta}{2}.} \quad (3.20)$$

Therefore for such a single-field model of inflation, one can see the equivalence between slow roll and the flatness of the potential:

$$\boxed{\text{(Single field, slow roll)} \iff \{\epsilon_V, |\eta_V|\} \ll 1,} \quad (3.21)$$

meaning that both the slope and the curvature of the scalar potential must be small in Planck mass units for single-field inflation to feature a slow-roll dynamics.

Example: quadratic inflation. This model, for which the scalar potential is that of a free scalar field and only contains a mass term, $V(\phi) = m^2\phi^2/2 \implies \epsilon_V = 2M_{\text{Pl}}^2/\phi^2$ (note the independence on m), can be solved exactly at leading order in slow roll, giving for example

$$\phi \approx \pm \sqrt{\phi_{\text{ini}}^2 - 4M_{\text{Pl}}^2(N - N_{\text{ini}})}. \quad (3.22)$$

Moreover, inflation stops at N_{end} corresponding to a field value $\phi(N_{\text{end}}) = \phi_{\text{end}}$, such that $\epsilon_V(\phi_{\text{end}}) \approx \epsilon(N_{\text{end}}) = 1$. One finds $\phi_{\text{end}} \approx \sqrt{2}M_{\text{Pl}}$ (although one should keep in mind that the slow-roll approximation breaks down exactly before and around that time), and therefore $\Delta N_{\text{tot}} = N_{\text{end}} - N_{\text{ini}} \approx \phi_{\text{ini}}^2/(4M_{\text{Pl}}^2) - 1/2$. One can thus rewrite the field evolution as $\phi \approx \pm \sqrt{\phi_{\text{end}}^2 + 4M_{\text{Pl}}^2(N_{\text{end}} - N)}$. Because $w = -1 + 2\epsilon/3 \approx -1$ during slow-roll inflation, one saw previously that the minimum amount of expansion needed to solve the flatness problem is $\Delta N_{\text{tot}} \gtrsim 60$, giving a condition on the initial field value: $|\phi_{\text{ini}}|/M_{\text{Pl}} \gtrsim 15.6$. Note that there is no condition on the initial field velocity, a feature that is shared by all slow-roll models of inflation as can be seen from Eq. (3.19). The extension of quadratic inflation to two-fields models of inflation, so-called double quadratic inflation, is studied at length in Chap. 9 together with the reheating mechanism.

3.2.2 Linear perturbations

So far, only the evolution of the homogeneous, background quantities, has been studied. Following cosmological perturbation theory explained in Chap. 2, one can follow how linear perturbations develop on top of this homogeneous picture.

Quadratic action

For this, one first finds the action that is quadratic in the matter and spacetime perturbations (intertwined in gauge-invariant perturbations), which only necessitates to expand each quantity in the action at linear order. Indeed if the action depends on a set of quantities $X_\alpha(t, \vec{x}) = \bar{X}_\alpha(t) + \delta X_\alpha(t, \vec{x})$, then its expansion up to quadratic order reads:

$$S[X] = \underbrace{S[\bar{X}]}_{S^{(0)}[\bar{X}]} + \underbrace{\frac{\delta S}{\delta X_\alpha} \Big|_{\bar{X}}}_{=0} \delta X_\alpha + \underbrace{\frac{1}{2} \frac{\delta^2 S}{\delta X_\alpha \delta X_\beta} \Big|_{\bar{X}}}_{S^{(2)}[\bar{X}, \delta X]} \delta X_\alpha \delta X_\beta + \dots, \quad (3.23)$$

where the first term is nothing but the background action, the second term vanishes by virtue of the background EoM, and the third term is the quadratic action that one wishes to compute here. From this equation, it is clear that if δX_α is expanded as $\delta X_\alpha = \delta X_\alpha^{(1)} + \delta X_\alpha^{(2)} + \dots$, then only $\delta X_\alpha^{(1)}$ is relevant to compute $S^{(2)}$. First, the scalar field is expanded as $\phi = \bar{\phi} + Q$ where $\bar{\phi}$ verifies the background EoM (3.16). Note that the question of covariance treated in Sec. 2.2.2 is trivial here since the field-space metric $G(\phi) = 1$ in the model (3.9). Next, one uses the ADM formalism to parameterise spacetime perturbations and chooses the spatially flat gauge in which one reminds that

$\psi_{\text{flat}} = E_{\text{flat}} = 0 = \hat{E}_i^{\text{flat}}$, and therefore $\nabla_i^{\text{flat}} = \partial_i$ and $R_{\text{flat}}^{(3)} = 0$. After plugging the solutions to the constraint equations of Eqs. (2.46)–(2.48) in the action rewritten as in Eq. (2.43), and simplifying with use of the background EoM, one finds the quadratic action of scalar and tensor perturbations in single-field inflation:

$$S_Q^{(2)} = \frac{1}{2} \int dt d^3 \vec{x} a^3 \left\{ \dot{Q}_{\text{flat}}^2 - \frac{(\partial Q_{\text{flat}})^2}{a^2} - \left[V_{,\phi\phi} - \frac{1}{a^3 M_{\text{Pl}}^2} \partial_t \left(\frac{a^3}{H} \dot{\phi}^2 \right) \right] Q_{\text{flat}}^2 \right\}, \quad (3.24)$$

$$S_\gamma^{(2)} = \frac{M_{\text{Pl}}^2}{8} \int dt d^3 \vec{x} a^3 \delta^{ik} \delta^{jl} \left[\dot{\gamma}_{ij} \dot{\gamma}_{kl} - \frac{(\partial \gamma_{ij}) \cdot (\partial \gamma_{kl})}{a^2} \right],$$

where for quantities X, Y , one has $(\partial X) \cdot (\partial Y) = \delta^{ij} \partial_i X \partial_j Y$, so that for example $(\partial Q_{\text{flat}})^2 = \delta^{ij} \partial_i Q_{\text{flat}} \partial_j Q_{\text{flat}}$. Notice that vector perturbations do not develop during single-field inflation, and actually this is the case in multifield inflation too.

Linear equations of motion and Sasaki-Mukhanov variables

The linear equations of motions for the perturbations Q_{flat} and γ are better understood in Fourier space. Thus, one first uses

$$Q_{\text{flat}}(t, \vec{x}) = \int \frac{d^3 \vec{k}}{(2\pi)^3} e^{i\vec{k} \cdot \vec{x}} Q_{\vec{k}}(t), \quad (3.25)$$

$$\gamma_{ij}(t, \vec{x}) = \int \frac{d^3 \vec{k}}{(2\pi)^3} e^{i\vec{k} \cdot \vec{x}} \sum_{\lambda=+,-} \gamma_{\vec{k}}^\lambda(t) \epsilon_{ij}^\lambda(\vec{k}),$$

where the two polarisations of gravitational waves, $\epsilon_{ij}^\lambda(\vec{k})$ corresponding to $\lambda \in \{+, -\}$ and verifying the transverse traceless conditions $\epsilon_{ii}^\lambda(\vec{k}) = 0 = k^i \epsilon_{ij}^\lambda(\vec{k})$ as well as $(\epsilon_{ij}^\lambda(-\vec{k}))^* = \epsilon_{ij}^\lambda(\vec{k})$ and $\epsilon_{ij}^\lambda(\vec{k}) \epsilon_{ij}^{\lambda'}(\vec{k}) = \delta_{\lambda\lambda'}$, have been introduced, together with the mode functions $Q_{\vec{k}}(t)$ in the scalar sector and $\gamma_{\vec{k}}^\lambda(t)$ in the tensor sector. Then, varying the quadratic actions in Eq. (3.24), one finds the linear EoM for the perturbations:

$$\ddot{Q}_{\vec{k}} + 3H\dot{Q}_{\vec{k}} + \left(M^2 + \frac{k^2}{a^2} \right) Q_{\vec{k}} = 0 \quad \text{with} \quad M^2 = V_{,\phi\phi} - \frac{1}{a^3 M_{\text{Pl}}^2} \partial_t \left(\frac{a^3}{H} \dot{\phi}^2 \right), \quad (3.26)$$

$$\ddot{\gamma}_{\vec{k}}^\lambda + 3H\dot{\gamma}_{\vec{k}}^\lambda + \frac{k^2}{a^2} \gamma_{\vec{k}}^\lambda = 0.$$

However, these are clearer when written in terms of conformal time τ such that $a d\tau = dt$, and in terms of canonically normalised perturbations, so-called

(Sasaki–Mukhanov variables): $v_{\vec{k}} = a Q_{\vec{k}}$ and $v_{\vec{k}}^\lambda = \frac{a}{2} M_{\text{Pl}} \gamma_{\vec{k}}^\lambda$.

(3.27)

Using $'$ to denote a derivative with respect to conformal time, one then has:

$$v_{\vec{k}}'' + \left(k^2 - \frac{z''}{z} \right) v_{\vec{k}} = 0, \quad (3.28)$$

$$v_{\vec{k}}^{\lambda''} + \left(k^2 - \frac{a''}{a} \right) v_{\vec{k}}^\lambda = 0,$$

where

$$z = aM_{\text{Pl}}\sqrt{2\epsilon} \implies \frac{z''}{z} = -a^2 V_{,\phi\phi} + \mathcal{H}^2 (2 + 5\epsilon - 2\epsilon^2 + 2\epsilon\eta) , \quad (3.29)$$

is the ratio between the Sasaki-Mukhanov variable $v = aQ_{\text{flat}}$ and the comoving curvature perturbation $\mathcal{R} = -\mathcal{H}v^\Psi$ defined in Eq. (2.36) when the matter content of the universe is a scalar field. Indeed, writing the stress-energy tensor associated to the Lagrangian (3.9) and recalling the definitions of the gauge-invariant velocity potential v^Ψ in Eq. (2.26), one finds that $v^\Psi = v^{(\text{gi})} - \Psi/\mathcal{H} = -Q^{(\text{gi})}/\bar{\phi}' - \Psi/\mathcal{H} = -Q_{\text{flat}}/\bar{\phi}'$ and therefore that

$$\boxed{\text{(Single field inflation:)} \quad \mathcal{R} = \frac{\mathcal{H}}{\bar{\phi}'} Q_{\text{flat}} = v/z .} \quad (3.30)$$

Note that, strictly speaking, $\mathcal{R}$ is not defined in an exact dS spacetime for which $\epsilon = 0 = z$. In general, z''/z is a complicated function of the background dynamics and the Sasaki-Mukhanov equations (3.28) must be solved numerically. However, there exists two regimes corresponding to $k^2 \gg Z''/Z$ (sub-horizon) and $k^2 \ll Z''/Z$ (super-horizon) for $Z \in \{z, a\}$, for which (approximate) analytical solutions can be found. Actually, one will see later that there are approximate, local, analytical solutions to these equations after expanding them at first order in slow-roll parameters. But first, one shall make explicit the links between inflation and quantum field theory in curved spacetime by discussing the initial conditions of such perturbations.

Initial conditions and canonical quantisation

During inflation, $Z''/Z \approx \mathcal{H}^2 = a^2 H^2$ and therefore the relative size between k^2 and Z''/Z goes from very big to very small when the mode $\vec{k}$ with wavenumber k crosses the horizon ($k = aH$). Initially, when this mode is very deep under the horizon, one can therefore consider the limit $k^2 \gg Z''/Z$ in the Sasaki-Mukhanov equations, which then describes the evolution of a massless oscillator in Minkowski spacetime (since this discussion is similar for scalar and tensor perturbations, in the following one focuses on scalar perturbations, though the reader should keep in mind that it also applies for tensors):

$$\text{(sub-horizon):} \quad v_{\vec{k}}'' + k^2 v_{\vec{k}} = 0 , \quad (3.31)$$

an equation whose solutions are linear combinations of two oscillating modes, $\propto e^{-ik\tau}$ and $\propto e^{ik\tau}$. This system can be described in the Hamiltonian formalism, $\pi_{\vec{k}} = v_{\vec{k}}'$, $\pi_{\vec{k}}' = -k^2 v_{\vec{k}}$, by the sub-horizon quadratic Hamiltonian:

$$H_{\text{sub}}^{(2)}(\tau) = \frac{1}{2} \int \frac{d^3 \vec{k}}{(2\pi)^3} \left[\pi_{\vec{k}}^2(\tau) + k^2 v_{\vec{k}}^2(\tau) \right] . \quad (3.32)$$

An important feature of inflation is that the initial conditions for cosmological perturbations can be chosen as the minimal quantum-zero-point fluctuations that exist in vacuum according to quantum physics. Bearing in mind that this is a choice and not a requirement, one shall see that a class of initial conditions can be chosen once the

perturbations are quantised. In order to do this, one promotes the classical Hamiltonian shown above to a quantum operator by requiring that the canonical variables v, π promoted to quantum operators, first in real space,

$$v(\tau, \vec{x}) \rightarrow \hat{v}(\tau, \vec{x}), \quad \pi(\tau, \vec{x}) \rightarrow \hat{\pi}(\tau, \vec{x}), \quad (3.33)$$

verify the canonical commutation relations at equal time τ :

$$[\hat{v}(\tau, \vec{x}), \hat{\pi}(\tau, \vec{y})] = i\delta^{(3)}(\vec{x} - \vec{y}), \quad (3.34)$$

where one shall remind that $\hbar = 1$ in this manuscript, and where brackets $[\cdot, \cdot]$ represent the quadratic form, commutation operator: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Then $\hat{H}_{\text{sub}}^{(2)}[\hat{v}_{\vec{k}}, \hat{\pi}_{\vec{k}}]$, where $\hat{v}_{\vec{k}}$ and $\hat{\pi}_{\vec{k}}$ are the Fourier transforms of $\hat{v}$ and $\hat{\pi}$, is a quantum operator and can be used to define the vacuum state as the one with minimum energy. Let one denote $|0\rangle$ the vacuum state, such that $\langle 0|\hat{H}_{\text{sub}}^{(2)}|0\rangle$ is minimised. The usual annihilation and creation operators, $\hat{a}_{\vec{k}}$ and $\hat{a}_{\vec{k}}^\dagger$ can be used in the Heisenberg picture to define the n -particles states of the theory, where for example $\hat{a}_{\vec{k}}^\dagger|0\rangle = |1_{\vec{k}}\rangle$ is the 1-particle state with momentum $\vec{k}$. Since they form a complete set of quantum states in the Hilbert space, any quantum operator can be decomposed in their basis, and therefore one can write:

$$\hat{v}_{\vec{k}}(\tau) = v_k(\tau)\hat{a}_{\vec{k}} + v_k^*(\tau)\hat{a}_{-\vec{k}}^\dagger, \quad \hat{\pi}_{\vec{k}}(\tau) = \pi_k(\tau)\hat{a}_{\vec{k}} + \pi_k^*(\tau)\hat{a}_{-\vec{k}}^\dagger, \quad (3.35)$$

where the fact that the so-called mode functions v_k, π_k depend only on the modulus k of $\vec{k}$, comes from the inspection of the equations of motion, Eq. (3.31) in the sub-horizon limit, but even Eq. (3.28) more generally, where the direction in which the vector $\vec{k}$ is pointing, never appears. The annihilation and creation operators must verify the following commutation relations:

$$[\hat{a}_{\vec{k}}, \hat{a}_{\vec{k}'}^\dagger] = (2\pi)^3 \delta^{(3)}(\vec{k} - \vec{k}'), \quad (3.36)$$

which, together with the canonical commutation relations (3.34), enforce the Wronskian of the two basis mode functions (v_k, v_k^*) to be fixed:

$$W(v_k, v_k^*) = v_k(v_k^*)' - v_k'v_k^* = i. \quad (3.37)$$

Now the vacuum state $|0\rangle$ can be explicitated in terms of the value of the mode function v_k , by minimising

$$\langle 0|\hat{H}_{\text{sub}}^{(2)}|0\rangle = \frac{\delta^{(3)}(0)}{2} \int \frac{d^3\vec{k}}{(2\pi)^3} \underbrace{(|v_k'|^2 + k^2|v_k|^2)}_{\omega_k}, \quad (3.38)$$

where the physical divergence $\delta^{(3)}(0)$ can be understood as a volume divergence. Therefore, although the total energy associated to $\hat{H}_{\text{sub}}^{(2)}$ is infinite, the spectral energy density

(per mode k , per volume, roughly ω_k) is finite can be minimised. For this, one parameterises the mode function as $v_k = r_k e^{i\theta_k}$ with $(r_k, \theta_k) \in \mathbb{R}$, in terms of which $\omega_k = r_k'^2 + r_k^2 \theta_k'^2 + k^2 r_k^2$. But, using the Wronskian condition (3.37), one actually gets

$$\begin{aligned} r_k^2 \theta_k' &= -1/2, \\ \omega_k(r_k, r_k') &= r_k'^2 + \frac{1}{4r_k^2} + k^2 r_k^2. \end{aligned} \quad (3.39)$$

Now, ω_k is extremised, $\partial\omega_k/\partial(r_k') = 0 = \partial\omega_k/\partial(r_k)$, giving:

$$\begin{aligned} r_k' &= 0, \\ r_k &= \frac{1}{\sqrt{2k}}, \\ \theta_k' &= -k \implies \theta_k = -k\tau + \varphi_k, \end{aligned} \quad (3.40)$$

whence we find that the vacuum state at the time τ , defined as the one with minimum energy, for a theory described by $H_{\text{sub}}^{(2)}$ corresponding to a massless oscillator in a Minkowski spacetime, is given by the following mode function:

$$(\text{Minkowski vacuum}): v_k^{\text{Minkowski}}(\tau) = \frac{1}{\sqrt{2k}} e^{-ik\tau + i\varphi_k}. \quad (3.41)$$

Note that although ω_k is finite for a given mode k for this minimum energy state, $\omega_k = k$, one recovers the well-know result that the total vacuum energy density (per volume but not per k mode) is formally divergent:⁴

$$\rho_{\text{vac}}^{\text{quantum}} = \frac{\langle 0 | \hat{H}_{\text{sub}}^{(2)} | 0 \rangle}{\delta^{(3)}(0)} = \frac{1}{16\pi^2} \int dk k^3 = \infty. \quad (3.42)$$

⁴Of course, this divergence should not be understood as physical, and rather comes from our ignorance about the high-energy physics. Indeed, the integral is UV-divergent, meaning that it is dominated by large values of the wavenumber k . But at the energy scales probed by such values of k , there is no guarantee that the physics is still described by the Hamiltonian $\hat{H}_{\text{sub}}^{(2)}$, and actually it is very unlikely that it is so. Therefore, a possible way out of this divergence is to regularise the integral by adding a so-called hard cut-off Λ , above which the integrand is supposed to vanish. Although there could be unknown physics at scales Λ smaller than the Planck scale, it is common and conservative to assume $\Lambda \sim M_{\text{Pl}}$, yeilding $\rho_{\text{vac}}^{\text{quantum}} \sim 10^{-2} M_{\text{Pl}}^4$. Even though finite, this result is problematic, as the current vacuum energy density as measured in our dark-energy-dominated, spatially flat universe, is

$$\rho_0 = \rho_{\text{c},0} = \rho_{\text{V},0} = 3\Omega_{\text{V},0}(H_0/M_{\text{Pl}})^2 \times M_{\text{Pl}}^4 \sim 10^{-122} M_{\text{Pl}}^4,$$

a value that is 120 orders of magnitude smaller than the above value quoted for $\rho_{\text{vac}}^{\text{quantum}}$, due to the huge gap between the energy scales $H_0 \sim 10^{-33} \text{eV}$ and $M_{\text{Pl}} \sim 10^{28} \text{eV}$. Of course, the total vacuum energy density is not just due to these quantum zero-point fluctuations, and one should add the classical energy density due to the ground states of fields at the minimum of their potentials, if not vanishing, as well as a possible bare cosmological constant from the description of gravity. The so-called cosmological constant problem comes from the high level of fine-tuning needed to counter-balance those three independent contributions, from values as high as M_{Pl}^4 to 120 orders of magnitude smaller. Note that different regularisation schemes than the hard cut-off one, such as dimensional regularisation, can help to diminish this tension but clearly not to solve it. For a comprehensive and pedagogical review on the cosmological constant problem, I recommend reading Ref. [163].

The idea now is to go away from the Minkowski spacetime which is only obtained as a limit in the infinite past for a given mode with wavenumber k , and to consistently define a vacuum during inflation, which therefore constitutes a first step towards quantum gravity, *i.e.* quantum field theory on a curved spacetime (indeed only the cosmological perturbations are treated in a quantum way, while the background is still classical and described only by general relativity).

Going back to the exact Sasaki–Mukhanov equations (3.28), and focusing again on scalar perturbations v_k only (where now v_k is the mode function associated to the quantum operator $\hat{v}_{\vec{k}}$), one can define an effective pulsation squared, $\omega_k^2(\tau) = k^2 - \frac{z''}{z}$, which is clearly time-dependent and converges to the flat spacetime limit k^2 when $\tau \rightarrow -\infty$. The issue with such a time-dependent setup is that there is not any more a particular quantum state that minimises the Hamiltonian energy for every time τ . For example one can still minimise the Hamiltonian, now given by $\hat{H}^{(2)}(\tau) = \int d^3\vec{k}/(2\pi)^3 [\pi_{\vec{k}}^2(\tau) + \omega_{\vec{k}}^2(\tau)v_{\vec{k}}^2(\tau)]$, but only at a fixed time τ_1 , which gives a mode function v_k^{min,τ_1} with initial conditions $v_k^{\text{min},\tau_1}(\tau_1) = [2\omega_k(\tau_1)]^{-1/2} e^{-i\omega_k(\tau_1)\tau_1 + i\varphi_k}$, and associated with a set of annihilation and creation operators $(\hat{a}_{\vec{k}}^{\tau_1}, \hat{a}_{\vec{k}}^{\tau_1\dagger})$. But at another time τ_2 , the minimised energy corresponds to another mode function v_k^{min,τ_2} which is not merely $v_k^{\text{min},\tau_1}(\tau_2)$, because of the time-dependence of $\omega_k(\tau)$. Therefore the associated set of annihilation and creation operators $(\hat{a}_{\vec{k}}^{\tau_2}, \hat{a}_{\vec{k}}^{\tau_2\dagger})$ does not coincide with the previous one, and the two vacuums are physically different. In particular, the vacuum at time τ_2 , $|0\rangle_{\tau_2}$, in general contains particles in the vacuum at time τ_1 , meaning that the annihilation operator $\hat{a}_{\vec{k}}^{\tau_1}$ does not annihilate $|0\rangle_{\tau_2}$: $\hat{a}_{\vec{k}}^{\tau_1}|0\rangle_{\tau_2} \neq 0$. This effect is well known as the gravitational production of particles in expanding spacetimes [164, 165] and can be explicitated by noting that, since $[v_k^{\text{min},\tau_1}, (v_k^{\text{min},\tau_1})^*]$ constitutes a basis for the mode functions, one can write:

$$\begin{aligned} v_k^{\text{min},\tau_2} &= \alpha_k v_k^{\text{min},\tau_1} + \beta_k (v_k^{\text{min},\tau_1})^*, \text{ or equivalently} \\ \hat{a}_{\vec{k}}^{\tau_1} &= \alpha_k^* \hat{a}_{\vec{k}}^{\tau_2} + \beta_k \hat{a}_{-\vec{k}}^{\tau_2\dagger} \quad \text{and} \quad \hat{a}_{\vec{k}}^{\tau_1\dagger} = \alpha_k \hat{a}_{\vec{k}}^{\tau_2\dagger} + \beta_k^* \hat{a}_{-\vec{k}}^{\tau_2}, \end{aligned} \quad (3.43)$$

with $(\alpha_k, \beta_k) \in \mathbb{C}^2$ the so-called Bogolyubov coefficient, because the quantum operator $\hat{v}_{\vec{k}}$ itself does not depend on such a choice:

$$\hat{v}_{\vec{k}}(\tau) = v_k^{\text{min},\tau_1}(\tau) \hat{a}_{\vec{k}}^{\tau_1} + \text{h. c.} = v_k^{\text{min},\tau_2}(\tau) \hat{a}_{\vec{k}}^{\tau_2} + \text{h. c.}, \quad (3.44)$$

where “h. c.” means Hermitian conjugate. Therefore one sees that the vacuum at τ_2 , $|0\rangle_{\tau_2}$, contains a number density of particles with momentum $\vec{k}$ in the vacuum at τ_1 ,

given by:⁵

$$n_k = \frac{\tau_2 \left\langle 0 \left| \hat{a}_{\vec{k}}^{\tau_1 \dagger} \hat{a}_{\vec{k}}^{\tau_1} \right| 0 \right\rangle_{\tau_2}}{\delta^{(3)}(0)} = |\beta_k|^2, \quad (3.45)$$

and that there seems to be no unique notion of vacuum in time-dependent backgrounds. This difficulty is however overcome in the situation at hand during inflation. Indeed, each mode with wavenumber k of cosmological interest, begins its evolution under the horizon, namely with dynamics dictated by $\hat{H}_{\text{sub}}^{(2)}$ equivalent to the Minkowski case. Therefore, even though one cannot define an unambiguous vacuum state for each mode k at any time τ , one can consider initial conditions for each mode, maybe at different times, that are consistent with the asymptotic, $k\tau \rightarrow -\infty$ Minkowskian limit where the vacuum state is unambiguous (since there the pulsation is time-independent, $\omega_k = k$) and given by Eq. (3.41). This procedure, consisting in defining the vacuum using only modes that are well under the horizon, corresponds to a choice called the:

(Bunch-Davies vacuum:) $v_k(\tau) \xrightarrow[k\tau \rightarrow -\infty]{} v_k^{\text{Minkowski}}(\tau) = \frac{1}{\sqrt{2k}} e^{-ik\tau + i\varphi_k},$

(3.46)

thus defining a unique set of annihilation and creation operators $(\hat{a}_{\vec{k}}^{\text{BD}}, \hat{a}_{\vec{k}}^{\text{BD}\dagger})$ for each k , as well as unique initial conditions for each mode during inflation, up to an irrelevant initial phase φ_k which is shared by all modes with wavenumber k .

Now that the quantum nature of cosmological perturbations has been specified, the linear equations of motion (3.28) are understood as operator equations for the quantum operators $\hat{v}_{\vec{k}}$. But by using the mode expansion (3.35) of these operators, and the fact that the annihilation and creation operators constitute a basis for the Hilbert space of the quantum states, one arrives at the following, final equations of motion for the mode functions:

(Sasaki–Mukhanov equations): $v_k'' + \left(k^2 - \frac{z''}{z}\right) v_k = 0,$
 $v_k^{\lambda''} + \left(k^2 - \frac{a''}{a}\right) v_k^{\lambda} = 0,$

(3.47)

which can be solved together with the initial conditions (3.46).

⁵However, because of the normalisation condition, Eq. (3.37), the Bogolyubov coefficients must verify:

$$|\alpha_k|^2 - |\beta_k|^2 = 1$$

and therefore, if the two times τ_1 and τ_2 are close enough, and if the effective frequency ω_k is only slowly varying, one finds that α_k must be close to 1 and β_k close to 0, meaning that in this *adiabatic* limit only few particles are created, since $n_k = |\beta_k|^2$. Thus, a huge particle production requires either a violation of adiabaticity or a long amount of time.

Solution in quasi-de Sitter spacetime

In the following, one derives analytical approximations for the solution of the Sasaki–Mukhanov equations by making an expansion at first order in slow-roll parameters. First, note that the expression (3.29) for z''/z is exact and is not such an expansion at second order. However simplifying it by keeping only terms at first order in slow-roll (denoted with the sign “ $\approx$ ”), $-a^2 V_{,\phi\phi} = -\eta_V(3 - \epsilon)\mathcal{H}^2 \approx (3\eta/2 - 6\epsilon)\mathcal{H}^2$ and therefore $z''/z \approx \mathcal{H}^2(2 - \epsilon + 3\eta/2)$. Moreover from the exact equation $d\mathcal{H}/d\tau = \mathcal{H}^2(1 - \epsilon)$, one finds the relation between the comoving Hubble factor and the quasi-de Sitter conformal time at first order in slow-roll parameters:

$$\mathcal{H} \approx -\frac{1 + \epsilon}{\tau}, \quad (3.48)$$

which enables one to recast the equations of motion in terms of τ only, in the slow-roll approximation, noting that $a''/a = \mathcal{H}^2(2 - \epsilon)$ (exact):

$$\begin{aligned} v_k'' + \left[k^2 - \frac{1}{\tau^2} \left(2 + 3\epsilon + 3\frac{\eta}{2} \right) \right] v_k &\approx 0, \\ v_k^{\lambda''} + \left[k^2 - \frac{1}{\tau^2} (2 + 3\epsilon) \right] v_k^\lambda &\approx 0. \end{aligned} \quad (3.49)$$

First, these equations can be solved in the sub-Hubble limit, where $k^2 \gg 1/\tau^2$, and for which one actually recovers the Bunch-Davies solutions (this can be done without the slow-roll approximation of course). The super-Hubble limit where $k^2 \ll 1/\tau^2$ is more subtle and indeed requires to use the slow-roll approximations. At zeroth order, the solutions to the equation $f'' - 2f/\tau^2 = 0$ are given as linear combinations of a mode $\propto \tau^2$ with decreasing amplitude, and another one $\propto -1/\tau$ with growing amplitude (remember that τ is growing from large negative values to 0^- during inflation). To go further in the analysis, one needs to assume that the slow-roll parameters themselves are slowly evolving, and one can only solve Eqs. (3.47) locally around a time of interest at which they are evaluated. Clearly, this time of interest corresponds to the time of Hubble crossing for the mode k , denoted as τ_k , *i.e.* corresponding to $k = \mathcal{H}(\tau_k)$. A useful notation for quantities evaluated at τ_k is also to write $*(k)$, whence for example $\mathcal{H}(\tau_k) = \mathcal{H}_{*(k)}$, where the k -dependence of the operation $*$ is sometimes not explicated but should not be forgotten. Around this time, it is consistent at first order in slow roll, to consider the following differential equations,

$$\begin{aligned} v_k'' + \left[k^2 - \frac{\nu_s^2 - 1/4}{\tau^2} \right] v_k &\approx 0, \\ v_k^{\lambda''} + \left[k^2 - \frac{\nu_t^2 - 1/4}{\tau^2} \right] v_k^\lambda &\approx 0, \end{aligned} \quad (3.50)$$

where

$$\nu_s^2 = \frac{9}{4} + 3\epsilon_* + \frac{3\eta_*}{2} \quad \text{and} \quad \nu_t^2 = \frac{9}{4} + 3\epsilon_*, \quad (3.51)$$

are positive constants only slightly deviating from $9/4$. These equations can then be solved exactly with use of Hankel functions, for example the mode function v_k of scalar fluctuations reads:

$$v_k(\tau) = \sqrt{-\tau} \left[A_k H_{\nu_s}^{(1)}(-k\tau) + B_k H_{\nu_s}^{(2)}(-k\tau) \right], \quad (3.52)$$

where A_k and B_k are constants of integration that are found by matching the above solution to the asymptotic initial Bunch-Davies vacuum. In order to do this, one recalls first the expansion of the Hankel function of the first kind in the small and large argument limits for ν real and positive,

$$(\nu > 0): \quad H_\nu^{(1)}(x) \xrightarrow{x \rightarrow 0} -\frac{i}{\pi} \Gamma(\nu) \left(\frac{2}{x} \right)^\nu \quad \text{and} \quad H_\nu^{(1)}(x) \xrightarrow{x \rightarrow \infty} \sqrt{\frac{2}{\pi x}} e^{i(x - \frac{\nu\pi}{2} - \frac{\pi}{4})}, \quad (3.53)$$

where Γ is the Euler gamma function, and the fact that $H_\nu^{(2)} = (H_\nu^{(1)})^*$, from which one infers for the mode function of scalar perturbations:

$$A_k = \frac{\sqrt{\pi}}{2} e^{i(\varphi_k + \frac{\pi}{2}\nu_s + \frac{\pi}{4})} \quad \text{and} \quad B_k = 0, \quad (3.54)$$

by comparing the small-argument expansion of Eq. (3.52) with the Bunch-Davies vacuum (3.46). Therefore, the final solution for v_k and its super-horizon, $-k\tau \rightarrow 0$ limit, are

$$\begin{aligned} v_k(\tau) &= \frac{\sqrt{-\pi\tau}}{2} e^{i(\varphi_k + \frac{\pi}{2}\nu_s + \frac{\pi}{4})} H_{\nu_s}^{(1)}(-k\tau) \\ &\xrightarrow{-k\tau \rightarrow 0} 2^{\nu_s-3/2} \frac{\Gamma(\nu_s)}{\Gamma(3/2)} \frac{1}{\sqrt{2k}} (-k\tau)^{1/2-\nu_s} e^{i(\varphi_k + \frac{\pi}{2}\nu_s - \frac{\pi}{4})}, \end{aligned} \quad (3.55)$$

and the solution for the tensor modes, v^λ , is formally the same with $\nu_s \rightarrow \nu_t$. It should remain clear however, that these solutions are only approximate around the time of Hubble crossing for the mode k that they describe. In particular, pushing their expressions to $-k\tau \rightarrow \infty$, as was done to find the constants A_k, B_k , is formally illegal and in practice the approximation is expected to be accurate for only a few e -folds before and after horizon crossing.

Power spectrum of the comoving curvature perturbation

Although the Sasaki-Mukhanov variables are useful because they verify differential equations that can be solved exactly, though locally in time with use of the Hankel functions, observable quantities are rather related to curvature perturbations ζ and $\mathcal{R}$ for the scalar sector, and to the comoving tensor modes γ for the tensor sector. The physics of linear fluctuations during single-field inflation can be summarized by the power spectra $P_{\mathcal{R}}(k)$ and $P_\gamma(k)$, of these fluctuations, which are the equal-time, two-point functions defined as quantum averages of the operators

$$\hat{\mathcal{R}}_{\vec{k}} = \frac{\hat{v}_{\vec{k}}}{z} \quad \text{and} \quad \hat{\gamma}_{ij}^{\vec{k}} = \frac{2}{aM_{\text{Pl}}} \sum_{\lambda=+, \times} \epsilon_{ij}^\lambda(\vec{k}) \hat{v}_{\vec{k}}^\lambda, \quad (3.56)$$

and thus reminiscent of their quantum nature:

$$\begin{aligned} \langle 0 | \hat{\mathcal{R}}_{\vec{k}}(\tau) \hat{\mathcal{R}}_{\vec{k}'}(\tau) | 0 \rangle &= (2\pi)^3 \delta^{(3)}(\vec{k} + \vec{k}') P_{\mathcal{R}}(k, \tau) \quad \text{with} \quad P_{\mathcal{R}}(k, \tau) = \frac{v_k v_k^*}{z^2}, \\ \langle 0 | \hat{\gamma}_{ij}^{\vec{k}}(\tau) \hat{\gamma}_{ij}^{\vec{k}'}(\tau) | 0 \rangle &= (2\pi)^3 \delta^{(3)}(\vec{k} + \vec{k}') P_{\gamma}(k, \tau) \quad \text{with} \quad P_{\gamma}(k, \tau) = \frac{8}{a^2 M_{\text{Pl}}^2} \sum_{\lambda=+, \times} v_k^{\lambda} (v_k^{\lambda})^*, \end{aligned} \quad (3.57)$$

where one used the polarisation conditions $\epsilon_{ij}^{\lambda}(\vec{k}) \left(\epsilon_{ij}^{\lambda'}(-\vec{k}) \right)^* = \epsilon_{ij}^{\lambda}(\vec{k}) \epsilon_{ij}^{\lambda'}(\vec{k}) = \delta_{\lambda\lambda'}$. Now, one needs to find expressions for a and z as functions of conformal time τ . For this, notice that up to first order in slow-roll, one finds from the expression $\mathcal{H} \approx -(1 + \epsilon)/\tau$ that, given a particular time τ_p , one has:

$$\frac{a}{a_p} \approx \left(\frac{-k\tau}{-k\tau_p} \right)^{-(1+\epsilon_p)} \implies a \approx (1 + \epsilon_*) \frac{k}{H_*} (-k\tau)^{-(1+\epsilon_*)}, \quad (3.58)$$

where in the second equality one has chosen the particular time to be the horizon exit for the mode k .⁶ Note also that $-(1 + \epsilon_*) = 1/2 - \nu_t$ and hence that a has the same time-dependence than v_k^{λ} on super-horizon scales. Getting $z(\tau)$ is slightly more intricate, and necessitates the resolution of the differential equation $z''/z = (\nu_s^2 - 1/4)/\tau^2$. One can look for solutions of the form $z = (-k\tau)^{\alpha}$ and finds the two possible such polynomial solutions, growing and decaying modes corresponding to $\alpha = 1/2 \mp \nu_s$, of which a general solution must be a linear combination. But one knows that $z \propto a\sqrt{\epsilon}$, and $a(\tau)$ only contains the growing mode, so from the slow variation of ϵ that cannot drive z too far from a , one deduces that:

$$z/z_p \approx \left(\frac{-k\tau}{-k\tau_p} \right)^{1/2-\nu_s} \implies z \approx (1 + \epsilon_*) \frac{k}{H_*} \sqrt{2\epsilon_*} M_{\text{Pl}} (-k\tau)^{1/2-\nu_s}, \quad (3.59)$$

whence one finds that both $\mathcal{R}_k$ and γ_k converge to constant values on super-horizon scales, which is an important general theorem of single-field inflation. Their dimensionless power spectra, defined as

$$\mathcal{P}_{\mathcal{R}} = \frac{k^3}{2\pi^2} P_{\mathcal{R}} \quad \text{and} \quad \mathcal{P}_{\gamma} = \frac{k^3}{2\pi^2} P_{\gamma}, \quad (3.60)$$

read

(Power spectra in single-field, slow-roll inflation):

$$\begin{aligned} \mathcal{P}_{\mathcal{R}}(k, \tau) &\underset{-k\tau \rightarrow 0}{=} \mathcal{P}_{\mathcal{R}}(k) \approx \frac{H_{*(k)}^2}{8\pi^2 \epsilon_{*(k)} M_{\text{Pl}}^2}, \\ \mathcal{P}_{\gamma}(k, \tau) &\underset{-k\tau \rightarrow 0}{=} \mathcal{P}_{\gamma}(k) \approx \frac{2H_{*(k)}^2}{\pi^2 M_{\text{Pl}}^2}, \end{aligned} \quad (3.61)$$

where one restored the k -dependence of the operation $*(k)$ that evaluates a quantity at the time of horizon crossing for the mode with wavenumber k , and kept only the

⁶For completeness, this equation can be reversed and gives $-k\tau \approx -k\tau_p (1 + \epsilon_p) (a/a_p)^{-1+\epsilon_p}$.

leading-order terms in slow roll. Therefore, although the power spectra converge to constant values and have no explicit dependence on k , they carry information about the background at the time τ_k of horizon crossing, and thus depend slightly on k . This scale-dependence can be parameterised by the scalar and tensor spectral indices, respectively defined as

$$n_s - 1 = \frac{\partial \ln \mathcal{P}_{\mathcal{R}}(k)}{\partial \ln k} \approx -2\epsilon_* - \eta_* , \quad (3.62)$$

$$n_t = \frac{\partial \ln \mathcal{P}_{\gamma}(k)}{\partial \ln k} \approx -2\epsilon_* . \quad (3.63)$$

Moreover, the tensor-to-scalar ratio r measures the relative amount of power in the tensor and scalar modes during inflation. In single-field, slow-roll inflation, one has the following consistency relation between the tensor-to-scalar ratio and the spectral index of tensor modes:

$$r = \frac{\mathcal{P}_{\gamma}}{\mathcal{P}_{\mathcal{R}}} \approx 16\epsilon_* \approx -8n_t . \quad (3.64)$$

All these quantities, $n_s - 1$, n_t , r , can be re-expressed in terms of the potential slow-roll parameters, ϵ_V and η_V with use of their approximations in the slow-roll regime: $\epsilon \approx \epsilon_V$ and $\eta \approx 4\epsilon_V - 2\eta_V$. Note also that rigorously, the spectral indices and tensor-to-scalar ratio are still k -dependent because they are expressed in terms of slow-roll parameters evaluated at τ_k . This dependence can be parameterised for example with the running of the spectral index, $\alpha_s = \partial n_s(k)/(\partial \ln k)$ which is a second-order quantity in terms of the slow-roll expansion, etc. But for definiteness, it is common to use a mode with fixed wavenumber, called the pivot scale k_{pivot} and corresponding to a typical cosmological scale measured in the CMB, to give a unique number for these quantities. In practice, to make the link between model-building and observations, one should specify the time $N_{\text{pivot}} = N_{*(k_{\text{pivot}})}$ (another possibility is to discuss the number of e -folds spent above the horizon and before the end of inflation for this particular scale, a quantity sometimes simply denoted N_*) at which the pivot scale exited the horizon, in order to make definite predictions on the theoretical side. But on the observational side, one is only given the value of k itself, and the total number of e -folds spent above the horizon for this mode, depends on the whole cosmological history between the end of inflation and the CMB emission. Although radiation-domination and matter-domination eras are well understood, there remains an uncertainty due to a reheating mechanism at the end of inflation to be precised. Either this mechanism is specified and N_* can be computed, or no assumption on the reheating phase is made and then N_* comes only as a theoretically constrained parameter to be measured by observations.

Note also that during slow-roll, using $\epsilon \approx \epsilon_V$, one finds the following approximate relation between the total field displacement $\Delta\phi = |\phi_{\text{end}} - \phi_{\text{ini}}|$ where the time “ini” is understood as 60 e -folds before horizon exit for the pivot scale, and the tensor-to-scalar ratio r , which is known as the:

$$\text{(Lyth bound): } \frac{\Delta\phi}{M_{\text{Pl}}} \sim \sqrt{\frac{r}{0.01}} , \quad (3.65)$$

which shows that a super-Planckian displacement, $\Delta\phi/M_{\text{Pl}} \gtrsim 1$, is required to hope observing directly primordial tensor modes in the near future, *i.e.* if $r \gtrsim 0.01$.

Example: quadratic inflation. Back to the example of quadratic inflation, where one finds that $\epsilon_V = \eta_V = 2M_{\text{Pl}}^2/\phi^2$, and choosing the pivot scale corresponding to $N_{\text{end}} - N_{\text{pivot}} = 60$, one finds approximate values for the potential slow-roll parameters with use of the slow-roll background trajectories: $\epsilon_V^{\text{pivot}} = \eta_V^{\text{pivot}} \approx 8.2 \times 10^{-3}$. Therefore $n_s^{\text{pivot}} \approx 0.967$ and $r_{\text{pivot}} \approx 0.13$, a latter value which is now in strong tension with latest CMB constraints, $r_{\text{pivot}} < 0.056$ at 95% confidence [38], see also Fig. 3.4 in the next section, Sec. 3.3.

Massive test scalar field in de Sitter

The computation of the power spectrum for the Sasaki-Mukhanov variables can be extended to test scalar field perturbations. By test scalar field, it is meant that the scalar field does not backreact on the geometry of spacetime. Of course, this can only be an approximation, but it can be justified, *e.g.* if inflation is driven by a scalar field ϕ and if there exists another field χ which is non-dynamical at the level of the background but still develops small perturbations whose effects on the spacetime perturbations remain negligible. Let such perturbations be called χ and suppose that they behave effectively as a canonically normalised massive field, hence:

$$\chi_k'' + \left(k^2 - \frac{a''}{a} + m_\chi^2 a^2 \right) \chi_k = 0, \quad (3.66)$$

where m_χ is an effective mass, and with $a = \mathcal{H}/H \approx -1/(\tau H)$ and $a''/a \approx 2/\tau^2$ assuming that the background is well described by a de Sitter spacetime (*i.e.* one works at zeroth order in slow-roll parameters and $a(t) \propto e^{Ht}$, with H a constant). Therefore, one can rewrite the above EoM as

$$\chi_k'' + \left[k^2 - \frac{\nu_\chi^2 - 1/4}{\tau^2} \right] \chi_k \approx 0, \quad \text{with } \nu_\chi^2 = \frac{9}{4} - \frac{m_\chi^2}{H^2}, \quad (3.67)$$

an expression in which H is supposed to be constant. The formal solution to this equation is exactly the same as (3.52), but to go further one needs to distinguish two cases.

- Light case.

Indeed, when $m_\chi < 3H/2$, then ν_χ is real and positive and the results for v_k readily apply to χ_k : assuming that the field χ also has Bunch-Davies initial conditions, one recovers Eq. (3.55), simply with the replacement $\nu_s \rightarrow \nu_\chi$. The power spectrum of the rescaled perturbations, $\tilde{\chi} = \chi/(aM_{\text{Pl}})$, then reads:

$$\frac{k^3}{2\pi^2} P_{\tilde{\chi}}(k, \tau) \Big|_{-k\tau \rightarrow 0} = \mathcal{P}_{\tilde{\chi}}(k, \tau) \Big|_{\nu_k \in \mathbb{R}^+} \approx \frac{H^2}{8\pi^3 M_{\text{Pl}}^2} (-k\tau)^{3-2\nu_\chi} [2^{\nu_\chi} \Gamma(\nu_\chi)]^2, \quad (3.68)$$

and has an amplitude similar to the one of tensor modes a short time after horizon crossing, but then decays due to the positive value of $3 - 2\nu_\chi$ in this regime.

- Heavy case.

But when $m_\chi > 3H/2$, then $\nu_\chi = i\mu_\chi$ is purely imaginary, $\mu_\chi \in \mathbb{R}^+$, and the qualitative behaviour of perturbations is very different. First, although the large-argument expansion of the Hankel function is similar for real and imaginary ν , assuming Bunch-Davies initial conditions for χ_k yields a very different constant of integration:

$$A_k = \frac{\sqrt{\pi}}{2} e^{-\frac{\pi}{2}\mu_\chi} e^{i(\varphi_k + \frac{\pi}{4})} \quad (\text{and } B_k = 0), \quad (3.69)$$

where one discovers an exponential suppression $e^{-\frac{\pi}{2}\mu_k}$ resembling a Boltzmann factor since $\mu_k \sim m_\chi/H$ in the limit of a heavy field, and where m_χ is an inertial term and H can be thought of as analogous to the temperature of de Sitter spacetime. Moreover, the small-argument expansion of the Hankel functions is qualitatively different:

$$(\mu > 0): \quad H_{i\mu}^{(1)}(x) \xrightarrow{x \rightarrow 0} -\frac{i}{\pi} \Gamma(i\mu) \left(\frac{x}{2}\right)^{-i\mu} + \frac{1}{i\mu \Gamma(i\mu)} \left(\frac{x}{2}\right)^{i\mu} [1 + \coth(\mu\pi)], \quad (3.70)$$

where major differences are, the presence of oscillations with k due to the $x^{i\mu}$ terms in the small-argument expansion of the Hankel function with imaginary argument, and the fact that they are more suppressed by powers of $-k\tau$:

$$\begin{aligned} \chi_k(\tau) &= \frac{\sqrt{-\pi\tau}}{2} e^{-\frac{\pi}{2}\mu_\chi} e^{i(\varphi_k + \frac{\pi}{4})} H_{\nu_\chi}^{(1)}(-k\tau) \\ &\xrightarrow{-k\tau \rightarrow 0} \frac{e^{-\frac{\pi}{2}\mu_\chi}}{2\sqrt{\pi k}} (-k\tau)^{1/2} \left\{ \Gamma(i\mu_\chi) \left(\frac{x}{2}\right)^{-i\mu_\chi} + \frac{\pi}{\mu_\chi \Gamma(i\mu_\chi)} \left(\frac{x}{2}\right)^{i\mu_\chi} [1 + \coth(\mu_\chi\pi)] \right\} e^{i(\varphi_k - \frac{\pi}{4})}. \end{aligned} \quad (3.71)$$

Collecting terms, one finds the very different behaviour of the power spectrum corresponding to heavy fluctuations ($m_\chi > 3H/2$), compared to the light case ($m_\chi < 3H/2$), in the super-horizon limit and once rescaled to $\tilde{\chi} = \chi/(aM_{\text{Pl}})$:

$$\begin{aligned} \frac{k^3}{2\pi^2} P_{\tilde{\chi}}(k, \tau) &\underset{-k\tau \rightarrow 0}{=} \mathcal{P}_{\tilde{\chi}}(k, \tau), \\ &\underset{\nu_k \in i\mathbb{R}}{\approx} \frac{H^2}{8\pi^3 M_{\text{Pl}}^2} e^{-\pi\mu_\chi} (-k\tau)^3 \left\{ \alpha(\mu_\chi) + \beta(\mu_\chi) \cos \left[2\mu_\chi \ln \left(\frac{-k\tau}{2} \right) + \varphi(\mu_\chi) \right] \right\}, \\ \text{with } \alpha(\mu_\chi) &= \frac{\pi}{\mu_\chi \sinh(\pi\mu_\chi)} (1 + e^{2\pi\mu_\chi}), \quad \beta(\mu_\chi) = \frac{\pi}{\mu_\chi} [1 + 2 \coth(\pi\mu_\chi)], \\ \text{and } \varphi(\mu_\chi) &= -\arg[\Gamma(i\mu_\chi)], \end{aligned} \quad (3.72)$$

where one used the property of the Euler gamma function, $|\Gamma(ib)|^2 = \pi/[b \sinh(\pi b)]$ for $b \in \mathbb{R}$. It is interesting to notice in this formula that the amplitude, the frequency and the phase of the $\ln(-k\tau/2)$ -oscillations depend on the mass parameter ν_χ , and that the power spectrum decays with time as $(-k\tau)^3$. Moreover, the oscillations are damped by the thermodynamics factor $e^{-\pi\mu_\chi}$, but there is a constant mode (in k , but still decaying with time), $\propto \pi/\mu_\chi$, that is not exponentially killed when μ_χ becomes quite larger than unity, see second term of $\alpha(\mu_\chi)$.

3.3 CMB observations and constraints on single-field models

Observations of the CMB not only constrain the background dynamics of inflation, $\Delta N_{\text{tot}} \gtrsim 60$, but also the statistics of linear fluctuations. Indeed, taking the power spectra at the end of inflation as initial conditions for the radiation-dominated and matter-dominated eras, Boltzmann codes like CMBFast [166], CAMB [167] and CLASS [168] can be used to evolve the probability density functions of the positions and momenta of particles in the early universe, and to predict the acoustic peaks in the temperature and polarisation spectra of the CMB. The physics of the CMB is extremely rich and I could not give enough credits to the physicists that helped understanding it, however in the spirit of keeping this thesis reasonably long, it shall not be further explained. The attitude in the following is rather to take the information on the inferred values of, or constraints on, the primordial parameters $(n_s, \alpha_s, r, \dots)$, as granted and explore their consequences in terms of model-building. Indeed, it is both a blessing and a curse that many different models of inflation succeed to provide the minimal amount of e -folds of expansion to solve both the horizon and the flatness problems, and even to predict accurately the values of n_s, r , etc. Therefore, it is of great importance to study in detail the constraints that cosmological observations put on these models that can be well-motivated or not in terms of high-energy physics. To put it in a nutshell, studying inflation amounts to studying physics beyond the Standard Model, at energy scales much larger than those accessible in particle accelerators on Earth, by taking full advantage of the great cosmic accelerator. This approach is extended in Chapter 5 to the CMB constraints on primordial non-Gaussianities and how they can help us to favour or rule out models of the very early universe. Rather than long sentences, one is invited to observe Fig. 3.4.

A few comments can be made, first about the figure, and then more generally about constraints on single-field, slow-roll inflation:

- A perfectly scale-invariant scalar power spectrum, $n_s = 1$, is ruled out at more than 7σ , and the deviation from 1 is very well measured: $n_s = 0.9649 \pm 0.0042$ at 68% confidence (1σ). It is a huge achievement of the simple single-field, slow-roll inflationary paradigm to predict such small but non-vanishing deviations from 1 (remember the typical example of quadratic inflation for which $n_s \approx 0.967$), and precise measurements of n_s enable one to distinguish amongst various models, *e.g.* “Low scale SB SUSY” models are excluded.
- Primordial gravitational waves have not been observed yet, as one is only given upper bounds on the tensor-to-scalar ratio: $r < 0.056$ at 95% confidence. This fact can be thought of as disappointing, since such observation would provide a smoking-gun evidence for a quantum generation of primordial perturbations, both of the scalar and tensor kinds, as predicted almost solely by cosmic inflation. But the constraints are so strong that they enable one to rule out a huge number of inflationary models, in particular so-called “large-field models” in which the scalar

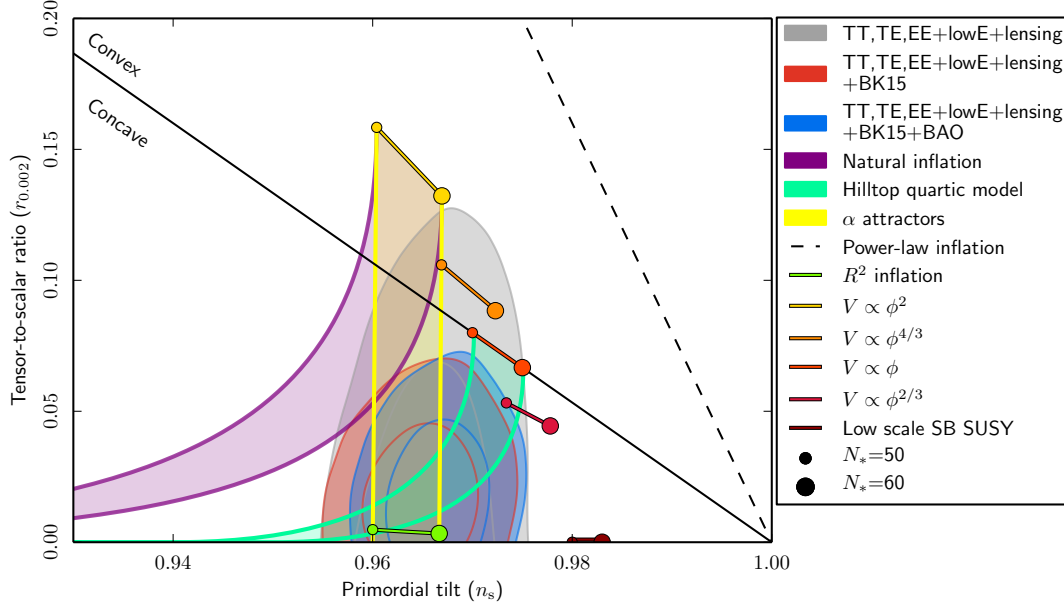


Figure 3.4: Planck 2018 constraints on single-field, slow-roll inflationary models: figure taken from [38]. The horizontal axis displays values of the scalar spectral index $n_s = 1 + \partial [\ln \mathcal{P}_{\mathcal{R}}(k)] / (\partial \ln k)$ while the tensor-to-scalar ratio $r = \mathcal{P}_{\gamma} / \mathcal{P}_{\mathcal{R}}$ is represented on the vertical axis. The grey, red and blue contours correspond to the values allowed after the Planck analysis, given respectively Planck CMB data [169] alone, Planck CMB data combined with the BICEP2/Keck Array (BK15) CMB data [170, 171], and Planck CMB data with BK15 data and BAO data from the 6dF [172] and SDSS [173, 174] large-scale structure experiments that help to break degeneracies with Λ CDM parameters. Predictions from a few single-field, slow-roll inflationary models are plotted on top of the Planck constraints, therefore making apparent which of them are ruled out, constrained, or fully consistent with cosmological observations. The time of horizon exit for the pivot scale $k_{\text{pivot}} = 0.002 \text{ Mpc}^{-1}$ used in this figure, is parameterised by N_* , and models that are excluded for some values of N_* but allowed for others, can be understood as having their reheating mechanism constrained [113]. For more details on the implications for model-building, see in the main text.

fields take super-Planckian values, $\phi_* > M_{\text{Pl}}$ and the first slow-roll parameter, ϵ_* , is not extremely small (such as the famous and simple quadratic inflation model: $\phi_* \sim 10M_{\text{Pl}}$, $\epsilon_* \sim 1 \times 10^{-2}$). Actually, all monomial potentials $V \propto \phi^p$ where $p \in \mathbb{R}^+$ are strongly disfavored by the combined (n_s, r) constraints. “Small-field models”, for which $\phi_* < M_{\text{Pl}}$ or “plateau models” that have a very flat potential, and models with concave rather than convex potentials, are generally favored by these constraints since they feature smaller values of ϵ_* and thus a smaller tensor-to-scalar ratio.

- Although not represented in this plot, the running of the spectral index, α_s is measured to be consistent with zero, an observation that is again in good agreement with the single-field, slow-roll picture where this quantity is a second-order one in the slow-roll expansion. The running of the running, $\partial\alpha_s/(\partial\ln k)$ is also constrained around a vanishing value.
- The amplitude of the scalar power spectrum, $A_s = \mathcal{P}_{\mathcal{R}}(k_{\text{pivot}})$ is also well measured, one has $A_s = 2.10 \times 10^{-9}$, which fixes the value of H_*^2/ϵ_* for single-field, slow-roll inflation. Since $\mathcal{P}_\gamma \propto (H_*/M_{\text{Pl}})^2$, the absence of detection of gravitational waves ($\mathcal{P}_\gamma < 0.056 \times 2.10 \times 10^{-9}$) provides us with an upper bound on the value of the Hubble parameter at the time of horizon exit for the pivot scale: $H_* < 7.6 \times 10^{-5} M_{\text{Pl}}$.

For completeness, the few inflationary models that are represented on Fig. 3.4, are spelled out here, but no comment is made on their motivations:

- Natural inflation: $V(\phi) = \Lambda^4 [1 + \cos(\phi/f)]$, where Λ is a mass scale that can be inferred from the measured value of A_s , and f is another mass scale often called the axion decay constant, that when varied together with the pivot-scale, horizon-exit time N_* , gives rise to the purple contour on Fig 3.4;
- Hilltop models: $V_p(\phi) = \Lambda^4 [1 - (\phi/\mu)^p]$, with $p \in \mathbb{R}$ and where Λ and μ are again mass scales. The hilltop quartic model simply corresponds to V_4 and varying both μ and N_* gives the green contour on Fig. 3.4 (hilltop quadratic, V_2 , is less favored by the Planck analysis);
- Power-law inflation has a different status, since it is rather defined as inflation happening with a scale factor growing as t^q with $q \in \mathbb{R}^+$. Exponential potentials like $V_q(\phi) = \Lambda^4 \exp\left(-\sqrt{2/q} \phi/M_{\text{Pl}}\right)$ can induce such background dynamics but overall these models are strongly disfavored because they predict a large tensor-to-scalar ratio except if $n_s \sim 1$, indeed one has the following relation: $n_s - 1 = -r/8$;
- α -attractors correspond to a class of models where the potential is stretched exponentially when going away from $\phi = 0$. E -models are a subset of these and feature of potential $V_\alpha(\phi) = \Lambda^4 \left[1 - \exp\left(\sqrt{2/(3\alpha)} \phi/M_{\text{Pl}}\right)\right]^2$. Interestingly, they provide a continuous description between the simplest quadratic inflation model for $\alpha \gg 1$

where $V(\phi) = m^2\phi^2/2$ and the Starobinsky inflation model for $\alpha = 1$. Varying both the dimensionless number α and N_* gives the yellow contour on Fig. 3.4;

- Starobinsky, or R^2 inflation, corresponds to the addition of a squared Ricci scalar in the Lagrangian of general relativity, which is a dimension-4 operator and therefore does not come with a mass scale as the Planck mass in front of the usual Einstein-Hilbert term R . Changing of frame, this theory can be rephrased in terms of pure GR with an additional scalar ϕ that features the following potential: $V(\phi) = \Lambda^4 \left[1 - \exp\left(\sqrt{2/3}\phi/M_{\text{Pl}}\right) \right]^2$, leading to universal predictions, $n_s - 1 = -2/N_*$ and $r = 12/N_*^2$, that are in excellent agreement with Planck constraints. This model is often quoted as the prototypical model of single-field slow-roll inflation that matches observations to a high degree of accuracy;
- Monomial potentials, $V_p(\phi) = \phi^p$ have already been commented, they are overall ruled out;
- The low-scale Spontaneously Broken Supersymmetry model corresponds to a potential $V(\phi) = \Lambda^4 [1 + \beta \ln(\phi/M_{\text{Pl}})]$ and predicts a too large n_s .

However, one should know that the above constraints are given for a very specific class of inflationary models: slow-roll (both $\epsilon, \eta \ll 1$), single-field (only one propagating scalar degree of freedom), with canonical kinetic terms ($-\partial_\mu\phi\partial^\mu\phi/2$ in the Lagrangian). Other kinds of models, sometimes better motivated, can be studied. First, transient violations of slow-roll, so-called features, can exist without ruining inflation and the overall quasi-exponential expansion of space, or models that feature a large and negative η with a small and decreasing ϵ (ultra-slow-roll) are fully consistent with the quasi-de Sitter dynamics but give very different observational predictions for the perturbations. Moreover, nothing tells us that there must be only one scalar field, and if there are several of them that are dynamical, then one must consider so-called multifield inflation, which is the main topic of this thesis, and also features a much different phenomenology. These scalar fields might have simple, canonical kinetic terms, but again this shall not come as a requirement but rather as a simplification, and one is let to consider non-canonical kinetic terms of the non-linear sigma models, see Eq. (2.10), that can lead to specific observational signatures, both at the level of linear perturbations and non-Gaussianities, see Chap. 4 and Chap. 5.

3.4 The effective field theory of inflation: a model-independent theory of fluctuations

Having explained and elucidated the degeneracy amongst the various possible single-field models, it would appear appealing to have a model-independent description of inflationary fluctuations. This is exactly the aim of the so-called Effective Field Theory of Inflation (EFTofI) [175, 176], which is briefly sketched in this Section following closely the spirit and sometimes the notations of this original paper.

As any Effective Field Theory (EFT), the EFToI relies on the symmetries of the system at hand to describe it in the most generic way. An important feature of the EFToI is that it describes only the inflationary fluctuations, and assumes that the background quantities are given functions of time. In particular, its aim is not to provide a mechanism for solving the horizon and flatness problems (any serious model of single-field slow-roll inflation does that), and it simply assumes a quasi-exponential expansion of the FLRW background spacetime, with $a(t) \propto e^{Ht}$ and $H(t)$ a given function of time that is slowly varying: $-\dot{H} \ll H^2$. This is both a strength and a weakness: it enables one to describe cosmological perturbations in a model-independent way, but that might not be realised in concrete models where a Lagrangian is specified and dictates both the background dynamics and the one of linear fluctuations in a consistent way.

3.4.1 Action in the unitary gauge

First, one shall note that the effect of having a dynamical scalar field with a non-vanishing velocity in a FLRW universe, is to spontaneously break the time diffeomorphism of de Sitter spacetime, due to a non-zero time derivative of the vacuum expectation value of the scalar field, $\dot{\phi} \neq 0$. Indeed, vacuum GR is invariant under all spacetime diffeomorphisms, but the presence of the scalar field $\phi(t, \vec{x}) = \bar{\phi}(t) + Q(t, \vec{x})$, perturbed at first order, reduces the number of spacetime symmetries of the inflationary universe compared to the maximally symmetric de Sitter spacetime. This statement is best seen in the transformation properties of the scalar field perturbations $Q(t, \vec{x})$ under such diffeomorphisms, see Sec. 2.3.3 for details. Under a linear transformation $\xi^\mu = (T, L^i)$ (such that $t \rightarrow \tilde{t} = t - T$ and $x^i \rightarrow \tilde{x}^i = x^i - L^i$ in the passive view that shall be used here), one finds from imposing that ϕ is a scalar, $\phi \rightarrow \tilde{\phi}$ with $\tilde{\phi}(\tilde{x}) = \phi(x)$, that at first order:

$$\tilde{Q}(t, \vec{x}) = Q(t, \vec{x}) + \dot{\bar{\phi}}(t)T(t, \vec{x}), \quad (3.73)$$

where it is clear that Q transforms non-linearly under time diffeomorphisms (meaning that $\tilde{Q}$ is not proportional to Q under a gauge transformation with $L^i = 0$) while it is still a scalar under spatial diffeomorphisms (meaning that $\tilde{Q} = Q$ under a gauge transformation with $T = 0$). It is always possible to choose a gauge which makes the correspondence between cosmic time t and the clock defined by the scalar field, $\phi(t, \vec{x})$: for this it is necessary to ask for vanishing perturbations of the scalar field on the hypersurfaces of constant t , meaning that $Q^{\text{unitary}}(t, \vec{x}) = 0$ in this gauge that one shall denote “unitary” by analogy with particle physics mechanisms. In this gauge, the dynamical scalar mode is therefore included in the description of the spacetime metric: $g_{\mu\nu}^{\text{unitary}}(t, \vec{x})$ must contain one scalar and two tensor dynamical degrees of freedom. Moreover, importantly $g_{\mu\nu}^{\text{unitary}}(t, \vec{x})$ is not invariant under time diffeomorphisms since it has eaten the scalar mode that transforms non-linearly. Note that until now, one was able to avoid writing down any Lagrangian, and (almost) only described the setup with words. But given the well-known saying “Physics is less fun without Lagrangians” of an old and wise physicist, one shall now write, in the spirit of EFTs, all possible operators that are compatible with the symmetries. Interestingly, as opposed to GR and other metric

theories with higher-order derivatives, the theory at hand can contain operators that are invariant under spatial diffeomorphisms but not time diffeomorphisms. Therefore, the resulting Lagrangian contains *a priori* many new terms besides the usual contractions of Riemann and metric tensors. Simply quoting the results of [176] without a proof, the most general action compatible with such symmetries and expressed in terms of independent quantities is

$$S = \int d^4x \sqrt{-g} F(g^{\mu\nu}, g^{00}, R_{\mu\nu\rho\sigma}, K_{ij}, \nabla_\mu; t), \quad (3.74)$$

where F is a generic function whose tensorial spacetime indices μ, ν etc., if any, must be evaluated on the time coordinate 0. In this expression, one reminds that $R_{\mu\nu\rho\sigma}$ is the usual 4-dimensional Riemann curvature of spacetime, g^{00} is nothing but the 0-0 component of the inverse spacetime metric $g^{\mu\nu}$, K_{ij} is the extrinsic curvature of the 3-dimensional hypersurfaces defined by the unit, timelike normal vector $n^\mu \propto \partial^\mu \tilde{t}$, with $\tilde{t}(\vec{x})$ the parametric function defining the hypersurfaces of constant ϕ (and therefore coinciding with t in the unitary gauge), see Sec. 2.4 for more details, with $\nabla_\mu(\cdot) = \partial_\mu(\cdot) + \Gamma^\cdots_{\mu\cdots} \times (\cdot)$ the usual covariant spacetime derivative, and t the cosmic time parameter. The action (3.74) can now be expanded around a FLRW background, with each tensorial quantity $X = \bar{X} + \delta X$, yielding [176]

$$\begin{aligned} S_{\text{unitary}} = \int d^4x \sqrt{-g} & \left[\frac{M_{\text{Pl}}^2}{2} R - (3 - \epsilon) H^2 M_{\text{Pl}}^2 - \epsilon H^2 M_{\text{Pl}}^2 g^{00} \right. \\ & + \frac{1}{2} M_2(t)^4 (\delta g^{00})^2 + \frac{1}{6} M_3(t)^4 (\delta g^{00})^3 + \frac{1}{24} M_4(t)^4 (\delta g^{00})^4 + \dots \\ & \left. - \frac{\bar{M}_1(t)^3}{2} \delta g^{00} \delta K - \frac{\bar{M}_2(t)^2}{2} (\delta K)^2 - \frac{\bar{M}_3(t)^2}{2} \delta K_j^i \delta K_i^j + \dots \right], \end{aligned} \quad (3.75)$$

where one used so-called tadpole cancellation, *i.e.* enforced that terms linear in the fluctuations (contained in the first three terms only) multiply the background Friedmann equations, to fix the function multiplying g^{00} and the term independent of the metric g inside the brackets (and thus equivalent to a time-varying cosmological constant $\Lambda(t) = (3 - \epsilon) H^2 M_{\text{Pl}}^2$ responsible for the quasi-exponential expansion of space). The dots stand for terms that are of higher order in derivatives and thus suppressed by powers of a higher energy scale, or of higher order in perturbations, or both.

3.4.2 Action for the pseudo-Goldstone π

The idea now is to restore explicitly the dynamical scalar mode which is included in the gravity sector in the unitary gauge, by evading the unitary gauge under a time diffeomorphism $t \rightarrow \tilde{t} = t - T(t, \vec{x})$, and describe the scalar mode by the gauge transformation T itself, which is promoted to a dynamical field: $T(x) \mapsto \tilde{\pi}(\tilde{x})$. This procedure is named a Stueckelberg transformation and the scalar field $\tilde{\pi}$ in this new gauge, that is therefore called a Stueckelberg field, must vanish in the unitary gauge by definition, meaning that it must transform as

$$\tilde{\tilde{\pi}}(\tilde{\tilde{x}}) = \tilde{\pi}(\tilde{x}) + \tilde{T}(\tilde{x}). \quad (3.76)$$

Looking at the law of transformation of the metric tensor under a change of coordinates, gives in particular $g^{00} \rightarrow \tilde{g}^{00}(\tilde{x}(x)) = \frac{\partial \tilde{t}(x)}{\partial x^\mu} \frac{\partial \tilde{t}(x)}{\partial x^\nu} g^{\mu\nu}(x)$, which after inversion enables one to express g^{00} in the action in terms of $\tilde{g}^{\mu\nu}(\tilde{x})$, $\tilde{\pi}(\tilde{x})$:⁷

$$g^{00}(x) = \left[(1 + \dot{\pi})^2 \tilde{g}^{00} + 2(1 + \dot{\pi}) \partial_i \tilde{\pi} \tilde{g}^{0i} + \tilde{g}^{ij} \partial_i \tilde{\pi} \partial_j \tilde{\pi} \right] \Big|_{\tilde{x}}. \quad (3.77)$$

Moreover, all functions of time like $H(t)$, $M_n(t)$, $\bar{M}_n(t)$, etc. are now evaluated at $\tilde{t} + \tilde{\pi}(\tilde{x})$, while $\sqrt{-g} d^4x$, R are of course invariant. *Forgetting for the moment the extrinsic curvature terms* $\propto \bar{M}_n$, one finds the action expressed in terms of the transformed fields and coordinates (one drops the tildes every where in this expression for simplicity):

$$\begin{aligned} S_\pi = \int d^4x \sqrt{-g} \Big\{ & \frac{M_{\text{Pl}}^2}{2} R - [3 - 2\epsilon(t + \pi)] H^2(t + \pi) M_{\text{Pl}}^2 \\ & - \epsilon(t + \pi) H^2(t + \pi) M_{\text{Pl}}^2 \left[1 + (1 + \dot{\pi})^2 g^{00} + 2(1 + \dot{\pi}) \partial_i \pi g^{0i} + g^{ij} \partial_i \pi \partial_j \pi \right] \\ & + \sum_{n=2}^{\infty} \frac{1}{n!} M_n^4(t + \pi) \left[1 + (1 + \dot{\pi})^2 g^{00} + 2(1 + \dot{\pi}) \partial_i \pi g^{0i} + g^{ij} \partial_i \pi \partial_j \pi \right]^n + \dots \Big\}, \end{aligned} \quad (3.78)$$

where now the dots stand for terms containing the extrinsic curvature or at least two Riemann tensors (that are invariant under the time diffeomorphism performed to get this action). The result (3.78) is quite complicated as in principle the pseudo-Goldstone π is interacting with the metric perturbations contained in g^{00} , g^{0i} and g^{ij} . Notice also that the brackets start at first order in perturbations: $1 + (1 + \dot{\pi})^2 g^{00} = -2\dot{\pi} + \delta g^{00} + 2\dot{\pi} \delta g^{00} - \dot{\pi}^2 + \dots$ up to second order, but one shall remind that the quasi-de Sitter background was chosen to enforce tadpole cancellation, and therefore the whole action actually begins at quadratic order in perturbations.

Decoupling limit

A dramatic simplification occurs in the so-called decoupling limit, for which the gravitational interactions of π , with metric perturbations δg , can be neglected. Before digging into the regime of validity of this assumption, one writes the action for π resulting from negligible mixed π - δg interactions:

$$\begin{aligned} S_\pi^{\text{decoupling}} = \int d^4x \sqrt{-g} \Big\{ & \sum_{n=2}^{\infty} \left[\frac{3M_{\text{Pl}}^2}{n!} \left(2H H^{(n)} - \frac{d^n(H^2)}{dt^n} \right) \pi^n - \frac{M_{\text{Pl}}^2}{(n-2)!} H^{(n-1)} \pi^{n-2} \left(\dot{\pi}^2 - (\partial_i \pi)^2 \right) \right. \\ & \left. + \frac{1}{n!} M_n^4(t + \pi) \left(-2\dot{\pi} - \dot{\pi}^2 + \frac{1}{a^2} (\partial_i \pi)^2 \right)^n \right] + \dots \Big\}, \end{aligned}$$

where one kept explicit the effect of the time-dependent background $H(t)$ and the fact that the operators M_n are evaluated at the shifted time $(t + \pi)$. Notice also that this

⁷The equivalent expression for δg^{00} is easily found as the background value $\bar{g}^{00} = -1$ is invariant under such transformation: $\delta g^{00}(x) = \left[1 + (1 + \dot{\pi})^2 \bar{g}^{00} + 2(1 + \dot{\pi}) \partial_i \tilde{\pi} \bar{g}^{0i} + \bar{g}^{ij} \partial_i \tilde{\pi} \partial_j \tilde{\pi} \right] \Big|_{\tilde{x}}.$

slow time-dependence manifests itself in the decoupling limit by letting π acquire a mass term, $m_\pi^2 = 3\dot{H}^2 M_{\text{Pl}}^2$,⁸ therefore showing that a conceptual leap has been made: time diffeomorphisms are now explicitly broken and π can be interpreted as pseudo-Goldstone boson (note that it would have been a Goldstone boson if the spacetime had remained exactly de Sitter, and the symmetry had only been spontaneously broken).

Actually, requiring that all background quantities are slowly varying functions of time (and thus that their time derivatives can be neglected, see *e.g.* Ref. [177] for the study of an example where such time-dependence cannot be neglected), one can simplify even more the action for π , which reads explicitly up to quartic order:

$$S_{\pi, \text{slow-varying}}^{\text{decoupling}} = \int d^4x \sqrt{-g} \left\{ \epsilon H^2 M_{\text{Pl}}^2 \left(\dot{\pi}^2 - \frac{(\partial_i \pi)^2}{a^2} \right) + 2M_2^4 \left[\dot{\pi}^2 + \dot{\pi} \left(\dot{\pi}^2 - \frac{(\partial_i \pi)^2}{a^2} \right) + \frac{1}{4} \left(\dot{\pi}^2 - \frac{(\partial_i \pi)^2}{a^2} \right)^2 \right] - \frac{4}{3} M_3^4 \left[\dot{\pi}^3 + \frac{3}{2} \dot{\pi}^2 \left(\dot{\pi}^2 - \frac{(\partial_i \pi)^2}{a^2} \right) \right] + \frac{2}{3} M_4^4 \dot{\pi}^4 + \dots \right\}, \quad (3.79)$$

which is often understood as *the* action of the single-field effective theory of inflation. One should now investigate the regime of validity of this result. If the M_n come as corrections to the slow-roll action in the first line, one finds that the dominant contribution to the kinetic terms of π is $\epsilon H^2 M_{\text{Pl}}^2$, which indicates that the canonically normalised π is $\pi_c = \sqrt{2\epsilon} H M_{\text{Pl}} \pi$. By using the decoupling limit, one neglected operators like

$$\epsilon H^2 M_{\text{Pl}}^2 \dot{\pi} \delta g^{00} \sim \sqrt{\epsilon} H \dot{\pi}_c \delta g_c^{00},$$

where one used $\delta g_c^{00} = M_{\text{Pl}} \delta g^{00}$ and used the slow-varying approximation to neglect the derivative of $\sqrt{\epsilon} H$. Comparing it to the slow-roll kinetic term $\dot{\pi}_c^2$ that was kept, and evaluating $\dot{\pi}_c \sim \omega \pi_c$ as well as $\pi_c \sim \delta g_c^{00}$, one finds that the decoupling limit is justified if

$$\omega \gg \Lambda_{\text{mix}}^{\text{SR}} = \sqrt{\epsilon} H. \quad (3.80)$$

If the kinetic term given by the operator M_2 was actually dominating the slow-roll contribution $\epsilon H^2 M_{\text{Pl}}^2$, one would instead infer that the canonically normalised π is $\pi_c = 2M_2^2 \pi$ and therefore by taking the decoupling limit one has neglected operators like

$$M_2^4 \dot{\pi} \delta g^{00} \sim \frac{M_2^2}{M_{\text{Pl}}} \dot{\pi}_c \delta g_c^{00},$$

⁸Be aware that π used here is not canonically normalised and his mass dimension is -1 . This explains why its mass squared is of dimension 6 instead of 2. It is straightforward but not particularly more illuminating to derive the mass of the canonically normalised pseudo-Goldstone $\pi_c = \sqrt{2\epsilon} H M_{\text{Pl}} \pi$: one needs to take the time derivative of this expression, square it and use integration by parts to remove the $\dot{\pi}_c \pi_c$ term, and add it to the contribution m_π^2 once rescaled. Roughly, the result is $m_{\pi_c}^2 \sim \epsilon H^2 + \dots$ where the dots stand for other slow-roll-suppressed contributions.

whence the decoupling limit is justified if

$$\omega \gg \Lambda_{\text{mix}}^{M_2} = \frac{M_2^2}{M_{\text{Pl}}}. \quad (3.81)$$

Thus, the decoupling limit is valid at energies higher than the the mixing scale Λ_{mix} , which therefore constitutes an IR cut-off for the resulting action. If the mixing scale is set by slow-roll interactions and $\Lambda_{\text{mix}} = \sqrt{\epsilon}H$, then one sees that the theory is only valid for modes that, either are still under the horizon, or have just exited it, and therefore the action (3.79) cannot describe the super-Hubble evolution of π . However, this is not a limitation of the EFToI, simply because one knows that in single-field inflation, there is the adiabatic mode ζ that is constant on super-horizon scales: one simply needs to make the connection between π and ζ just after horizon crossing. As one shall see, there is also a UV cut-off for the theory set by $\epsilon, H, M_{\text{Pl}}$ and the speed of sound c_s^2 that is defined in the following.

Speed of sound and Wilson coefficients of derivative interactions

The action (3.79) can be rewritten in terms of a speed of sound for the linear propagation of the π fluctuations, and of Wilson coefficients encoding the strength of leading-order interactions in the decoupling limit. Still up to fourth order in perturbations, collecting coefficients in front of given operators, one indeed finds:

$$\begin{aligned} S_{\pi, \text{slow-varying}}^{\text{decoupling}} = \int d^4x \sqrt{-g} \epsilon H^2 M_{\text{Pl}}^2 \left\{ \frac{1}{c_s^2} \left(\dot{\pi}^2 - c_s^2 \frac{(\partial_i \pi)^2}{a^2} \right) - \left(\frac{1}{c_s^2} - 1 \right) \left(\frac{A}{c_s^2} \dot{\pi}^3 + \dot{\pi} \frac{(\partial_i \pi)^2}{a^2} \right) \right. \\ \left. + \left(\frac{1}{c_s^2} - 1 \right) \left[\frac{B}{c_s^4} \dot{\pi}^4 + \left(1 + \frac{3A}{2c_s^2} \right) \dot{\pi}^2 \frac{(\partial_i \pi)^2}{a^2} + \frac{((\partial_i \pi)^2)^2}{4a^4} \right] \right\}, \quad (3.82) \end{aligned}$$

with the speed of sound c_s , given by

$$\frac{1}{c_s^2} - 1 = \frac{2M_2^4}{\epsilon H^2 M_{\text{Pl}}^2}, \quad (3.83)$$

assumed to be positive and thus smaller than 1, and where the RHS coincides with $2 \left(\Lambda_{\text{mix}}^{M_2} / \Lambda_{\text{mix}}^{\text{SR}} \right)^2$ and can be understood as measuring the relative strength of the single-field slow-roll term and its leading-order correction set by the mass scale M_2 . Moreover, one defined the Wilson coefficients A, B as:⁹

$$\begin{aligned} \frac{A}{c_s^2} &= -1 + \frac{2}{3} \left(\frac{M_3}{M_2} \right)^4, \\ \frac{4B}{c_s^4} &= 1 - 4 \left(\frac{M_3}{M_2} \right)^4 + \frac{4}{3} \left(\frac{M_4}{M_2} \right)^4, \end{aligned} \quad (3.84)$$

⁹Note that this definition of A matches the one of the WMAP [178] team, while more recent data analysis like the one of Planck [39] rather use a parameter $\tilde{c}_3 = -(M_3/M_2)^4$ which is simply related to A as $\tilde{c}_3 = -3/2(1 + A/c_s^2)$.

that set the size of the bispectrum and of the trispectrum, to be defined in Chap. 5, of the EFToI. An important outcome of the EFToI is that the sizes of interactions are partially set by the non-linear realisation of time diffeomorphisms, and thus are not independent one from the others. For example, the $\dot{\pi}(\partial_i\pi)^2$ cubic interaction depends only on c_s^2 : the more reduced is the speed of sound, the stronger are the interactions. This holds even true for the $((\partial_i\pi)^2)^2$ quartic interactions, and the $\dot{\pi}^2(\partial_i\pi)^2$ interactions are set by the quadratic and cubic Lagrangians. Actually at each order n in the perturbations, only the $\dot{\pi}^n$ interaction has a strength that does not depend on the lower-order terms.

Power spectrum of the curvature perturbation with a reduced speed of sound

First, one needs to find the linear relation between the comoving curvature perturbation $\mathcal{R}$ and the pseudo-Goldstone π , in order to connect predictions from the EFToI to observable quantities like $\mathcal{P}_{\mathcal{R}}$, the power spectrum of $\mathcal{R}$. In order to find it, one must remember that π is the residual from a time diffeomorphism use to leave the unitary gauge, and that in the π -gauge the metric perturbations are neglected in the decoupling limit. Therefore in the π -gauge, the spatial metric does not have scalar perturbations: $g_{ij}^\pi = a^2(\delta_{ij} + \gamma_{ij})$, which corresponds in the language of cosmological perturbations described in Chap 2, to the flat gauge: $\psi_{\text{flat}} = 0 = E_{\text{flat}}$. Now performing the inverse gauge transformation back to the unitary gauge where the fundamental scalar field ϕ had no perturbations (and thus where scalar perturbations may coincide with their values in the comoving gauge defined previously in this manuscript, remember that $Q_{\text{com}} = 0$ if the matter content of the universe is a single scalar field $\phi = \bar{\phi} + Q$), ξ^μ with $T = -\pi$, one finds from the law of transformation of ψ , Eq. (2.19) (be careful that now one is performing a gauge transformation in cosmic time t and not conformal time τ , hence $\mathcal{H}$ there is H here), that $\psi_{\text{unitary}} = H\pi$ while $E_{\text{unitary}} = 0$ and therefore $g_{ij}^{\text{unitary}} = a^2[\delta_{ij}(1 - 2H\pi) + \gamma_{ij}]$, which indeed coincides partially (up to the perturbation $E_{\text{com}} \neq 0$) with g_{ij}^{com} provided the identification

$$\boxed{\text{(Comoving curvature perturbation in the EFToI): } \mathcal{R} = -H\pi.} \quad (3.85)$$

The power spectrum of the mode π_k slightly after sound horizon crossing (corresponding to $kc_s = aH$), can be easily computed if the decoupling limit is assumed to be well valid up to that point. Indeed, once π has been rescaled, $\pi \rightarrow v_\pi = \sqrt{2\epsilon}HM_{\text{Pl}}/c_s \times \pi$, v_π are massless (in the slow-varying approximation) perturbations fluctuating in a quasi-de Sitter background, and one can use the results of Sec. 3.2 up to the fact that the speed of sound might deviate from 1, a technical issue that is tackled by formally replacing $k \rightarrow kc_s$. One knows that the power spectrum of the massless, canonically normalised v_π must be $P_{v_\pi} \approx \frac{H_*^2}{2k^3 c_{s*}^3}$ where one simply used the replacement mentioned above for the momenta, although a subtle difference is that now the time of evaluation denoted by the subscript $*$ (note the difference with $*$ used for horizon crossing) is the *sound horizon* crossing time, *i.e.* corresponding to $kc_s = aH$ which is expected to happen before Hubble crossing. This gives a dimensionless power spectrum $\mathcal{P}_{v_\pi} = k^3/(2\pi)^2 P_{v_\pi} \approx \frac{H_*^2}{4\pi^2 c_{s*}^3}$

and therefore $\mathcal{P}_{\mathcal{R}} = H_*^2 \mathcal{P}_\pi \approx \frac{c_{s*}^2}{2\epsilon_* M_{\text{Pl}}^2} \mathcal{P}_{v_\pi}$ is:

(Power spectrum of the curvature perturbation in the EFToI): $\mathcal{P}_{\mathcal{R}}(k) \approx \frac{H_*^2}{8\pi^2 \epsilon_* c_{s*} M_{\text{Pl}}^2}.$

(3.86)

Note the extra factor $1/c_{s*}$ compared to the standard result of slow-roll inflation, meaning that the scalar power spectrum is boosted by a reduced speed of sound due to the operator $\propto M_2$. Moreover, this results in an extra term in the scalar spectral index (and quantities are evaluated at a slightly different time),

$$n_s - 1 \approx -2\epsilon_* - \eta_* - s_* \quad \text{with} \quad s = \frac{\dot{c}_s}{H c_s}. \quad (3.87)$$

Since the propagation of gravitational waves is not affected by the operators $\propto M_n$, $\mathcal{P}_\gamma = 2H_*^2/(\pi^2 M_{\text{Pl}}^2)$, the tensor-to-scalar ratio is both reduced by a factor of the speed of sound and is sensitive to the slow evolution of H between sound horizon crossing and horizon crossing (but this results in a second-order correction in slow-roll parameters, except if the speed of sound is very small and those two events are separated by many e -folds of expansion, since $N_* - N_* \sim \ln(c_{s*}^{-1})$):

$$r \approx 16\epsilon_* c_{s*} \times \underbrace{\left(\frac{H_*}{H_*}\right)^2}_{\approx 1 + 2\epsilon_* \ln(c_{s*}^{-1})} \approx 16\epsilon_* c_{s*}. \quad (3.88)$$

Of relevant energy scales

This paragraph discusses the relevant energy scales in the theory at hand, and follows the spirit and the notations of Ref. [179].

Symmetry-breaking scale. First, the symmetry-breaking scale Λ_b sets the energy above which the invariance under time diffeomorphisms of the theory must be restored, giving a clear UV-cutoff to the EFToI. Looking at the conserved charge under such symmetry for the free theory (quadratic part) of Eq. (3.79), one can show that it is well-defined only when $\omega \gg \Lambda_b$, with [179]

$$\Lambda_b^4 = 2\epsilon H^2 M_{\text{Pl}}^2 c_s, \quad (3.89)$$

meaning that the symmetry is broken on scales $\omega < \Lambda_b$. Note that evaluated with the usual single-field inflationary background, one finds $\Lambda_b = \dot{\phi}^2 c_s$ which matches the intuition that it is the clock defined by the background field $\dot{\phi}(t)$ that breaks the de Sitter time diffeomorphisms. Moreover, the scalar power spectrum reads roughly $\mathcal{P}_{\mathcal{R}} \sim (H_*/\Lambda_{b*})^4$, exceeding one if the “energy of the experiment” H_* gets larger than Λ_{b*} and therefore evading the regime of validity of cosmological perturbation theory.

Strong-coupling scale and new physics. But the practical UV-cutoff for calculations with the EFToI may be well below Λ_b , at another scale Λ_* called the strong-coupling scale. Indeed, unitarity bounds on the tree-level scattering of the π fields with two cubic interactions, $\pi\pi \rightarrow \pi\pi$, indicate that computations using Eq. (3.79) can be trusted only for energies $\omega \ll \Lambda_*$ with Λ_* set by the strength of the cubic couplings [180]:

$$\Lambda_{*,\dot{\pi}(\partial\pi)^2}^4 = 16\pi^2\epsilon H^2 M_{\text{Pl}}^2 \frac{c_s^5}{(1-c_s^2)^2}, \quad (3.90)$$

$$\Lambda_{*,\dot{\pi}^3}^4 = \frac{\Lambda_{*,\dot{\pi}(\partial\pi)^2}^4}{A^2}. \quad (3.91)$$

The same bounds are obtained by requiring that loop corrections to the free propagation of π fields, $\pi \rightarrow \pi$, are negligible compared to the tree-level result. Note that in single-field, slow-roll inflation with canonical kinetic terms, $c_s = 1$ and therefore the strong coupling scale is formally pushed towards infinity and the theory never becomes strongly coupled. Therefore, predictions from such models may be trusted up to the symmetry-breaking scale Λ_b . Once the speed of sound is less than unity, and more particularly when $c_s \ll 1$, the strong coupling scale becomes relevant and one should be careful not to use the current formalism beyond its regime of validity. However note that the strong coupling scale needs not be a strong limitation of the EFToI in general, which relies on the spontaneous breaking of time diffeomorphisms, but rather reflects the fact that the action (3.79) must not be trusted beyond Λ_* for concrete calculations, and needs to be completed. Such UV completions may include additional degrees of freedom or higher-derivative terms like the ones contained in the extrinsic curvature, which must become relevant around an energy scale said *of new physics* lower than the strong coupling scale: $\Lambda_{\text{new}} < \Lambda_*$. An example a such UV-completion is given in [2] with the careful study of generic two-field models of inflation for which one of the two perturbations has a large mass, $m_s^2 \gg H^2$, and can therefore be integrated out, leading to an effective single-field theory of the kind (3.79) where new physics (the heavy fluctuations) become relevant at the energy scale $\Lambda_{\text{new}}^2 = m_s^2 c_s^2$.

Naturalness. An important statement that the EFToI enables one to make, is that the coefficients $A, B, \dots$ in Eq. (3.79), are *naturally* of order 1. What naturally means in this context of Effective Field Theory, is that radiative corrections to the action can only change these bare parameters by a relative amount of order unity. As an example, one can look at the $\dot{\pi}^3$ coupling which gets a loop correction from a diagram including three $\dot{\pi}(\partial\pi)^2$ vertices (that are always there because of the non-linearly realised symmetry, remember the strength of this interaction is $c_s^{-2} - 1$). With rough estimates and in the $c_s \ll 1$ limit, one finds such one-loop correction to give rise to a new contribution [179] $\tilde{M}_3^4 \dot{\pi}^3$ with $\tilde{M}_3^4 = \mathcal{O}(1)\Lambda_{*,\dot{\pi}(\partial\pi)^2}^4/c_s^9$, thus yielding a new effective parameter $A/c_s^2 \rightarrow A/c_s^2 + \mathcal{O}(1)/c_s^2$ which therefore shows that A of order 1 is radiatively stable. Moreover, would A be much smaller than 1, for example $A \sim c_s^2 \ll 1$, then pushing the EFT up to the strong-coupling scale $\Lambda_{*,\dot{\pi}^3}$ would induce large corrections of order $1/c_s^2$, see Eq. (3.91), and would therefore violate unitarity bounds from $\pi\pi \rightarrow \pi\pi$ scattering

amplitudes. As an example, in DBI inflation [181, 182], a particular single-field model of inflation with a non-linear kinetic term and which is tuned to be radiatively stable, one exactly has $A = -1$, and $B = 5/4$.

Extrinsic curvature and dispersion relation

Under the Stueckelberg transformation and in the decoupling limit, one can find the law of transformation of the extrinsic curvature in the unitary gauge action [183]. Together with the equivalent law for δg^{00} , one has

$$\delta g^{00} \rightarrow -2\dot{\pi} - \dot{\pi}^2 + \frac{1}{a^2} (\partial_i \pi)^2, \quad (3.92)$$

$$\begin{aligned} \delta K_j^i \rightarrow & \left(\dot{H}\pi + \frac{1}{2}\ddot{H}\pi^2 \right) \delta_j^i - (1 - \dot{\pi})\partial^i \partial_j \pi + \partial^i \dot{\pi} \partial_j \pi + \partial^i \pi \partial_j \dot{\pi} \\ & - H \left[\partial^i \pi \partial_j \pi - \frac{\delta_j^i}{2a^2} (\partial_k \pi)^2 \right] + \mathcal{O}((\partial\pi)^3). \end{aligned} \quad (3.93)$$

In the slow-varying approximation, one can neglect the terms proportional to the derivatives of H in the above expression, and find that δK_j^i , transformed in the π -gauge, begins at the order of two spatial derivatives. Indeed, keeping only terms quadratic in π to see the effect of the extrinsic curvature on the free propagation, and forgetting its impact on interactions, one needs to consider only $\bar{M}_{1,2,3}$ used above in (3.75),¹⁰ and finds after integrating by part the term $-a\bar{M}_1\dot{\pi}\partial^2\pi$:

$$S_{\delta K}^{(2)} = \int d^4x \sqrt{-g} \left[-\frac{\bar{M}_1^3 H}{2} \frac{(\partial_i \pi)^2}{a^2} - \frac{\bar{M}^2}{2} \frac{(\partial^2 \pi)^2}{a^4} \right], \quad (3.94)$$

with $\bar{M}^2 = \bar{M}_2^2 + \bar{M}_3^2$. From this, one understands that the effect of $\bar{M}_1$ is to change the linear dispersion relation $\omega = kc_s$ by shifting

$$c_s^2 = c_{s,(0)}^2 \rightarrow c_s^2 = c_{s,(0)}^2 \left[1 + \frac{\bar{M}_1^3 H}{2\epsilon H^2 \bar{M}_{\text{Pl}}^2} \right], \quad (3.95)$$

where $c_{s,(0)}^2$ is given by Eq. (3.83), while the effect of $\bar{M}_{2,3}$ is to induce a non-linear correction to the dispersion relation:

$$c_s^2 = c_{s,(0)}^2 \rightarrow c_s^2(k) = c_{s,(0)}^2 \left[1 + \frac{k^2}{a^2} \frac{\bar{M}^2}{2\epsilon H^2 \bar{M}_{\text{Pl}}^2} \right], \quad (3.96)$$

¹⁰Indeed, other terms containing the extrinsic curvature can only appear either with more powers of δK or of δg^{00} , which both begin at first order in perturbations. Note however that they have a different status: the operators with more powers of δK will contain even more spatial derivatives and be irrelevant at the energy scale of inflation, while the infinite tower of operators

$$- \sum_{n=1}^{\infty} \frac{(\bar{M}_n^{(\delta g)})^3}{(n+1)!} (\delta g^{00})^n \delta K,$$

with $\bar{M}_1^{(\delta g)} = \bar{M}_1$ but otherwise $\bar{M}_{n>1}^{(\delta g)} \neq \bar{M}_{n>1}$, contains terms with just two spatial derivatives at any order in the $(\partial\pi)^n$ expansion that are therefore *a priori* relevant to compute n -point functions of π .

two effects that can add one to the other. Therefore, the terms $\propto \bar{M}_{n \geq 2}$ can be understood as high-energy corrections to the action (3.79), relevant only for modes that are deep inside the horizon, $k/(aH) > \sqrt{\epsilon} M_{\text{Pl}}/\bar{M}_{n \geq 2}$, and can be neglected around the time of horizon crossing except in the extreme cases where $\bar{M}_{n \geq 2} \rightarrow M_{\text{Pl}}$. Note also that if the effects coming from the extrinsic curvature cannot be neglected, the regime of validity of the decoupling limit Λ_{mix} is set by barred mass scales $\bar{M}_{1,2,3}$ rather than $\Lambda_{\text{mix}}^{\text{SR}}$ or $\Lambda_{\text{mix}}^{M_2}$.

Links with other theories of inflation

The Effective Field Theory of Inflation provides an agnostic parameterisation of the physics of linear fluctuations and of leading interactions during single-field inflation. In particular, it encapsulates several known examples:

- Single-field, slow-roll inflation with canonical kinetic terms and at leading order in the slow-roll parameters, is recovered by setting $M_n = \bar{M}_n = 0$ and therefore $c_s^2 = 1$, $A = B = 0$ in Eq. (3.82), see also the primordial power spectrum (3.86). The fact that interactions disappear completely in this limit can be interpreted as the almost vanishing of non-Gaussianities in these simple models. See Chap. 5 for more details, and in particular how the cubic interactions are suppressed by slow-roll parameters at quadratic order in these cases;
- Keeping only the M_n but setting the $\bar{M}_n = 0$, one recovers so-called $P(X, \phi)$ models of inflation, also called k -inflation [184, 185], *i.e.* corresponding to Lagrangians that are generic functions of the kinetic term $X = -1/2 \partial_\mu \phi \partial^\mu \phi$ and the scalar field value ϕ , provided an identification between the derivatives of the function P and the parameters c_s^2 , A and B . In this thesis, it has been shown explicitly that these theories also correspond to a particular limit of multifield models of inflation at the level of fluctuations, when the fields' perturbations that are orthogonal to the background trajectory, so-called entropic perturbations, are sufficiently heavy that they can be integrated out hence yielding a single-field effective theory for fluctuations, see Refs. [2, 5] and Sec. 5.3. Again this holds provided an identification between c_s^2 and A on one side, and the multifield parameters (bending of the trajectory, scalar potential, field-space curvature, etc.) on the other side;
- Looking at the effect of the extrinsic curvature, $\bar{M}_{n \geq 2}$, amounts to studying higher-derivative models of inflation, where the Lagrangian can depend on ϕ and its first derivative as in $P(X, \phi)$ theories, but also on the second derivative $\partial^2 \phi$. They have not been particularly investigated in this thesis, but they could represent an interesting avenue to extend the works mentioned in the previous point, and in particular to push the regime of validity of the single-field EFT after integrating out heavy entropic perturbations, to higher energy scales where the dispersion relation $\omega(k)$ becomes non-linear.

Chapter 4

Multifield inflation: exploring implications from high-energy physics

In this chapter, one encounters for the first time in this thesis, explicit equations for the dynamics of multifield inflation, at the level of the background and linear fluctuations. But first, Sec. 4.1 motivates the study of these models of inflation featuring several fundamental scalar degrees of freedom, both from a fundamental perspective based on bottom-up and top-down approaches, as well as from a phenomenological perspective. The formalism specific to multifield inflation is then reviewed, but only shortly as it is constantly used and often re-explained in the subsequent chapters and sections, in particular those that include the published papers on this subject during my thesis, see for example Secs. 5.2–5.3, as well as Sec. 7.2. When possible, the reader is referred to specific parts of these sections for details, in order to avoid having twice the same information at different places.

In Sec. 4.2, after showing the background equations of motion, the dynamics of linear fluctuations are made explicit, and particular emphasis is given on the usefulness to handle equations that are manifestly covariant, not only with respect to spacetime coordinates x^μ , but also with respect to field-space coordinates ϕ^I . Multifield canonical variables are identified and it is explained how to quantise the multifield system of perturbations. Power spectra of effectively massless scalar fields in de Sitter spacetime, and the resulting power spectrum for the comoving curvature perturbation, are computed and the zeroth order effect coming from a non-trivial field space is exhibited.

Then Sec. 4.3 introduces the important notions of adiabatic and entropic perturbations in multifield inflation, which are commonly used in this thesis. Their coupled dynamics are shown, which notably enables one to derive expressions for the power spectrum of the comoving curvature perturbation on large scales during multifield inflation in a slow-varying approximation, although for the purpose of displaying concrete results, the number of fields is taken to be $N_{\text{field}} = 2$ (Ref. [5] displayed in Sec. 5.3.2 generalises these notions to any number of scalar fields). In order to introduce important phenom-

ena for the current thesis, this section also includes an analysis of the relevant mass scales in two-field inflationary setups with non-canonical kinetic terms: in particular the notions of sub-Hubble and effective super-Hubble masses of entropic fluctuations are explained, and it is shown how they can exhibit negative values causing multifield instabilities which leave interesting observational imprints.

4.1 Motivations

In this section, motivations for the study of inflation beyond the single-field paradigm are given. Rather than strict arguments against single-field inflation which might well describe our actual Universe, these consist in my opinion in theoretical guidelines that one should keep in mind when studying early universe physics.

4.1.1 Indirect motivations: limitations of the single-field picture

First, indirect motivations for the study of multifield inflation come from the limitations of the slow-roll, single-field picture, that one shall here investigate upon. In order to do this, one must first remember the strong theoretical constraints on such models of the early universe based on CMB observations, and more particularly on the derivatives of the scalar potential for the inflaton, $V(\phi)$. Indeed, remember that for standard slow-roll inflation to proceed, one needs to meet the two conditions $\epsilon_V, \eta_V \ll 1$, meaning that both the slope and the curvature of the scalar potential must be small in Planck mass units. In particular, those constraints put into question the *naturalness* of slow-roll, single-field inflation, as it seems that two dimensionless parameters of the model must be fine-tuned to small values. This problem of naturalness can be exemplified with the so called η -problem that is summarised in the following. Moreover, recent years have seen the quick growth of a discipline aiming at eliminating low-energy (at the scale of inflation) effective field theories that do not possess a UV completion at higher energy scales where a quantum theory of gravity must apply: the so-called *swampland program* that is also in tension with the simplest single-field paradigm and is shortly mentioned here too.

The η -problem(s).

Consider a single-field slow-roll model of inflation, with a scalar field ϕ that has standard kinetic terms and a potential $V(\phi)$, and is minimally coupled to Einstein gravity. This theory might well exist as an EFT valid at the energy scale of inflation, with the slow-roll Lagrangian

$$\mathcal{L}_{\text{sr}}(\phi) = \frac{M_{\text{Pl}}^2}{2} R - \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - V_{\text{sr}}(\phi). \quad (4.1)$$

But according to EFT principles, all operators compatible with the symmetries of the problem should be written in an EFT expansion, possibly with unknown Wilson coefficients, even if truncated at a given order in derivatives. In the following, one shall focus

on the leading two-derivative order, but consider the addition of higher-dimensional operators suppressed by the scale of new physics to some power, conservatively supposed here to be the Planck mass, of the form:

$$O(\phi) = -V_{\text{sr}}(\phi) \sum_{n=1}^{\infty} \frac{\lambda_n}{n!} \frac{\phi^n}{M_{\text{Pl}}^n}, \quad (4.2)$$

where λ_n are Wilson coefficients that should be expected to be of order unity. As an example, if ϕ is supposed to have a $\mathbb{Z}_2$ symmetry, then the scalar potential should be an even function of ϕ , and only the even terms $n = 2p$ with $p \in \mathbb{N}^*$ should be kept in the operator $O(\phi)$. Now if you believe in the power of EFTs to describe physics at a given energy scale (and you probably should), it means that the actual dynamics of inflation should be derived from the EFT Lagrangian $\mathcal{L}_{\text{EFT}}(\phi) = \mathcal{L}_{\text{sr}}(\phi) + O(\phi)$. Taking the example of the $\mathbb{Z}_2$ -symmetric Lagrangian for simplicity (but the argument below is valid more generically), one finds in particular the effective scalar potential

$$V_{\text{eff}}(\phi) = V_{\text{sr}}(\phi) \left(1 + \sum_{p=1}^{\infty} \frac{\lambda_{2p}}{(2p)!} \frac{\phi^{2p}}{M_{\text{Pl}}^{2p}} \right), \quad (4.3)$$

to yield a new η_V -parameter:

$$\begin{aligned} \eta_{V,\text{eff}} &= \eta_{V,\text{sr}} + \lambda_2 + 2\sqrt{2\epsilon_{V,\text{sr}}} \lambda_2 \frac{\phi}{M_{\text{Pl}}} + \frac{\lambda_4 - \lambda_2^2}{2} \frac{\phi^2}{M_{\text{Pl}}^2} + \mathcal{O}\left(\sqrt{2\epsilon_{V,\text{sr}}} \frac{\phi^3}{M_{\text{Pl}}^3}, \frac{\phi^4}{M_{\text{Pl}}^4}\right) \\ &\simeq \lambda_2 + \frac{\lambda_4 - \lambda_2^2}{2} \frac{\phi^2}{M_{\text{Pl}}^2} + \mathcal{O}\left(\frac{\phi^4}{M_{\text{Pl}}^4}\right), \end{aligned} \quad (4.4)$$

where in the second line one has completely neglected the terms containing $\sqrt{\epsilon_{V,\text{sr}}}$, $\eta_{V,\text{sr}}$ since they should be small compared to the Wilson coefficients $\lambda_{2p} \sim 1$.

This result is quite important and deserves some comments. First, it shows that the “bare” $\eta_{V,\text{sr}}$ parameter is *a priori* very different from the “renormalised one” $\eta_{V,\text{eff}}$ that should be measured with experiments: it actually gets corrected by the infinite set of fundamental operators $\lambda_{2p}\phi^{2p}/M_{\text{Pl}}^{2p}$, $p \geq 1$ even though only a few terms have been kept in the above expression. In order to refine the analysis, one should now distinguish two inflationary scenarios.

- Small-field inflation, corresponding to a background field displacement of order $\Delta\phi \lesssim M_{\text{Pl}}$. In that case, it is clear that only the dimension-6 operator, $V(\phi)\lambda_2\phi^2/M_{\text{Pl}}^2$ is relevant for the renormalisation of η_V , since all the other ones result in contributions that are suppressed as $\phi^{2p}/M_{\text{Pl}}^{2p} \ll 1$. But since λ_2 is expected to be of order unity as a Wilson coefficient in an EFT expansion, the end value of the effective η_V parameter is

$$\eta_{V,\text{eff}} \sim 1,$$

which is already in tension with the slow-roll requirement $\eta_V \ll 1$ in order to sustain enough e -folds of inflation.

- Large-field inflation, corresponding to a background field displacement of order $\Delta\phi \gtrsim M_{\text{Pl}}$. This case is even more dramatic, since then *all* fundamental operators, even of dimension strictly larger than six, are relevant to find the actual value of $\eta_{V,\text{eff}}$, and adding them results in higher and higher values. Without assuming further symmetries and a particular scaling of the numbers λ_{2p} , it is then impossible to quote a precise value for the curvature of the effective potential, but

$$\eta_{V,\text{eff}} \gg 1,$$

which is of course now in complete disagreement with the slow-roll requirement $\eta_V \ll 1$.

Here the non-renormalisable operator $O(\phi)$ has been assumed to be present simply because it is allowed by the symmetries of the problem, but in principle even the renormalisable potential $V_{\text{sr}}(\phi)$ receives radiative corrections that can spoil the smallness of η , therefore displaying the two faces of the η -problem.¹ Either way, the conclusion is that the required value for η_V is *unnaturally* small as it necessitates a fine-tuning of the Wilson coefficient λ_2 in small-field inflation, and a whole hierarchy of relations amongst the other λ_{2p} in large-field inflation (like $\lambda_4 = \lambda_2^2$ in the example above), hence possibly pointing towards extra physics beyond the single-field, slow-roll paradigm. Moreover, note that one has been conservative in assuming that the non-renormalisable operators are suppressed by the Planck scale, although the scale of the new physics Λ could be consistently quite smaller, $\Lambda \ll M_{\text{Pl}}$, which would therefore strengthen even more the mentioned discrepancies. This thesis exhibits in Sec. 5.2 a particular multifield example where the usual η -problem described here might be evaded,² since it allows to have a long enough period of inflation even though the curvature of the potential *in Planck mass units* is large and therefore there is no contradiction with having $\eta_V > 1$ any more: this is made possible by having a strongly bent background trajectory in field space, thus making the effective curvature of the potential along the trajectory smaller than in the radial direction, see Ref. [1] for more details.

Swampland conjectures: insights from quantum gravity.

The *swampland program* has recently received a renewed attention and is still subject to controversies. It is not the goal of this very short paragraph to review it in full glory,

¹Note that these radiative corrections can be negligible if an internal symmetry is assumed for the renormalisable potential, by asking $V_{\text{sr}}(\phi)$ to be invariant under $\phi \rightarrow \phi + C$ where C is a constant: so-called shift-symmetry. However, there is no reason for this symmetry to hold true in a consistent UV-completion, and therefore the above arguments with the non-renormalisable operator O still applies even in this particular case. Moreover, assuming a supersymmetric action (that nevertheless must be broken by the time-dependent inflationary background) only diminishes the trouble to radiative corrections of order $\Delta\eta \sim 1$, that are again supplemented by non-renormalisable interactions.

²Usual in the sense of the single-field case for which the potential cannot be naturally flat in *Planck mass units*, but it has not been investigated in details how would the η -problem translate in this different case of a curved field space where a new mass scale M may play an important role: should the potential be flat in *units of the curvature of the field space*? If yes, then the η -problem is still there...

nor to assess its accuracy or the precise constraining power that it may have on model-building. Rather, one shall try to understand its general spirit and the guidelines that it may provide. Based on the fact that many different models of inflation are compatible with CMB observations, the idea of the swampland program is to reduce the volume of possible descriptions of the early universe from the theoretical side. Indeed, many models of inflation simply consist in *assuming* particular forms of the potential and/or of the kinetic terms, and a minimal-or-not coupling to gravity, and checking which values of the free parameters are compatible with observations, if any. Even though this procedure is not wrong *per se*, one could easily forget that such “low-energy” theories must emerge as the result of coarse-graining a finer, higher-energy fundamental theory. Actually, since general relativity is non-renormalisable, one expects such UV theory to exist at least at the Planck scale, where quantum effects should appear in gravitational interactions. As it is well known, one is not yet provided with a complete and consistent theory of quantum gravity, even though many important progresses have been made in the last fifty years, but there have been attempts to propose as generically as possible some criteria for a low-energy EFT not to fall into the so-called swampland, *i.e.* the plethora of single-field EFTs that do not possess a UV completion resembling what one expects in quantum gravity. Here one shall encounter the swampland de Sitter conjecture and the swampland distance conjecture, in simplified forms.

- Based on the experience that stable de Sitter spacetimes are difficult to build in quantum gravity frameworks, the swampland de Sitter conjecture has been proposed and subsequently refined [186–188], and can be summarised by the following requirements for a single-field inflationary model not to be in the swampland:

$$\sqrt{2\epsilon_V} > c, \text{ or } \eta_V < -c', \quad (4.5)$$

where $c \sim 1$ and $c' \sim 1$ are two positive numbers of order unity. The conjecture therefore states that if the slope of the potential is small and $\sqrt{2\epsilon_V} < 1$, then the curvature of the potential must be large and negative, and conversely a small curvature of the potential (or large and positive) $\eta_V > -1$, implies that the slope of the potential must be large. Clearly, usual setups of slow-roll, single-field inflation with both $\epsilon_V, \eta_V \ll 1$, are all in contradiction with the swampland de Sitter conjecture. This conjecture also applies to multifield models of inflation provided a redefinition of the parameters ϵ_V, η_V , but this point shall not be developed here and the interested reader is referred to Sec. 5.2 where the concrete multifield setup of [1] is shown to respect the two-field version of the de Sitter swampland conjecture. Actually, it has been argued more generally that the swampland de Sitter conjecture was only compatible with multifield inflation featuring strongly bent background trajectories [189].

- Moreover, it is believed that the spectrum of light particles that are therefore dynamical and relevant at a given energy scale for inflation, is unstable against super-Planckian field displacements [190]. Put it otherwise, a given low-energy EFT around an initial location ϕ_{ini} in field space, is only valid inside a sphere with

radius $d \times M_{\text{Pl}}$ with $d \sim 1$ a positive number of order unity, such that the theory makes sense only for field-space displacements $\Delta\phi$ that verify:

$$\frac{\Delta\phi}{M_{\text{Pl}}} < d, \quad (4.6)$$

which therefore constitutes the so-called swampland distance conjecture that has been proposed and subsequently refined in, *e.g.*, Refs. [191–193]. The swampland distance conjecture is not in contradiction with single-field, slow-roll inflation, provided it is realised in small-field scenarios, and is actually compatible with the absence of observation so far of primordial gravitational waves on CMB scales, since combined with the Lyth bound, see Eq. (3.65), it gives $r \lesssim 0.01 \times d^2$. Contrarily, a detection of r in the near future would mean that slow-roll, single-field inflation is in contradiction with the swampland distance conjecture.

Although the exact form of the swampland conjectures is still under debate, and in particular more precise values for the order unity numbers c, c', d under investigation, and even if generic proofs of these conjectures have not yet been exhibited, they provide one with a strong theoretical guideline: a low-energy EFT of inflation should have a UV completion (in quantum gravity or not). This guideline is so far understood to be in contradiction with the simplest slow-roll, single-field picture, while still being compatible with multifield inflation, therefore making multi-scalar models theoretically interesting candidates for the description of the early universe.

4.1.2 Direct motivations for multi-scalar inflation

Importantly, there are direct motivations for the study of multifield inflation, both from a theoretical, top-down approach, and from a phenomenological perspective. These are shortly reviewed in the following.

Quantum gravity again: a plethora of scalar fields.

Although the invocation of a precise theory of quantum gravity is far from needed to motivate the study of multifield inflation, it is instructive to consider seriously the implications of a fundamental description of spacetime in a quantum framework, as a necessary UV-completion of the effective theory that is inflation. Indeed, even though inflation occurs at an energy scale $H \ll M_{\text{Pl}}$, one has seen that its dynamics crucially depend on the physics up to the Planck scale. So far, the most successful quantum framework for gravity has been string theory, and in the following one reviews shortly how string inflation arises and how its phenomenology coincides in practice with the study of multifield inflation. The reader shall be aware that no effort has been made to render this paragraph rigorous nor self-contained, in particular no precise statement about string theory is made, and only the main ingredients and conclusions are outlined. Most of its inspiration has been taken from [32]

In what follows, one considers the context of supergravity, *i.e.* the low-energy limit of supersymmetric string theory in ten dimensions, where therefore only the interactions

of the massless modes of the fundamental closed strings (that otherwise have a mass spectrum related to the string scale M_s), with possibly additional open string states, are considered in a consistent $1/M_s$ expansion. Different sectors of supersymmetric string theory can arise depending on the choice of chirality for the spacetime spectrum, which leads to the famous five superstring theories: types IIB and IIA corresponding respectively to chiral and non-chiral spectra, type I describing unoriented strings and the two heterotic string theories $SO(32)$ and $E_8 \times E_8$ for hybrids of superstrings and bosonic strings. For definiteness, one considers here the supergravity limit of type IIB string theory which is described by the fundamental modes of the massless string spectrum:

- G , the symmetric tensor mode corresponding to the $10d$ spacetime metric;
- B_2 , a two-form analog to the electromagnetic field strength in Maxwell theory;
- Φ , a scalar mode called the *dilaton*, that completes the description of the *universal* modes of superstring theory;
- C_0, C_2, C_4 , respectively a scalar, a two-form and a four-form that are distinctive of the type IIB string theory.

Alternatively, the $2p$ -forms can be described by the $(2p+1)$ -fluxes with $F_{2p+1} = dC_{2p}$ for $p = 0, 1, 2$ and $H_3 = dB_2$, and the duals $\tilde{F}_3$ and $\tilde{F}_5$. These fields that are living on the full ten-dimensional spacetime manifold, may be supplemented by *localised* objects, such as Dp -branes which are p -dimensional objects charged under the form C_{p+1} and on which open strings attach and have Dirichlet boundary conditions (their endpoints can freely move in the direction tangential to the brane but not leave it by moving in the transverse one), hence the letter D.

Although providing a useful theoretical framework for high-energy computations, superstring theory (and even supergravity), as ten-dimensional theories do not immediately describe the cosmological spacetime observed in our Universe, which seems to be of dimension four, only... Therefore, one must consider the possibility of compactifying the extra six dimensions as internal dimensions (the case of large extra dimensions is not treated here) inaccessible to observations at our energy scales. This procedure, called dimensional compactification, can be summarised as follows:

$$\mathcal{M}_{10} = \mathcal{M}_4 \times X_6, \quad (4.7)$$

where $\mathcal{M}_{10}$ is the fundamental ten-dimensional manifold, $\mathcal{M}_4$ is the four-dimensional cosmological spacetime, and X_6 is the six-dimensional manifold that is compactified as an internal space. The effective theory on the four-dimensional manifold $\mathcal{M}_4$ of relevance for inflation and that results from this operation, highly depends on the details of the compactification scheme, amongst which the geometrical features of X_6 as well as the presence or not of localised sources like D-branes in the original theory on $\mathcal{M}_{10}$, play an important role. Irrespective of details of how inflation arises, the important outcome of this procedure is that one is inevitably left on the four-dimensional manifold with a plethora of scalar fields, that effectively describe the dynamics of the internal

manifold X_6 , as well as the $2p$ -forms and localised sources in ten dimensions, that have been integrated out. For example, the compactification of Calabi-Yau orientifolds with $\mathcal{N} = 1$ supersymmetry in type IIB string theory but without localised sources, results in a number of scalars:

- C_0 and Φ have been preserved as fundamental scalars of the theory restricted to the sub-manifold $\mathcal{M}_4$, and can be combined as the complex *axiodilaton* $\tau = C_0 + ie^{-\Phi}$;
- b_α, c_α arise as projections of the two-forms B_2 and C_2 under the orientifold action,³ and their numbers coincide with the dimension of the odd eigenspace of the corresponding cohomology group, they can be combined to form the 2-form scalars $G_\alpha = c_\alpha - \tau b_\alpha$;
- θ_i are similar projections of the four-form C_4 , but this time their number coincides with the dimension of the even eigenspace of the corresponding cohomology group;
- t^I are called the *Kähler moduli* and correspond to the allowed deformations of the six-dimensional metric $\hat{g}$ on X_6 , they can be understood as the volume of fundamental two-cycles on X_6 and can be combined quadratically with a three-form c_{ijk} projecting on the even subspace, to form four-cycle volumes $\tau_i = c_{ijk} t^j t^k$ that themselves are combined with the θ_i to define the *complexified four-cycle volumes* $T_i = \tau_i + i\theta_i + \mathcal{O}(G_\alpha)$ where $\mathcal{O}(G_\alpha)$ is another contribution proportional to the 2-form scalars G_α ;
- ξ^A , so-called *complex structure moduli* describe the dynamics of the complex structure of X_6 .

Clearly, just from the closed string sector, many scalar fields arise as an effective, low energy, theory of quantum gravity. Note that adding open strings and localised sources such as Dp-branes typically leads to the consideration of even more scalar fields. But an important issue with this procedure so far, is that the scalar fields that were initially massless are still not provided with a potential: they are therefore free to change configurations up to the point to ruining the compactification scheme itself. In order to provide a satisfactory compactification, one should therefore specify how the fields are stabilised, a procedure called *moduli stabilisation*. On the compact space X_6 the various form-fields can be endowed with non-trivial background profiles, a proceeding called *flux compactification* [194] and resulting in a scalar potential for the four-dimensional sector, *e.g.* for the axiodilaton and the complex structure moduli, but actually not for the Kähler moduli which may however receive contributions from other, non-perturbative effects coming from the Dp-branes. Note that the many discrete choices of such fluxes and non-perturbative effects result in the famous large quantity of possible vacua in string theory. Then, the exact spectrum of these four-dimensional scalar fields should be computed: the heavy ones can be integrated out while at least one direction should

³Orientifolding refers to applying an involutive symmetry transformation to X_6 together with a reversal of the string orientation, and retaining only the states from the original spectrum on X_6 that are invariant under this procedure.

be found to be light in order to sustain inflation for long enough. But typically, several scalar fields with masses $m_i \lesssim 3H/2$ and therefore (close-to-)dynamical will remain in the low-energy field theory, therefore corresponding effectively to the study of multifield inflation.

Actually, many single-field models inspired from such stringy considerations are fundamentally multifield, and the mass spectrum has simply been truncated: this is the case of natural inflation [195, 196] which displays a fundamental axion featuring a discrete shift symmetry $\theta \rightarrow \theta + (2\pi)f$ with f the so-called axion decay constant, and a cosine potential protected from radiative corrections, as well as the famous DBI model [182, 197] with particular non-canonical kinetic terms at non-linear order in derivatives, to prevent them from renormalisation. Indeed, the *axions* such as θ_i mentioned above are usually numerous just from the closed string sector, and can in some approximation be shown to be described by a Lagrangian of the type [198, 199]:

$$\mathcal{L} = -\frac{1}{2}M_{\text{Pl}}^2 K_{ij} \partial_\mu \theta^i \partial^\mu \theta^j - \frac{1}{2} M_{ij} \theta^i \theta^j, \quad (4.8)$$

where K_{ij} is called the Kähler metric and M_{ij} is a mass matrix whose spectrum can be statistically known in the large N_{field} limit thanks to random matrix theory [200] and therefore phenomenological consequences can be computed in a statistical way [59]. As for single-field DBI inflation, its interpretation in terms of a UV-completion is the description of the radial evolution of a D3-brane moving at a relativistic pace in the ten-dimensional manifold $\mathcal{M}_{10}$, but in general the effective potential in $\mathcal{M}_4$ should also depend on the angular coordinates on $\mathcal{M}_{10}$, therefore leading to the more generic multifield model, so-called *multifield DBI inflation* [47, 50, 201–203].

To put it in a nutshell, considering the effects of quantum gravity at the energy scale of inflation, at least implies the study of often several dynamical scalar fields, a situation that is tackled phenomenologically by multifield inflation.

An agnostic search for the inflationary particle content: scalar fields and beyond.

*La prière de l'agnostic: “Ô Dieu, s’il y a un Dieu, sauve mon âme si j’ai une âme”.*⁴

Ernest Renan

But actually, even without resorting to arguments based on quantum gravity, multifield inflation should be studied just because it is one of the possible descriptions of the early universe. Indeed, even in the absence of a precise description of gravity in a quantum framework from which to deduce a precise number of fields, with a given spectrum of spins, masses and interactions, multifield inflationary models with both kinetic and potential interactions, simply constitute the most generic possibility at lowest order in derivatives and for non-spinning particles. Of course, one could go further and study the most general scalar theories taking into account all orders in derivatives, so-called generalised multifield $P(X^{IJ}, \phi)$ models where $X^{IJ} = \partial_\mu \phi^I \partial^\mu \phi^J$, or the effects of

⁴Translation: *Prayer of an agnostic: “O God, if there is a God, save my soul if I have a soul”.*

spinning particles during inflation, either usual fermionic spin-1/2 particles, gauge fields or even exotic bosonic and fermionic states with arbitrary spins, and actually each of these domains has its own dedicated literature. But there has been an effort to unify the above studies once a background evolution is assumed, the so-called *cosmological collider program*, that aims at discovering the spectrum of masses and spins of extra particles beyond the usual comoving curvature perturbation $\mathcal{R}$ that is the only dynamical quantity in single-field inflation. These studies have undertaken different names depending on the techniques that are used, the kinds of particles that are probed, and on which observational imprint they focus, such as the Quasi-Single Field inflation scenario, the cosmological collider program, or more recently the cosmological bootstrap (see, *e.g.* Refs. [51, 52, 63, 67, 73, 76, 204, 205]). But all of them rely on the same principle: being agnostic about the particle content and trying to infer as generic predictions as possible within a regime of validity that enables one to probe the spectrum of extra particles during inflation. To put it in a nutshell, being an inflationary agnostic I would therefore pray:

“O inflationary scalar fields, if there are scalar fields during inflation, tell me your masses if you have masses”.

4.2 Dynamics of multifield inflation

In the following, independently of the exact motivation, one considers that inflation can be described by the following theory,

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{Pl}}^2}{2} R - \frac{1}{2} g^{\mu\nu} G_{IJ}(\phi) \partial_\mu \phi^I \partial_\nu \phi^J - V(\phi) \right], \quad (4.9)$$

consisting in the standard Einstein-Hilbert action for general relativity to describe gravity, and a set of scalar fields ϕ^I with $I \in \{1, \dots, N_{\text{field}}\}$ that can have both potential $V(\phi)$ and kinetic $G_{IJ}(\phi)$ interactions, in the matter sector. Focusing now on the phenomenological side, the goal is to derive observational predictions that are specific to these models, and hopefully find relevant astrophysical and cosmological imprints of their interactions in the primordial universe.

In order to do this, one uses cosmological perturbation theory as explained in Chap. 2, in particular the scalar fields are expanded at second order, $\phi^I(t, \vec{x}) = \bar{\phi}^I(t) + Q^I(t, \vec{x}) - \Gamma^I_{JK} Q^J(t, \vec{x}) Q^K(t, \vec{x})/2$, see Eq. (2.15), in terms of the covariant perturbations Q^I , and spacetime perturbations are parameterised using the ADM formalism.

4.2.1 Background

Generalities. At the level of the background, homogeneous scalar fields, the action reads (one forgets the bar superscript in order to simplify notations):

$$S_\phi^{(0)} = \int d^4x a^3 \left[\frac{1}{2} G_{IJ} \dot{\phi}^I \dot{\phi}^J - V(\phi) \right], \quad (4.10)$$

while the Friedmann equations (1.11) become in this multifield setup a generalisation of the single-field case (3.14):

$$\boxed{3M_{\text{Pl}}^2 H^2 = \frac{1}{2} \dot{\sigma}^2 + V(\phi) \quad \text{and} \quad \dot{H} = -\frac{\dot{\sigma}^2}{2M_{\text{Pl}}^2}, \quad \text{where} \quad \dot{\sigma}^2 = G_{IJ} \dot{\phi}^I \dot{\phi}^J} \quad (4.11)$$

is the total squared velocity in field space (note that the “field” σ itself, defined as the time integral of $\dot{\sigma}$, can be understood as a curvilinear coordinate in field space, and therefore is not uniquely defined). Taking the Euler-Lagrange equations associated with the background action (4.10) yields the following equations of motion for the homogeneous scalar fields:

$$\boxed{D_t \dot{\phi}^I + 3H \dot{\phi}^I + G^{IJ} V_{,J} = 0, \quad \text{with} \quad D_t \dot{\phi}^I = \ddot{\phi}^I + \Gamma^I_{JK} \dot{\phi}^J \dot{\phi}^K} \quad (4.12)$$

the field-space-covariant, time derivative, and $V_{,J} = \partial V / \partial \phi^J$. Indeed, remember that although ϕ^I are coordinates in field space, their time derivatives $\dot{\phi}^I$ are vectors, and that the simple derivative of a vector is not a vector in general: one should rather use the associated covariant derivative. Eq. (4.12) is the first example where an equation is found to be consistently expressed in a manifestly covariant way (meaning that each of the terms in the equation is covariant on its own without the need to mix it with another one), and in the remaining of this thesis a particular effort has been made to always follow this rule of principle, which actually allows to check the consistency of the derived equations.

The first Hubble slow-roll parameter is found to be

$$\boxed{\epsilon = -\dot{H}/H^2 = \frac{\dot{\sigma}^2}{2H^2 M_{\text{Pl}}^2},} \quad (4.13)$$

and the second Hubble slow-roll parameter, η , also takes a form similar to the single-field case with the formal replacement $\dot{\phi} \rightarrow \dot{\sigma}$:

$$\boxed{\eta = 2(\epsilon - \delta) \quad \text{with} \quad \delta = -\frac{\ddot{\sigma}}{H\dot{\sigma}}.} \quad (4.14)$$

Note however that a huge novelty is that the requirements that $\epsilon \ll 1$ in order to indeed have an inflationary phase, and $\eta \ll 1$ for it to last long enough, only put bounds on the relative size of the total kinetic and potential energies, $\dot{\sigma}^2 < V(\phi)$, and of the total acceleration and velocity $|\ddot{\sigma}/(H\dot{\sigma})| \ll 1$. Thus in general, one cannot assume in multifield inflation that the individual accelerations $D_t \dot{\phi}^I$ are negligible (but of course each component I of the total velocity must remain small): rather, they can be large but compensate each others. As one shall see, this corresponds to situations where the background trajectory in field space is strongly bent, a scenario that recently attracted much attention [1, 77–79, 206]. Moreover, there is no unique identification between the Hubble parameters ϵ, η on one hand, and the potential slow-parameters ϵ_V, η_V on the

other hand, which again results in more freedom: in general, the scalar potential needs not be flat nor have a small curvature in multifield setups. These features are particularly appealing when considered together with the high-energy constraints mentioned in the previous section. Indeed, multifield inflation may provide a quasi-exponential expansion of space without violating the swampland conjectures and still being compatible with a large η_V parameter, possibly evading the η -problem.

However in situations where the scalar potential is flat enough, the scalar fields may be all slowly rolling and the background trajectory solved analytically. Indeed, assuming that $D_t \dot{\phi}^I \ll 3H \dot{\phi}^I$, one finds the corresponding generalised slow-roll equations of motion (denoted by the symbol “ $\approx$ ”):

$$\dot{\phi}^I \approx -\frac{G^{IJ}V_{,J}}{3H}, \quad (4.15)$$

which may be integrated explicitly, easily or not depending on if the RHS depends on other fields than the I^{th} one. An explicit example of an analytical resolution of the background EoM in two-field inflation where a generalised slow-roll approximation is used, is given in Sec. 9.1. But in general, this generalised slow-roll is not verified and one must resort to a numerical resolution even for the background equations of motion.

4.2.2 Linear perturbations

Quadratic action and linear equations of motion. The dynamics of linear fluctuations are ruled by the quadratic action, which may be found *e.g.* in the flat gauge in terms of the fluctuations Q_{flat}^I , exactly in the same way as in the single-field case. For this, one needs to expand explicitly the action (4.9) at second order in scalar fields and spacetime perturbations parameterised in the ADM formalism. Once the constraint equations are solved, see Eqs. (2.46)–(2.48), and plugged back in the quadratic action, one finds:

$$S^{(2)} = \frac{1}{2} \int d^4x a^3 \left[\left(G_{IJ} D_t Q_{\text{flat}}^I D_t Q_{\text{flat}}^J - \frac{(\partial Q_{\text{flat}}^I) \cdot (\partial Q_{\text{flat}}^J)}{a^2} \right) - M^2_{IJ} Q_{\text{flat}}^I Q_{\text{flat}}^J \right], \quad (4.16)$$

$$\text{with } M^2_{IJ} = V_{;IJ} - R_{IJKL} \dot{\phi}^K \dot{\phi}^L - \frac{1}{a^3 M_{\text{Pl}}^2} D_t \left(\frac{a^3}{H} \dot{\phi}_I \dot{\phi}_J \right).$$

Note that the covariant perturbations Q^I are vectors of the field space, and hence have the same status as the background time derivatives $\dot{\phi}^I$, therefore their simple time derivatives are not covariant and must be corrected by including the usual term $\propto \Gamma^I_{JK}$ to go from ∂_t to D_t . In addition to these covariant kinetic terms, it is interesting to investigate the quantities contained in M^2_{IJ} , the squared mass matrix of inflationary perturbations. The first term $V_{;IJ}$ is the covariant Hessian matrix of the potential, where the semicolon denotes a field-space-covariant derivative: $V_{;IJ} = D_J(V_{,I}) = V_{,IJ} - \Gamma^K_{IJ} \dot{\phi}^J V_{,K}$ since $V_{,I}$ is a contravariant vector, and where $V_{,IJ} = \partial^2 V / (\partial \phi^I \partial \phi^J)$. The second contribution to the mass matrix is purely geometrical, and depends on some contractions of the Riemann tensor *of the field space* along background fields’ velocities, while the third

one, inversely proportional to the squared Planck mass, comes from the backreaction of the metric fluctuations induced by the scalar fields and may be suppressed by slow-roll parameters in reasonable cases. Note that each of the three contributions is symmetric under the exchange of I, J indices, hence the squared mass matrix is symmetric.

Going first to Fourier space, the linear equations of motion for the fluctuations are found by writing down the Euler-Lagrange equations associated with the quadratic action (4.16) (one forgets the subscript “flat” in the following for simplicity):

$$D_t D_t Q_k^I + 3H D_t Q_k^I + \left(\frac{k^2}{a^2} \delta_J^I + M_J^{2I} \right) Q_k^J = 0, \quad (4.17)$$

where one recalls that internal indices I may be lowered or raised with the field-space metric G_{IJ} (evaluated on the background for these equations that are linear in perturbations), as an example $M_J^{2I} = G^{IK} M_{KJ}^2$. It is clear from these equations that the linear perturbations mix with each others due to two physical effects: the curvature of the field space via the covariant time derivatives, and the mass matrix (which notably contains contributions from the covariant hessian of the potential and the Riemann curvature of the field space, that need not be diagonal). The analytical resolution of these equations is usually impossible, and one shall resort to numerical implementations to solve them. However, under an assumption of a slowly-evolving background, it is possible after changing variables to a locally inertial frame (in field space) and diagonalising the mass matrix, to recast Eq. (4.17) as independent linear second-order differential equations with constant coefficients around the time of horizon crossing. This somehow heavy formalism shall not be introduced here, but the interested reader is referred to Sec. 7.2, part 5.3, where they shall find as a side result of the article [5], such kind of analytical approximation.

But actually, before solving any equation, one should be careful about the quantisation of system, which enables one, not only to find relevant initial conditions, but also to define correctly the mode functions that are needed to compute observational quantities. Indeed, the multifield quantisation is more complex, or richer, than its single-field counterpart. In particular as one shall see, although one can identify a set of N_{field} quantum annihilation and creation operators $(\hat{a}_k^A, \hat{a}_k^{A,\dagger})$ defining an equivalent Bunch-Davies vacuum, they need not coincide with each of the scalar fields’ fluctuations Q^I (note the different indices).

Multifield canonical variables. In order to quantise scalar fields’ perturbations, one must first identify canonical variables, a path that can be summarized by the following diagram [44, 207]:

$$Q^I \longrightarrow Q^\alpha = e_I^\alpha Q^I \longrightarrow v^\alpha = a Q^\alpha \longrightarrow u^\alpha = (R^{-1})^\alpha_\beta v^\beta \xrightarrow{\text{Quantisation}} \hat{u}^\alpha. \quad (4.18)$$

The quantities e_α^I are called vielbeins of the field space and define a local orthogonal frame (whose indices are raised and lowered as $e_I^\alpha = \delta^{\alpha\beta} G_{IJ} e_\beta^J$), as

$$\delta^{\alpha\beta} e_\alpha^I e_\beta^J = G^{IJ} \quad \text{and} \quad G_{IJ} e_\alpha^I e_\beta^J = \delta_{\alpha\beta}. \quad (4.19)$$

Note that since by definition vielbeins define a local orthogonal frame, the indices α, β , etc. can be raised and lowered with the Euclidean metric $\delta_{\alpha\beta}$ and therefore the up or down position has no particular meaning. The requirement that these relations are verified at any time along the background trajectory implies that they must be conserved quantities with respect to the covariant derivative D_t , which therefore implies $D_t(e_\alpha^I e_\beta^J) = 0$, *i.e.* the existence of an anti-symmetric matrix Ω such that $D_t e_\alpha^I = \Omega_\alpha^\beta e_\beta^I$. But then, which anti-symmetric matrix Ω is used, is only a matter of choice and results in an interesting freedom for how to describe perturbations in multifield setups. A famous choice of vielbeins corresponds to the local adiabatic-entropic basis which shall be reviewed in the next section, Sec. 4.3, and for which the entries of Ω can be understood as turning rates of the background trajectories, so-called “curvatures” in mathematical studies of parametric curves in any dimension. Another simple choice is the one of “parallel-transported” vielbeins, for which $\Omega = 0$ and therefore $D_t e_\alpha^I$ is vanishing; they shall be used soon to simplify the quantisation procedure. The perturbations Q^α are nothing but the projections of the initial fields’ fluctuations Q^I along the directions defined by this local inertial frame, and the v^α are just rescalings of the Q^α needed to remove the Hubble friction term in the linear equations of motion expressed in comoving time.

R is a matrix that is effectively changing the local frame as $e_\alpha^I \rightarrow \tilde{e}_\alpha^I = R^\beta_\alpha e_\beta^I$, and where the new set of quantities $\tilde{e}_\alpha^I$ are again vielbeins of the field space provided R is an orthogonal matrix: $R^{-1} = R^T$. In order to obtain rotated fluctuations $u^\alpha = R_\beta^\alpha v^\beta$ with canonical kinetic terms at each instant of time, the orthogonal matrix R can be chosen to verify:

$$\dot{R}^\alpha_\beta = - (e_I^\alpha D_t e_\gamma^I) R^\gamma_\beta = -\Omega_\gamma^\alpha R^\gamma_\beta \text{ and } R^\alpha_\beta(t_{\text{ini}}) = \delta_\beta^\alpha. \quad (4.20)$$

Actually, the rotated vielbeins $\tilde{e}_\alpha^I$ for this particular choice of matrix R , verify

$$D_t \tilde{e}_\alpha^I = \dot{R}^\beta_\alpha e_\beta^I + R^\beta_\alpha D_t e_\beta^I = \left(-\Omega_\gamma^\beta R^\gamma_\alpha + R^\gamma_\alpha \Omega_\gamma^\beta \right) e_\beta^I = 0, \quad (4.21)$$

and therefore correspond to the choice of anti-symmetric matrix $\tilde{\Omega} = 0$: they are the parallel-transported vielbeins mentioned above. Given those considerations, one may use the simpler, more straightforward path to canonical variables u^α [208]:

$$\boxed{Q^I \longrightarrow u^\alpha = a e_I^\alpha Q^I \text{ with } D_t e_\alpha^I = 0 \xrightarrow{\text{Quantisation}} \hat{u}^\alpha.} \quad (4.22)$$

And indeed, using these parallel-transported vielbeins e_I^α , switching to conformal time, one finds the quadratic action for the variables u^α to be:

$$S^{(2)} = \frac{1}{2} \int d\tau \frac{d^3 \vec{k}}{(2\pi)^3} \left\{ \delta_{\alpha\beta} u_k'^\alpha u_k'^\beta - \left[\left(k^2 - \frac{a''}{a} \right) \delta_{\alpha\beta} + a^2 M^2_{\alpha\beta} \right] u_k^\alpha u_k^\beta \right\}, \quad (4.23)$$

with $M^2_{\alpha\beta} = e_\alpha^I e_\beta^J M^2_{IJ}$,

which therefore shows that the perturbations u^α now mix only via the non-trivial, time-dependent mass matrix projected in the local basis defined by the parallel-transported vielbeins, $M^2_{\alpha\beta}$. Indeed the Euler-Lagrange equations for the action (4.23) give

$$u''_{\vec{k}}{}^\alpha + \left[\left(k^2 - \frac{a''}{a} \right) \delta_{\alpha\beta} + a^2 M^2_{\alpha\beta} \right] u_{\vec{k}}{}^\beta = 0, \quad (4.24)$$

which are the multifield counterparts of the single-field Sasaki-Mukhanov equation.

Multifield canonical quantisation. The quantisation of the canonical variables u^α that were just identified then follows a path similar to the one of single-field inflation. In particular, a set of annihilation and creation operators is identified, and a Bunch-Davies vacuum is defined with sub-horizon modes. Looking at the sub-horizon limit of Eq. (4.24), one simply recovers N_{field} copies of the quantum harmonic oscillator: defining the canonical conjugate momentum $\pi_\alpha = u'_\alpha$ of u^α in this limit, one finds the classical Hamiltonian $H_{\text{sub}}^{(2)}$ and immediately promotes it to a quantum operator by requiring that the canonical variables themselves are promoted to quantum operators, first in real space,

$$u^\alpha(\tau, \vec{x}) \rightarrow \hat{u}^\alpha(\tau, \vec{x}), \quad \pi_\alpha(\tau, \vec{x}) \rightarrow \hat{\pi}_\alpha(\tau, \vec{x}), \quad (4.25)$$

that must verify the canonical commutation relations at equal time τ :

$$[\hat{u}^\alpha(\tau, \vec{x}), \hat{\pi}_\beta(\tau, \vec{y})] = i\delta^\alpha_\beta \delta^{(3)}(\vec{x} - \vec{y}). \quad (4.26)$$

Defining the quantum operators $\hat{u}^\alpha_{\vec{k}}, \hat{\pi}_{\alpha\vec{k}}$ as the Fourier transforms of the real-space ones, one can decompose them in the basis of quantum states of the Hilbert space made of the annihilation and creation operators $(\hat{a}^A_{\vec{k}}, \hat{a}^{\dagger A}_{\vec{k}})$ defining the n -particles states of the quantum theory. For example $\hat{a}^{\dagger A}_{\vec{k}}|0\rangle = |1^A_{\vec{k}}\rangle$ is the state with one particle A with wavenumber $\vec{k}$ obtained by acting with the creation operator on the vacuum $|0\rangle$ that minimises the quadratic quantum Hamiltonian. The most general decomposition of the canonical operators on this basis of quantum states is the following:

$$\boxed{\hat{u}^\alpha_{\vec{k}}(\tau) = \sum_{A=1}^{N_{\text{field}}} u^\alpha_{A,k}(\tau) \hat{a}^A_{\vec{k}} + u^{*\alpha}_{A,k}(\tau) \hat{a}^{\dagger A}_{-\vec{k}}, \quad \hat{\pi}_{\alpha\vec{k}}(\tau) = \sum_{A=1}^{N_{\text{field}}} \pi_{\alpha A,k}(\tau) \hat{a}^A_{\vec{k}} + \pi^*_{\alpha A,k}(\tau) \hat{a}^{\dagger A}_{-\vec{k}}}, \quad (4.27)$$

where it is of utmost importance that for each fixed value of α , $\hat{u}^\alpha$ can have non-vanishing components along different quantum oscillators labelled by A , which therefore results in not only N_{field} but actually N_{field}^2 mode functions u^α_A to follow for each wavenumber with modulus k . From now on, the sum over A -type indices will be implicit when they are repeated, just like with other indices. Enforcing these fundamental oscillators to be independent,

$$[\hat{a}^A_{\vec{k}}, \hat{a}^{\dagger B}_{\vec{k}'}] = (2\pi)^3 \delta^{AB} \delta^{(3)}(\vec{k} - \vec{k}'), \quad (4.28)$$

imposes the following conditions on the mode functions u_A^α :

$$u_{A,k}^\alpha (u_{A,k}^{*\beta})' - u_{A,k}'^\alpha u_{A,k}^{*\beta} = i\delta^{\alpha\beta}. \quad (4.29)$$

The vacuum state $|0\rangle$ is found by minimising the quadratic Hamiltonian using the above mode functions, which is obtained in the sub-horizon, Minkowskian limit, by:

$$u_{A,k}^{\alpha, \text{Minkowski}}(\tau) = \frac{1}{\sqrt{2k}} e^{-ik\tau} U^\alpha_A, \quad (4.30)$$

where U is an arbitrary unitary matrix that is irrelevant both for the quantisation procedure and the computation of observables such as power spectra, etc., and therefore can be chosen as $U^\alpha_A = \delta^\alpha_A$ for convenience, meaning that at initial times when interactions are suppressed, each mode function u^α can be chosen to be aligned with a single quantum oscillator labelled by A . Therefore more generally, taking into account the time evolution of the mode functions and the mixing between the various fields' fluctuations, one can still define a vacuum with a generalised Bunch-Davies procedure, *i.e.* by requiring that:

(Multifield Bunch-Davies vacuum): $u_{A,k}^\alpha(\tau) \xrightarrow[k\tau \rightarrow -\infty]{} u_{A,k}^{\alpha, \text{Minkowski}}(\tau) = \frac{\delta_A^\alpha}{\sqrt{2k}} e^{-ik\tau},$

(4.31)

which uniquely fixes the set of quantum operators $(\hat{a}_k^A, \hat{a}_k^{\dagger A})$ that are used, and provides consistent initial conditions for the N_{field}^2 mode functions u_A^α . Given those initial conditions and the multifield Sasaki-Mukhanov equations for the N_{field}^2 mode functions, which read

(Multifield Sasaki-Mukhanov equations):
 $u_{A,k}^{\prime\prime\alpha} + \left[\left(k^2 - \frac{a''}{a} \right) \delta_{\alpha\beta} + a^2 M^2_{\alpha\beta} \right] u_{A,k}^\beta = 0,$

(4.32)

the full system of linear equations can be solved, although almost always numerically only. In particular, remember that a difficulty comes from the mass matrix projected in the vielbeins' basis, $M^2_{\alpha\beta}$, which to be known first requires to solve for the vielbeins themselves from the parallel-transport equation, $\dot{e}_\alpha^I = -\Gamma^I_{JK} \dot{\phi}^J e_\alpha^K$. Then, the fields' fluctuations in the flat gauge can be retrieved by remembering that $\hat{Q}^I = e_\alpha^I \hat{u}^\alpha/a$, and therefore that the mode functions read $Q_A^I = e_\alpha^I u_A^\alpha/a$.

A final note is that in practice, the multifield canonical quantisation procedure is often only implicit, and it is common to simply read that the fields' fluctuations Q^I in the flat gauge and their conjugate momenta P_I , are promoted to quantum operators as:

$$[\hat{Q}^I(t, \vec{x}), \hat{P}_J(t, \vec{y})] = i\delta_J^I \delta^{(3)}(\vec{x} - \vec{y}), \quad (4.33)$$

and decomposed in Fourier space into the basis $(\hat{a}_k^A, \hat{a}_k^{\dagger A})$ with corresponding mode functions Q_A^I , etc. This procedure is of course correct, but it is well justified only once

the canonical quantisation using the u^α fluctuations with canonical kinetic terms and no mixing on sub-Hubble scales, has been invoked. Therefore, the equations of motion to be solved can equivalently be the N_{field} copies:

$$D_t D_t Q_{A,k}^I + 3H D_t Q_{A,k}^I + \left(\frac{k^2}{a^2} \delta_J^I + M_J^{2I} \right) Q_{A,k}^J = 0, \quad (4.34)$$

with initial conditions given by

$$Q_{A,k}^\alpha(\tau) \xrightarrow[k\tau \rightarrow -\infty]{} \delta_A^\alpha \frac{1}{a\sqrt{2k}} e^{-ik\tau}, \quad (4.35)$$

where one reminds that $Q_A^I = e_\alpha^I Q_A^\alpha$, with e_α^I the solution of the parallel-transport at times τ when the mode k was deep in the horizon.

Power spectra. Power spectra of the fields' fluctuations in the flat gauge, $P_Q^{IJ}(k, \tau)$ are given by the quantum two-point functions:

$$\langle 0 | \hat{Q}_k^I(\tau) \hat{Q}_{k'}^J(\tau) | 0 \rangle = (2\pi)^3 \delta^{(3)}(\vec{k} + \vec{k}') P_Q^{IJ}(k, \tau), \text{ with } P_Q^{IJ}(k, \tau) = Q_{A,k}^I(\tau) Q_{A,k}^{*J}(\tau), \quad (4.36)$$

and the corresponding dimensionless power spectra are simply defined by

$$\mathcal{P}_Q^{IJ}(k, \tau) = \frac{k^3}{2\pi^2} P_Q^{IJ}(k, \tau). \quad (4.37)$$

Moreover, the comoving curvature perturbation $\mathcal{R}$ is related to the fields' fluctuations in the flat gauge as

(Comoving curvature perturbation in multifield inflation): $\mathcal{R} = \frac{H}{\dot{\sigma}^2} \dot{\phi}_I Q_{\text{flat}}^I,$

(4.38)

which means its power spectrum is given by:

$$\mathcal{P}_{\mathcal{R}}(k, \tau) = \frac{H^2}{\dot{\sigma}^4} \dot{\phi}_I \dot{\phi}_J \mathcal{P}_Q^{IJ}(k, \tau), \quad (4.39)$$

and therefore selects only the symmetric part of $\mathcal{P}_Q^{IJ}$, showing that the power spectrum of the comoving curvature perturbation is always real.

Massless scalar fields in de Sitter. Just for concreteness, one considers the particular case of effectively massless scalar fields in de Sitter spacetime, whence $M_{\alpha\beta}^2 = 0$ and $a''/a = 2a^2 H^2$. Then, the multifield Sasaki-Mukhanov equations in the local orthogonal frames are all decoupled and can be solved separately, giving eventually up to an irrelevant phase:

$$Q_{A,k}^\alpha(\tau) = \frac{\delta_A^\alpha}{\sqrt{2k}} e^{-ik\tau} \left(1 - \frac{i}{k\tau} \right). \quad (4.40)$$

Note that in this much simplified case, no mixing at all is taken into account in the local orthogonal frame, which explains why each field perturbation Q^α remains aligned with its initial quantum mode labelled by A . However this is not the case in the initial field space coordinates, since the vielbeins e_α^I will mix those contributions one with the others. But actually, the vielbeins disappear from the expression of the power spectra, since $Q_A^I Q_A^J \propto e_\alpha^I \delta_A^\alpha e_\beta^J \delta_A^\beta = G^{IJ}$, and one finds explicitly the dimensionless power spectra on super-horizon scales:

$$\mathcal{P}_Q^{IJ}(k, \tau) \underset{-k\tau \rightarrow 0}{=} \mathcal{P}_Q^{IJ}(k) = \left(\frac{H}{2\pi}\right)^2 G^{IJ}, \quad (4.41)$$

where one used the relation $\tau = -(aH)^{-1}$ which is exact in de Sitter spacetime. Notice that although no mass effect at all is taken into account, using vielbeins enabled one to describe at the zeroth order, the geometry of the field space which is obviously encoded in the inverse field-space metric G^{IJ} . More complicated effects, such as the ones due to the Riemann curvature of the field space and contributing to the mass matrix, were however neglected and thus do not appear in the final result.

In that case, the power spectrum of the curvature perturbation is simply

$$\mathcal{P}_\mathcal{R}(k, \tau) \underset{-k\tau \rightarrow 0}{=} \mathcal{P}_\mathcal{R}(k) = \frac{H^2}{8\pi^2 \epsilon M_{\text{Pl}}^2}. \quad (4.42)$$

Note that strictly speaking this quantity is divergent in the limit $\epsilon = 0$, a feature which is due to the absence of a well-defined curvature perturbation $\mathcal{R}$ in de Sitter spacetime, exactly like in the single-field case. However Eq. (4.42) indeed gives the correct result at leading order, for massless scalar fields in quasi-de Sitter spacetime, provided the replacement $H \rightarrow H_*$ and $\epsilon \rightarrow \epsilon_*$, which therefore shows that in this case, the multifield power spectrum is formally the same as the single-field one.

4.3 The adiabatic-entropic decomposition

In this section, one focuses on the particular case $N_{\text{field}} = 2$, which is obviously the first non-trivial case where multifield effects arise, to define the adiabatic-entropic basis and corresponding perturbations, together with the main results concerning this formalism.

4.3.1 A new parameterisation.

Adiabatic-entropic vielbeins and background EoM. As already mentioned, using vielbeins that define a locally orthogonal frame along the background trajectory, can be useful to follow the evolution of perturbations in multifield setups. One therefore defines first the adiabatic vielbein as

$$e_\sigma^I = \frac{\dot{\phi}^I}{\dot{\sigma}}, \quad (4.43)$$

from which the entropic vielbein is defined as the unit vector orthogonal to it (and whose direction can be specified by fixing the orientation of the local basis), e_s^I such that the set (e_α^I) with $\alpha \in \{\sigma, s\}$, verifies the vielbeins' conditions (4.19). The covariant derivatives of these vectors of the field space can be parameterised as:

$$D_t e_\sigma^I = H \eta_\perp e_s^I, \quad D_t e_s^I = -H \eta_\perp e_\sigma^I, \quad (4.44)$$

where $H \eta_\perp$, sometimes denoted $\dot{\theta}$ or ω , can be understood as the covariant rate of turn of the background trajectory on the curved field-space manifold. More particularly, the dimensionless parameter $\eta_\perp$ and called the *bending*, measures the acceleration perpendicular to the background trajectory, hence its notation, and provides a dimensionless measure of the deviation of the background trajectory from a geodesic of the field space. Indeed, in situations where the background trajectory coincides with such geodesic, $D_t \dot{\phi}^I = 0$ and therefore $D_t e_\sigma^I = 0$, implying that the bending vanishes. Note also that the statement “geodesic deviation” is covariant and applies to any kind of field-space manifold irrespective of its geometry, while “bending” or “perpendicular acceleration” can be confusing in curved field spaces.

The background equations of motion for the scalar fields can already be written in the adiabatic-entropic basis, simply by replacing $\dot{\phi}^I = \dot{\sigma} e_\sigma^I$, and keeping tracks of the vielbeins' projection, giving in the two-field case under consideration:

$$\ddot{\sigma} + 3H\dot{\sigma} + V_{,\sigma} = 0, \quad V_{,s} + \dot{\sigma} H \eta_\perp = 0, \quad (4.45)$$

where one defined the projections $V_{,\alpha} = e_\alpha^I V_{,I}$. In particular, note that there is apparently a single effective dynamical background field, $\dot{\sigma}$, which evolves in a very similar fashion to the single-field case with a Hubble friction term and a potential force, even though one actually has to follow the dynamics of the vielbeins (e_σ^I, e_s^I) too. Moreover, the derivative of the potential in the direction perpendicular to the trajectory is simply proportional to the bending parameter $\eta_\perp$, from which it is clear that this second equation describes the “equilibrium” in a non-inertial frame, where the inertial force $\propto \eta_\perp$ is counterbalanced by the slope of the potential in the orthonormal direction. Although already illuminating for the description of the background dynamics, the usefulness of the adiabatic-entropic basis is better seen when studying perturbations.

Linear perturbations in the adiabatic-entropic basis. The linear equations of motion in the flat gauge, written in terms of the fields' fluctuations Q_{flat}^I , can be rewritten in terms of the adiabatic and entropic fields' fluctuations in the flat gauge, respectively defined as

$$Q_\sigma^{\text{flat}} = e_{\sigma I} Q_{\text{flat}}^I, \quad \text{and} \quad Q_s^{\text{flat}} = e_{s I} Q_{\text{flat}}^I, \quad (4.46)$$

giving [44, 47, 209]:

$$\begin{aligned}\ddot{Q}_\sigma^{\text{flat}} + 3H\dot{Q}_\sigma^{\text{flat}} + \left(\frac{k^2}{a^2} + m_\sigma^2\right) Q_\sigma^{\text{flat}} &= \frac{d}{dt} \left(2H\eta_\perp Q_s^{\text{flat}} \right) - 2 \left(\frac{V_{;\sigma}}{H\dot{\sigma}} - \epsilon \right) H^2 \eta_\perp Q_s^{\text{flat}}, \\ \ddot{Q}_s^{\text{flat}} + 3H\dot{Q}_s^{\text{flat}} + \left(\frac{k^2}{a^2} + m_s^2\right) Q_s^{\text{flat}} &= -2\dot{\sigma}\eta_\perp \frac{d}{dt} \left(\frac{H}{\dot{\sigma}} Q_\sigma^{\text{flat}} \right),\end{aligned}\tag{4.47}$$

with the adiabatic mass

$$\frac{m_\sigma^2}{H^2} = \frac{V_{;\sigma\sigma}}{H^2} - \eta_\perp^2 - \frac{1}{a^3 H^2 M_{\text{Pl}}^2} \frac{d}{dt} \left(\frac{a^3 \dot{\sigma}^2}{H} \right),$$

and the entropic mass including the geometrical contribution:

(Entropic mass in two-field inflation): $\frac{m_s^2}{H^2} = \frac{V_{;ss}}{H^2} - \eta_\perp^2 + \epsilon R_{\text{fs}} M_{\text{Pl}}^2,$

(4.48)

where $V_{;ss} = e_s^I e_s^J V_{;IJ}$ and R_{fs} is the Ricci scalar of the field space. These equations are enlightening. But before commenting them, it should be noted that the adiabatic field's fluctuation in the flat gauge, Q_σ^{flat} , is simply proportional to the comoving curvature perturbation $\mathcal{R}$, since

$\mathcal{R} = \frac{H}{\dot{\sigma}} Q_\sigma^{\text{flat}},$

(4.49)

and therefore one is interested in making predictions for the value of Q_σ^{flat} at the end of inflation. Moreover, Q_s^{flat} coincides at the linear order with the fluctuation $Q_s = e_{sI} Q^I$ (where Q^I is simply the covariant perturbation of ϕ^I before any gauge is chosen) in any gauge since under a linear gauge transformation $\xi^\mu = (T, L_i)$, one has $Q_s \rightarrow Q_s + e_{sI} \dot{\phi}^I T = Q_s$, because by definition of the adiabatic-entropic basis $e_{sI} e_\sigma^I = 0$. In particular, $Q_s^{\text{flat}} = Q_s^{\text{com}}$ in the comoving gauge and at the linear order, which is denoted $\mathcal{F}$ in Sec. 5.3.⁵ Of course, this is not the case for $Q_\sigma = e_{\sigma I} Q^I$ that can for example vanish after a gauge transformation with $T = -Q_\sigma/\dot{\sigma}$, that coincides approximately with the comoving gauge, therefore $Q_\sigma^{\text{com}} = 0$, see again Sec. 5.3 for details.

Going back to Eqs. (4.47), a few comments should be made. First, the adiabatic perturbation fluctuates with a mass that can be rewritten in terms of the background slow-roll parameters, indeed one finds:⁶

$$\frac{m_\sigma^2}{H^2} = -\frac{3}{2}\eta + \frac{1}{2}\epsilon\eta - \frac{1}{4}\eta^2 - \frac{1}{2}\epsilon_3\eta,\tag{4.50}$$

⁵Note however that crucially this is true only at the linear order in perturbation theory relevant to describe the physics of linear fluctuations as is done in this Chapter, and that the entropic field does transform under spacetime diffeomorphisms at second and higher order, see *e.g.* [210]. This justifies different notations Q_s^{flat} , $\mathcal{F}$, etc. for the values of the entropic field's fluctuations in different gauges when non-linear effects are taken into account, such as when non-Gaussianities are computed. Here, we will simply denote it Q_s since there is no ambiguity at the linear level.

⁶A few useful, exact formulas concerning the adiabatic sector, *i.e.* the multifield background, are

from which it is clear that Q_σ^{flat} is almost massless in slowly varying situations where $\epsilon, \eta, \epsilon_3 \ll 1$, and that its mass is actually independent of the bending parameter $\eta_\perp$. Actually at leading order in slow-roll parameters, $m_\sigma^2 \approx -3\eta/2$ is very small but usually negative (an exception may be the ultra-slow-roll case or another non-attractor behaviour with $\eta < 0$), showing that Q_σ^{flat} is actually slightly growing with time. But the adiabatic equation of motion can be rewritten directly in terms of the comoving curvature perturbation $\mathcal{R} = (2\epsilon)^{-1/2} Q_\sigma^{\text{flat}}/M_{\text{Pl}}$, for which one finds many cancellations in the mass term, until finding a new LHS in Eq. (4.47): $\ddot{\mathcal{R}} + (3 + \eta)H\dot{\mathcal{R}} + (k^2/a^2)\mathcal{R} = \dots$, consistently with the expectation that $\mathcal{R}$ should be exactly massless.

What also appears clearly in the linear EoM written in the adiabatic-entropic basis is that the adiabatic and entropic perturbations are coupled, and therefore that their masses are not the only relevant scales in the situation at hand, indeed note that this coupling is parameterised by the size of the bending parameter $\eta_\perp$; in particular when the background trajectory follows a geodesic of the field space, $\eta_\perp = 0$ and their dynamics are then decoupled. Actually, noting that $V_{,\sigma}/(H\dot{\sigma}) = -3 + \epsilon - \eta/2$, one can rewrite the RHS of the adiabatic equation of motion as just one total derivative term. Switching for the variable $\mathcal{R}$ everywhere, one finds:

$$\ddot{\mathcal{R}} + (3 + \eta)H\dot{\mathcal{R}} + \frac{k^2}{a^2}\mathcal{R} = \frac{1}{a^3\epsilon M_{\text{Pl}}} \frac{d}{dt} \left(a^3 \sqrt{2\epsilon} H \eta_\perp Q_s \right), \quad (4.51)$$

$$\ddot{Q}_s + 3H\dot{Q}_s + \left(\frac{k^2}{a^2} + m_s^2 \right) Q_s = -2\sqrt{2\epsilon} H M_{\text{Pl}} \eta_\perp \dot{\mathcal{R}}. \quad (4.52)$$

When $\eta_\perp = 0$ the dynamics is effectively single-field, and one recovers the well-known result that $\mathcal{R}$ is conserved on super-horizon scales, indeed Eq. (4.51) then reduces to $\dot{\mathcal{R}} + (3 + \eta)H\mathcal{R} \simeq 0$ which is solved by an almost exponentially decaying $\mathcal{R}$, and therefore $\mathcal{R}$ converges to a constant value. However in general situations the bending is not vanishing and in that case, the constancy of $\mathcal{R}$ on super-horizon scales is violated as it constantly receives contributions from the entropic field whose dynamics must therefore be carefully studied.

Few comments have been made so far on the evolution of the entropic field, but now that one understood that its dynamics can be crucial to determine the statistics of $\mathcal{R}$ at the end of inflation, they shall be investigated. First, Q_s fluctuates with a mass squared given by Eq. (4.48), where one reads three independent contributions. The first contribution, $V_{;ss}/H^2$, is simply the projection of the covariant Hessian of the potential along the entropic direction that is by definition perpendicular to the background trajectory,

gathered here for the reader willing to check the calculations presented in this section:

$$\begin{aligned} \frac{V_{;\sigma\sigma}}{H^2} &= 3\epsilon - 3\frac{\ddot{\sigma}}{H\dot{\sigma}} - \frac{\ddot{\sigma}}{H^2\dot{\sigma}} + \eta_\perp^2, \text{ with} \\ \frac{\ddot{\sigma}}{H\dot{\sigma}} &= -\epsilon + \frac{\eta}{2}, \text{ and } \frac{\ddot{\sigma}}{H^2\dot{\sigma}} = 2\epsilon^2 + \frac{1}{4}\eta^2 - \frac{5}{2}\epsilon\eta + \frac{1}{2}\epsilon_3\eta, \text{ with } \epsilon_3 = \dot{\eta}/(H\eta), \text{ moreover} \\ \frac{1}{a^3 H^2 M_{\text{Pl}}^2} \frac{d}{dt} \left(\frac{a^3 \dot{\sigma}^2}{H} \right) &= 6\epsilon + 2\epsilon\eta - 2\epsilon^2, \text{ where one used everywhere } \dot{\sigma} = \sqrt{2\epsilon} H M_{\text{Pl}}. \end{aligned}$$

and corresponds to the usual mass of orthogonal fluctuations that one knows from classical dynamics. In reasonable situations, one would expect it to be positive, although its amplitude can vary a lot depending on the exact model at hand. The second contribution, $-\eta_\perp^2$, vanishes along geodesics and is therefore interpreted as the mass induced by the non-inertial motion in field space. Note that this contribution is importantly always negative, and that its amplitude can be large in situations where there is a strong bending, $\eta_\perp^2 \gg 1$, potentially destabilising the background trajectory, see Sec. 4.3.3 for more details. The third contribution, $\epsilon R_{\text{fs}}/M_{\text{Pl}}^2$, is geometrical: it depends not on the scalar potential, but on the field-space metric, and more precisely on the scalar curvature of the field space, encoded in R_{fs} . It vanishes for flat field spaces, but brings a positive or negative contribution in respectively spherical-like or hyperbolic-like field spaces. This geometrical contribution has been somehow overlooked in the past, but regained interest in the last years with the unveiling of the geometrical destabilisation of inflation [211] happening in negatively curved field spaces and that is reviewed in Sec. 4.3.3. A particular effort of this thesis has been to assess the observational consequences of a curved field space, whose contribution to the mass of entropic fluctuations plays an important role.

But studying m_s^2 is not sufficient to determine the linear dynamics of Q_s , since it is coupled to the adiabatic mode $Q_\sigma^{\text{flat}} \leftrightarrow \mathcal{R}$ via the bending, and in general the coupled system should be solved together and numerically to yield the correct solution. An exception arises on super-horizon scales, for which the dynamics can be approximately solved analytically, a situation that shall now be reviewed and used to predict the power spectra at the end of two-field inflation.

4.3.2 Super-Hubble evolution and power spectra at the end of inflation

Super-Hubble EoM in the adiabatic-entropic basis. On super-horizon scales, the adiabatic equation of motion, Eq. (4.51) indeed simplifies to:

$$\frac{d}{dt} \left[a^3 \sqrt{\epsilon} \left(\sqrt{\epsilon} \dot{\mathcal{R}} - \sqrt{2} \frac{H \eta_\perp}{M_{\text{Pl}}} Q_s \right) \right] = \mathcal{O} \left(\frac{k^2}{a^2} \right), \quad (4.53)$$

which can therefore be integrated as

$$\dot{\mathcal{R}}_k \underset{\frac{k}{a} \ll H}{=} \sqrt{\frac{2}{\epsilon}} \frac{H \eta_\perp}{M_{\text{Pl}}} Q_{s,k} + \frac{K_k}{a^3 \sqrt{\epsilon}}, \quad (4.54)$$

where K_k is a constant of integration that quickly becomes irrelevant since its contribution redshifts roughly as a^{-3} . Assuming that this exponentially decaying term has become negligible, one can plug the above expression for $\dot{\mathcal{R}}$ in the entropic EoM, which

gives the

(Super-Hubble evolution of Q_s in two-field inflation):

$$\ddot{Q}_s + 3H\dot{Q}_s + m_{s,\text{eff}}^2 Q_s = 0, \quad \text{with the} \quad (4.55)$$

(Effective mass of super-Hubble entropic perturbations:)

$$\frac{m_{s,\text{eff}}^2}{H^2} = \frac{m_s^2}{H^2} + 4\eta_\perp^2 = \frac{V_{;ss}}{H^2} + 3\eta_\perp^2 + \epsilon R_{\text{fs}} M_{\text{Pl}}^2, \quad (4.56)$$

where now the bending contribution is always positive. Importantly, the entropic EoM does not depend explicitly on the adiabatic perturbation on super-horizon scales, and therefore it can be solved alone. Moreover, all the physics except the usual Hubble friction $\propto H$ (note that the quantum oscillations $\propto k^2/a^2$ have been consistently neglected), is encoded in the effective mass of super-Hubble entropic fluctuations, $m_{s,\text{eff}}^2$, which is a given function of the two-field background and therefore sets the time scale after which the entropic perturbations are damped by the expansion of space.⁷ Once the super-Hubble evolution of Q_s has been solved (potentially analytically in slowly varying situations, or numerically in more involved cases), the end value of $\mathcal{R}$ is easily found by solving for the

(Super-Hubble evolution of $\mathcal{R}$ in two-field inflation): $\dot{\mathcal{R}}_k \stackrel{\frac{k}{a} \ll H}{=} 2H\eta_\perp \mathcal{S}_k, \quad (4.57)$

where one defined the

(Dimensionless entropic perturbation): $\mathcal{S} = \frac{H}{\dot{\sigma}} Q_s. \quad (4.58)$

Actually, rewriting the effective large-scale entropic EoM in terms of this rescaled entropic perturbation gives:

$$\ddot{\mathcal{S}}_k + (3 + \eta) H \dot{\mathcal{S}}_k + (m_{s,\text{eff}}^2 - m_\sigma^2) \mathcal{S}_k \stackrel{\frac{k}{a} \ll H}{=} 0, \quad (4.59)$$

which can be solved in an overdamped approximation, denoted by the symbol “ $\approx$ ” in the following and consisting in neglecting $\ddot{\mathcal{S}}$:⁸

⁷This is true in the usual cases where $m_{s,\text{eff}}^2$ is strictly positive. A strictly negative value of $m_{s,\text{eff}}^2$, a situation that can be encountered in negatively curved spaces when ϵ grows larger than a critical value [211], means that the background trajectory is unstable and that perturbation theory is ill-defined on this particular background, and should be replaced by a new perturbation theory on the actual background. An exactly vanishing value of $m_{s,\text{eff}}^2$, possible only if the field space assumes a particular shift-symmetry, has been investigated in so-called “orbital inflation” scenario: ultralight entropic perturbations freeze on super-Hubble scales and due to a non-zero bending $\eta_\perp$, constantly feed the evolution of $\mathcal{R}$ which therefore quickly forgets its initial value at horizon crossing [212–214]; this scenario should lead to strongly correlated adiabatic and entropic perturbations at the end of inflation. Do they survive through the reheating phase?

⁸A justification of this approximation is given here. Consider a slow-varying background, a situation that is less restrictive than assuming an overdamped regime for the perturbations, and most often

$$\dot{\mathcal{S}}_k \approx -\frac{m_{s,\text{eff}}^2 - m_\sigma^2}{(3+\eta)H} \mathcal{S}_k \implies \mathcal{S}_k \approx \mathcal{S}_{k,*} \exp \left[-\frac{m_{s,\text{eff}}^2 - m_\sigma^2}{(3+\eta)H} t \right], \quad (4.60)$$

where $\mathcal{S}_{k,*}$ is the value of the rescaled entropic perturbation at the time of horizon crossing for the modes with wavenumber k .

Overdamped approximation and correlated adiabatic-entropic perturbations.

Within this approximation, it is therefore possible to write the law of evolution of the two-field perturbations' system on super-Hubble scales as [215]:

$$\frac{d}{dt} \begin{pmatrix} \mathcal{R} \\ \mathcal{S} \end{pmatrix} \approx \begin{pmatrix} 0 & \alpha H \\ 0 & \beta H \end{pmatrix} \begin{pmatrix} \mathcal{R} \\ \mathcal{S} \end{pmatrix}, \quad (4.61)$$

where one saw that

$$\alpha = 2\eta_\perp, \quad \text{and} \quad \beta = -\frac{m_{s,\text{eff}}^2 - m_\sigma^2}{(3+\eta)H^2}. \quad (4.62)$$

matched in usual inflationary scenarios independently of the dynamics of linear fluctuations. Then, one can find the solutions of the entropic EoM on large scales, Eq. (4.59), by looking at the effective frequency ω_{t_0} such that $\mathcal{S}_{t_0} \sim \exp(i\omega_{t_0} t)$ around a fixed time t_0 , and where for consistency $d\omega_{t_0}/dt_0 \ll \omega_{t_0}^2$, a situation that corresponds to a WKB approximation. One finds that ω (one forgets the subscript t_0 in the following) should verify

$$-\omega^2 + iH(3+\eta)\omega + m_{s,\text{eff}}^2 - m_\sigma^2 = 0,$$

an equation that possesses two branches of solution depending on the value of the effective mass of the rescaled entropic perturbations.

- Either it is heavy, $(m_{s,\text{eff}}^2 - m_\sigma^2)/H^2 > (3+\eta)^2/4$, and

$$\omega_\mp = \frac{(3+\eta)H}{2} \left[i \pm \sqrt{\frac{4}{(3+\eta)^2 H^2} (m_{s,\text{eff}}^2 - m_\sigma^2) - 1} \right],$$

including the usual Hubble friction damping term $\propto i$, as well as the super-Hubble oscillations of underdamped massive fields. In that case, the overdamped regime is not applicable and one cannot neglect $\dot{\mathcal{S}}$ in the large-scale entropic EoM. Notice however that in this case the envelope of the oscillations is quickly decaying and therefore the feeding of $\mathcal{R}$ by the entropic perturbation $\mathcal{S}$ is localised around the time of horizon crossing only, and may be completely negligible.

- Either it is light, $(m_{s,\text{eff}}^2 - m_\sigma^2)/H^2 < (3+\eta)^2/4$, and

$$\omega_\mp = i \frac{(3+\eta)H}{2} \left[1 \pm \sqrt{1 - \frac{4}{(3+\eta)^2 H^2} (m_{s,\text{eff}}^2 - m_\sigma^2)} \right],$$

where now the Hubble friction term is supplemented by an extra friction for the decaying mode ω_- , and slowed down by a negative friction for the “growing mode” ω_+ . The decaying mode then quickly becomes negligible and one can approximate $\mathcal{S}_k \approx \mathcal{S}_{k,*} \exp(-\omega_+ t)$, which therefore generalises Eq. (4.60) to intermediate cases, and which is exactly recovered in the very light limit $(m_{s,\text{eff}}^2 - m_\sigma^2)/H^2 \ll (3+\eta)^2/4$, yielding $\omega_+ \simeq (m_{s,\text{eff}}^2 - m_\sigma^2)/[(3+\eta)H]$ in this overdamped regime.

This first-order differential system can easily be solved, yielding

$$\begin{pmatrix} \mathcal{R}(t) \\ \mathcal{S}(t) \end{pmatrix} \approx \begin{pmatrix} 1 & T_{\mathcal{RS}}(t_*, t) \\ 0 & T_{\mathcal{SS}}(t_*, t) \end{pmatrix} \begin{pmatrix} \mathcal{R}_* \\ \mathcal{S}_* \end{pmatrix}, \quad (4.63)$$

with

$$\begin{aligned} T_{\mathcal{RS}}(t_*, t) &= \int_{t_*}^t dt' T_{\mathcal{SS}}(t_*, t') \alpha(t') H(t'), \\ T_{\mathcal{SS}}(t_*, t) &= \exp \left(\int_{t_*}^t dt' \beta(t') H(t') \right), \end{aligned} \quad (4.64)$$

two positive transfer functions. Therefore the final power spectra read:

$$\begin{aligned} \mathcal{P}_{\mathcal{RR}}(t) &\approx \mathcal{P}_{\mathcal{RR}}(t_*) + 2T_{\mathcal{RS}}(t_*, t) \mathcal{P}_{\mathcal{RS}}(t_*) + T_{\mathcal{RS}}^2(t_*, t) \mathcal{P}_{\mathcal{SS}}(t_*), \\ \mathcal{P}_{\mathcal{RS}}(t) &\approx T_{\mathcal{SS}}(t_*, t) \mathcal{P}_{\mathcal{RS}}(t_*) + T_{\mathcal{RS}}(t_*, t) T_{\mathcal{SS}}(t_*, t) \mathcal{P}_{\mathcal{SS}}(t_*), \\ \mathcal{P}_{\mathcal{SS}}(t) &\approx T_{\mathcal{SS}}^2(t_*, t) \mathcal{P}_{\mathcal{SS}}(t_*). \end{aligned} \quad (4.65)$$

Notice that a non-zero cross-correlation between adiabatic and entropic modes can arise both from sub-Hubble mechanisms that have not been investigated here (via the initial condition $\mathcal{P}_{\mathcal{RS}}(t_*)$) and from the super-Hubble feeding of $\mathcal{R}$ that is under study in this paragraph. The relative amount of cross-correlation can be parameterised by an angle Δ defined as

(Adiabatic-entropic correlation): $\cos(\Delta) = \frac{\mathcal{P}_{\mathcal{RS}}}{\sqrt{\mathcal{P}_{\mathcal{RR}} \mathcal{P}_{\mathcal{SS}}}}.$

(4.66)

This angle Δ , that can be defined without resorting to any analytical approximation and computed numerically by solving for the full super-Hubble evolution of the system $(\mathcal{R}, \mathcal{S})$, can also be found approximately in simple situations.

As an example, one shall consider that the two-field system is composed of very light scalar fields ϕ^1, ϕ^2 with negligible sub-Hubble interactions. Around the time of horizon crossing, each perturbation Q^1, Q^2 (in the flat gauge) should have a power spectrum given by $\mathcal{P}_Q^{11} \simeq \mathcal{P}_Q^{22} \simeq [H_*/(2\pi)]^2$ and no cross-correlation, $\mathcal{P}_Q^{12} = 0$. Therefore, initial conditions for the super-Hubble evolution are in this simple scenario,

$$\mathcal{P}_{\mathcal{RR}}(t_*) \simeq \frac{H_*^2}{8\pi\epsilon_* M_{\text{Pl}}^2}, \quad \mathcal{P}_{\mathcal{SS}}(t_*) \simeq \frac{H_*^2}{8\pi\epsilon_* M_{\text{Pl}}^2}, \quad \text{and } \mathcal{P}_{\mathcal{RS}}(t_*) \simeq 0, \quad (4.67)$$

giving explicitly for the angle Δ ,

$$\cos(\Delta) \simeq \frac{T_{\mathcal{RS}}}{\sqrt{1 + T_{\mathcal{RS}}^2}}. \quad (4.68)$$

Notice that $0 \leq \cos(\Delta) < 1$ meaning that the super-Hubble evolution alone can only correlate adiabatic and entropic perturbations. Moreover in that case, one finds that the relative amount of entropic power is

$$\beta_{\text{iso}} = \frac{\mathcal{P}_{\mathcal{SS}}}{\mathcal{P}_{\mathcal{RR}} + \mathcal{P}_{\mathcal{SS}}} \simeq \frac{T_{\mathcal{SS}}^2}{1 + T_{\mathcal{RS}}^2 + T_{\mathcal{SS}}^2}. \quad (4.69)$$

In the limit where $\eta_\perp = 0$, *i.e.* $\alpha = 0$, *i.e.* $T_{\mathcal{RS}} = 0$, one recovers the usual result that there cannot be correlated adiabatic and entropic perturbations, $\cos(\Delta) = 0$, and that the relative amount of entropic modes with respect to adiabatic ones is simply set by the relative size of the difference between the effective entropic mass on large scales $m_{s,\text{eff}}^2$ and the adiabatic mass m_σ^2 , compared to the Hubble parameter H^2 as encoded in the parameter β .

Spectral indices and violation of Maldacena's consistency relation. The spectral indices of adiabatic and entropic power spectra can be expressed in terms of the parameters α and β evaluated at horizon exit, as well as the correlation angle Δ of late-time perturbations that one can hope to measure. Indeed, keeping in mind the simple scenario of light non-interacting scalar fields on sub-Hubble scales for which

$$\begin{aligned}\mathcal{P}_{\mathcal{RR}}(t) &\approx \mathcal{P}_{\mathcal{RR}}(t_*) [1 + T_{\mathcal{RS}}^2(t_*, t)] , \\ \mathcal{P}_{\mathcal{RS}}(t) &\approx \mathcal{P}_{\mathcal{RR}}(t_*) T_{\mathcal{RS}}(t_*, t) T_{\mathcal{SS}}(t_*, t) , \\ \mathcal{P}_{\mathcal{SS}}(t) &\approx \mathcal{P}_{\mathcal{RR}}(t_*) T_{\mathcal{SS}}^2(t_*, t) ,\end{aligned}\tag{4.70}$$

one finds the spectral indices to be

$$\begin{aligned}n_{\mathcal{RR}} - 1 &\approx (n_{\mathcal{RR},*} - 1) + \frac{1}{H_*(1 - \epsilon_*)} \frac{\partial \ln(1 + T_{\mathcal{RS}}^2)}{\partial t_*} , \\ n_{\mathcal{RS}} &\approx n_{\mathcal{RR},*} + \frac{1}{H_*(1 - \epsilon_*)} \frac{\partial \ln(T_{\mathcal{RS}} T_{\mathcal{SS}})}{\partial t_*} , \\ n_{\mathcal{SS}} &\approx n_{\mathcal{RR},*} + \frac{1}{H_*(1 - \epsilon_*)} \frac{\partial \ln(T_{\mathcal{SS}}^2)}{\partial t_*} ,\end{aligned}\tag{4.71}$$

where one used the relation $d \ln(k/k_{\text{pivot}}) = H_*(1 - \epsilon_*) dt$, and where $n_{\mathcal{RR},*} = 1 - 2\epsilon_* - \eta_*$ is the spectral index of the adiabatic curvature power spectrum evaluated at the time of horizon crossing and corresponding to the usual one of single-field, slow-roll inflation. $n_{\mathcal{RR}} - 1 = n_s - 1$ is the resulting spectral index for the comoving curvature perturbation power spectrum at the end of inflation and is constrained by CMB observations. Moreover, the derivatives of the transfer function with respect to the time of horizon crossing, and responsible for deviations from the single-field scale dependence, are given at leading order in the slow-varying approximation by:

$$\frac{1}{H_*} \frac{\partial T_{\mathcal{RS}}}{\partial t_*} = -\alpha_* - \beta_* T_{\mathcal{RS}} , \quad \text{and} \quad \frac{1}{H_*} \frac{\partial T_{\mathcal{SS}}}{\partial t_*} = -\beta_* T_{\mathcal{SS}} ,\tag{4.72}$$

which allows one to rewrite the scalar spectral index of the comoving curvature perturbation as

(Approximate scalar spectral index in two-field inflation):
 $n_s - 1 \approx -2\epsilon_* - \eta_* - \alpha_* \sin(2\Delta) - 2\beta_* \cos^2(\Delta) ,$

(4.73)

and similarly for the other spectral indices.

Primordial gravitational waves are not affected by the presence of scalar fluctuations at the linear order, and therefore the tensor-to-scalar ratio reads:

$$r = \frac{\mathcal{P}_\gamma}{\mathcal{P}_{\mathcal{R}\mathcal{R}}} \approx r_* \sin^2(\Delta) , \quad (4.74)$$

where r_* is the tensor-to-scalar ratio at the time of horizon crossing and corresponds to the usual single-field, slow-roll one which verifies the consistency relation $r_* \approx -8n_t \approx 16\epsilon_*$. Therefore in two-field models of inflation, one has in general:

$$\boxed{\text{(Violation of the single-field consistency relation): } r \approx -8n_t \sin^2(\Delta) ,} \quad (4.75)$$

which shows that even less primordial gravitational waves than in single-field inflation should be expected at CMB scales (given the observed value of scalar perturbations A_s) in two-field inflationary setups and at the level of a linear analysis.

4.3.3 Possible multifield instabilities

Having investigated quite generally the effects of the entropic mode on the adiabatic one in simple scenarios (slow variation, overdamped regime, light scalar fields with negligible sub-Hubble interactions, etc.), the current section now aims at giving an introduction for a more involved phenomenology based on multifield instabilities, that may leave interesting observational imprints.

Geometrical destabilisation of inflation

The geometrical destabilisation of inflation [211] is a generic scenario in multifield models of inflation that feature a negatively curved field space. In that case, the Ricci scalar of the field space is negative and reads $R_{\text{fs}} \sim -1/M^2$ with possible field-dependent coefficients, but always scaling as the inverse of a new mass scale M that is typically expected to lie in the range:

$$H \ll M \ll M_{\text{Pl}} . \quad (4.76)$$

As an example, the hyperbolic plane is a two-dimensional space that can be described by a diagonal field-space metric $G_{IJ}(\varphi, \chi)$, defining distances on the curved manifold as:

$$d\sigma^2 = \left(1 + \frac{2\chi^2}{M^2}\right) d\varphi^2 + \frac{2\sqrt{2}\chi}{M} d\varphi d\chi + d\chi^2 \implies R_{\text{fs}} = -\frac{4}{M^2} . \quad (4.77)$$

Suppose inflation is taking place along the $\chi = 0$ line of the two-dimensional field space, thanks to a slow-roll potential in the ϕ -direction, $V_{\text{sr}}(\phi)$, and a stabilized potential in the second, χ -direction, $V_{\text{stable}}(\chi)$ that can for example read simply $V_{\text{stable}}(\chi) = m^2 \chi^2/2$. Then, using the adiabatic-entropic basis, one finds that the effective entropic mass on super-Hubble scales, $m_{s,\text{eff}}^2$, reads in H units [77]:

$$\frac{m_{s,\text{eff}}^2}{H^2} = \frac{V_{;ss}}{H^2} + 3\eta_\perp^2 + \epsilon R_{\text{fs}} M_{\text{Pl}}^2 = \frac{m_h^2}{H^2} - 4\epsilon \frac{M_{\text{Pl}}^2}{M^2} , \quad (4.78)$$

where one supposes that $V_{;ss}$ is only slowly varying and can be approximated by the mass scale $m_h^2 > 0$, and used $\eta_\perp = 0$ since $\chi = 0$ is a geodesic of the negatively curved field space. The geometrical destabilisation of inflation happens if the second term, with a negative sign, overcomes the first, positive one. This situation is met if at some time:

$$\epsilon > \epsilon_c = \frac{M^2}{4M_{\text{Pl}}^2} \frac{m_h^2}{H_c^2}, \quad (4.79)$$

a condition that initially is assumed not to hold whence the stable background dynamics described above. But if ϵH^2 is a growing function of time, *i.e.* if $\eta - 2\epsilon > 0$, a situation that is typically the case in slow-roll single-field inflation for example,⁹ then one finds a critical time before the end of inflation at which $H = H_c$ and $\epsilon = \epsilon_c$, even for reasonable values of the parameters, say $m_h \sim 10H_c$ and $M \sim 10^{-2}M_{\text{Pl}}$ for definiteness, and at which the background is destabilised: $\epsilon_c \sim 2.5 \times 10^{-3}$ for these particular values. Note that by pushing the mass scale M down to the Hubble scale, $M \sim H$, even a background trajectory stabilised by an orthogonal potential as steep as $m_h \sim M_{\text{Pl}}$ would become unstable before the end of inflation around $\epsilon_c \sim 0.25$. On the contrary, by saturating the bound to $M \sim M_{\text{Pl}}$ (thus making the field space almost flat), it becomes difficult to destabilise the background trajectory unless it is initially not very stable, *i.e.* $m_h \lesssim 2H$ only. Therefore, the geometrical destabilisation of inflation is expected to happen generically in moderately negatively curved field spaces, except if a very strongly stabilising potential is present in the χ -direction.

To summarise, as long as ϵ_c is found to be smaller than unity, there must be a time before the end of inflation from which the background trajectory becomes unstable. Indeed in that case one finds that $m_{s,\text{eff}}^2$ is negative and therefore that entropic perturbations grow exponentially fast even on super-Hubble scales, hence quickly leaving the regime of validity of perturbation theory even for modes that describe very long wavelengths. This can be understood in the language of dynamical systems as a sign that the background trajectory at $\chi = 0$ has become repulsive and that perturbation theory must be defined along another, more stable background trajectory at $\chi \neq 0$. This follow-up after geometrical destabilisation has been investigated in [77, 216–218]: inflation then keeps proceeding along the new orbit but away from the potential valley at $\chi = 0$, and with a non-vanishing geodesic deviation $\eta_\perp$, therefore dubbed *sidetracked* inflation.

Transient tachyonic instability

In the previous paragraph, one understood that the geometry of the field space may displace the background trajectory from the naive one at the minimum of the potential valley, to a sidetracked path where three competing effects are at play and must be considered together: potential forces, curvature of the field space, inertia from the bending. In the following, one assumes that inflation proceeds in such a way in a two-dimensional

⁹Indeed, one knows that in that case $n_s - 1 = -2\epsilon_* - \eta_* = -0.035$ while $r = 16\epsilon_* < 0.056$, hence $\epsilon_* < 0.0035$ and therefore $\eta_* > 0.0315$, so one has the approximate relation $\eta > 9\epsilon$ at the time of horizon exit for the CMB scales.

field space, and that the background trajectory is now stable, *i.e.* that $m_{s,\text{eff}}^2 > 0$. But still, along this *strongly non-geodesic* path with $\eta_\perp \gg 1$, an interesting transient instability can develop for each Fourier mode with wavenumber k . Concrete setups of this kind have been exhibited and studied *e.g.* in [1, 77–79, 219, 220], and provide an interesting framework to evade the η -problem and verify the de Sitter swampland conjecture as explained in Sec. 4.1.1. Now, have a look at the sub-Hubble dynamics, on scales where the relevant mass scale for entropic fluctuations is not $m_{s,\text{eff}}^2$ but $m_s^2 = m_{s,\text{eff}}^2 - 4H^2\eta_\perp^2$:

$$\frac{m_s^2}{H^2} = \frac{V_{;ss}}{H^2} - \eta_\perp^2 + \epsilon R_{\text{fs}} M_{\text{Pl}}^2 = \frac{m_h^2}{H^2} - \eta_\perp^2 - 4\epsilon \frac{M_{\text{Pl}}^2}{M^2}, \quad (4.80)$$

with the same notations as in the previous paragraph. As can be seen, even though large-scale entropic fluctuations are stable, a large value of the the bending can lead to a negative entropic mass squared on small scales. As an example, suppose the background trajectory is quite stable, $m_{s,\text{eff}}^2/H^2 \sim 100$ due to the interplay between the negatively curved field space,¹⁰ the potential and the bending which contributes with $\eta_\perp \sim 10$. Then $m_s^2/H^2 \sim -300$ is large and negative, thus resulting in an exponential growth of entropic modes on sub-Hubble scales. The coupling between adiabatic and entropic modes being parameterised by the bending $\eta_\perp$, the growth of $\mathcal{S}$ is very efficiently shared with $\mathcal{R}$, which therefore also grows simultaneously on sub-Hubble scales.

But this instability is not as catastrophic as the one of geometrical destabilisation, since it is well bounded in time in both directions for a given wavenumber k , or seen differently bounded in the IR and the UV for a given time t . Indeed, as the scale k^{-1} is approaching the comoving Hubble radius $\mathcal{H}$, the interactions between entropic and adiabatic modes are such that the effective mass scale of entropic fluctuations rather becomes $m_{s,\text{eff}}^2$ which receives *positive* contributions from the bending and is well positive: the instability gradually stops and eventually entropic modes decay on super-Hubble scales while $\mathcal{R}$ quickly approaches an asymptotic value. In the other direction, deep on sub-Hubble scales, there is a time before which the quantum oscillations k^2/a^2 overcome the negative value of the small-scale entropic mass m_s^2 , thus making the effective frequency $\omega^2(k) = k^2/a^2 + m_s^2$ positive and stabilising the dynamics of entropic modes. In the comoving wavenumber domain, k/a , and for a given time t , the instability is bounded by an IR cutoff around H^{-1} (actually $|c_s|/H$ where c_s is an effective speed of sound for the curvature perturbation), while the UV one is given by $\sqrt{|m_s^2|}$. For more precise statements, and a comparison between analytical and numerical results, the interested reader is referred to Sec. 5.2 where the original article [1] on this topic is presented, and the interesting observational consequences are explained together with the conclusions that one can make for model-building in this kind of scenario.

¹⁰In this paragraph, the discussion is restricted to negatively curved field spaces to bridge together the two kinds of instabilities of this Section, since geometrical destabilisation can only happen with such a negative field-space curvature, but nothing forbids to have the transient tachyonic instability in a flat (or even positively curved) field space, the only requirement being then that $\eta_\perp^2 > V_{;ss}/H^2$ (respectively that $\eta_\perp^2 > V_{;ss}/H^2 + 4\epsilon M_{\text{Pl}}^2/M^2$ in the case where $R_{\text{fs}} = 4/M^2$).

Chapter 5

Primordial non-Gaussianities as a probe of extra particle content

In the previous chapter, the background and linear dynamics of inflation were extended to the multifield case, and key phenomenological effects such as the feeding of the co-moving curvature perturbation $\mathcal{R}$ by the entropic one $\mathcal{S}$ on super-horizon scales, and its consequences, have been investigated. This chapter aims at pursuing the detailed analysis of multifield inflation in the context of non-linear dynamics, and more precisely of the computation of non-Gaussianities in multifield inflation, which can indeed feature a very rich phenomenology, potentially enabling to discriminate amongst inflationary models.

First, the rather long Sec. 5.1 explains the basics of primordial non-Gaussianities, starting from their definition in terms of correlation functions and how to compute them with either the in-in formalism or the δN -formalism. The standard lore that single-field inflation with canonical kinetic terms produces a negligible amount of such non-Gaussianities is extensively explained, but particular cases possibly evading this standard scenarios are also explored: excited initial states, higher-derivative corrections and predictions from the Effective Field Theory of Inflation. The analysis is then extended to the multifield case for which the phenomenology is richer but potentially more model-dependent: however one discusses generic features such as equilateral non-Gaussianities coming from sub-horizon interactions, the local shape arising after a long period of super-hubble interactions, and the particularly promising squeezed limit of the bispectrum that enables one to probe the spectrum of extra particles content beyond *the* inflaton of the single-field picture.

Then, Sec. 5.2 goes into the details of the research done during this thesis and presents Ref. [1] where a large class of two-field models featuring a negatively curved field space and a strongly bent background trajectory, is shown to give rise to large and flattened non-Gaussianities at any order in the correlation functions. An analytical description using the important single-field effective theory obtained from integrating the heavy entropic perturbation is derived and explained, and the overall treatment is supported by a first-principle, exact numerical resolution of the two-field system including linear

fluctuations but also the bispectrum.

These interesting findings motivate a thorough re-analysis of non-Gaussianities in multifield inflation with curved field space and Sec. 5.3 displays a computation of the cubic order action describing interactions in the two-field case, see Sec. 5.3.1 which presents Ref. [2], which is extended to any number N_{field} of scalars, see Sec. 5.3.2 which presents Ref. [3], directly in terms of the comoving curvature perturbation and the entropic perturbation(s). The geometrical effects coming from the curved field space are explained, both at the level of the full multifield cubic action, and in the corresponding single-field effective theory that can be obtained if (all) the entropic perturbation(s) is (are) heavy and can be integrated out, therefore strengthening our general understanding of primordial non-Gaussianities in the multifield case. The differences between the two-field case and the higher dimensional one are stressed.

5.1 Formalism and generalities

The expression “primordial non-Gaussianities” refers to effects that make the Probability Density Function (PDF) of a given fluctuating primordial quantity, deviating from Gaussian statistics. It is often meant to describe deviations from Gaussianity in the scalar sector, and more particularly of the statistics of the comoving curvature perturbation $\mathcal{R}$ (often confused with ζ , and this confusion shall be nurtured in the articles presented in this Chapter), but of course it can be applied to other scalar fields such as the entropic perturbation $\mathcal{S}$ in two-field inflation, the tensor modes $\gamma_{\pm}$ of primordial gravitational waves and all kinds of cross-correlation beyond the two-point function and connected higher n -point functions. In this section, one focuses on the computation of the observable n -point functions of the comoving curvature perturbation $\mathcal{R}$ in single-field and multifield inflation, and emphasis is given on the links between physical situations and resulting non-Gaussianities.

5.1.1 Correlation functions as a parameterisation of Non-Gaussianities

Generalities

Correlation functions represent the full Probability Density Function (PDF) as they constitute the basis coordinates of the characteristic function which is the Fourier transform of the PDF and therefore contains the same statistical information. These probabilistic features are shortly reviewed here, and in particular it is explained how the connected n -point functions beyond the two-point function can be used as a diagnosis of the Gaussianity of the underlying statistical distribution.

A bit of probability theory on the real line. Consider a random variable X , assumed to take continuous values in $\mathbb{R}$ for simplicity in this paragraph. Its PDF may be written $f_X(x)$ and by definition contains the whole statistical information about X . Now, consider its characteristic function, which is denoted $\varphi_X(t)$ and corresponds to the

complex conjugate of the Fourier transform of f_X :

$$\varphi_X(t) = \int dx e^{itx} f_X(x), \quad (5.1)$$

and is therefore equally suitable to describe the statistics of X . Interestingly, φ_X is actually the generating function for the moments of X , *i.e.* one can deduce all moments of X just by differentiating φ_X :

$$\langle X^n \rangle = \int dx x^n f_X(x) = \frac{1}{i^n} \varphi_X^{(n)}(0), \quad (5.2)$$

where $\varphi_X^{(n)}(0)$ is the n -th derivative of $\varphi_X(t)$ evaluated at the origin. This proves that $\langle X^n \rangle$, the moments of X , are equally suitable to describe the statistics of X , since one has indeed:

$$f_X(x) = \frac{1}{2\pi} \int dt e^{-itx} \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \langle X^n \rangle. \quad (5.3)$$

Suppose that $X_g \sim \mathcal{N}(\mu, \sigma^2)$, *i.e.* that X_g follows a Gaussian distribution centered on μ and with standard deviation σ . Then, one knows that:

$$f_{X_g}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \implies \varphi_{X_g}(t) = e^{i\mu t - \frac{\sigma^2 t^2}{2}}, \quad (5.4)$$

from which the moments can be calculated and of course only depend on μ and σ^2 :

$$\langle X_g \rangle = \mu, \langle X_g^2 \rangle = \mu^2 + \sigma^2, \langle X_g^3 \rangle = \mu^3 + 3\mu\sigma^2, \langle X_g^4 \rangle = \mu^4 + 6\mu^2\sigma^2 + 3\sigma^4, \dots \quad (5.5)$$

This redundancy of description between the first and second moment and the higher-order ones for a Gaussian distribution can be avoided if one uses the cumulants of X rather than their moments. Cumulants are simply defined as the connected pieces of the moments, and carry exactly the same statistical information, they can be found from the logarithm of the characteristic function $K_X(t) = \ln[\varphi_X(t)]$, since then:

$$\kappa_n^X = \frac{1}{i^n} K_X^{(n)}. \quad (5.6)$$

In particular, one finds for the Gaussian distribution:

$$K_{X_g}(t) = i\mu t - \frac{\sigma^2 t^2}{2} \implies \kappa_1^{X_g} = \langle X_g \rangle = \mu, \kappa_2^{X_g} = \langle X_g^2 \rangle - \langle X_g \rangle^2 = \sigma^2, \kappa_{n \geq 3}^{X_g} = 0, \quad (5.7)$$

where the exact cancellation of the cumulants of order three or more is only true for Gaussian distributions. To put it in a nutshell, the cumulants of X , that coincide with its connected correlation functions $\langle X^n \rangle_c$, uniquely determine the statistics of X , and the cumulants of order equal or larger than three measure deviations from Gaussian statistics: these are the non-Gaussianities of interest in this Chapter.

Cosmological perturbations. In cosmology, statistical fluctuations are defined such that they are vanishing on average, *i.e.* they have no mean. Moreover, one understands from observations and even requires for the consistency of perturbation theory, that their statistics must be close to Gaussian. If they are perfectly Gaussian, then their statistics is uniquely determined by their two-point functions only: these are the power spectra of linear fluctuations. But if they have a small non-Gaussian component, this should be visible in their higher-order cumulants, *i.e.* the connected pieces of their correlation functions of order three and more. Importantly in inflation, non-Gaussianities are a signal of interactions in the early Universe: measuring them would provide a substantial amount of information concerning early universe physics. In particular, one has understood in the previous Chapters 3–4 that different models often lead to similar predictions for the observable power spectrum. The three-point function, connected four-point function, and higher-order connected correlations therefore constitute an incredible opportunity to disentangle different models by having different observational predictions, hopefully compared to data some day and therefore discriminating amongst the possible cosmological histories. In the following, one explains how to compute these correlation functions beyond the power spectrum, during inflation.

Quantum calculation: the interaction picture

Suppose your system is described by quantum operators that can be $\left(\hat{Q}_{\text{flat}}^I\right)_I$ the fields' perturbations in the flat gauge, or $\left(\hat{\mathcal{R}}, \hat{\mathcal{F}}^\alpha\right)_\alpha$ with $\alpha \in \{1, \dots, N_{\text{field}} - 1\}$ labelling the entropy perturbations beyond the adiabatic comoving curvature perturbation. To encapsulate these possibilities, in the following they will simply be denoted $\hat{\psi}_i$ with $i \in \{1, \dots, N_{\text{field}}\}$, with their canonically conjugate momenta p_{ψ_i} . In cosmology, one is interested in computing correlation functions of these fields, *i.e.* vacuum expectation values of quantum operators $\hat{\mathcal{O}}\left(\hat{\psi}_i(t), \hat{p}_{\psi_i}(t)\right)$ constructed out of them, at a given time t of interest. The situation is quite different from particle physics, where one computes *scattering amplitudes* between asymptotic initial and final states corresponding to the vacuums of the free theory, respectively $|\text{in}\rangle$ and $|\text{out}\rangle$. But such S-matrix is strictly speaking not defined in time-dependent spacetimes as in cosmology, for which one cannot impose asymptotic conditions in the far future where fields keep interacting at least gravitationally. Therefore, rather than in-out amplitudes, cosmologists compute time-dependent in-in amplitudes, where the asymptotic initial state is often taken to be the Bunch-Davies vacuum: $|\text{in}\rangle \rightarrow |0\rangle$.¹ To conclude, the object of interest is:

$$\left\langle \text{in} \left| \hat{\mathcal{O}}\left(\hat{\psi}_i(t), \hat{p}_{\psi_i}(t)\right) \right| \text{in} \right\rangle, \quad (5.8)$$

which shall be denoted in a simpler way in the following: $\langle \hat{\mathcal{O}}(t) \rangle$.

¹See the discussion in Sec. 5.1.2 about excited initial states where deviations from the Bunch-Davies vacuum at early times, is allowed. Actually in that case, the excited initial state can be expressed in terms of the Bunch-Davies vacuum by redefining simultaneously the mode function $\mathcal{R}$ and the fundamental oscillator $\hat{a}$, schematically as $\mathcal{R}_{\text{BD}}\hat{a}_{\text{excited}} \rightarrow \mathcal{R}_{\text{excited}}\hat{a}_{\text{BD}}$ with a Bogolyubov transformation.

In the Heisenberg picture, the time evolution of the quantum operators is set by the full quantum Hamiltonian $\hat{H}(\hat{\psi}_i(t), \hat{p}_{\psi_i}(t); t)$ of the perturbations ψ_i and p_{ψ_i} , that, if it is not simply quadratic, yields complicated non-linear equations of motion including all interactions of the theory:

$$\frac{d}{dt}\hat{\psi}_i = i [\hat{H}, \hat{\psi}_i] , \quad \text{and} \quad \frac{d}{dt}\hat{p}_{\psi_i} = i [\hat{H}, \hat{p}_{\psi_i}] , \quad (5.9)$$

where the brackets $[,]$ denote the usual quantum commutator. In general these equations are too hard to be solved, at least in order to keep track of an analytical result, and the cunning cosmologist must resort to the use of *interaction picture fields*, $\hat{\psi}_i^I$ and $\hat{p}_{\psi_i}^I$, that are evolved with a simpler Hamiltonian called the free Hamiltonian $\hat{H}_{\text{free}}$. For this purpose, the full Hamiltonian is split into two pieces, the free one that will give equations of motion for the interaction picture fields that can be solved analytically, and a complicated one encoding the remaining interactions, $\hat{H}_{\text{int}}$, that shall be taken into account only perturbatively in the computation of the correlation functions:

$$\boxed{\hat{H} = \hat{H}_{\text{free}} + \hat{H}_{\text{int}} .} \quad (5.10)$$

It is a common choice to use the full quadratic Hamiltonian as the free one, $\hat{H}^{(2)} = \hat{H}_{\text{free}}$, because it corresponds to linear equations of motion that one can hope to solve analytically, and encodes non-perturbatively all these linear effects, while all non-linear effects are taken into account perturbatively in $\hat{H}_{\text{int}} = \hat{H}^{(3)} + \hat{H}^{(4)} + \dots$. This is typically the situation that one often encounters in single-field inflation and is well justified because cubic and higher-order interactions are negligible compared to the quadratic terms yielding the linear evolution. However it should be emphasized that the interaction picture is nothing but a choice, and different schemes can be used depending on the physical situation at hand. For example in multifield inflation, even the linear equations of motion derived from the full quadratic action, can be hard to solve analytically, and if some of the quadratic terms are smaller than others, they may be treated perturbatively as interactions in $\hat{H}_{\text{int}}$ rather than in the free Hamiltonian, a situation therefore described by $\hat{H}^{(2)} = \hat{H}_{\text{free}} + \delta\hat{H}^{(2)}$ and $\hat{H}_{\text{int}} = \delta\hat{H}^{(2)} + \hat{H}^{(3)} + \hat{H}^{(4)} + \dots$, an example of this kind being provided in Sec. 5.1.3. This being said, the interaction picture fields are by definition evolved with the free Hamiltonian *evaluated with the interaction picture fields* $\hat{H}_{\text{free}}^I = \hat{H}_{\text{free}}(\hat{\psi}_i^I, \hat{p}_{\psi_i}^I)$:

$$\boxed{\frac{d}{dt}\hat{\psi}_i^I = i [\hat{H}_{\text{free}}^I, \hat{\psi}_i^I] , \quad \text{and} \quad \frac{d}{dt}\hat{p}_{\psi_i}^I = i [\hat{H}_{\text{free}}^I, \hat{p}_{\psi_i}^I] ,} \quad (5.11)$$

and are related to the full fields by a unitary operator $\hat{U}$:

$$\hat{\psi}_i^I = \hat{U}^\dagger \hat{\psi}_i \hat{U} , \quad \hat{p}_{\psi_i}^I = \hat{U}^\dagger \hat{p}_{\psi_i} \hat{U} \implies \hat{\mathcal{O}}^I = \hat{\mathcal{O}}(\hat{\psi}_i^I, \hat{p}_{\psi_i}^I) = \hat{U}^\dagger \hat{\mathcal{O}} \hat{U} , \quad (5.12)$$

where for the last equality one has supposed that the operator $\hat{\mathcal{O}}$ can be decomposed as a series in $\hat{\psi}_i, \hat{p}_{\psi_i}$. Knowing the law of evolution of the full quantum operators and

the interaction picture ones, constrains the unitary operator $\hat{U}$ to verify the following operator differential equation:

$$\left[\cdot, \hat{U}^\dagger \frac{d}{dt} \hat{U} \right] = i \left[\cdot, \hat{H}_{\text{int}}^I \right], \quad (5.13)$$

where the dot $\cdot$ means that the operator can be applied to either $\hat{\psi}_i^I$ or $\hat{p}_{\psi_i}^I$, $\forall i$, and where $\hat{H}_{\text{int}}^I$ is evaluated on the interaction picture fields: $\hat{H}_{\text{int}}^I = \hat{H}_{\text{int}}(\hat{\psi}_i^I, \hat{p}_{\psi_i}^I) = \hat{U}^\dagger \hat{H}_{\text{int}}(\hat{\psi}_i, \hat{p}_{\psi_i}) \hat{U}$. Note that to find this differential equation one had to use the fact that $\hat{U}$ is unitary, *i.e.* that $\hat{U}^\dagger = \hat{U}^{-1}$ and therefore that $d\hat{U}^\dagger/dt = -\hat{U}^\dagger (d\hat{U}/dt) \hat{U}^\dagger$. Since $(\hat{\psi}_i^I, \hat{p}_{\psi_i}^I)$ constitute a complete set of quantum states in the Hilbert space, one can say that:

$$\frac{d}{dt} \hat{U} = i \hat{U} \hat{H}_{\text{int}}^I, \quad (5.14)$$

with the asymptotic condition $\hat{U}(t) \xrightarrow[t \rightarrow -\infty]{} \hat{1}$ obtained by asking that interactions are switched off in the far past, and therefore that the full and interacting fields initially coincide. This equation can be formally solved and yields

$$\hat{U}(t) = \bar{T} \left(e^{i \int_{-\infty}^t dt' \hat{H}_{\text{int}}^I(t')} \right), \quad (5.15)$$

with $\bar{T}$ the anti-time ordering operator, and where one used $-\infty^+$ to denote that the time integral should be deformed in the complex plane above the real axis, $t \rightarrow t + i\epsilon$ with $\epsilon > 0$, in order to effectively turn off interactions in the distant past, a procedure that enables one to project the vacuum of the interacting theory $|\text{in}\rangle$ onto the vacuum of the free theory defined by $\hat{H}_{\text{free}}^I$, $|0\rangle$, which can be chosen to be the Bunch-Davies vacuum. Therefore, $\langle \hat{\mathcal{O}}(t) \rangle = \langle \text{in} | \hat{\mathcal{O}}(t) | \text{in} \rangle = \langle \text{in} | \hat{U} \hat{\mathcal{O}}^I(t) \hat{U}^\dagger | \text{in} \rangle$, giving the master formula of the in-in formalism:

$$\boxed{\langle \hat{\mathcal{O}}(t) \rangle = \left\langle 0 \left| \bar{T} \left(e^{i \int_{-\infty}^t dt' \hat{H}_{\text{int}}^I(t')} \right) \hat{\mathcal{O}}^I(t) T \left(e^{-i \int_{-\infty}^t dt'' \hat{H}_{\text{int}}^I(t'')} \right) \right| 0 \right\rangle}, \quad (5.16)$$

where the hermitian conjugate of the operator U involves the time-ordering operator $T = \bar{T}^\dagger$ and with $-\infty^-$ denoting a deformation of the contour of integration below the real axis, $t \rightarrow t - i\epsilon$ with $\epsilon > 0$. Note that the deformation of the time integrals in the complex plane, as encoded in the notations $-\infty^\pm$, enabled one to replace $|\text{in}\rangle \rightarrow |0\rangle$. This exact expression can hardly be solved, and must in practice be expanded in powers of $\hat{H}_{\text{int}}^I$ corresponding to a diagrammatic expansion of the computation *à la Feynman*.

In particular, the first terms are given by:

$$\begin{aligned} \langle \hat{\mathcal{O}}(t) \rangle &= \langle 0 | \hat{\mathcal{O}}^I(t) | 0 \rangle + i \int_{-\infty}^t dt' \langle 0 | \left(\hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) - \hat{\mathcal{O}}^I(t) \hat{H}_{\text{int}}^I(t') \right) | 0 \rangle \\ &\quad - \int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' \langle 0 | \left(\hat{H}_{\text{int}}^I(t'') \hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) + \hat{\mathcal{O}}^I(t) \hat{H}_{\text{int}}^I(t') \hat{H}_{\text{int}}^I(t'') \right) | 0 \rangle \\ &\quad + \int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' \langle 0 | \hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) \hat{H}_{\text{int}}^I(t'') | 0 \rangle + \dots \end{aligned} \quad (5.17)$$

This expression can be rewritten in several useful ways. The first one is called the *nested commutators form*, and requires to rewrite the integral of the third line, over a square in the time domain, as the sum of two triangle integrals in the time domain:

$$\begin{aligned} &\int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' \langle 0 | \hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) \hat{H}_{\text{int}}^I(t'') | 0 \rangle \\ &= \int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' \langle 0 | \left(\hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) \hat{H}_{\text{int}}^I(t'') + \hat{H}_{\text{int}}^I(t'') \hat{\mathcal{O}}^I(t) \hat{H}_{\text{int}}^I(t') \right) | 0 \rangle, \end{aligned}$$

which enables one to write:

$$\begin{aligned} \langle \hat{\mathcal{O}}(t) \rangle &= \langle 0 | \hat{\mathcal{O}}^I(t) | 0 \rangle + i \int_{-\infty}^t dt' \langle 0 | \left[\hat{H}_{\text{int}}^I(t'), \hat{\mathcal{O}}^I(t) \right] | 0 \rangle \\ &\quad - \int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' \langle 0 | \left[\hat{H}_{\text{int}}^I(t''), \left[\hat{H}_{\text{int}}^I(t'), \hat{\mathcal{O}}^I(t) \right] \right] | 0 \rangle + \dots \end{aligned} \quad (5.18)$$

where the higher-order terms contained in ... can actually be made explicit, giving the exact nested commutators formula:

$$\boxed{\langle \hat{\mathcal{O}}(t) \rangle = \sum_{n=0}^{\infty} i^n \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n \langle 0 | \left[\hat{H}_{\text{int}}^I(t_n), \left[\hat{H}_{\text{int}}^I(t_{n-1}), \dots, \left[\hat{H}_{\text{int}}^I(t_1), \hat{\mathcal{O}}^I(t) \right] \dots \right] \right] | 0 \rangle}. \quad (5.19)$$

Using hermiticity of the interaction hamiltonian, $\left(\hat{H}_{\text{int}}^I \right)^\dagger = \hat{H}_{\text{int}}^I$, and of the observable operator made of the fundamental operators $\hat{\psi}_i^I$ and $\hat{p}_{\psi_i}^I$, $\left(\hat{\mathcal{O}}^I \right)^\dagger = \hat{\mathcal{O}}^I$, one can simplify the nested commutators as, *e.g.*,

$$\begin{aligned} i \langle 0 | \left[\hat{H}_{\text{int}}^I(t'), \hat{\mathcal{O}}^I(t) \right] | 0 \rangle &= i \langle 0 | \left\{ \hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) - \left(\hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) \right)^\dagger \right\} | 0 \rangle \\ &= -2 \text{Im} \left(\langle 0 | \hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) | 0 \rangle \right) \end{aligned} \quad (5.20)$$

This enables one to write the in-in formula in terms of explicitly real quantities only,

which I therefore call the *real form*, and whose first terms read:

$$\begin{aligned} \langle \hat{\mathcal{O}}(t) \rangle = & \langle 0 | \hat{\mathcal{O}}^I(t) | 0 \rangle - 2 \int_{-\infty}^t dt' \operatorname{Im} \left(\langle 0 | \hat{H}_{\text{int}}^I(t') \hat{\mathcal{O}}^I(t) | 0 \rangle \right) \\ & - 2 \int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' \operatorname{Re} \left\{ \langle 0 | \left(\hat{H}_{\text{int}}^I(t'') \left[\hat{H}_{\text{int}}^I(t'), \hat{\mathcal{O}}^I(t) \right] \right) | 0 \rangle \right\} + \dots, \end{aligned} \quad (5.21)$$

where later on in the calculation the real part can be written as the product of two imaginary parts due to the remaining commutator that is anti-hermitian.

Note that this quantum in-in formalism can be used to compute n -point functions during inflation, at tree level but also with loops.

Classical calculation: the δN -formalism

Although the in-in formalism is completely generic and can be used in any situation, it is sometimes unnecessarily complicated. Indeed, it requires a careful manipulation of quantum operators that do not commute one with the others, of nested time integrals that need to be regulated in the UV (the $\pm i\epsilon$ -prescriptions), and the knowledge of analytical formulae for the interaction picture fields both on small and large scales. But a simplification occurs upon horizon crossing as indeed perturbations are expected to lose their quantum behaviour around that time (this can be seen, *e.g.* by looking at the ratio between the commutator and the anti-commutator of two quantum perturbations, that is rapidly decaying above the horizon). Then, they can simply be treated as complex-valued real numbers and the physics of these large-scale linear fluctuations become close to the background dynamics, as described by the δN -formalism [26, 40, 221–224] that is shortly reviewed here. This enables one to estimate the final non-Gaussianities if their initial conditions around the time of horizon crossing are otherwise known, or if they can be neglected.

Separate universe approach. The δN -formalism relies on the *separate universe approach* [225, 226] to treat large-scale fluctuations during inflation: as perturbations exit the decreasing comoving Hubble radius $\mathcal{H}^{-1}$, they must stop interacting by causality and therefore each of them evolves separately in a way similar to the background but affected by their initial conditions. Consider a wavenumber k , corresponding to a physical wavelength $\lambda(t) = 2\pi/k \times a(t)$ which is stretched from a microscopic size to a super-Hubble one by the quasi-exponential expansion of the Universe, and denote t_{ini} a time corresponding to a few e -folds after horizon exit for this mode k , typically for which $\lambda(t_{\text{ini}}) = 10H_{\text{ini}}^{-1}$ for example. What will eventually make our observable Universe therefore consists at that time t_{ini} in a collection of patches denoted by $p \in \{1, \dots, n_{\text{patches}}\}$,

with a typical size $\lambda(t_{\text{ini}})$ and that evolve independently until they re-enter the horizon in the radiation-domination or matter-domination era. Then, the statistics of the observable Universe can be recollected from the statistics of the individual patches. In each patch p , the evolution is dictated only by the background dynamics and the initial conditions at the time t_{ini} . See Fig. 5.1 for a schematic understanding of the situation.

δN and the curvature perturbation. Now, in each patch the spacetime geometry should be locally homogeneous and isotropic, since they each constitute their own Universe, and therefore the metric can be described by:

$$ds^2 = -dt^2 + a_p^2(t)d\vec{x}^2, \quad (5.22)$$

where a_p is a local scale factor. Zooming out to very large scales encapsulating many of these individual patches, this amounts to defining a local scale factor in a continuous description, $\tilde{a}(t, \vec{x}_p) = a_p(t) \rightarrow \tilde{a}(t, \vec{x})$, that one knows how to describe from cosmological perturbation theory: forgetting vector and tensor perturbations, and partially fixing the scalar gauge by requiring that $E = 0$ using the scalar part of the spatial gauge freedom, one has at non-linear order:

$$\tilde{a}(t, \vec{x}) = a(t)e^{\psi(t, \vec{x})}. \quad (5.23)$$

Therefore, the statistics of the patches on such large scales are only described by the curvature perturbation ψ , which matches our understanding that this is the relevant observational quantity. More precisely, it is possible to relate the local amount of total expansion, *i.e.* the local e -folding number between the initial time t_{ini} and an arbitrary time t , defined as

$$N(t, t_{\text{ini}}; \vec{x}) = \int_{t_{\text{ini}}}^t \frac{d\tilde{a}(t, \vec{x})}{\tilde{a}(t, \vec{x})}, \quad (5.24)$$

that coincides with $N = \int \tilde{H} dt$ where $\tilde{H} = \dot{\tilde{a}}/\tilde{a}$ is a local Hubble parameter, to the gauge-invariant curvature perturbation ζ . First, note that the integral can be formally computed:

$$N(t, t_{\text{ini}}; \vec{x}) = \psi(t, \vec{x}) - \psi(t_{\text{ini}}, \vec{x}) + \ln \left[\frac{a(t)}{a(t_{\text{ini}})} \right], \quad (5.25)$$

Then, remember that time diffeomorphisms have not been fixed yet, and therefore that the statements “at time t ” or “at time t_{ini} ” are ambiguous and depend on the choice of time slicing. Consider two different such ways to define the time slicings at the final stages, from an initial time slicing t_{ini} defined by choosing flat hypersurfaces. The first way, denoted A , consists in defining the final time slicing with uniform energy density hypersurfaces, while the second way, denoted B , consists in choosing spatially flat hypersurfaces again. By definition, this corresponds that:

$$\begin{aligned} \psi_A(t, \vec{x}) &= \psi_{\text{uni}}(t, \vec{x}) = -\zeta(t, \vec{x}), & \psi_A(t_{\text{ini}}, \vec{x}) &= \psi_{\text{flat}}(t_{\text{ini}}, \vec{x}) = 0, \\ \psi_B(t, \vec{x}) &= \psi_{\text{flat}}(t, \vec{x}) = 0, & \psi_B(t_{\text{ini}}, \vec{x}) &= \psi_{\text{flat}}(t_{\text{ini}}, \vec{x}) = 0, \end{aligned} \quad (5.26)$$

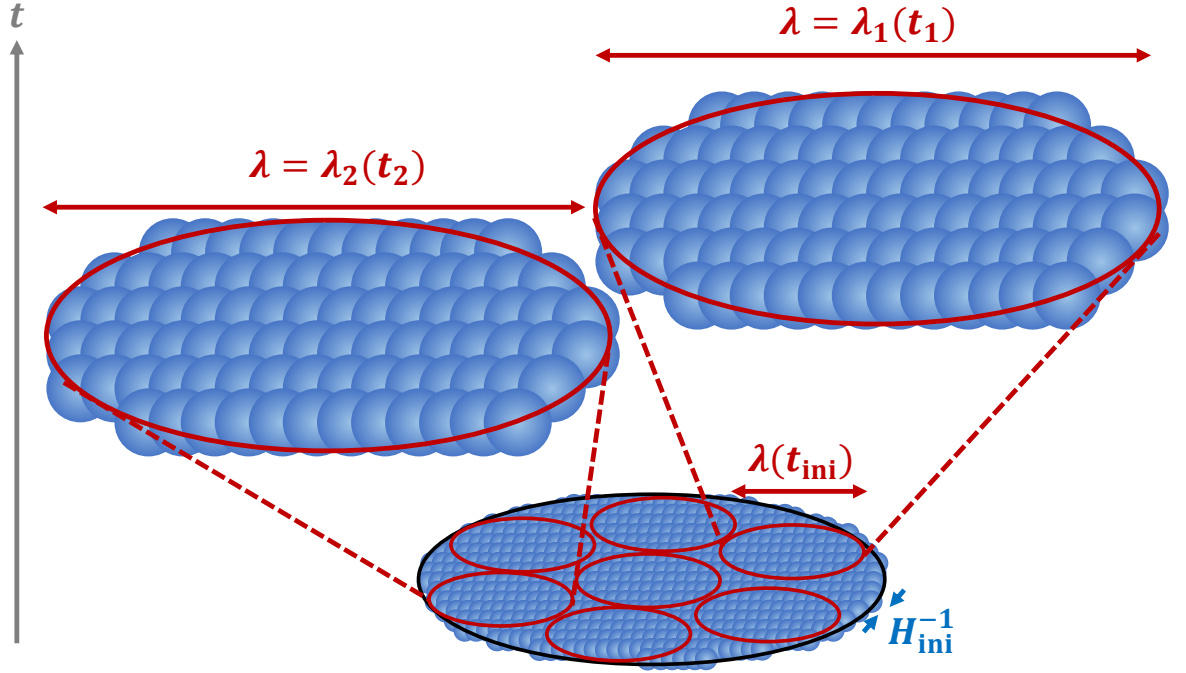


Figure 5.1: Evolution of our observable universe in its early inflationary stage. At the time t_{ini} , what will make our observable universe (circled in black) is made of several patches of typical size $\lambda(t_{\text{ini}})$ (circled in red), where $\lambda(t)$ is the physical wavelength of a fluctuation of cosmological interest. Each of these patches contains a few Hubble patches of size H_{ini}^{-1} (the blue balls). Since in this picture the initial time slicing coincides with the spatially flat hypersurfaces, all patches have exactly the same size at the initial time t_{ini} . However quantities describing the matter content (typically scalar fields during inflation) may assume different values in different patches and therefore the cosmological evolution of the independent patches are different. For example, one finds that the time t_p at which the patch p becomes of a given fixed size λ , depends on the patch: an equivalent statement is that at the same final time t , there will be a large-scale modulation of the scale factor, *i.e.* a curvature perturbation. This reasoning is the bedrock of the separate universe approach and the δN -formalism.

therefore meaning that the difference in e -folding number between the final uniform energy density hypersurfaces and the *unperturbed history* (indeed note that N_B does not depend on the spatial coordinate $\vec{x}$), $\delta N(t, \vec{x}) = N_A(t, t_{\text{ini}}; \vec{x}) - N_B(t, t_{\text{ini}})$ is:

$$\boxed{(\delta N\text{-formalism}): \delta N(t, \vec{x}) = -\zeta(t, \vec{x}) .} \quad (5.27)$$

δN and the initial conditions for the fields' perturbations. Using the discrete description, one knows that the evolution of the patch p can solely be determined by its initial conditions. In the context of inflation, these are the values of the scalar fields $\phi^I(t_{\text{ini}}, \vec{x})$ on the initial slice t_{ini} that coincides with spatially flat hypersurfaces, therefore for which $\phi^I(t_{\text{ini}}, \vec{x}) = \bar{\phi}^I(t_{\text{ini}}) + Q_{\text{flat}}^I(t_{\text{ini}}, \vec{x}) + \Gamma^I_{JK} Q_{\text{flat}}^J(t_{\text{ini}}, \vec{x}) Q_{\text{flat}}^K(t_{\text{ini}}, \vec{x}) + \dots$, for the perturbed history, where Q_{flat}^I are the gauge-invariant perturbations of a general multifield inflation model, coinciding with the fields' perturbations in the spatially flat gauge used here. On the other hand, the unperturbed history N_B can only depend on the homogeneous values of the scalar fields at the initial time. Therefore one can write the time evolution of both the perturbed history N_A and the unperturbed one N_B , as a unique background function N of different initial conditions:

$$N_A(t, t_{\text{ini}}; \vec{x}) = N[\phi^I(t_{\text{ini}}, \vec{x}); t] , \quad N_B(t, t_{\text{ini}}) = N[\bar{\phi}^I(t_{\text{ini}}); t] , \quad (5.28)$$

thus enabling one to express the curvature perturbation on the final uniform energy density hypersurfaces as:

$$\boxed{\begin{aligned} & \text{(Curvature perturbation from the } \delta N\text{-formalism):} \\ & -\zeta(t, \vec{x}) = \sum_{n=1}^{\infty} N_{I_1 \dots I_n}(t) Q_{\text{flat}}^{I_1}(t_{\text{ini}}, \vec{x}) \dots Q_{\text{flat}}^{I_n}(t_{\text{ini}}, \vec{x}) , \\ & \text{where } N_{I_1 \dots I_n}(t) = \left. \frac{D^n N}{D\phi^{I_1} \dots D\phi^{I_n}} \right|_{\bar{\phi}^I(t_{\text{ini}}); t} , \end{aligned}} \quad (5.29)$$

where D denotes the field-space covariant derivative.

Statistics of the comoving curvature perturbation $\mathcal{R}$. Remembering that on large scales one has $\zeta \simeq -\mathcal{R}$, one can therefore deduce the large-scale statistics of $\mathcal{R}(t, \vec{x})$ from the statistics of the fields' perturbations in the flat gauge just after horizon exit $Q_{\text{flat}}^I(t_{\text{ini}}, \vec{x})$ and the dependence of the background dynamics on the initial values of the homogeneous scalar fields, as encoded in the multi-derivatives function $N_{I_1 \dots I_n}$. Going back to Fourier space, and up to quartic order in perturbation theory, one finds

for example:

$$P_{\mathcal{R}}(k) = N_I N_J P_{Q_{\text{ini}}}^{IJ}(k), \quad (5.30)$$

$$B_{\mathcal{R}}(k_1, k_2, k_3) = N_I N_J N_K B_{Q_{\text{ini}}}^{JK}(k_1, k_2, k_3) \\ + N_I N_{JK} N_L [P_{Q_{\text{ini}}}^{IK}(k_1) P_{Q_{\text{ini}}}^{JL}(k_2) + 2 \text{ perm.}] , \quad (5.31)$$

$$T_{\mathcal{R}}(\vec{k}_i) = N_I N_J N_K N_L T_{Q_{\text{ini}}}^{JKL}(\vec{k}_i) \\ + N_{IJ} N_K N_L N_M [P_{Q_{\text{ini}}}^{IK}(k_1) B_{Q_{\text{ini}}}^{JLM}(k_{12}, k_3, k_4) + 11 \text{ perm.}] \\ + N_{IJ} N_{KL} N_M N_N [P_{Q_{\text{ini}}}^{JL}(k_{13}) P_{Q_{\text{ini}}}^{IM}(k_3) P_{Q_{\text{ini}}}^{KN}(k_4) + 11 \text{ perm.}] \\ + N_{IJK} N_L N_M N_N [P_{Q_{\text{ini}}}^{IL}(k_2) P_{Q_{\text{ini}}}^{JM}(k_3) P_{Q_{\text{ini}}}^{KN}(k_4) + 3 \text{ perm.}] . \quad (5.32)$$

The physical interpretation of these equations is pretty intuitive.

- The final power spectrum $P_{\mathcal{R}}$ is given by the linear background evolution as dictated by the single-derivative function N_I , of the Gaussian statistics of the fluctuating fields Q_{flat}^I at the initial time t_{ini} .
- The final bispectrum $B_{\mathcal{R}}$ receives two contributions. The first one is simply given by the linear super-Hubble evolution of the initial bispectrum of the Q_{flat}^I and is reminiscent from the quantum interactions of the scalar fields. The second one is due to the non-linear super-Hubble evolution as dictated by the double-derivative function N_{IJ} , of the Gaussian properties of the scalar fields at the initial time, and can therefore be interpreted as classical, local interactions.
- The final trispectrum $T_{\mathcal{R}}$ receives four contributions, but the two last ones are similar: they result from two kinds of non-linear evolution, given by the triple-derivative function N_{IJK} and the square of the double-derivative one, of the Gaussian statistics of the Q^I on super-Hubble scales, and therefore correspond also to local interactions. The first contribution comes from the linear evolution of the initial trispectrum of the Q^I , while the second one mixes the non-linear evolution on super-Hubble scales and the initial non-Gaussian statistics of the Q^I described by their bispectrum; hence they both carry information about the quantum interactions on sub-Hubble scales.

Of course, this scheme can be extended to any order in perturbation theory, and in principle the super-Hubble, classical contribution to any n -point function can be calculated solely from the derivatives of the function N and the Gaussian statistics of the Q^I just after horizon exit. I plan in the future to implement a numerical approach to solve these equations at a high order in perturbation theory and for multifield inflationary setups.

5.1.2 Primordial non-Gaussianities in single-field inflation

First, primordial non-Gaussianities in the context of single-field, slow-roll inflation with Bunch-Davies initial states, are computed following Maldacena's seminal work [227],

and using the exact in-in formalism. Then, the computation is extended to more exotic situations: excited initial states and higher-derivative corrections in $P(X, \phi)$ inflation. Finally, insights from the EFT of inflation are discussed.

Generalities

Non-Gaussianities in single-field inflation can be computed from the in-in master formula (5.16) where the free evolution of the interacting fields is described with the full quadratic Lagrangian

$$\mathcal{L}^{(2)}(\mathcal{R}, \dot{\mathcal{R}}) = a^3 \epsilon M_{\text{Pl}}^2 \left[\dot{\mathcal{R}}^2 - \frac{(\partial \mathcal{R})^2}{a^2} \right], \quad (5.33)$$

from which the canonical conjugate momentum of $\mathcal{R}$ is identified,

$$p_{\mathcal{R}} = \frac{\partial \mathcal{L}^{(2)}}{\partial \dot{\mathcal{R}}} = 2a^3 \epsilon M_{\text{Pl}}^2 \dot{\mathcal{R}}. \quad (5.34)$$

Therefore the free Hamiltonian density, chosen here to coincide with the full quadratic one, reads:

$$\begin{aligned} \mathcal{H}_{\text{free}}(\mathcal{R}, p_{\mathcal{R}}) &= \mathcal{H}^{(2)}(\mathcal{R}, p_{\mathcal{R}}) = \dot{\mathcal{R}}[p_{\mathcal{R}}] p_{\mathcal{R}} - \mathcal{L}^{(2)}(\mathcal{R}, \dot{\mathcal{R}}[p_{\mathcal{R}}]) \\ &= a^3 \epsilon M_{\text{Pl}}^2 \left[\left(\frac{p_{\mathcal{R}}}{2a^3 \epsilon M_{\text{Pl}}^2} \right)^2 + \frac{(\partial \mathcal{R})^2}{a^2} \right], \end{aligned} \quad (5.35)$$

where in the first line $\dot{\mathcal{R}}[p_{\mathcal{R}}]$ should be understood as expressed explicitly in terms of the momentum $p_{\mathcal{R}}$ by inverting Eq. (5.34). With this choice of interaction scheme, the interaction picture field $\mathcal{R}^I$ follows the classical equations derived from the full quadratic Lagrangian only, *i.e.* the usual linear dynamics of single-field inflation:

$$\mathcal{E}_{\mathcal{R}^I} = -\frac{1}{a^3 \epsilon M_{\text{Pl}}^2} \frac{\delta S^{(2)}}{\delta \mathcal{R}} \Big|_{\mathcal{R}^I} = 0 \iff \ddot{\mathcal{R}}^I + (3 + \eta) H \dot{\mathcal{R}}^I - \frac{\partial^2 \mathcal{R}^I}{a^2} = 0, \quad (5.36)$$

which can also be rewritten in terms of a rescaled momentum χ defined by,

$$p_{\mathcal{R}} = 2a M_{\text{Pl}}^2 \partial^2 \chi, \quad (5.37)$$

and that can be formally inverted as $\chi = a^2 \epsilon \partial^{-2} \dot{\mathcal{R}}$, and in terms of which

$$\mathcal{E}_{\mathcal{R}^I} = \frac{\partial^2}{\epsilon a^2} (\dot{\chi}^I + H \chi^I - \epsilon \mathcal{R}^I) = 0. \quad (5.38)$$

Now the cubic, quadratic and higher-order Hamiltonians should be computed and evaluated at the values taken by the interacting field $\mathcal{R}^I$ and its canonical conjugate momentum $p_{\mathcal{R}}^I$, since the interaction scheme corresponds to:

$$\hat{H}_{\text{int}}^I = \hat{H}_I^{(3)} + \hat{H}_I^{(4)} + \dots, \quad (5.39)$$

in order to compute the n -point functions of single-field inflation that read at tree-level in the quantum computation:

$$\begin{aligned}
\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \rangle &= \langle 0 | \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I | 0 \rangle = (2\pi)^3 \delta^{(3)}(\vec{k}_1 + \vec{k}_2) P_{\mathcal{R}^I}(k_1), \quad (5.40) \\
\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \rangle &= \underbrace{\langle 0 | \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I \hat{\mathcal{R}}_{\vec{k}_3}^I | 0 \rangle}_{=0} + 2\text{Im} \left[\langle 0 | \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I \hat{\mathcal{R}}_{\vec{k}_3}^I \int_{-\infty}^t dt' \hat{H}_I^{(3)}(t') | 0 \rangle \right], \\
\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \hat{\mathcal{R}}_{\vec{k}_4} \rangle_c &= \underbrace{\langle 0 | \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I \hat{\mathcal{R}}_{\vec{k}_3}^I \hat{\mathcal{R}}_{\vec{k}_4}^I | 0 \rangle_c}_{=0} + 2\text{Im} \left[\langle 0 | \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I \hat{\mathcal{R}}_{\vec{k}_3}^I \hat{\mathcal{R}}_{\vec{k}_4}^I \int_{-\infty}^t dt' \hat{H}_I^{(4)}(t') | 0 \rangle \right] \\
&\quad + 2\text{Re} \left\{ \left\langle 0 \left| \int_{-\infty}^t dt' [\hat{H}_I^{(3)}(t'), \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I \hat{\mathcal{R}}_{\vec{k}_3}^I \hat{\mathcal{R}}_{\vec{k}_4}^I] \int_{-\infty}^{t'} dt'' \hat{H}_I^{(3)}(t'') \right| 0 \right\rangle \right\}, \\
&\quad \dots
\end{aligned}$$

The subscript $_c$ denotes that only the connected component of the corresponding correlation function has been retained, *e.g.*,

$$\begin{aligned}
\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \hat{\mathcal{R}}_{\vec{k}_4} \rangle_c &= \langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \hat{\mathcal{R}}_{\vec{k}_4} \rangle - (\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \rangle \langle \hat{\mathcal{R}}_{\vec{k}_3} \hat{\mathcal{R}}_{\vec{k}_4} \rangle + 2 \text{ perm.}) \quad (5.41) \\
&= \langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \hat{\mathcal{R}}_{\vec{k}_4} \rangle - (\langle \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I \rangle \langle \hat{\mathcal{R}}_{\vec{k}_3}^I \hat{\mathcal{R}}_{\vec{k}_4}^I \rangle + 2 \text{ perm.}),
\end{aligned}$$

where “+ 2 perm.” means that the two cyclic permutations different from the one that is explicitly shown, should be added (here the three permutations correspond to the three ways one can form two pairs with four objects: once one pair is formed, there is no choice left for the second one). By definition of the interacting picture where the free evolution is dictated by the quadratic Hamiltonian only, both the three-point function and the connected four-point function of the interacting fields, vanish. Of course, the total four-point function of the interacting fields $\mathcal{R}^I$ has a non-vanishing non-connected part due to its Gaussian statistics, but this contribution is subtracted in the trispectrum that is defined in terms of the *connected* four-point function of $\mathcal{R}$ only. See the diagrammatic expansion in Fig. 5.2 corresponding to the first n -point functions of single-field inflation at tree level, and note in particular the presence of two different channels contributing to the trispectrum: the contact diagram and the scalar-exchange one.

The route towards the computation of non-Gaussianities in single-field inflation is therefore the following, and can easily be adapted to other cases:

- Compute $\hat{H}_{\text{free}} = \hat{H}^{(2)}$ in order to find the equation of motion verified by the interaction picture field $\hat{\mathcal{R}}^I$. This was already done in Chapter 4, though with a Lagrangian formalism, as indeed one understood that $\hat{\mathcal{R}}^I$ with this interaction scheme is simply the linear comoving curvature perturbation that verifies the usual linear equations of single-field inflation;
- Compute $\hat{H}_{\text{int}} = \hat{H}^{(3)} + \hat{H}^{(4)} + \dots$ in order to feed the RHS of Eq. (5.40). In practice, for a given n -point function, the leading-order term in powers of $\hat{H}_{\text{int}}$, *i.e.* the tree-level result, only necessitates the knowledge of $\hat{H}_I^{(k)}$ with $k \in \{3, \dots, n\}$. Therefore



Figure 5.2: Two-point, three-point, and four-point functions at tree level in single-field inflation with the following interaction scheme: $\hat{H}_{\text{free}} = \hat{H}^{(2)}$ and $\hat{H}_{\text{int}} = \hat{H}^{(3)} + \hat{H}^{(4)} + \dots$. A blue line represents a free propagator of the interacting field $\mathcal{R}^I$ while the black dots denotes an interaction vertex.

to compute the bispectrum it is enough to know $\hat{H}^{(3)}$, for the trispectrum $\hat{H}^{(3)}$ and $\hat{H}^{(4)}$, etc.;

- Compute the vacuum expectation values of the time-dependent quantum operators by developing them on the fixed basis of annihilation and creation operators that act in a simple way on the vacuum state $|0\rangle$, with the time-dependent mode function $\mathcal{R}^I(t)$ verifying the linear equations of motion $\mathcal{E}_{\mathcal{R}^I} = 0$, and express the correlation functions in terms of (real and imaginary parts of) integrals of complex-valued functions instead of quantum operators.
- Solve the equation of motion analytically in order to manipulate explicit expression of $\mathcal{R}^I(t)$, and perform the time integrals as explicitly as possible, potentially with some approximation such as a slowly evolving background.

Shape functions

One begins by defining the bispectrum of the comoving curvature perturbation $\mathcal{R}$:

$$\boxed{\text{(Bispectrum of } \mathcal{R}\text{): } \langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \rangle = (2\pi)^3 \delta^{(3)}(\vec{k}_1 + \vec{k}_2 + \vec{k}_3) B_{\mathcal{R}}(k_1, k_2, k_3)}, \quad (5.42)$$

where momentum conservation enforces the vectors $\vec{k}_i$ to close in a triangle in Fourier space. Note however that much more freedom on the vectorial dependence of the modes is left compared to the two-point function, indeed in order to describe a triangle it is necessary and sufficient to specify three real numbers: the three lengths of the sides k_1, k_2, k_3 , or any independent combinations of them like the total perimeter $K = k_1 + k_2 + k_3$ and any two of the other lengths or of the ratios like $x_2 = k_2/k_1$ and $x_3 = k_3/k_1$, or two lengths and an angle, etc. The shape dependence of the bispectrum is described by the function $\mathcal{S}$ which is dimensionless and defined in a way similar to the dimensionless power spectrum:

$$\boxed{\text{(Bispectrum shape): } \mathcal{S}(k_1, k_2, k_3) = \frac{(k_1 k_2 k_3)^2}{(2\pi)^4 A_S^2} B_{\mathcal{R}}(k_1, k_2, k_3)}, \quad (5.43)$$

with $A_s = 2.10 \times 10^{-9}$ the observed value of the dimensionless power spectrum at the pivot scale in the CMB. It is then useful to introduce standard shapes of the bispectrum, to which a given model may coincide with or not.

A first phenomenologically motivated shape is the one of *local* non-Gaussianities, which are defined in real space as follows:

$$\mathcal{R}(x) = \mathcal{R}_g(x) + \frac{3}{5} f_{\text{NL}}^{\text{loc}} (\mathcal{R}_g(x)^2 - \langle \mathcal{R}_g(x)^2 \rangle) , \quad (5.44)$$

where $\mathcal{R}_g(x)$ is a random variable with Gaussian statistics that are uniquely defined in terms of its two-point function, coinciding with the one of the non-Gaussian variable $\mathcal{R}(x)$. Going to Fourier space, one finds that such non-Gaussian variable would have a bispectrum of the form:

$$B_{\mathcal{R}}^{\text{loc}}(k_1, k_2, k_3) = \frac{6}{5} f_{\text{NL}}^{\text{loc}} (P_{\mathcal{R}_g}(k_1)P_{\mathcal{R}_g}(k_2) + 2 \text{ perm. }) . \quad (5.45)$$

Neglecting the small scale-dependence of the power spectrum, $\propto (n_s - 1)$, one finds that the corresponding bispectrum shape is simply $f_{\text{NL}}^{\text{loc}} \times \mathcal{S}_{\text{loc}}$, with

$$\boxed{\text{(Local shape): } \mathcal{S}_{\text{loc}} = \frac{3}{10} \left(\frac{k_3^2}{k_1 k_2} + 2 \text{ perm. } \right)} . \quad (5.46)$$

Some models of inflation may feature a bispectrum with a shape function resembling the local one, but others may not, and therefore it is useful to define other shapes, in particular that are better theoretically motivated.

For this, one first defines the *equilateral* shape as the one that is largest when the Fourier modes form an equilateral triangle and therefore all describe the same scale,

$$\boxed{\text{(Equilateral shape): } \mathcal{S}_{\text{eq}} = \left(\frac{k_1}{k_2} + 5 \text{ perm. } \right) - \left(\frac{k_3^2}{k_1 k_2} + 2 \text{ perm. } \right) - 2} , \quad (5.47)$$

where the 5 non-displayed permutations correspond to the other ratios k_i/k_j with $i \neq j$, and the overall amplitude has been chosen such that $\mathcal{S}_{\text{eq}}(k, k, k) = 1$.

It also proves useful to define an *orthogonal* shape, which may arise naturally in DBI Galileon inflation (see *e.g.* Ref. [228] and subsequent works), as:

$$\boxed{\text{(Orthogonal shape): } \mathcal{S}_{\text{orth}} = 3 \left[\left(\frac{k_1}{k_2} + 5 \text{ perm. } \right) - \left(\frac{k_3^2}{k_1 k_2} + 2 \text{ perm. } \right) - 8/3 \right]} , \quad (5.48)$$

again such that $\mathcal{S}_{\text{orth}}(k, k, k) = 1$. The word “orthogonal” has the following meaning: one can define a scalar product in the space of the shape functions, by writing them at a fixed total scale K and parameterising their shape dependencies with $x_2 = k_2/k_1$ and $x_3 = k_3/k_1$ after arranging momenta such that $k_3 \leq k_2 \leq k_1$, meaning that the triangle inequality is verified:

$$0 \leq 1 - x_2 \leq x_3 \leq x_2 \leq 1 . \quad (5.49)$$

Then, the scalar product between two shapes $\mathcal{S}_1$ and $\mathcal{S}_2$ is defined as:

$$\mathcal{S}_1 \cdot \mathcal{S}_2 = \int_{1/2}^1 dx_2 \int_{1-x_2}^{x_2} dx_3 S_1(1, x_2, x_3) S_2(1, x_2, x_3). \quad (5.50)$$

The orthogonal shape has been defined such that $\mathcal{S}_{\text{orth}} \cdot \mathcal{S}_{\text{eq}} \simeq 0$ and therefore enables one to describe many bispectrum shapes as a linear combination of the equilateral and the orthogonal ones, as the latter is both peaking on equilateral triangles with a positive sign, and on flattened ones, corresponding to saturating the bound $x_3 \sim 1 - x_2$, with a negative sign. The *flattened* shape, corresponding to a bispectrum that is maximal only on these flattened triangle configurations, and that can be found in single-field models of inflation with excited initial states [229–231] as well as multifield ones with imaginary speed of sound [1, 77–79, 206], is an example of such linear combination: $\mathcal{S}_{\text{flat}} = (\mathcal{S}_{\text{eq}} - \mathcal{S}_{\text{orth}})/2$. It is also customary to define the *cosine* between two bispectrum shapes, simply as the normalised scalar product between them:

$$\cos(\mathcal{S}_1, \mathcal{S}_2) = \frac{\mathcal{S}_1 \cdot \mathcal{S}_2}{\sqrt{(\mathcal{S}_1 \cdot \mathcal{S}_1)(\mathcal{S}_2 \cdot \mathcal{S}_2)}}, \quad (5.51)$$

which enables one to handle a dimensionless and amplitude-free notion of correlation between bispectrum shapes in the $[-1, 1]$ range. These few but important bispectrum shapes are represented in Fig. 5.3.

The trispectrum and its shape function can also be defined as:

(Trispectrum and its shape):

$$\left\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \hat{\mathcal{R}}_{\vec{k}_4} \right\rangle_c = (2\pi)^3 \delta^{(3)}(\vec{k}_1 + \vec{k}_2 + \vec{k}_3 + \vec{k}_4) T_{\mathcal{R}}(k_1, k_2, k_3, k_4, k_{12}, k_{34})$$

$$\mathcal{T}(k_1, k_2, k_3, k_4, k_{12}, k_{34}) = \frac{(k_1 k_2 k_3 k_4)^3}{(2\pi)^6 A_s^3} T_{\mathcal{R}}(k_1, k_2, k_3, k_4, k_{12}, k_{34}),$$

(5.52)

where now the shapes of quadrangles in Fourier space can be parameterised with six real numbers, the norms of the wave vectors, $k_{1,2,3,4}$, as well as the norms of the diagonals of the quadrangles $k_{12} = |\vec{k}_1 + \vec{k}_2|$ and $k_{34} = |\vec{k}_3 + \vec{k}_4|$.

Single-field bispectrum and its consistency relation in the squeezed limit

Cubic action. Maldacena first computed in full generality the cubic order action of single-field inflation with canonical kinetic terms, a minimal coupling to Einstein gravity, and any kind of scalar potential $V(\phi)$ [227]. Because this computation is extended to

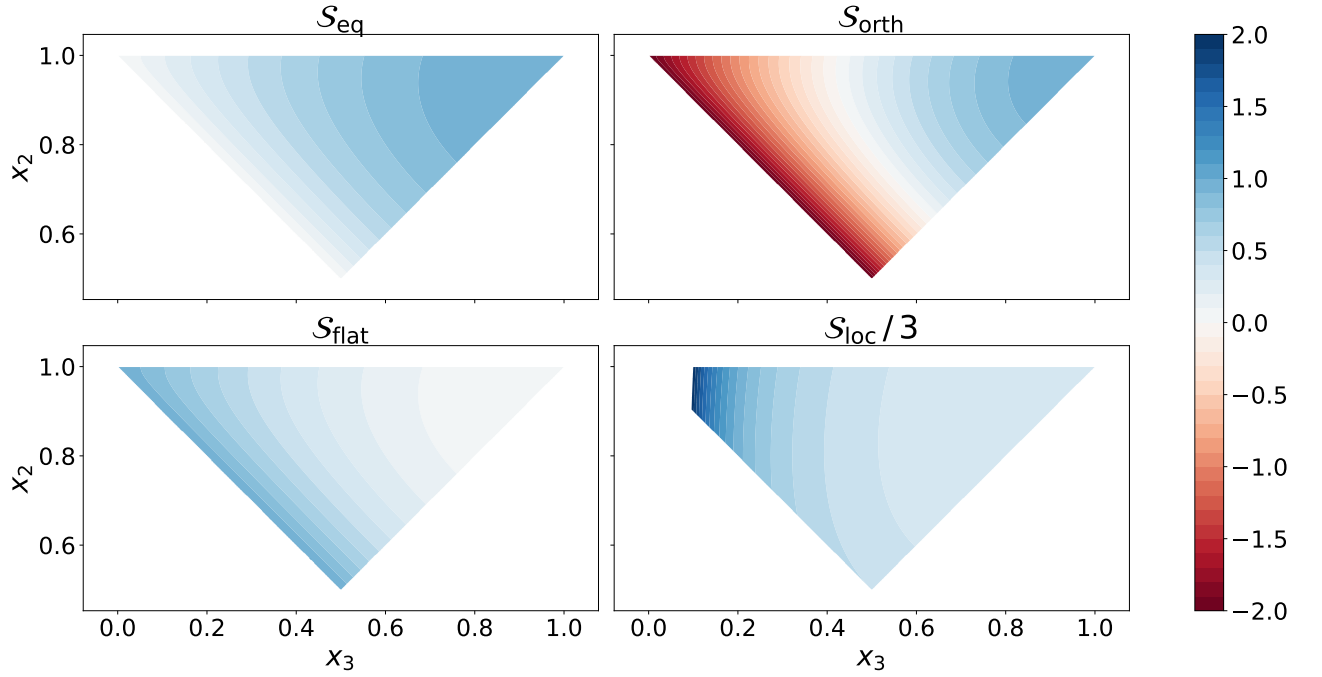


Figure 5.3: Bispectrum shapes $S_i(1, x_2, x_3)$ at an overall scale K as introduced in the main text. The equilateral shape peaks with value unity on equilateral triangles, $x_2 \rightarrow 1, x_3 \rightarrow 1$, the orthogonal shape too but it also drops to negative values with order unity on flattened triangles $x_3 \rightarrow 1 - x_2$. The flattened shape is a linear combination of the two previous ones and peaks with value unity on... flattened triangles. The local shape has been divided by three for representation purposes: it not only peaks but diverges in the squeezed limit $x_2 \rightarrow 1, x_3 \rightarrow 0$.

the case of two scalar fields in Sec. 5.3.1 and N_{field} ones in Sec. 5.3.2, see Refs. [2, 3], with non-canonical kinetic terms and any scalar potential, and because it is explained in great detail there, one simply quotes the final result here:

$$\mathcal{L}^{(3)} = M_{\text{Pl}}^2 a^3 \left[\epsilon(\epsilon - \eta) \dot{\mathcal{R}}^2 \mathcal{R} + \epsilon(\epsilon + \eta) \mathcal{R} \frac{(\partial \mathcal{R})^2}{a^2} - \frac{2}{a^4} (\partial \mathcal{R}) (\partial \chi) \partial^2 \chi \right] + \mathcal{D} + \mathcal{E}, \quad (5.53)$$

where:

$$\begin{aligned} \mathcal{D} = & -M_{\text{Pl}}^2 \partial_t \left[9H a^3 \mathcal{R}^3 - \frac{a}{H} (1 - \epsilon) \mathcal{R} (\partial \mathcal{R})^2 + a^3 \frac{\epsilon}{H} \mathcal{R} \dot{\mathcal{R}}^2 + \frac{1}{6aH^3} \mathcal{R} (\mathcal{R}_{,ij} \mathcal{R}_{,ij} - (\partial^2 \mathcal{R})^2) \right. \\ & \left. - \frac{1}{2aH^2} \mathcal{R} (\mathcal{R}_{,ij} \chi_{,ij} - \partial^2 \mathcal{R} \partial^2 \chi) + \frac{1}{2aH} \mathcal{R} (\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2) \right] \quad (5.54) \\ \mathcal{E} = & a^3 \frac{2\epsilon M_{\text{Pl}}^2}{H} \mathcal{E}_{\mathcal{R}} \left[\dot{\mathcal{R}} \mathcal{R} - \frac{1}{4a^2 H} ((\partial \mathcal{R})^2 - \partial^{-2} \partial_i \partial_j (\partial_i \mathcal{R} \partial_j \mathcal{R}) - 2H (\partial \mathcal{R} \partial \chi - \partial^{-2} \partial_i \partial_j (\partial_i \mathcal{R} \partial_j \chi))) \right]. \end{aligned}$$

A few comments should be made at this stage. First, it is clear that $\mathcal{R}$ has no non-derivative cubic interaction, as it should be at any order actually in order for $\mathcal{R}$ to remain radiatively massless. The variable χ is just a useful notation but of course depends only on $\mathcal{R}$ in this single-field setup: there is no other degree of freedom, see Eq. (5.37). All cubic interactions are explicitly suppressed by at least two powers of the slow-roll parameters (remember that $\partial^2 \chi \propto p_{\mathcal{R}} \propto \epsilon \dot{\mathcal{R}}$), even though Eq. (5.53) is an exact result and not a systematic slow-roll expansion. This is far from being a trivial result, as naively expanding the action at cubic order in $\mathcal{R}$ yields cubic interactions that do not feature explicitly such slow-roll suppression, and only a detailed analysis of the redundancy of the obtained operators, using integrations by parts and the linear equations of motion that the interaction picture fields verify, enable one to show precise cancellations between the leading-order pieces and hence leaving only the slow-roll suppressed terms beginning at second order. Therefore, a crude estimate of the bispectrum with the bulk Lagrangian is given by the non-linearity parameter $f_{\text{NL}} \sim \mathcal{L}^{(3)} / (\mathcal{R} \mathcal{L}^{(2)}) \sim \mathcal{O}(\epsilon, \eta)$, which shows that the bispectrum of single-field inflation is suppressed by at least one power of the slow-roll parameters and therefore negligibly small. This statement is made more explicit in the following.

Boundary terms. Moreover, there has been quite a common mistake in the interpretation of the boundary terms $\mathcal{D}$ and remaining linear equations of motion $\mathcal{E}$ arising from the manipulations needed to render explicit the sizes of the interactions [232], beginning with the seminal article of Maldacena.² Because in the interaction picture, the interaction Hamiltonian is evaluated on the interaction field $\mathcal{R}^I$ that does verify the linear

²Note that the final bulk action of Maldacena's result [227] differs from the one quoted here by terms $\propto \epsilon \eta$. This simply corresponds to a choice of taking into account these terms in the boundary action rather than in the bulk one. The displayed form of the action in this thesis is such that the boundary terms give a total vanishing contribution in the super-horizon limit of single-field inflation, see the

equations of motion $\mathcal{E}_{\mathcal{R}^I} = 0$, the contribution $\mathcal{E}$ does identically vanish in the in-in master formula and never plays a role in the computation of the correlation functions at any order. But the boundary terms in $\mathcal{D}$ do in general participate to the three-point function and to the final bispectrum, even though their contributions are suppressed in standard scenarios, as one can see simply with the following argument (the interested reader is referred to Sec. 5.3.1 and Ref. [2] for more details). Let one write $\mathcal{D}(t) = -\partial_t \mathcal{B}(t)$, which therefore gives by assuming that interactions are switched off in the distant past, that the time integral of $\mathcal{D}$ has simply been replaced by an evaluation of $-\mathcal{B}$ at the upper limit of the integral. Thus the contribution from $\mathcal{D}$ does not vanish in general, even though not all terms in $\mathcal{B}$ contribute to a given correlation function. For example, in the three-point function of $\mathcal{R}$, the commutator form is useful to see that the contribution from $\mathcal{D}$ (which comes in the Hamiltonian with a sign opposite to the one in the Lagrangian),

$$\left\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \right\rangle(t) \supset i \left\langle 0 \left| \left[\hat{\mathcal{B}}^I(t), \hat{\mathcal{R}}_{\vec{k}_1}^I(t) \hat{\mathcal{R}}_{\vec{k}_2}^I(t) \hat{\mathcal{R}}_{\vec{k}_3}^I(t) \right] \right| 0 \right\rangle, \quad (5.55)$$

is non-zero only for the terms in $\hat{\mathcal{B}}^I$ that involve the canonically conjugate momentum $\hat{p}_{\mathcal{R}}^I$, *i.e.* that are proportional to the time derivative $\dot{\mathcal{R}}^I$. In single-field inflation, one identifies two such contributions with operators in $\mathcal{B}$ of the form $\mathcal{R}^2 p_{\mathcal{R}}$ and $\mathcal{R} p_{\mathcal{R}}^2$. For example, going to Fourier space, the first of these terms reads

$$\begin{aligned} \hat{\mathcal{B}} \supset \int \frac{d^3 \vec{k}_a d^3 \vec{k}_b d^3 \vec{k}_c}{(2\pi)^9} \delta^{(3)}(\vec{k}_a + \vec{k}_b + \vec{k}_c) \frac{b(\vec{k}_a, \vec{k}_b, \vec{k}_c)}{4a^2 H^2} \hat{\mathcal{R}}_{\vec{k}_a} \hat{\mathcal{R}}_{\vec{k}_b} \hat{p}_{\vec{k}_c}^{\mathcal{R}}, \\ \text{with } b(\vec{k}_a, \vec{k}_b, \vec{k}_c) = \vec{k}_b^2 - \frac{(\vec{k}_b \cdot \vec{k}_c)^2}{\vec{k}_c^2} \end{aligned} \quad (5.56)$$

that can be symmetrised under $(\vec{k}_a \leftrightarrow \vec{k}_b)$ without loss of generality (note also that by writing momentum conservation, $\vec{k}_b \cdot \vec{k}_c = (k_a^2 - k_b^2 - k_c^2)/2$, therefore showing that b is actually only a function of the norms $k_{1,2,3}$), thus giving a non-vanishing contribution to the bispectrum of $\mathcal{R}$:

$$\left\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \right\rangle'(\tau) \supset -\frac{b(k_1, k_2, k_3)}{2a^2 H^2} P_{\mathcal{R}^I}(k_1, \tau) P_{\mathcal{R}^I}(k_2, \tau) + 2 \text{ perm.} , \quad (5.57)$$

where a primed correlation function means that the factor $(2\pi)^3 \delta^{(3)}(\vec{k}_1 + \vec{k}_2 + \vec{k}_3)$ has been divided out. But note that although one can be interested in the value of the

discussion just below. The form displayed by Maldacena is equally correct: his boundary contribution is non-vanishing in the super-horizon limit, therefore making the difference between our bulk actions. The error of Maldacena lies elsewhere, by him completely ignoring the boundary terms but keeping the terms proportional to the linear equations of motion, and estimating their size by a field redefinition. By chance (but this is not a suprise since terms proportional to linear equations of motion and in the boundary contribution come from the same manipulations and are not independent), the computed correction with this procedure coincides with the correct computation of the non-zero boundary contribution and forgetting the identically vanishing linear equations of motion applied to the interaction picture fields.

bispectrum at any time τ , the observable bispectrum is the one at the end of inflation, when all the modes with wavenumbers $k_{1,2,3}$ are well above the horizon, and therefore $k_i^2/a^2 \ll H^2$. In this limit, $b(k_i)/(a^2 H^2) \ll 1$ and the computed contribution is negligible. It is also possible to show that the second term in $\mathcal{B}$ *a priori* contributing to the bispectrum of $\mathcal{R}$, proportional to the operator $\mathcal{R}p_{\mathcal{R}}^2$, gives a final contribution of the form

$$\left\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \right\rangle'(\tau) \supset -\frac{c(k_1, k_2, k_3)}{2a^3 \epsilon H M_{\text{Pl}}^2} P_{\mathcal{R}^I}(k_1, \tau) \text{Re} \left(P_{\mathcal{R}^I p_{\mathcal{R}}^I} \right)(k_2, \tau) + 5 \text{ perm.} \quad , \quad (5.58)$$

with $c(k_i)$ an order-one dimensionless function of the wavenumbers, and where $P_{\mathcal{R}^I p_{\mathcal{R}}^I}$ is the cross-power spectrum of $\mathcal{R}^I$ with its linear canonical conjugate momentum $p_{\mathcal{R}}^I$. This contribution is again negligible in the super-horizon limit, as can be seen by recalling that $p_{\mathcal{R}}^I = 2aM_{\text{Pl}}^2 \partial^2 \chi^I$ and therefore that

$$\frac{P_{\mathcal{R}^I p_{\mathcal{R}}^I}}{2a^3 \epsilon H M_{\text{Pl}}^2} = \frac{k^2}{a^2 H^2} \frac{H}{\epsilon} P_{\mathcal{R}^I \chi^I} \xrightarrow{k \ll aH} 0.$$

Therefore one has proven that the boundary terms are negligible for the computation of the three-point function of $\mathcal{R}$ in single-field inflation, but only on super-horizon scales. However this is not true in general on sub-horizon scales, and even on super-horizon scales the boundary terms may contribute in multifield inflation, see Ref. [2] in Sec. 5.3.1.

Single-field bispectrum in a slow-varying approximation. Boundary terms being negligible in single-field inflation on super-horizon scales, and terms proportional to linear equations of motion being vanishing when evaluated with the interaction picture fields as they should, only the bulk cubic Lagrangian remains and gives the observed value of the bispectrum at the end of inflation for the large scales that relevant in CMB observations. One can compute explicitly the three-point function by using the mode-decomposition of $\hat{\mathcal{R}}^I$ in conformal time τ as:

$$\hat{\mathcal{R}}_{\vec{k}}^I(\tau) = \mathcal{R}_{\vec{k}}^I(\tau) \hat{a}_{\vec{k}} + \mathcal{R}_{\vec{k}}^{I*}(\tau) \hat{a}_{-\vec{k}}^\dagger, \quad (5.59)$$

where the mode function verifies the standard linear EoM (5.36) that, if a Bunch-Davies initial state is assumed, is solved by:

$$\mathcal{R}_{\vec{k}}^I(\tau) = \frac{H}{M_{\text{Pl}} \sqrt{4\epsilon k^3}} (1 + ik\tau) e^{-ik\tau} \implies \mathcal{R}_{\vec{k}}^{I'}(\tau) = \frac{H}{M_{\text{Pl}} \sqrt{4\epsilon k^3}} k^2 \tau e^{-ik\tau} - aH \left(\epsilon + \frac{\eta}{2} \right) \mathcal{R}_{\vec{k}}^I(\tau). \quad (5.60)$$

For example, the contribution from the first term in Eq. (5.53) can now be computed using *e.g.* the real form of the in-in formula, giving (one reminds the simple relation between the cubic Hamiltonian and Lagrangian, $\mathcal{H}^{(3)}(\mathcal{R}^I, p_{\mathcal{R}}^I) = -\mathcal{L}^{(3)}(\mathcal{R}^I, \dot{\mathcal{R}}^I[p_{\mathcal{R}}^I])$, the reader being however warned that such relation does not hold true from the quartic order):

$$\left\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \right\rangle'(\tau) \supset 4M_{\text{Pl}}^2 \text{Im} \left\{ \left[\mathcal{R}_{\vec{k}_1}^{I*} \mathcal{R}_{\vec{k}_2}^{I*} \mathcal{R}_{\vec{k}_3}^{I*} \right](\tau) \int_{-\infty^+}^{\tau} d\tau' [a^2 \epsilon (\epsilon - \eta) \mathcal{R}_{\vec{k}_1}^{I'} \mathcal{R}_{\vec{k}_2}^{I'} \mathcal{R}_{\vec{k}_3}^I](\tau') \right\} + 2 \text{ perm.} \quad (5.61)$$

To go further and perform the time integral explicitly, one needs to use a slow-varying approximation, which enables one to replace in the above expressions $(H, \epsilon, \eta) \rightarrow (H_*, \epsilon_*, \eta_*)$ with a star denoting evaluation at horizon crossing, as well as to neglect the second term $\propto (\epsilon + \eta/2)$ in the formula giving $\mathcal{R}_k''(\tau)$. This gives at lowest non-vanishing order in derivatives of the background, for this particular contribution to the shape function $\mathcal{S}$ evaluated at the end of inflation for simplicity (*i.e.* at $k_i\tau \rightarrow 0, \forall i$, even though the corresponding equation at any time τ is easily obtained):

$$\mathcal{S}(k_1, k_2, k_3) \supset \frac{\epsilon - \eta}{4} \frac{k_1 k_2}{k_3} \frac{K + k_3}{K^2} + 2 \text{ perm.} , \quad (5.62)$$

with $K = k_1 + k_2 + k_3$ the overall scale, *i.e.* the perimeter of the triangle in Fourier space, and where the stars were omitted for simplicity. The computation of the contributions from the two other bulk cubic interactions is left for the reader, and the final result [227] is only displayed:

$$\mathcal{S}(k_1, k_2, k_3) = \frac{\epsilon}{8} \left(\frac{k_1}{k_2} + 5 \text{ perm.} \right) + \frac{\eta - \epsilon}{8} \left(\frac{k_3^2}{k_1 k_2} + 2 \text{ perm.} \right) + \frac{\epsilon}{K} \left(\frac{k_1 k_2}{k_3} + 2 \text{ perm.} \right) . \quad (5.63)$$

Note that it can be rewritten in terms of the local and equilateral shapes, as

$$\mathcal{S} = \frac{5}{12}(\eta + 2\epsilon)\mathcal{S}_{\text{loc}} + \frac{\epsilon}{8}\mathcal{S}_{\text{eq}} + \frac{\epsilon}{2}\mathcal{S}_{\text{remaining}} , \quad (5.64)$$

where the remaining contribution can be written explicitly and actually seems to resemble the equilateral shape, although slightly boosted on isosceles configurations.

Independently of these details, two very important conclusions can be drawn:

- The bispectrum of single-field inflation with Bunch-Davies initial states and a slowly varying background, is suppressed by slow-roll parameters for every configuration, therefore making it unobservably small.
- Its *squeezed* limit, corresponding to $k_3 \ll k_2 \sim k_1$, is given by the contribution $\propto \mathcal{S}_{\text{loc}}$ corresponding to local non-Gaussianities, see Eq. (5.45), with

$$f_{\text{NL}}^{\text{loc}} = \frac{5}{12}(1 - n_s) . \quad (5.65)$$

This result can actually be shown to be completely generic to single-clock models of inflation where an adiabatic limit is reached on super-horizon scales, independently of the exact background dynamics or the considered interactions [233]. Because it relates the scale-dependence of the power spectrum to the amplitude of the squeezed limit of the bispectrum in single-field inflation, it is called a *single-field consistency relation* and reads

(Single-field bispectrum in the squeezed limit):

$$\lim_{k_3 \ll k_2 \sim k_1} B_{\mathcal{R}}(k_1, k_2, k_3) = (1 - n_s) P_{\mathcal{R}}(k_1) P_{\mathcal{R}}(k_3) , \quad (5.66)$$

therefore implying that if a non-Gaussian signal were measured in the squeezed limit of the primordial bispectrum, then all attractor single-field models of inflation would be ruled out.³

Higher-order n -point functions

The primordial trispectrum may be parameterised as

$$T_{\mathcal{R}}(\vec{k}_i) = \tau_{\text{NL}} (P_{\mathcal{R}}(k_{12})P_{\mathcal{R}}(k_2)P_{\mathcal{R}}(k_3) + 11 \text{ perm. }) \\ + \frac{54}{25} g_{\text{NL}} (P_{\mathcal{R}}(k_1)P_{\mathcal{R}}(k_2)P_{\mathcal{R}}(k_3) + 3 \text{ perm. }) , \quad (5.67)$$

where this definition of the non-linearity parameters τ_{NL} and g_{NL} , *a priori* $\vec{k}_i$ -dependent, is motivated by the particular case of local non-Gaussianities extended to a higher order:

$$\mathcal{R}(x) = \mathcal{R}_g(x) + \frac{3}{5} f_{\text{NL}}^{\text{loc}} (\mathcal{R}_g(x)^2 - \langle \mathcal{R}_g(x)^2 \rangle) + \frac{9}{25} g_{\text{NL}}^{\text{loc}} \mathcal{R}_g^3(x) , \quad (5.68)$$

with $f_{\text{NL}}^{\text{loc}}$ and $g_{\text{NL}}^{\text{loc}}$ two $\vec{k}_i$ -independent numbers, and which corresponds to a trispectrum of the form (5.67) in Fourier space with:

$$\tau_{\text{NL}} = \left(\frac{6}{5} f_{\text{NL}}^{\text{loc}} \right)^2 , \text{ and } g_{\text{NL}} = g_{\text{NL}}^{\text{loc}} . \quad (5.69)$$

Equipped with these definitions, a few interesting results regarding non-Gaussianities as probed by the four-point function and higher-order correlation functions in single-field inflation with Bunch-Davies initial states and in a slow-varying approximation, are now displayed without proofs.

- At horizon exit, the dimensionless trispectrum is small since scalar sub-Hubble scalar interactions are all suppressed by slow-roll parameters in single-field inflation, in particular an estimation with the in-in formalism of the quartic interaction shows that $\tau_{\text{NL}} \lesssim \mathcal{O}(\epsilon)$ [242], although a contribution from the graviton-exchange diagram (similar to the scalar-exchange diagram of Fig. 5.2 but with the straight internal scalar propagator replaced by a wavy one corresponding to a graviton,

³Exceptions to this rule seem to be single-field models of inflation that feature a non-attractor dynamics, such as an ultra-slow-roll phase, for which it was found that the squeezed limit of the bispectrum results in $f_{\text{NL}}^{\text{loc}} = 5/2$ due to the absence of an adiabatic limit on super-horizon scales [234], and would therefore result in an observable signal in the near future. But actually, it seems that any way the squeezed limit of the observable single-field bispectrum is identically vanishing at leading order in derivatives due to local observer effects initially forgotten, a result first shown in the case of attractor models both analytically [235, 236] and numerically [237] although a non-vanishing second-order correction $\propto (k_3/k_1)^2$ was found [238], and later extended to non-attractor scenarios [239] and to an equivalent collapsed shape of the trispectrum [240]. Note however that in a recent work [241], it was claimed that the cancellation mentioned above would only be valid in an exactly infinite wavelength limit, $k_3 = 0$ and therefore unphysical, implying a possibly small but non-vanishing signal, which revived the thrilling debate on the squeezed limit of the single-field primordial bispectrum.

and where the two cubic interactions are mixing scalar and tensor perturbations, *e.g.* such as $\dot{\mathcal{R}}^2\gamma$) boosts this signal to $\tau_{\text{NL}} \sim \mathcal{O}(r)$ [243], where $r = 16\epsilon$ is the value of tensor-to-scalar ratio in single-field slow-roll inflation.

- A larger contribution from the trispectrum may come from super-Hubble interactions when all relevant cosmological modes are outside the horizon and therefore must interact locally. Using the δN -formalism applied to single-field inflation, this results in local non-Gaussianities as described by Eq. (5.68) with $\tau_{\text{NL}} = (6f_{\text{NL}}^{\text{loc}}/5)^2$ and $g_{\text{NL}} = g_{\text{NL}}^{\text{loc}} = \mathcal{O}(\epsilon, \eta)^2$ [224], reminding that $f_{\text{NL}}^{\text{loc}} \propto 1 - n_s$ is obtained in the squeezed limit of the single-field bispectrum. Thus in single-field inflation the super-Hubble contribution to the trispectrum is even smaller than the sub-Hubble one and is therefore unobservably small.
- Just like the fact that the squeezed limit of the bispectrum must be simply proportional to $1 - n_s$ and two powers of the power spectrum, there exists relations between soft limits of higher-order correlation functions in single-field inflation. Actually, one of them has just been evoked: in the *collapsed* limit of the trispectrum, taking one of the diagonals of the quadrangle to vanish in Fourier space, *e.g.* $k_{12} \rightarrow 0$, one can show without assuming a particular background and in a model-independent way that [205]:

$$\tau_{\text{NL}}(\vec{k}_i) \xrightarrow{k_{12} \rightarrow 0} \left(\frac{6}{5}f_{\text{NL}}^{\text{loc}}\right)^2. \quad (5.70)$$

Note however that this result relies on the assumption of a strictly single degree of freedom, and is broken once interactions with other particles are taken into account, like other scalar fields in multifield inflation but also just the graviton that must be present even in single-field inflation, and corresponds to saturating a more general inequality that must be satisfied for any super-Hubble evolution generating a bispectrum with $f_{\text{NL}} = 5B_{\mathcal{R}}(k_1, k_2, k_3)/(6P_{\mathcal{R}}(k_1)P_{\mathcal{R}}(k_2) + 2 \text{ perm.})$ and a trispectrum with a τ_{NL} parameter, and called the *Suyama-Yamaguchi bound* [244], reading:

$$\tau_{\text{NL}} \geq \left(\frac{6}{5}f_{\text{NL}}\right)^2. \quad (5.71)$$

A sketch of a proof is given in Sec. 5.1.3 about primordial non-Gaussianities in multifield inflation. It is possible to generalise these soft limits to higher-order correlation functions, and at next-to-leading-order in the soft momenta (such as k_{12} in the above example), see *e.g.* Refs. [245–249].

Excited initial states

Suppose that the initial state cannot be described by the Bunch-Davies vacuum, *i.e.* that the set of annihilation and creation operators $(\hat{a}_{\vec{k}}, \hat{a}_{-\vec{k}}^\dagger)$ on which the quantum perturbation $\hat{\mathcal{R}}_{\vec{k}}^I$ is decomposed, does not correspond to $(\hat{a}_{\vec{k}}^{\text{BD}}, \hat{a}_{-\vec{k}}^{\text{BD}\dagger})$ that respectively

annihilate $|0\rangle$ and create the 1-particle states of the theory. However the mode function $\mathcal{R}^I$ in this basis should still correspond to the solution of the linear EoM set by the free Hamiltonian, and in particular for $\hat{H}_{\text{free}} = \hat{H}^{(2)}$, one still has $\mathcal{R}_k^I(t) = H \times \left(M_{\text{Pl}} \sqrt{4\epsilon k^3}\right)^{-1} \times (1 + ik\tau) e^{-ik\tau}$. But for practical calculations, it is easier to work with the usual annihilation and creation operators that can be recovered under the following identities:

$$\begin{aligned}\hat{\mathcal{R}}_k^I(\tau) &= \mathcal{R}_k^I(\tau) \hat{a}_{\vec{k}} + \mathcal{R}_k^{I*}(\tau) \hat{a}_{-\vec{k}}^\dagger \\ &= \mathcal{R}_{k,\text{excited}}^I(\tau) \hat{a}_{\vec{k}}^{\text{BD}} + \mathcal{R}_{k,\text{excited}}^{I*}(\tau) \hat{a}_{-\vec{k}}^{\text{BD}\dagger},\end{aligned}\quad (5.72)$$

where the excited initial quantum states can be related to the Bunch-Davies vacuum by a Bogolyubov transformation,

$$\hat{a}_{\vec{k}} = \alpha_k^* \hat{a}_{\vec{k}}^{\text{BD}} + \beta_k \hat{a}_{-\vec{k}}^{\text{BD}\dagger} \quad \text{and} \quad \hat{a}_{\vec{k}}^\dagger = \alpha_k \hat{a}_{\vec{k}}^{\text{BD}\dagger} + \beta_k^* \hat{a}_{-\vec{k}}^{\text{BD}}, \quad (5.73)$$

therefore implying that

$$\mathcal{R}_{k,\text{excited}}^I = \frac{H}{M_{\text{Pl}} \sqrt{4\epsilon k^3}} \left[\alpha_k^* (1 + ik\tau) e^{-ik\tau} + \beta_k^* (1 - ik\tau) e^{ik\tau} \right]. \quad (5.74)$$

Note that the standard Bunch-Davies case is recovered in the limit $\alpha_k = 1, \beta_k = 0$ which indeed corresponds to the intuition since the number of initial particles in the Bunch-Davies vacuum with wavenumber k is $n_k = |\beta_k|^2$. Requiring for consistency of the perturbation theory that these particles do not backreact strongly on the background puts bounds on $|\beta_k|^2$ and therefore enables one to treat the second mode in Eq. (5.74) as a small correction [230]. Taking into account such correction at the linear order in β_k , *e.g.* in the last mode function $\mathcal{R}_{k_3}^I(\tau')$ of the explicitly shown permutation in Eq. (5.61), would yield a new contribution within the time integral, of the form

$$\mathcal{S}(k_1, k_2, k_3) \supset \frac{\epsilon - \eta}{4} \frac{k_1 k_2}{k_3} \times \underbrace{\text{Im} \left(\beta_{k_3} \int_{-\infty^+}^0 d\tau' (1 - ik_3 \tau') e^{-i\tilde{k}_3 \tau'} \right)}_{= \text{Re}(\beta_{k_3}) (\tilde{k}_3 - k_3)/\tilde{k}_3^2}, \quad (5.75)$$

with $\tilde{k}_3 = k_1 + k_2 - k_3$, which therefore results in a large contribution in the limit $\tilde{k}_3 \rightarrow 0$ corresponding to flattened triangles [229–231]. Note that the apparent $1/\tilde{k}_3^2$ divergence in exact flattened configurations is spurious and explicitly disappears if a cutoff scale $-\tau_c = 1/k_m$ is used, as it indeed brings an additional contribution with the exact opposite divergence in the limit $\tilde{k}_3 \rightarrow 0$ thus making the sum of the two divergences large but finite, and $\propto_{\tilde{k}_3 \rightarrow 0} \text{Re}(\beta_{k_3}) k_1 k_2 / (k_3 k_m)$.

Non-canonical kinetic structure

Single-field slow-roll inflation with canonical kinetic terms is interesting to study *per se*, but for the reasons mentioned in Sec. 4.1 it would be valuable to understand how non-Gaussianities can arise in more general scenarios. In this paragraph (and the following

one), the particle content is still restricted to a single degree of freedom, but a more generic structure is allowed. Here, one considers the so-called k -inflationary setups [184, 185], consisting in allowing a non-canonical kinetic structure to the matter Lagrangian, *i.e.*

$$S = \frac{1}{2} \int d^4x \sqrt{-g} [M_{\text{Pl}}^2 R + 2P(X, \phi)] , \text{ with } X = -\frac{1}{2} \partial_\mu \phi \partial^\mu \phi , \quad (5.76)$$

and where $P(X, \phi)$ is a generic function of X and ϕ . The canonical kinetic structure of slow-roll inflation is recovered for the particular choice $P = X - V(\phi)$, as well as a famous example of higher-derivative model, DBI inflation [181, 182] for $P(X, \phi) = \Lambda^4 / f(\phi) \sqrt{1 - f(\phi) X / \Lambda^4} - V(\phi)$. Expanding the total action in perturbations in the comoving gauge, using the ADM formalism to find generalised constraint equations, it is possible to compute the quadratic and cubic Lagrangians of k -inflation, which read in conformal time [185, 229, 232, 250]:

$$S^{(2)} = \int d^3\vec{x} d\tau a^2 \frac{\epsilon}{c_s^2} \left[\mathcal{R}'^2 - c_s^2 (\mathcal{R})^2 \right] \quad (5.77)$$

$$S^{(3)} = \int d^3\vec{x} d\tau a^2 \left[\frac{g_1}{a} \mathcal{R}^3 + g_2 \mathcal{R} \mathcal{R}'^2 + g_3 \mathcal{R} (\partial \mathcal{R})^2 + g_4 \mathcal{R}' (\partial_j \mathcal{R}) (\partial_j \partial^{-2} \mathcal{R}') \right. \\ \left. + g_5 \partial^2 \mathcal{R} (\partial_j \partial^{-2} \mathcal{R}') (\partial_j \partial^{-2} \mathcal{R}') \right] , \quad (5.78)$$

with

$$g_1 = \frac{\epsilon}{H c_s^4} \left(1 - c_s^2 - 2 \frac{\lambda c_s^2}{\Sigma} \right) , \quad g_2 = \frac{\epsilon}{c_s^4} [-3(1 - c_s^2) + \epsilon - \eta] \\ g_3 = \frac{\epsilon}{c_s^2} [(1 - c_s^2) + \epsilon + \eta - 2s] , \quad g_4 = \frac{\epsilon^2}{2c_s^4} (\epsilon - 4) , \quad g_5 = \frac{\epsilon^3}{4c_s^4} , \quad (5.79)$$

with

$$c_s^2 = \frac{P_{,X}}{P_{,X} + 2X P_{,XX}} , \quad s = \frac{\dot{c}_s}{H c_s} , \quad \Sigma = \frac{\epsilon H^2}{c_s^2} , \quad \lambda = X^2 P_{,XX} + \frac{2}{3} X^3 P_{,XXX} . \quad (5.80)$$

From the quadratic action, one can infer the linear behaviour of the comoving curvature perturbation in the interaction picture with such a generic speed of sound c_s^2 , and from the cubic action one can compute the bispectrum shape in terms of the five parameters $c_s^2, \lambda/\Sigma, \epsilon, \eta, s$. This program was first performed at leading order in a slow-varying approximation [250] and later extended to next order [229, 232]. Rather than carrying exhaustively this calculation, one simply notes that in a slow-varying approximation, the above action reduces to the one expected from the decoupling limit of the EFT of Inflation, although one first needs to perform a few manipulations to eliminate a redundant operator in Eq. (5.77), as explicited *e.g.* in Sec. 4.2 of Ref. [77], therefore meaning that the EFToI should encapsulate the main features of the bispectrum in $P(X, \phi)$ inflation (see Ref. [232] for analytical expressions of the next-order corrections as well as a thorough analysis of the possible shapes and amplitudes in k -inflation),

provided the following rules of replacement:

$$c_s^2 \longrightarrow c_s^2, \quad \frac{2\lambda}{\Sigma} \longrightarrow -\left(\frac{1}{c_s^2} - 1\right) A, \quad \text{and } \epsilon, \eta, s \longrightarrow 0. \quad (5.81)$$

Therefore one now turns to the study of non-Gaussianities in the EFT of Inflation.

Insights from the EFT of Inflation

The Effective Field Theory of Inflation [175, 176], reviewed in Sec. 3.4, is a powerful tool to easily compute primordial non-Gaussianities in a generic way from the self-interactions of the Goldstone boson π of broken time diffeomorphisms, though neglecting its mixing with gravity. It encapsulates the leading-order interactions of the previously mentioned situations, slow-roll inflation and k -inflation, and even enables one to go further by taking into account the higher-derivative effects coming from the extrinsic curvature terms. But since the goal of this paragraph is only to be pedagogical, one will dismiss the extrinsic curvature for this discussion and focus on the decoupling limit of the EFT of Inflation at lowest order in derivatives and after a slow-varying approximation has been made, *i.e.* the starting point is Eq. (3.82), which is recalled here (though truncated at cubic order) :

$$S^{(2)} + S^{(3)} = \int d^4x \sqrt{-g} \epsilon H^2 M_{\text{Pl}}^2 \left[\frac{1}{c_s^2} \left(\dot{\pi}^2 - c_s^2 \frac{(\partial_i \pi)^2}{a^2} \right) - \left(\frac{1}{c_s^2} - 1 \right) \left(\frac{A}{c_s^2} \dot{\pi}^3 + \dot{\pi} \frac{(\partial_i \pi)^2}{a^2} \right) \right] \quad (5.82)$$

First, one remembers that already at the level of the quadratic action, a non-trivial speed of sound $c_s^2 < 1$ appears, thus changing the dynamics of linear fluctuations. Still in the slow-varying approximation, solving the linear equations of motion for the interaction picture Goldstone boson π^I and remembering the linear relation to convert it in the adiabatic comoving curvature perturbation, $\mathcal{R}^I = -H_* \pi^I$, one finds a new expression for the fundamental mode function:

$$\mathcal{R}_k^I(\tau) = \frac{H_*}{M_{\text{Pl}} \sqrt{4\epsilon_* c_{s*} k^3}} (1 + i k c_{s*} \tau) e^{-i k c_{s*} \tau} \implies \mathcal{R}_k^{I'}(\tau) = \frac{H_*}{M_{\text{Pl}} \sqrt{4\epsilon_* c_{s*} k^3}} k^2 c_{s*}^2 \tau e^{-i k c_{s*} \tau}, \quad (5.83)$$

where the star denotes evaluation at sound horizon crossing, defined by $k c_{s*} = (aH)_*$.

Then, non-Gaussianities can be computed explicitly. But first, one can make a rough guess of the size of the bispectrum by estimating the non-linearity parameter:

$$f_{\text{NL}} \sim \frac{\mathcal{L}^{(3)}}{\mathcal{R} \mathcal{L}^{(2)}} \sim \mathcal{O} \left(\frac{1}{c_s^2} - 1 \right) + \mathcal{O} \left[\left(\frac{1}{c_s^2} - 1 \right) A \right] \quad (5.84)$$

where one used the approximation around sound horizon $\mathcal{R}_k^{I'} \sim k c_{s*} \mathcal{R}_k^I$, and from which it is clear that large non-Gaussianities can arise in single-field inflation provided scalar perturbations propagate with a small speed of sound, $c_s^2 \ll 1$. Indeed, remember that natural values for the Wilson coefficient A are of order unity and therefore it is unlikely that the amplitude of the bispectrum is significantly boosted by this coefficient only.

However, the precise value of A can crucially affect the shape of the bispectrum, but such statement requires a finer analysis. The big success of the EFToI is that it enables one to describe in a very simple way the dominant interactions, and indeed to cubic order only two operators need to be used to compute the bispectrum: $\mathcal{R}^3$ and $\mathcal{R}'(\partial\mathcal{R})^2$. These two contributions can be computed explicitly, consistently at leading order in the slow varying approximation. For example, the one from the pure time-derivatives interactions is very easy to find and reads

$$\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \hat{\mathcal{R}}_{\vec{k}_3} \rangle' \supset 12 \frac{\epsilon M_{\text{Pl}}^2}{H} \frac{A}{c_s^2} \left(\frac{1}{c_s^2} - 1 \right) \text{Im} \left\{ [\mathcal{R}_{k_1}^{I*} \mathcal{R}_{k_2}^{I*} \mathcal{R}_{k_3}^{I*}] \int_{-\infty^+}^0 d\tau' [a \mathcal{R}_{k_1}^{I'} \mathcal{R}_{k_2}^{I'} \mathcal{R}_{k_3}^{I'}] (\tau') \right\}, \quad (5.85)$$

where the three cyclic permutations of the $\vec{k}_i$ pairs are equivalent and were therefore simply added, and which gives the corresponding contribution to the shape function (the second contribution is algebraically more complicated because of the spatial derivatives, but it is straightforward to compute it and its final form is therefore shown without further explanation):

$$\mathcal{S}_{\mathcal{R}^3} = \frac{3A}{2} \left(\frac{1}{c_s^2} - 1 \right) \frac{k_1 k_2 k_3}{K^3}, \quad (5.86)$$

$$\mathcal{S}_{\mathcal{R}'(\partial\mathcal{R})^2} = \left(\frac{1}{c_s^2} - 1 \right) \frac{1}{k_1 k_2 k_3} \left[-\frac{1}{K} \sum_{i>j} k_i^2 k_j^2 + \frac{1}{2K^2} \sum_{i \neq j} k_i^2 k_j^3 + \frac{3}{2K^3} \prod_i k_i^2 + \frac{1}{8} \sum_i k_i^3 \right].$$

First, one confirms the rough estimates of the size of the non-Gaussianities in the EFToI, boosted by the inverse speed of sound squared. More into the details, both contributions are individually close to the equilateral shape $\mathcal{S}_{\text{eq}}$, but their added combination can deviate quite substantially from it when the coefficient A approaches a particular value. Indeed, evaluating the total shape function on the exact equilateral configuration, one finds:

$$\mathcal{S}(1, 1, 1) = \frac{1}{18} \left(\frac{1}{c_s^2} - 1 \right) \left(A - \frac{17}{4} \right), \quad (5.87)$$

from which it is clear that for $A \simeq 17/4$ the equilateral shape cannot represent the bispectrum of the EFToI. Indeed, around this value of A , the bispectrum shape is more correlated with the orthogonal one [180]. To give a concrete example, in DBI inflation one has $A = 1$ and therefore the bispectrum signal peaks on equilateral configurations, with order unity amplitude if $c_s^2 \sim 0.1$. Barring this cancellation for values of $A \simeq 17/4$, what one has learnt is that kinetic interactions at lowest order result in a mostly equilateral bispectrum.

5.1.3 Primordial non-Gaussianities in multifield inflation

It is difficult to obtain generic analytical results for primordial non-Gaussianities in multifield inflation. Instead, in this section one encounters various physical situations in order to develop some intuition about and understanding of the non-linear mechanisms

in these more complicated scenarios. Except otherwise stated, one has in mind in this section, non-linear sigma models of inflation which feature both a scalar potential and kinetic interactions described by a field-space metric G_{IJ} .

Interactions above the horizon and local non-Gaussianities

First, if all the scalar fields perturbations, *e.g.* the Q^I in the flat gauge, are very light, one has learnt in Sec. 4.2.2 that after horizon crossing they have developed standard two-point functions:

$$P_Q^{IJ}(k) = \frac{2\pi^2}{k^3} \left(\frac{H_*}{2\pi} \right)^2 G^{IJ}. \quad (5.88)$$

Therefore, such models of multifield inflation seem to be simply N_{field} copies of single-field inflation so far (however note the presence of the non-trivial field-space metric inverse, G^{IJ}). But the super-Hubble evolution in multifield inflation is much less trivial than in the single-field scenarios since the curvature perturbation is sourced and does not necessarily reach an adiabatic limit. Therefore, even weak interactions may accumulate for super-Hubble perturbations during the remaining of the inflationary history. Neglecting the contribution from the intrinsic bispectrum of the scalar field just after horizon crossing, an assumption that may be justified if all the light scalar fields are almost decoupled under the horizon, one can focus on the second contribution to the bispectrum of $\mathcal{R}$ in Eq. (5.31) that was found with the δN -formalism:

$$B_{\mathcal{R}}(k_1, k_2, k_3) \simeq N_I N_{JK} N_L [P_Q^{IK}(k_1) P_Q^{JL}(k_2) + 2 \text{ perm.}] . \quad (5.89)$$

In that case, it means that the observable bispectrum is purely the result of the non-linear evolution above the horizon as described by the second-order derivative N_{JK} , of Gaussian random fields Q^I with statistics described by P_Q^{IJ} . Using that $P_Q^{IJ}(k) = G^{IJ} P_Q(k) = G^{IJ} / (N_K N^K) \times P_{\mathcal{R}}(k)$ with $P_Q(k)$ the single-field power spectrum and where one has used the formula for the power spectrum in the δN formalism, Eq. (5.30), one therefore finds that the bispectrum shape coincides with the local form $\mathcal{S}_{\text{loc}}$, with an overall amplitude

$$f_{\text{NL}}^{\text{loc}} = \frac{5}{6} \frac{N^I N_{IJ} N^J}{(N_K N^K)^2}. \quad (5.90)$$

But this should not come as a surprise, since dominant interactions were assumed to come from the super-horizon evolution when spatial derivatives are negligible, and therefore must take place locally in space by definition, thus correlating small and large scales in Fourier space (indeed, remember that the local shape peaks in the squeezed limit where $k_3 \ll k_2 \sim k_1$). With a similar reasoning, the trispectrum is in that case well approximated too, by the non-linear evolution above the horizon of the Gaussian fields Q^I , and its expression with the δN -formalism, Eq. (5.32), can be simplified to:

$$\begin{aligned} T_{\mathcal{R}}(\vec{k}_i) &\simeq N_{IJ} N_{KL} N_M N_N [P_Q^{JL}(k_{13}) P_Q^{IM}(k_3) P_Q^{KN}(k_4) + 11 \text{ perm.}] \\ &\quad + N_{IJK} N_L N_M N_N [P_Q^{IL}(k_2) P_Q^{JM}(k_3) P_Q^{KN}(k_4) + 3 \text{ perm.}] , \end{aligned} \quad (5.91)$$

which also corresponds to a local shape in this approximation, and therefore for which the non-linearity parameters $\tau_{\text{NL}}, g_{\text{NL}}$ are $\vec{k}_i$ -independent:

$$\tau_{\text{NL}} = \frac{N^I N_{IJ} N^{JK} N_K}{(N_L N^L)^3}, \quad \text{and} \quad g_{\text{NL}} = \frac{25}{54} \frac{N_{IJK} N^I N^J N^K}{(N_L N^L)^3}. \quad (5.92)$$

However, note that since there can be in general a non-trivial mixing between first-order and second-order terms in the expression for τ_{NL} , one does not recover *a priori* the proportionality between τ_{NL} and $(f_{\text{NL}}^{\text{loc}})^2$.⁴ Actually, using the Cauchy-Schwarz inequality, it is possible to show the Suyama-Yamaguchi inequality [244] that has already been mentioned once in this thesis:

$$\tau_{\text{NL}} \geq \left(\frac{6}{5} f_{\text{NL}}^{\text{loc}} \right)^2, \quad (5.93)$$

with a bound that is saturated if and only if the vectors N^I coincide with the eigenvectors of the matrix N_{IJ} , as is trivially the case when there is only one field direction. These expressions for $f_{\text{NL}}^{\text{loc}}, \tau_{\text{NL}}, g_{\text{NL}}$ were successively found in Refs. [223, 224, 251] for canonical kinetic terms ($G_{IJ} \delta_{IJ}$).

Sub-horizon interactions and equilateral non-Gaussianities

Local non-Gaussianities may arise in multifield inflation if sub-horizon interactions are negligible, as explained in the previous paragraph. However this is not true in general since one had to assume that all the fields were almost massless and that their mutual couplings were negligible. Using two-field inflation as a prototypical example, with perturbations decomposed in the adiabatic-entropic basis, and once a generalised comoving gauge is chosen, in which $E_{\text{com}} = 0, \psi_{\text{com}} = \mathcal{R}, Q_{\sigma}^{\text{com}} = 0, Q_s^{\text{com}} = \mathcal{F}$ (note that here one has carefully used a different notation, $\mathcal{F}$, to denote the entropic perturbation in this gauge, not to confuse it with the one in the flat gauge, Q_s^{flat} , as such differences matter at the second order in perturbation theory that is relevant for the computation of the bispectrum). The linear EoM are the ones presented in Sec. 4.3, and more precisely Eq. (4.51) with $Q_s^{\text{flat}} \rightarrow \mathcal{F}$ that is justified at the linear order. One will now discuss qualitatively the features of some particular cases of interest.

- When the entropic field is very heavy, see Sec. 5.3 for more precise quantitative statements, but what one has in mind is typically $m_s^2 \gg H^2, k^2/a^2$, it is possible to integrate it out of the theory as is easily seen from the linear EoM for $\mathcal{F}$, which reads in this massive limit and at leading order in m_s^{-2} :

$$\mathcal{F} \simeq -2\sqrt{2}\epsilon\eta_{\perp} \frac{H M_{\text{Pl}}}{m_s^2} \dot{\mathcal{R}}, \quad (5.94)$$

⁴Note that in the limit of single-field, slow-roll inflation, one finds straightforwardly that $\tau_{\text{NL}} = (6f_{\text{NL}}^{\text{loc}}/5)^2$, and that the scaling of the non-linearity parameters as determined by the first derivatives of N with respect to the initial field ϕ , coincides with the expected amplitudes from in-in calculations: $f_{\text{NL}}^{\text{loc}} \sim \mathcal{O}(\epsilon, \eta), g_{\text{NL}} \sim \mathcal{O}[(\epsilon, \eta, \epsilon_3)^2]$. But of course, a careful computation of the exact coefficients would add up the missing terms of similar amplitude coming from the sub-Hubble interactions that were neglected here, because what one had in mind in this paragraph were larger contributions from the super-horizon evolution in multifield inflation.

whence $\mathcal{F}$ simply becomes a constrained quantity, just like the lapse and the shift. This result is far from trivial since it means that the two-field model effectively behaves as a single-field one. However, the fact that $\mathcal{F}$ is integrated out and not just truncated from the spectrum of particles relevant for inflation, will impact the dynamics of $\mathcal{R}$ which therefore may deviate from the single-field, slow-roll behaviour with canonical kinetic terms. Note also that the second degree of freedom is only integrated out at the level of the perturbations, and that *a priori* the background trajectory remains purely multifield. That is why the resulting theory is called a *single-field effective theory of fluctuations*. Replacing $\mathcal{F}$ as a function of $\mathcal{R}$ every where in the action results in a breaking of Lorentz invariance for the comoving curvature perturbation at the level of linear fluctuations already, as it then develops a speed of sound smaller than unity [49, 55, 62, 179, 252]:

$$\frac{1}{c_s^2} - 1 = \frac{4H^2\eta_\perp^2}{m_s^2}. \quad (5.95)$$

When the bending is small, $\eta_\perp^2 \ll m_s^2/H^2$, the deviation of c_s^2 from unity is however completely negligible, which means that the two-field system is actually behaving as a single-field, slow-roll one: primordial non-Gaussianities are negligible. But when the bending is sizeable (remember that rigorously m_s^2 has a negative contribution from $\eta_\perp^2$ and therefore can become negative if the bending dominates over the two other contributions; here one still assumes the standard case where $m_s^2 > 0$ even though $\eta_\perp^2 \gg 1$), the deviation of c_s^2 from unity is large and one typically expects to find large non-Gaussianities in equilateral (or orthogonal) configurations, as in the case of higher-derivatives model of single-field inflation that was treated above.⁵

- When the entropic field is very light, there is another regime of validity in which it may be integrated out, but that results this time in a modified dispersion relation for $\mathcal{R}$. In that case, $m_s^2 \ll H^2, k^2/a^2$ and before horizon exit the linear EoM for $\mathcal{F}$ may be approximately solved in the same way as shown above provided the formal replacement $m_s^2 \rightarrow k^2/a^2$. Therefore, this results in a k -dependent speed of sound for $\mathcal{R}$:

$$\frac{1}{c_s^2(k)} - 1 = \frac{4H^2\eta_\perp^2}{k^2/a^2}. \quad (5.96)$$

Again, when the bending is small (or simply when the corresponding mode is still very deep in the horizon), $\eta_\perp^2 \ll k^2/(a^2H^2)$, one recovers the standard single-field behaviour and small non-Gaussianities. However if the bending is sizeable, there

⁵This discussion has dismissed the effect of integrating out $\mathcal{F}$ in the cubic action, and has not considered explicitly the resulting cubic self-interactions for $\mathcal{R}$. This is done consistently and exhaustively for all cubic interactions in Ref. [2], see Sec. 5.3.1, where we have shown that also at the cubic level, one recovers a $P(X)$ -like action, provided the identification shown in eq. (5.81) where now the parameter A is not a unknown Wilson coefficient as in the EFToI but is rather derived from the two-field UV completion and depends on the full multifield features: bending of the background trajectory, mass of the entropic field, curvature of the field space, etc.

may be a regime in sub-Hubble scales for which $\eta_{\perp}^2 \gg k^2/(a^2 H^2) \gg 1$ and the deviation of c_s^2 from unity is large and dominated by the term $\propto k^2$, therefore resulting in a non-linear dispersion relation $\omega(k) \propto k^2$. This interesting but peculiar regime is also met in the so-called ghost inflation scenario [253], and in the EFToI [176, 254] when extrinsic curvature terms are taken into account as one understood in Sec. 3.4. The consequences of this non-linear dispersion relation for the primordial power spectrum and non-Gaussianities have been further studied in Refs. [61, 179, 255], although to my humble knowledge no exhaustive analysis of the resulting cubic self-interactions of $\mathcal{R}$ in this regime has been made so far. The resulting adiabatic mode function has a very peculiar form due to an order-one logarithmic derivative of the speed of sound under the horizon, $s \sim -1$, and a gradient term $\propto k^4$ instead of k^2 . It is generically expected to result in a bispectrum shape mostly equilateral although slightly correlated with the orthogonal one [179]. A concrete two-field setup with a curved field space and exhibiting a single-field effective theory with such non-linear dispersion relation, can be found in Ref. [77] where the exact bispectrum is computed numerically and found to precisely coincide with the equilateral shape.

Probing the squeezed limit: the cosmological collider

Setup. The squeezed limit of the bispectrum in multifield inflation is particularly interesting because it provides a non-trivial example where an analytical understanding is possible, although only in a perturbative way as is explained below, and demonstrates clearly how primordial non-Gaussianities may be used as a cosmological collider: the signal in this limit depends strongly on the mass (and spin, if any) of the extra particle, which one may hope to measure in the future. The literature on the topic is huge, for a partial selection of interesting articles see *e.g.* Refs. [51, 52, 63, 67, 73, 76, 204, 205], and the current paragraph does not aim at reproducing all known results in a faithful way.

Rather, one focuses on one of the main features of the bispectrum of two-field inflation, that can be analytically computed using the in-in formalism, in the particular framework called Quasi-Single-Field inflation [51, 52]. For this, one begins with the quadratic two-field Lagrangian for $\mathcal{R}, \mathcal{F}$ that were defined in the previous paragraph, and which reads:

$$\mathcal{L}^{(2)} = a^3 \left[\epsilon M_{\text{Pl}}^2 \left(\dot{\mathcal{R}}^2 - \frac{(\partial \mathcal{R})^2}{a^2} \right) + \frac{1}{2} \left(\dot{\mathcal{F}}^2 - \frac{(\partial \mathcal{F})^2}{a^2} - m_s^2 \mathcal{F}^2 \right) + 2\sqrt{2}\epsilon M_{\text{Pl}} H \eta_{\perp} \dot{\mathcal{R}} \mathcal{F} \right]. \quad (5.97)$$

Importantly, the free Hamiltonian is *not* chosen to coincide exactly with the quadratic one, as no generic analytical solution of the coupled linear EoM is known when the mixing $\propto \eta_{\perp}$ is not vanishing. Therefore, one decomposes $\mathcal{H}^{(2)} = \mathcal{H}_{\text{free}} + \mathcal{H}_{\text{int}}^{(2)}$ with:

$$\mathcal{H}_{\text{int}}^{(2)} = -\sqrt{\frac{2}{\epsilon}} \frac{H \eta_{\perp}}{M_{\text{Pl}}} p_{\mathcal{R}} \mathcal{F}. \quad (5.98)$$

The interaction picture mode functions, $\mathcal{R}^I$ and $\mathcal{F}^I$ can be found by solving the linear EoM *without* the mixing $\propto \eta_\perp$ since it was removed in the definition of the free Hamiltonian. Even in this simplified picture, one must use a slow-varying approximation around the time of horizon crossing in order to find explicit formulae, that read:

$$\mathcal{R}_k^I(\tau) = \frac{H}{\sqrt{4\epsilon M_{\text{Pl}} k^3}} (1 + ik\tau) e^{-ik\tau}, \quad (5.99)$$

$$\mathcal{F}_k^I(\tau) = \frac{\sqrt{\pi}}{2} e^{i(\nu-1/2)\frac{\pi}{2}} H(-\tau)^{3/2} H_\nu^{(1)}(-k\tau), \quad (5.100)$$

where one reminds that:⁶

$$\nu = \left(\frac{9}{4} - \frac{m_{s,\text{eff}}^2}{H^2} \right)^{1/2}, \quad (5.101)$$

is either real and positive for a light entropic perturbation or purely imaginary (with positive imaginary part) for a heavy one, and $H_\nu^{(1)}$ is the Hankel function of the first kind with parameter ν .

The cubic order Hamiltonian is also taken into account as part of the interaction Hamiltonian in order to compute the bispectrum of the model in a perturbative setup, which therefore gives:

$$\mathcal{H}_{\text{int}} = \mathcal{H}_{\text{int}}^{(2)} + \mathcal{H}^{(3)}. \quad (5.102)$$

Correction to the power spectrum. Note that this particular interaction scheme allows for quadratic interactions for the interaction picture fields $\mathcal{R}^I, \mathcal{F}^I$. In particular, the master in-in formula gives *tree-level* contributions to the power spectrum of $\mathcal{R}$ that come from inserting an even number of quadratic interaction Hamiltonians $\hat{H}_I^{(2)} = \hat{H}_{\text{int}}^{(2)}(\mathcal{R}^I, \mathcal{F}^I)$. The leading-order correction corresponds to a scalar-exchange diagram which is shown in Fig. 5.4, and that one shall denote $\left\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \right\rangle_{(2)}$ since it begins at quadratic order in $\hat{H}_I^{(2)}$. Although this result concerns only the Gaussian statistics of

⁶Why is it $m_{s,\text{eff}}^2$ and not m_s^2 which appears in the definition of ν that is relevant for $\mathcal{F}^I$? The answer is subtle, but first note that *a priori* the question is not relevant: the difference between those two mass scales is $4H^2\eta_\perp^2$ which has to be negligible by consistency of the perturbative expansion. However, if one is interested in the limit where $\eta_\perp$ reaches the boundary of this regime of validity, say $\eta_\perp \lesssim 1$, the difference might matter. Remember that the splitting between free part and interaction terms is made at the level of the Hamiltonian, and not of the Lagrangian, a fact that has the following consequence. In the Hamiltonian, the mass term for $\mathcal{F}$ is actually $m_{s,\text{eff}}^2/2 \times \mathcal{F}^2$, but there is also the mixing term $-\sqrt{2\epsilon}H\eta_\perp/M_{\text{Pl}} \times \mathcal{F}p_{\mathcal{R}}$ where crucially $\dot{\mathcal{R}}$ is thus not the only contribution to the conjugate momentum $p_{\mathcal{R}}$ in the full theory: $p_{\mathcal{R}} \supset \sqrt{\epsilon}M_{\text{Pl}}H\eta_\perp\mathcal{F}$. The Hamilton equations then result in an EoM for $\mathcal{F}$ with a mass term $\propto m_s^2$ once both effects are taken into account, consistently with the Lagrangian description as it should. But in the interaction scheme, the conjugate momentum of $\mathcal{R}^I$ is simply given by $\dot{\mathcal{R}}^I$ since now the mixing term is treated as an interaction, $p_{\mathcal{R}}^I \propto \dot{\mathcal{R}}^I$, and therefore the EoM for $\mathcal{F}^I$ has a mass term $\propto m_{s,\text{eff}}^2$ and ν can only involve $m_{s,\text{eff}}^2$.

$\mathcal{R}$, it shown here how to compute it. The two-point function at tree level is given by:

$$\begin{aligned} \langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \rangle &= \langle 0 | \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I | 0 \rangle + 2\text{Re} \left\{ \left\langle 0 \left| \int_{-\infty}^t dt' [\hat{H}_I^{(2)}(t'), \hat{\mathcal{R}}_{\vec{k}_1}^I \hat{\mathcal{R}}_{\vec{k}_2}^I] \int_{-\infty}^{t'} dt'' \hat{H}_I^{(2)}(t'') \right| 0 \right\rangle \right\}, \\ &+ \dots, \end{aligned} \quad (5.103)$$

where the $\dots$ begin at fourth order in $\hat{H}_I^{(2)}$. Note also that at the same, quadratic order in $\hat{H}_I^{(2)}$, there is a loop diagram with two internal $\mathcal{F}$ -propagators starting and finishing at two cubic vertices of the form $\mathcal{R}\mathcal{F}^2$ that must be there in the cubic Lagrangian. But loops shall not be considered in the following, and one rather focuses on tree-level calculations. More explicitly, one finds the quadratic correction $\langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \rangle_{(2)}$ in a slow-varying approximation to be:

$$\begin{aligned} \langle \hat{\mathcal{R}}_{\vec{k}_1} \hat{\mathcal{R}}_{\vec{k}_2} \rangle_{(2)} &= (2\pi)^3 \delta^{(3)}(\vec{k}_1 + \vec{k}_2) 16\epsilon M_{\text{Pl}}^2 H^2 \eta_{\perp}^2 \int_{-\infty}^0 d\tau' a^3(\tau') \int_{-\infty}^{\tau'} d\tau'' a^3(\tau'') \times \\ &\quad \underbrace{\text{Re} [2\mathcal{F}_{k_1}^{I*}(\tau'') \mathcal{F}_{k_1}^I(\tau') \mathcal{R}_{k_1}^I \mathcal{R}_{k_1}^{I*}(\tau'') (\mathcal{R}_{k_1}^I \mathcal{R}_{k_1}^{I*}(\tau') - \mathcal{R}_{k_1}^{I*} \mathcal{R}_{k_1}^I(\tau'))]}_{-4\text{Im}(\mathcal{R}_{k_1}^I \mathcal{R}_{k_1}^{I*}(\tau')) \text{Im}[\mathcal{F}_{k_1}^{I*}(\tau'') \mathcal{F}_{k_1}^I(\tau') \mathcal{R}_{k_1}^I \mathcal{R}_{k_1}^{I*}(\tau'')]} \end{aligned} \quad (5.104)$$

where as anticipated one was able to use the anti-hermiticity of the remaining quantum commutator to write the result as a product of two imaginary parts. Then inserting the explicit mode functions $\mathcal{R}_k^I(\tau), \mathcal{F}_k^I(\tau)$ shown in Eq. (5.99), and making the changes of variable $x = -k_1\tau', y = -k_1\tau''$, one eventually gets the corrected dimensionless power spectrum:

$$\begin{aligned} \mathcal{P}_{\mathcal{R}} &= \frac{H^2}{8\pi^2\epsilon M_{\text{Pl}}^2} (1 + \mathcal{C}), \quad \text{with} \\ \mathcal{C} &= 4\eta_{\perp}^2 \pi e^{-\pi\text{Im}(\nu)} \times \text{Im} \left[\int_0^{\infty} dx x^{-1/2} \sin(x) H_{\nu}^{(1)}(x) \int_x^{\infty} dy y^{-1/2} e^{-iy} \left(H_{\nu}^{(1)}(y) \right)^* \right]. \end{aligned} \quad (5.105)$$

Of course, a consistency requirement is that the correction is small, $\mathcal{C} \ll 1$, which is indeed enforced by $\eta_{\perp} \ll 1$ coming from the necessity to have $\int dt \hat{H}_I^2(t) \ll 1$ in the perturbative expansion of the in-in formalism. Otherwise, an infinite amount of diagrams would need to be computed. Also, all background quantities were supposed to be constant around the time of horizon crossing that participates the most to the power spectrum for a given mode k_1 . Note eventually that the final contribution has an exponential suppression, $e^{-\pi\text{Im}(\nu)}$ for a massive entropic perturbation reaching the threshold $m_{s,\text{eff}}^2/H^2 \geq 9/4$, as indeed in that case it is exponentially decaying in the super-horizon limit, as already discussed at several places in this thesis. For all these reasons, the overall contribution from the entropic field to the adiabatic power spectrum in this setup, is negligible compared to the single-field counterpart. However, there is a well-know quantity that single-field inflation is known not to produce any observable

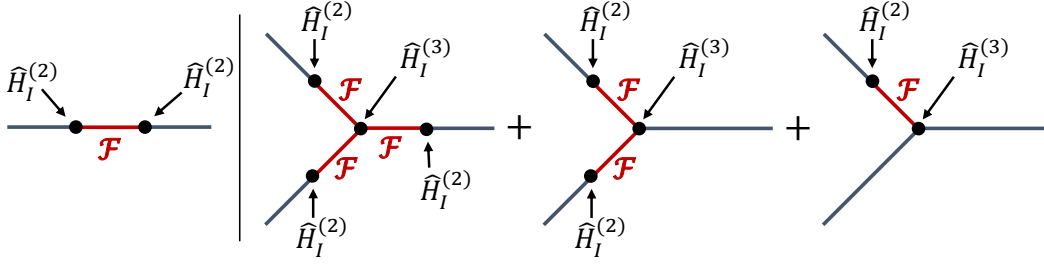


Figure 5.4: Leading-order, tree-level contributions to the two-point and three-point functions from exchanges of a virtual entropic perturbation $\mathcal{F}$. (Left panel:) The largest tree-level contribution to the power spectrum from the exchange of a single scalar particle, that is fully computed in the main text. (Right panel:) The three kinds of cubic interactions giving the largest contributions and resulting in the three different diagrams that are represented. From left to right one has: $\mathcal{F}^3$ cubic interaction with three quadratic mixings, $\mathcal{F}^2\mathcal{R}$ with two quadratic mixings, $\mathcal{F}\mathcal{R}^2$ with one quadratic mixing. They *a priori* all contribute to the final bispectrum, but in the text one focuses on the first of the three only.

signal for: primordial non-Gaussianities, and more particularly the squeezed limit of the bispectrum, and therefore the correction coming from the interaction scheme, might actually end up being the dominant one.

Bispectrum: generalities and the squeezed limit. *A priori*, all kinds of two-field cubic interactions between $\mathcal{R}$ and $\mathcal{F}$, as explicated in Ref. [2], should be taken into account in the computation of the bispectrum, resulting in the different tree-level diagrams represented in Fig. 5.4. Historically the considered interaction is, following the notations used in this thesis:

$$H_{\text{int}}^{(3)} \supset a^3 V_{;sss} \mathcal{F}^3. \quad (5.106)$$

Counting all possible permutations shows that ten independent terms contribute to the three-point function just from this cubic interaction, combined as it should with three quadratic ones. It is much beyond the scope of this paragraph to list them and compute them explicitly, so instead one will simply jump to the result found in the literature. First, the whole shape has been computed numerically in the case of a real ν , *i.e.* for $0 \leq m_{s,\text{eff}}^2/H^2 \leq 9/4$, and interestingly enough interpolates between the equilateral shape for large values of the entropic mass, and the local shape for lighter cases [51, 52]. This corresponds to the qualitative expectation from the analysis presented in the previous paragraph about sub-Hubble interactions between adiabatic and entropic perturbations: if the mass is of order H , it decays quickly around horizon exit and therefore interactions are maximal when all modes are exiting at the same time, *i.e.* at equilateral configurations, while when it is very light, interactions keep happening for some time after horizon exit, locally in real space and therefore making the bispectrum closer to the local shape. The full numerical result lies in between those two shapes,

and the overall amplitude of the signal can be estimated by looking at the value of the bispectrum shape at the exact equilateral configuration semi-analytically [52],

$$\mathcal{S}(k, k, k) = -\frac{9}{10}\alpha(\nu)\frac{V_{;sss}}{H}\eta_{\perp}^3 A_s^{-1/2}, \quad (5.107)$$

where both $\eta_{\perp}, V_{;sss}/H \ll 1$ as required by the consistency of the perturbative scheme, $A_s = 2.10 \times 10^{-9}$ is the dimensionless scalar power spectrum, and $\alpha(\nu)$ is a numerical factor that needs a careful numerical integration to be found: it is a monotonically increasing function of ν , starting at $\alpha(0) \sim 0.2$ and then slowly increasing ($\alpha(0.8) \sim 1$) before blowing up for very light fields ($\alpha(1) \sim 10$ and $\alpha(1.35) \sim 300$), see Fig. 8 of Ref. [52] (The formal divergence as $\nu \rightarrow 1.5$ is unphysical and rather signals that perturbative control is lost because of cumulative effects from the frozen entropic perturbation on large scales). Because of the rather large value $A_s^{-1/2} = 2.2 \times 10^4$, the overall amplitude of the bispectrum can be large even in the controlled perturbative regime corresponding to $\eta_{\perp}, V_{;sss}/H \ll 1$, therefore making it observable. If the entropic field is light, then the function $\alpha(\nu)$ boosts the signal even more.

Importantly, the squeezed limit of the bispectrum can be estimated analytically. Although there is still an overall k -independent factor to be determined numerically because consisting in several integrals of Hankel functions, the scaling behaviour in the squeezed limit is explicitly dependent on the mass of the entropic field, therefore making the probe of the bispectrum in the squeezed limit the equivalent of a particle collider in cosmology. For a real ν , one finds [52]:

$$\mathcal{S}(k_1, k_2, k_3)_{k_3 \ll k_2 \sim k_1} \simeq -\frac{2}{3\pi}s(\nu)\frac{V_{;sss}}{H}\eta_{\perp}^3 A_s^{-1/2} \left(\frac{k_1}{k_3}\right)^{\nu-1/2}, \quad (5.108)$$

where $s(\nu)$ is monotonically increasing from $\nu > 1/2$ ($s(0.5) \sim 3, s(1) \sim 12$, for more details see Fig. 9 of Ref. [52]), for which the squeezed limit of the bispectrum is enhanced by the squeezing parameter $\kappa = k_3/k_1 \ll 1$ to a negative power: $\mathcal{S} \propto \kappa^{1/2-\nu}$, making it again potentially observable. To be precise, the squeezed limit of the bispectrum almost coincides with the local shape in this limit, but strictly speaking the squeezing power-law behaviour is different because of the parameter ν , and therefore may be called a *quasi-local* shape.

In Ref. [63], the authors not only considered more generic quadratic and cubic interactions between $\mathcal{R}$ and a second scalar field σ not as much constrained as the entropic field $\mathcal{F}$, in the spirit of a multi-field EFT of inflation, but also generalised the computation of the bispectrum to a potentially imaginary ν parameter. Actually, a simple way to extend the result to such heavy extra particles, is simply to analytically continue the result of the bispectrum in the squeezed limit, Eq. (5.108), to complex values of ν . In terms of the $x_i = k_i/k_1 \leq 1$, the result is therefore [63]:

$$\mathcal{S}(1, 1, \kappa)_{\kappa \ll 1} \propto \sqrt{\kappa} \cos [\text{Im}(\nu) \log(\kappa) + \varphi(\nu)], \quad (5.109)$$

where $\varphi(\nu)$ is a ν -dependent but k -independent phase. In the case of a heavy extra particle, one can see that the squeezing parameter actually decreases the amplitude of

the signal in the squeezed limit (consistently with the fact that the bispectrum shape should rather coincide with an equilateral one in this limit). But very interestingly, the signal is now modulated by a long-wavelength in the κ -domain, with a frequency directly given by the mass of the heavy field: $\text{Im}(\nu) = \sqrt{m_{s,\text{eff}}^2/H^2 - 9/4}$. A detection of such modulated signal in the bispectrum would be a smoking-gun evidence for the presence of an extra particle beyond the inflaton, and would even provide a measurement of the mass of this extra particle! Of course, one could, and should, worry that the overall amplitude of the signal would be weak because of the squeezing that plays against its observation. Although this is true, there may remain a hope that the above result roughly holds true at the limit of the regime of validity of perturbation theory, where $\eta_\perp, V_{;sss}/H^2 \lesssim 1$, therefore making the signal large enough to be observed even in this squeezed limit. For numerical works that go beyond the perturbative coupling, see Refs. [256, 257].

Extensions. The general idea that probing the squeezed limit of the bispectrum amounts to building a cosmological collider, has been further developed in the so-called *cosmological collider* program [67], where it has been extended to more general particles than the scalar fields usually studied in inflation: spinning particles and gauge fields were also added to the description, resulting in an additional line-of-sight dependence of the signal, $\propto P_s(\vec{k}_1 \cdot \vec{k}_3)$ where P_s is the s -th Legendre polynomial. See also Ref. [73] on the topic of spinning particles, where the squeezed limit is cleverly considered from the beginning, which enables one to avoid many of the difficulties of the initial QSF setup. Building on these discoveries, recent years have seen the emergence of a new field of research in theoretical primordial cosmology, the so-called *cosmological bootstrap* program [76] aiming at constraining the possible forms of the inflationary correlation functions at the end of inflation by directly imposing the symmetries of a (quasi-) de Sitter space, as well as physical principles such as unitarity and locality, at the final boundary of the inflationary epoch, without describing the full time evolution in the bulk spacetime. Although this domain is new, it is rapidly developing, and many new results have been found that were not known at the beginning of my thesis.

Moreover, I am currently extending the QSF setup to more than one entropic field as parameterised in my recent work [3], together with S. Aoki, S. Renaux-Petel and M. Yamaguchi. Interesting physical effects may arise due to non-trivial interactions in the entropic sector, that are then transferred to the adiabatic curvature perturbation due to the quadratic mixing. Stay tuned!

5.1.4 Observational constraints

This short paragraph mentions very quickly how CMB observations by the Planck satellite enable one to place constraints on the amount of primordial non-Gaussianities. Indeed, they have not been detected so far. The results from the Planck analysis [39] are summarised in Table 5.1.4.

Parameter	$f_{\text{NL}}^{\text{loc}}$	$f_{\text{NL}}^{\text{eq}}$	$f_{\text{NL}}^{\text{ortho}}$	$g_{\text{NL}}^{\text{loc}}$
Value	-0.9 ± 5.1	-26 ± 47	-38 ± 24	$(-5.8 \pm 6.5) \times 10^4$

5.2 Transient tachyonic instability and enhanced non-Gaussianities in flattened configurations (article)

If the squeezed limit of the bispectrum is undoubtedly of utmost interest, both for its theoretical and phenomenological features, its overall amplitude may well be unobservably small, even in multifield inflation due to the dependence on the squeezing parameter for an extra heavy field, and the possible smallness of the coupling constants. In particular, the formalism presented above with the in-in formalism, requires $\eta_{\perp} \ll 1$ for the perturbation scheme to remain valid. Although this may be justified in certain circumstances, the resulting bispectrum does not encapsulate the *large bending* regime described by $\eta_{\perp} \gg 1$, which had been so far only handled numerically. In Ref. [1],

J. Fumagalli, S. Garcia-Saenz, L. Pinol, S. Renaux-Petel, J. Ronayne. 2019, HYPER NON-GAUSSIANITIES IN INFLATION WITH STRONGLY NONGEODESIC MOTION, *Physical Review Letters (PRL)* 123, 201302,

that is reproduced below, we investigated both analytically and numerically such multifield scenarios featuring a background trajectory with a *large geodesic deviation*, and found that they generically lead to a transient, tachyonic instability on sub-Hubble scales as described in Sec. 4.3.3. Importantly, the instability is bounded both in the UV and in the IR at a given time, or equivalently for a given mode the instability is only transient. This ensures that there is no fundamental instability at the level of the full theory, and we checked that perturbative control is still verified. But interestingly, we found both analytically and numerically that the bispectrum of these multifield setups has a shape that correlates most with a flattened shape, in the same spirit as the excited initial states explained in Sec. 5.1.2. A major difference though, is that this flattened shape is the main contribution to the total shape of the bispectrum, and its amplitude is overall much larger, typically $f_{\text{NL}}^{\text{flat}}$ ranges from 10 to 100 depending on the details of the model at hand. Around that time and just after, Refs. [79, 206] confirmed those findings.

The numerical treatment relies on **PyTransport** [70, 72, 74], a code that evolves two-point and three-point correlation functions of the full multifield theory and exhibits the shape and amplitude of the bispectrum of $\mathcal{R}$ at the end of inflation. Because this is one of the main results of the paper, this figure is reproduced here. The representation is slightly different from the one that was used in this thesis since the wavenumbers forming a triangle in Fourier space with perimeter K have a shape parameterised by two numbers α, β : $k_1 = K/2 \times (1 - \beta)$, $k_2 = K/4 \times (1 + \alpha + \beta)$, $k_3 = K/4 \times (1 - \alpha + \beta)$.

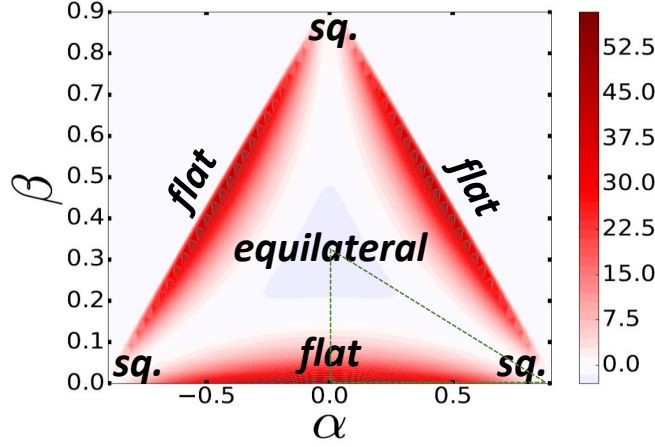


Figure 5.5: Amplitude and shape of the bispectrum in a prototypical model of “hyper-inflation”, *i.e.* a two-field model of inflation with a negatively curved field space and a strongly non-geodesic motion. The (α, β) -plane is annotated to help reading it: “sq.” stands for squeezed triangle, “flat” for flattened triangles, “equilateral” for equilateral triangle. The bispectrum has a shape correlating most with the flattened shape and, ordering the wavenumbers as $k_3 \leq k_2 \leq k_1$ to avoid redundancies (corresponding to $\alpha \geq 0$ and $\beta \leq (1 - \alpha)/3$, *i.e.* only the 1/6-th of the total figure situated at the bottom right corner delimited by the green dashed line), the largest amplitude is reached for triangles with $\alpha = \beta = 0$ corresponding to $k_3 = k_2 = k_1/2$, with $f_{\text{NL}}^{\text{flat}} \simeq 50$. For comparison, evaluating the shape in the equilateral configuration gives $f_{\text{NL}}^{\text{eq}} \simeq -1$, while it is vanishing in the squeezed limit as expected from the single-field effective theory and the fact that $m_{s,\text{eff}}^2/H^2 \gg 1$.

Therefore the figure is annotated in order to explain to which triangle corresponds a given region in the (α, β) -plane.

Although this numerical approach is extremely powerful, it does not grasp the interesting physics at hand, and moreover does not allow the computation of higher-order correlations. That is why we used and further developed a novel analytical approach, initiated in Refs. [77, 78], where the entropic field is integrated out as it was explained around Eq. (5.95), making use of the fact that the *absolute value* of m_s^2 is large, even though m_s^2 itself is actually negative, therefore leading to an exponential amplification of the entropic modes, that is efficiently transferred to the adiabatic sector thanks to the large coupling $\eta_\perp$. This results in a single-field effective theory for $\mathcal{R}$ which features an *imaginary* speed of sound, reminiscent from the full two-field instability. Using this EFT, we were able to analytically compute the leading-order piece to the bispectrum, a computation that clearly shows the similarities with the case of excited initial states and the appearance of the boosted configurations due to terms inversely proportional to $\tilde{k}_3 = k_1 + k_2 - k_3$ for example. Moreover, we have analytically estimated the size of

all n -point functions and showed that they were all maximal at generalised “flattened” shapes.

Besides this interesting phenomenology, these models can be interesting theoretically, since a strong bending scenario is what is required in order to respect the swampland conjectures [189]. Moreover, they enable the Universe to inflate for a sufficiently long amount of time, even though the potential is not flat in Planck mass units, a potentially interesting feature regarding the η -problem as reviewed in Sec. 4.1.1.

The original article as published in PRL is now displayed, together with its Appendix.⁷ The notations used are close to the ones of this thesis but not completely: in the article we use ζ to denote the comoving curvature perturbation which has been consistently written $\mathcal{R}$ in this thesis, and the entropic perturbation in the flat gauge is Q_s there while it corresponds more precisely to Q_s^{flat} .

⁷In this article (and the following ones), I have chosen to keep the Introduction, Conclusion and Bibliography as they are in the published version, in order not to break it (them) down in pieces that are not self-contained. I apologise for any redundancy.

Hyper-Non-Gaussianities in Inflation with Strongly Nongeodesic Motion

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Several recent proposals to embed inflation into high-energy physics rely on inflationary dynamics characterized by a strongly nongeodesic motion in negatively curved field space. This naturally leads to a transient instability of perturbations on sub-Hubble scales, and to their exponential amplification. Supported by first-principles numerical computations, and by the analytical insight provided by the effective field theory of inflation, we show that the bispectrum is enhanced in flattened configurations, and we argue that an analogous result holds for all higher-order correlation functions. These “hyper-non-Gaussianities” thus provide powerful model-independent constraints on nonstandard inflationary attractors motivated by the search for ultraviolet completions of inflation.

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Introduction.—Negatively curved field space plays a crucial role in modern embeddings of inflation in high-energy physics. Nonlinear sigma models with a hyperbolic target space arise naturally in top-down realizations of inflation, particularly within supergravity, giving rise to the α -attractor class of models (see, e.g., Refs. [1–3]). Independently of the question of their ultraviolet completions, nonminimal kinetic terms of the hyperbolic type lead to interesting dynamics, allowing for nontrivial inflationary trajectories characterized by a strongly nongeodesic motion [4–7]. This in turn relaxes the conditions of slow-roll to allow for potentials that are steep in Planck units [8,9], a welcome feature in view of the eta problem and the recently much discussed swampland conjectures [10–12]. Lastly, internal field spaces with negative curvature are at the origin of the phenomenon of geometrical destabilization [13–17], in which noninflationary degrees of freedom, even heavy ones, can dramatically affect the fate of inflation.

A concrete scenario in which the consequences of a hyperbolic field space have been studied is the proposal of “hyperinflation” [18], which has recently been under scrutiny [19,20]. The intuitive picture of this setup is that of an inflationary trajectory corresponding to a circular motion around the minimum of a (circularly symmetric) scalar potential. The hyperbolic geometry is crucial to compensate for the loss of angular velocity to the Hubble friction, allowing inflation to last long enough, even if the potential is too steep to inflate along a radial trajectory.

Within this circumstance, hyperinflation proceeds along a strongly nongeodesic trajectory, and a striking outcome is an exponential growth of the curvature power spectrum around the time of Hubble crossing, and the corresponding suppression of the tensor-to-scalar ratio. With such an amplification, assessing the size of nonlinear effects in this setup appears to be crucial, while previous studies have restricted their attention to the analysis of linear fluctuations.

In this context, this Letter presents a general framework to study non-Gaussianities in the presence of strongly nongeodesic motion typical of hyperbolic-type geometry, highlighting how this naturally leads to “hyper-non-Gaussianities.” For definiteness we concentrate on the specific example of hyperinflation as a particularly interesting playground to analyze the effects of the nontrivial field space in this class of models. However our results are formulated in general terms and have a broad range of applicability. Essentially, they indicate that in negatively curved field space, inflationary models with strongly nongeodesic motion are characterized by an enhanced non-Gaussian signal, both for the bispectrum and for all higher-point correlation functions, that can easily lead to tensions with experimental bounds. These model-independent constraints sharpen the range of allowed theoretical constructions, and are of utmost importance in view of the intense current efforts to build nonstandard inflationary scenarios in agreement with quantum gravity conjectures.

Hyperinflation.—The starting point is an action for two scalar fields $\varphi^I = (\phi, \theta)$ with noncanonical kinetic term minimally coupled to gravity:

$$S = \int d^4x \sqrt{-g} \left(\frac{M_{\text{Pl}}^2}{2} R - \frac{1}{2} G_{IJ} \nabla^\mu \varphi^I \nabla_\mu \varphi^J - V(\varphi) \right). \quad (1)$$

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The matrix G_{IJ} defines a metric in the internal field space parametrized by the coordinates φ^I , in this case the hyperbolic plane of curvature $-2/M^2$, and is assumed to have the form

$$G_{IJ}d\varphi^I d\varphi^J = d\phi^2 + M^2 \sinh^2\left(\frac{\phi}{M}\right) d\theta^2. \quad (2)$$

Moreover, the potential is assumed to depend only on the “radial” field ϕ , $V = V(\phi)$, with $V' > 0$.

Consider now an inflationary background characterized by homogeneous fields $\phi(t)$ and $\theta(t)$, and a quasi-de Sitter spacetime metric with scale factor $a(t)$ and Hubble parameter $H(t) = \dot{a}/a$, with t the cosmological time. Hyperinflation corresponds to a nonstandard attractor solution of the action (1), with small parameters $\epsilon \equiv -\dot{H}/H^2 \simeq 3MV'/2V$ and $\eta \equiv \dot{\epsilon}/H\epsilon \simeq 2\epsilon - 3MV''/V'$, that arises under the conditions

$$\frac{3M}{M_{\text{Pl}}} < \frac{M_{\text{Pl}} V'}{V} \ll \frac{M_{\text{Pl}}}{M}, \quad \frac{M|V''|}{V'} \ll 1. \quad (3)$$

More precisely, the equation of motion $\ddot{\phi} + 3H\dot{\phi} - M \sinh(\phi/M) \cosh(\phi/M) \dot{\theta}^2 + V'(\phi) = 0$ admits a solution with $\dot{\phi} \simeq -3MH$, independently of the slope of the potential. Defining $h^2 \equiv [V'(\phi)/MH^2] - 9$, a positive quantity for hyperinflation solutions [see Eq. (3)], one has $h^2/9 + 1 \simeq \epsilon_V/\epsilon \simeq \eta_V/(2\epsilon - \eta)$, where $\epsilon_V = \frac{1}{2}M_{\text{Pl}}^2(V'/V)^2$ and $\eta_V = M_{\text{Pl}}V''/V$ are the standard potential “slow-roll” parameters, not necessarily small here. In hyperinflation, potentials that verify the swampland de Sitter conjecture (in its refined version [21,22]) should obey either $\epsilon_V \geq \mathcal{O}(1)$ or $-\eta_V \geq \mathcal{O}(1)$, corresponding, respectively, to a steep slope or steep negative curvature in Planck units. From the above relations, one deduces that a prolonged phase of hyperinflation supported by such potentials is necessarily characterized by $h^2 \gg 1$ (see also Ref. [20]). We will concentrate on this theoretically most interesting regime, which, as we will see, corresponds to a strongly nongeodesic motion. Actually, as emphasized recently in a model-independent manner [9], the latter feature is necessary in order to inflate on potentials whose slope is steep in Planck units, and it is also a characteristic feature of the sidetracked models studied in Ref. [6].

Strongly nongeodesic motion and dynamics of linear perturbations.—Let us now consider linear fluctuations. We employ gauge invariant variables Q^I that coincide with the field fluctuations $\delta\varphi^I$ in the spatially flat gauge, and perform a decomposition in terms of the adiabatic and entropic modes Q_σ and Q_s , defined as the projection of Q^I in the direction tangential and perpendicular to the background trajectory respectively, the inner product being defined by the field space metric G_{IJ} (see, e.g., Ref. [23] for a review of perturbation theory in multifield inflation). The adiabatic mode can be expressed as

$Q_\sigma = (\dot{\sigma}/H)\zeta$, with the definition $\dot{\sigma} \equiv \sqrt{G_{IJ}\dot{\varphi}^I\dot{\varphi}^J}$, and where ζ is the comoving curvature perturbation. The equation of motion for the entropic perturbation is given by

$$\ddot{Q}_s + 3H\dot{Q}_s + \left(\frac{k^2}{a^2} + m_s^2\right)Q_s = -2\dot{\sigma}\eta_\perp\dot{\zeta}, \quad (4)$$

where k is the Fourier wave number, we introduced

$$\eta_\perp \equiv -\frac{V_{,ss}}{H\dot{\sigma}}, \quad m_s^2 \equiv V_{,ss} - H^2\eta_\perp^2 + \epsilon H^2 R_{\text{fs}} M_{\text{Pl}}^2. \quad (5)$$

Here $V_{,s}$ and $V_{,ss}$ stand for the projections in the entropic direction of the first and second (field-space covariant) derivatives of the potential, respectively, and R_{fs} is the field space scalar curvature. The “bending” parameter $\eta_\perp$ is physically important as it gives a measure of the deviation of the background trajectory from a geodesic in field space [24]. A strongly nongeodesic motion is characterized by $\eta_\perp^2 \gg 1$, resulting in a large negative contribution to the entropic mass m_s^2 , something that a negatively curved field space only reinforces. Without a stabilization from the potential, a large negative m_s^2/H^2 is thus a built-in feature of these models. Although unusual, this property is not *a priori* in contradiction with the requirement of a stable background. Indeed, on super-Hubble scales $k/a \ll H$ one has $\dot{\zeta} = 2H^2\eta_\perp/\dot{\sigma}Q_s$, and (4) yields an uncoupled equation for Q_s , now with a different effective mass $m_{s(\text{eff})}^2 \equiv m_s^2 + 4H^2\eta_\perp^2$, to which the bending contributes positively.

Specifying this general discussion to hyperinflation, we find, to leading-order in the slow-varying approximation,

$$\eta_\perp^2 \simeq h^2, \quad m_s^2 \simeq -2H^2h^2, \quad m_{s(\text{eff})}^2 \simeq 2H^2h^2. \quad (6)$$

As anticipated, a strongly nongeodesic motion corresponds to $h^2 \gg 1$. In this situation, the large and *positive* $m_{s(\text{eff})}^2/H^2$ implies a rapid decay of Q_s on super-Hubble scales and the conservation relation $\dot{\zeta} \simeq 0$. The decay of homogeneous perturbations $Q_s(k=0)$ is a proof that the background solution of hyperinflation is indeed a stable attractor. On the contrary, the large and *negative* m_s^2/H^2 signals a transient instability of fluctuations on sub-Hubble scales, observed also in some sidetracked inflationary models [6] and earlier in Refs. [25,26]. These considerations can be checked numerically. In Fig. 1 we consider the same background as studied in Ref. [19], for the quadratic potential $V(\phi) = \frac{1}{2}m^2\phi^2$ with $m = M = 10^{-2}M_{\text{Pl}}$. We display the time dependence of the dimensionless curvature ($\mathcal{P}_\zeta$) and entropic ($\mathcal{P}_S = H^2/\dot{\sigma}^2\mathcal{P}_{Q_s}$) power spectra, for the scale k_{55} that crosses the Hubble radius 55 e -folds before the end of inflation, which we take as the CMB pivot scale. The normalization factor is the “standard” result $\mathcal{P}_0 = H^2/(8\pi^2\epsilon M_{\text{Pl}}^2)_{k_{55}=aH}$. Soon after “entropic mass crossing” the exponential growth of entropic fluctuations caused by the

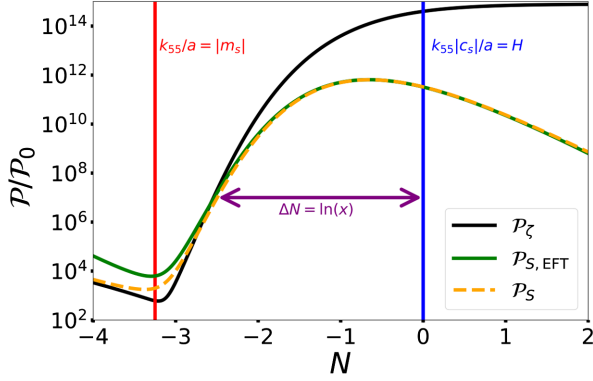


FIG. 1. Adiabatic ($\mathcal{P}_\zeta$) and entropic ($\mathcal{P}_S$) power spectra as functions of the number of e -folds, for the representative model detailed in the main text. The spectra are evaluated for the scale k_{55} that crosses the Hubble radius 55 e -folds before the end of inflation, at $N = 0$ in the plot. $\mathcal{P}_{S,EFT}$ is the entropic power spectrum deduced from the relation (8).

tachyonic instability feeds the adiabatic perturbation, before entropic fluctuations decay and the curvature perturbation becomes constant. The transient instability results in an exponentially small tensor-to-scalar ratio $r = 3.6 \times 10^{-16}$.

Bispectrum.—We now turn to the numerical calculation of the bispectrum in hyperinflation. (See, e.g., Refs. [27,28] for recent reviews on primordial non-Gaussianities, and Ref. [29] for the most recent observational constraints from the Planck Collaboration.) The results have been obtained with PyTransport 2.0 [30,31], a code based on the transport approach to compute two- and three-point correlation functions in multifield models with curved field space (see also CppTransport [32–34]). Figure 2 is a plot of the reduced bispectrum $f_{NL}(k_1, k_2, k_3)$ for the same representative model as above, as a function of the variables (α, β) defined by $k_1 = (3k_{55}/4)(1 + \alpha + \beta)$, $k_2 = (3k_{55}/4)(1 - \alpha + \beta)$, and $k_3 = (3k_{55}/2)(1 - \beta)$. The resulting bispectrum is quite unlike what is usually found in inflationary models with a Bunch-Davies vacuum state. In particular, hyperinflation generates a non-Gaussian signal that is peaked near flattened triangle configurations, i.e., the ones with $k_1 \simeq k_2 + k_3$ (the edges in Fig. 2), which is typical of excited initial states. Explicitly, we find

$$f_{NL}^{\text{eq}} = -2.0, \quad f_{NL}^{\text{flat}} = 53.8, \quad (7)$$

where the two parameters simply denote the evaluation of the reduced bispectrum, respectively, at $k_1 = k_2 = k_3$ and at the representative flattened configuration $k_2 = k_3 = k_1/2$. Although we have presented results for the particular case of a quadratic potential and for a specific set of parameters, we remark that the qualitative outcome—a strong non-Gaussian signal in flattened configurations—is quite robust. We find, for instance, $f_{NL}^{\text{flat}} \simeq 25$ for a Starobinsky-type potential and $f_{NL}^{\text{flat}} \simeq 100$ for a quartic potential, while $f_{NL}^{\text{eq}} = O(1)$ in each case.

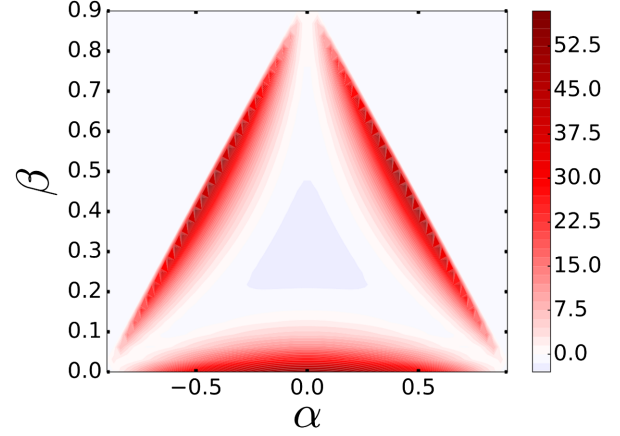


FIG. 2. Shape dependence $f_{NL}(\alpha, \beta)$, at fixed overall scale $k_1 + k_2 + k_3 = 3k_{55}$, for the same model as in Fig. 1. The characteristic feature of the bispectrum is its dominant signal near flattened configurations. Note that the equilateral configuration corresponds to the point $(\alpha, \beta) = (0, 1/3)$.

Effective single-field description.—In a standard setup with a single light degree of freedom, heavy entropic fluctuations can be integrated out to yield an EFT for the adiabatic mode (see, e.g., Refs. [25,35–38]). In the type of models we consider, the entropic field is heavy but *tachyonic*, yet the procedure can be carried out equivalently to the standard case, as explained in Ref. [39]. In slowly evolving backgrounds and in the regime $k^2/a^2 \ll |m_s^2|$, one finds

$$Q_s = -2 \frac{\dot{\sigma}\eta_\perp}{m_s^2} \dot{\zeta}, \quad (8)$$

which results in an effective quadratic action for the curvature perturbation:

$$S_{\text{eff}}^{(2)} = \int d\tau d^3x a^2 \epsilon M_{\text{Pl}}^2 \left[\frac{\zeta'^2}{c_s^2} - (\vec{\nabla} \zeta)^2 \right], \quad (9)$$

where $\tau \simeq -1/(aH)$ is the conformal time, $\zeta' \equiv d\zeta/d\tau$, and the speed of sound c_s is defined by

$$\frac{1}{c_s^2} \equiv 1 + \frac{4H^2 \eta_\perp^2}{m_s^2} = \frac{m_{s(\text{eff})}^2}{m_s^2}. \quad (10)$$

An imaginary sound speed is thus a model-independent consequence of a tachyonic entropic mass ($m_s^2 < 0$) and a stable background ($m_{s(\text{eff})}^2 > 0$). For instance, in hyperinflation we find $c_s^2 \simeq -1$. In this class of models, the curvature perturbation thus propagates with a “wrong sign” dispersion relation: $\omega^2 = -|c_s|^2 k^2 \simeq -k^2$. Accordingly, the mode functions do not oscillate but rather grow or decay exponentially, affecting all wave modes k up to the cutoff of the EFT—what in the two-field theory was a tachyonic

instability affecting low-energy modes has become in the EFT a gradient-type instability to which the whole spectrum is sensitive. Such a theory is not *a priori* catastrophic, as the corresponding instability is only transient. However, our results will ultimately bound the amplification of fluctuations.

It will prove useful to introduce the dimensionless parameter x such that the wave modes k described by the effective theory satisfy $k|c_s|/a < xH$. Its dependence on models' parameters is $x \sim |c_s|/m_s/H$, where the numerical factor in the right should be somewhat smaller than unity. Quantitatively, x can be determined by examining when the power spectrum of the entropic fluctuation computed in the full theory matches the one deduced from Eq. (8), which is the central relation from which the EFT derives. One can see in Fig. 1 that the two become in very good agreement less than one e -fold after entropic mass crossing, corresponding to $x \sim 10$ in this example. The general solution of the linear equation of motion reads, for $c_s^2 < 0$,

$$\zeta_k(\tau) = \left(\frac{2\pi^2}{k^3}\right)^{1/2} \alpha [e^{k|c_s|\tau+x} (k|c_s|\tau-1) - \rho e^{i\psi} e^{-(k|c_s|\tau+x)} (k|c_s|\tau+1)], \quad (11)$$

where we omit the mild k dependence of (α, ρ, ψ) for simplicity, and we stress that it only applies for $k|c_s|\tau + x \geq 0$. The parameter ρ sets the relative amplitude of the exponentially decaying mode compared to the growing one at the time marking the validity of the EFT (and ψ is a phase difference), while α can be taken to be real and parametrizes their overall amplitude. [The amplitude of the decaying mode is necessarily nonzero, as the quantization condition entails the relation $2\alpha^2\rho \sin(\psi)|c_s| = \mathcal{P}_0$.] The final value of the curvature power spectrum $\mathcal{P}_\zeta = \alpha^2 e^{2x}$ [assuming very conservatively that $\rho \lesssim \mathcal{O}(1)$] depends on the initial conditions of the EFT. Although these can in principle be determined by matching to the full computation of $\mathcal{P}_\zeta(\tau)$, interestingly, this is not needed to study higher-order correlation functions, to which we now turn.

The cubic action of the EFT of inflationary perturbations [40,41] reads (at lowest order in derivatives and in the slow-varying approximation):

$$S_{\text{eff}}^{(3)} = \int d\tau d^3x \frac{a\epsilon M_{\text{Pl}}^2}{H} \left(\frac{1}{c_s^2} - 1\right) \left[\zeta'(\vec{\nabla}\zeta)^2 + \frac{A}{c_s^2} \zeta'^3 \right], \quad (12)$$

where A is a dimensionless constant of order 1 that can be computed from the full theory [42]. Although the interactions in Eq. (12) are standard, the behavior of the mode function (11) is not, and the computation of the bispectrum is nontrivial [39]. Contrary to what a naive power counting would indicate, one finds that the reduced

bispectrum does not feature an exponential enhancement by e^{2x} , like the power spectrum. Instead, it is independent of x for near equilateral configurations, with

$$f_{NL}^{\text{eq}} \simeq \frac{10}{9} \left(\frac{1}{|c_s|^2} + 1 \right) \left(\frac{13A}{6} - \frac{5}{24} \right). \quad (13)$$

Given the result $c_s^2 \simeq -1$ in hyperinflation, we have the analytical prediction that $f_{NL}^{\text{eq}} = \mathcal{O}(1)$, in agreement with the numerical results. Away from the equilateral limit, one finds a dependence of f_{NL} on the cutoff scale xH (with the exception of the squeezed limit, which can be shown to verify the single-clock consistency relation via standard arguments). Akin to models with excited initial states (see, e.g., Refs. [43–47]) the constructive interferences between two growing and one decaying mode result in a magnification of the signal near flattened configurations $k_1 \simeq k_2 + k_3$,

$$f_{NL}^{\text{flat}} \simeq \frac{1}{192} \left(\frac{1}{|c_s|^2} + 1 \right) [39(A-1) + 12x^2 + 4(A+1)x^3], \quad (14)$$

and a global shape with a large overlap with the orthogonal template (except for values of $A \simeq -1$) [39]. With $x^2 \sim h^2 \gg 1$ in hyperinflation with strongly nongeodesic motion (e.g., $x^2 \sim 100$ in our example), we conclude that flattened non-Gaussianities are large in this type of model, again in agreement with the full two-field numerical results (see the Supplemental Material [48] for a quantitative comparison).

Higher-order correlation functions.—We have seen that the single-field effective theory of perturbations with imaginary sound speed can unambiguously predict the striking features of the reduced bispectrum, thus providing a valuable device to gain analytical insight into the complex multifield dynamics of models with large negative entropic mass. But from a pragmatic perspective, the real power of the EFT approach is that it can go beyond the reach of current numerical methods, as we now show by providing an estimate of higher-order correlation functions in this class, including hyperinflation. Like for the bispectrum, for $n \geq 4$, the reduced connected n -point function $\langle \zeta^n \rangle / \langle \zeta^2 \rangle^{n-1}$ does not feature an exponential amplification [49]. (This has been shown in Ref. [49] using the EFT put forward in the first version of this work.) In spite of this, we find that some flattened configurations for the trispectrum and higher-point correlators are enhanced by powers of the parameter x , essentially due to the same phenomenon of constructive interferences between growing and decaying modes that occurs for the bispectrum.

Focusing on the dominant contributions in the large x limit, one can find an explicit derivation of the trispectrum in the Supplemental Material [48], where we also give further details of our estimate for the higher-point functions

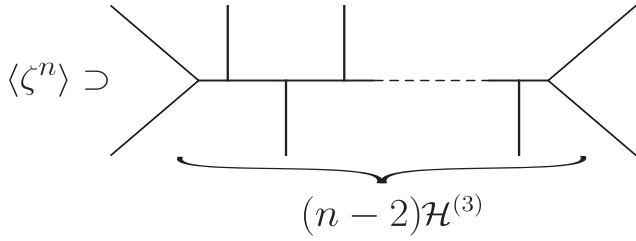


FIG. 3. Dominant contribution to the connected n -point correlation function of ζ .

and characterize which flattened shapes are enhanced. Following the *in-in* formalism [50], the computation of the n -point correlator can be organized as a sum of connected Feynman diagrams with n external lines, and with each insertion of the interaction Hamiltonian corresponding to a vertex. We find that a diagram with v vertices contributes as $\langle \zeta^n \rangle / \langle \zeta^2 \rangle^{n-1} \propto x^{2n+v-4}$ for the maximally enhanced flattened configurations. This contribution is largest when $v = n - 2$, corresponding to diagrams of the type shown in Fig. 3, with $(n - 2)$ insertions of the cubic Hamiltonian, yielding the estimate

$$\frac{\langle \zeta^n \rangle}{\langle \zeta^2 \rangle^{n-1}} \sim \left[\left(\frac{1}{|c_s|^2} + 1 \right) x^3 \right]^{n-2}. \quad (15)$$

Notice that, despite the rapid growth of the correlation functions as n increases, the theory is nevertheless under perturbative control for observationally relevant models. Indeed, perturbativity is guaranteed provided $\langle \zeta^n \rangle / \langle \zeta^2 \rangle^{n-1} \mathcal{P}_\zeta^{(n-2)/2} \sim (f_{NL}^{\text{flat}} A_s^{1/2})^{n-2} \lesssim 1$, which is a weaker requirement than meeting the observational bounds on the bispectrum.

Discussion.—In negatively curved field space, and in the absence of a stabilizing effect from the potential in the direction perpendicular to the background trajectory, a strongly nongeodesic motion in field space automatically induces a transient instability of fluctuations on sub-Hubble scales. Under these general circumstances, we can make use of an effective field theory for the curvature perturbation that naturally explains the exponential amplification of the power spectrum. Moreover, it predicts a reduced bispectrum whose characteristics are in striking agreement with first-principles numerical computations in the full theory: order-one non-Gaussianities in equilateral configurations, and a magnification near flattened ones. However, contrary to the power spectrum, the reduced bispectrum is not exponentially amplified. We have moreover argued that an analogous outcome holds for all higher-order reduced correlation functions, namely, a hierarchical enhancement for particular flattened shapes proportional to a power of the instability rate. When the latter is very large, these hyper-non-Gaussianities lead to tensions with observational constraints, as exemplified by models

of hyperinflation that satisfy the de Sitter swampland conjecture.

Our model-independent results severely bound the magnitude of a large negative entropic mass. Hence, it results in a powerful selection criterion on models with negatively curved field space and a strongly nongeodesic motion that have been receiving much attention recently. Namely, at least some stabilizing effect by the potential is needed to counterbalance the otherwise strongly tachyonic mass of entropic fluctuations on sub-Hubble scales. This compensating effect can be large, to the extent that $|m_s^2/H^2| \ll 1$ or $m_s^2/H^2 \gg 1$, which are well understood situations. It can also be mild, resulting again in a negative entropic mass, but not parametrically larger than the Hubble scale (a feature shared by hyperinflation with a moderate degree of bending). Without hierarchy, an EFT cannot be rigorously derived, but we expect our results to give a qualitatively correct picture, i.e., an enhancement of the bispectrum in flattened configurations, and similarly for the trispectrum. Thus, our results pave the way for future studies about the role of field-space geometry in the dynamics of inflation, and particularly in how nongeodesic motion of inflationary attractors can lead to novel signatures that can be probed with current and next-generation experiments.

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Hyper non-Gaussianities in inflation with strongly non-geodesic motion

Supplemental Material

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A. Comparison between analytical and numerical bispectra

In this first supplemental material we provide further details on the comparison of the results for the bispectrum as computed numerically in the full two-field theory and analytically in the single-field EFT. In the main text we have quoted the reduced bispectrum f_{NL} in the equilateral and squashed configurations (the latter being representative of more general flattened configurations): Eq. (7) gives the numerical results (for the specific set of parameters $m = M = 10^{-2} M_{\text{Pl}}$) while Eqs. (13) and (14) give the approximate analytical formulae as derived from the EFT.

The EFT formulae depend on c_s , A and x , which are unknown parameters within the EFT and must be determined either from the knowledge of the UV completion (the hyperinflation model in this case) or through a matching calculation. The speed of sound is easily computed in the two-field theory from the standard result (10), which gives $c_s^2 \simeq -1$ in hyperinflation, as indicated in the main text. For the constants A and x it is easier to perform a matching given the knowledge of the full numerical bispectrum. Remembering that the EFT result for f_{NL} is more accurate for the equilateral configuration [38], we compare f_{NL}^{eq} in Eqs. (7) and (13) to find

$$A \simeq -0.33. \quad (16)$$

On the other hand, the computation of x is necessarily less accurate, since x is precisely what defines the regime of validity of the EFT. In the text we showed how the value of x may be estimated from the entropic power spectrum, which produced the result $x \sim 10$.

We now make this estimate for x more precise by comparing the full analytical and numerical bispectra. Fig. 4 displays the one-dimensional slice of $f_{NL}(\alpha, \beta)$ that ranges from $f_{NL}(0, 0) \equiv f_{NL}^{\text{flat}}$ to $f_{NL}(0, 1/3) \equiv f_{NL}^{\text{eq}}$, where for the EFT prediction we have used $x = 10$ and $x = 11$. It is clear that the estimate derived from the 2-point statistics provides a quantitatively good match for the bispectrum. As expected, the dependence on x is only important near the flattened configuration, and we judge the value $x \simeq 10$ as a slightly better fit to the numerical data in view of the fact that the EFT prediction for f_{NL}^{flat} is expected to be less accurate than for f_{NL}^{eq} .

Fig. 5 is the full plot of the reduced bispectrum derived from the EFT, using the value $x = 10$ and $A = -0.33$ as in (16). Although we have used a single one-dimensional

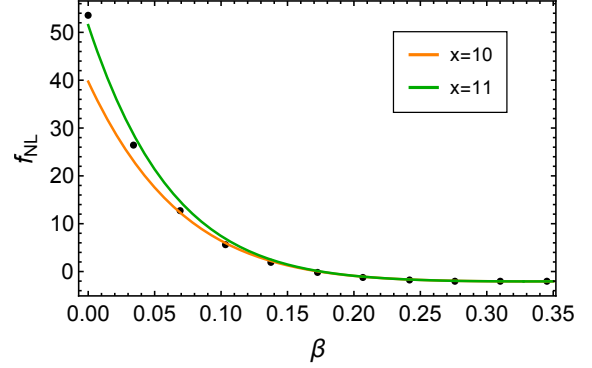


FIG. 4. Graph of the function $f_{NL}(0, \beta)$ corresponding to a one-dimensional slice of the reduced bispectrum. The points are the numerical data, and the curves show the analytical EFT results for $c_s^2 = -1$, $A = -0.33$ and two different values of x .

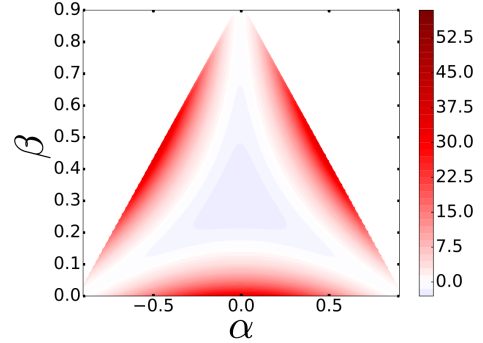


FIG. 5. Shape dependence $f_{NL}(\alpha, \beta)$ derived analytically in the EFT of single-field inflation, for $x = 10$ and $A = -0.33$. Observe the very good agreement with the full numerical result Fig. 2 in the main text.

slice of f_{NL} for the estimation of x and A , one can see an overall excellent agreement for the global shape of the bispectrum between the analytical and numerical results (see Fig. 2 in the main text).

Incidentally, even though the evaluation of the EFT coefficient A via a matching computation is perfectly sufficient, it is worth remarking that it also concords with the analytical prediction inferred from the two-field UV completion. Applying the results of Ref. [48] to the model of hyperinflation, we find

$$A = -\frac{1}{3} - \frac{1}{6(9 + h^2)} \frac{MV'''}{H^2}. \quad (17)$$

For the simple quadratic potential that we used in this Letter we have $V''' = 0$. This yields $A = -1/3$, in perfect agreement with the matching calculation.

B. Estimation of the trispectrum and higher-point correlation functions

In this second supplemental material we derive explicitly the trispectrum for the shape configurations that dominate in the limit of large x , focusing on a specific type of vertex for simplicity. We then generalize the calculation to estimate the reduced n -point function and derive Eq. (15). For this, we use that the n -point correlator is given by the *in-in* formula [47]

$$\langle \zeta^n \rangle = \sum_{j=0}^{\infty} i^j \int_{\tau_0}^0 d\tau_1 a(\tau_1) \int_{\tau_0}^{\tau_1} d\tau_2 a(\tau_2) \cdots \int_{\tau_0}^{\tau_{j-1}} d\tau_j a(\tau_j) \times \langle 0 | [H_I(\tau_j), \cdots [H_I(\tau_1), \zeta_I^n] \cdots] | 0 \rangle, \quad (18)$$

where the subscript I refers to the interaction picture, H_I is the interaction Hamiltonian, and we have introduced the ultraviolet cutoff $\tau_0 = -x/(k_m |c_s|)$ to regularize the time integrals (with k_m the largest among the external momenta), consistent with the fact that the EFT is only valid after a certain time.

1. Trispectrum from ζ'^3 interaction

We begin by defining

$$\mathcal{T}(k_1, k_2, k_3, k_4, k_{12}, k_{13}) = \frac{\langle \zeta_{\vec{k}_1} \zeta_{\vec{k}_2} \zeta_{\vec{k}_3} \zeta_{\vec{k}_4} \rangle (k_1 k_2 k_3 k_4)^{9/4}}{(2\pi)^9 \delta(\sum_i \vec{k}_i) A_s^3}, \quad (19)$$

as a dimensionless measure of the reduced 4-point correlation function. As usual, because of isotropy the trispectrum can be parametrized in terms of the magnitudes k_i of the momenta plus two of the sums $k_{ij} \equiv |\vec{k}_i + \vec{k}_j|$, which we choose to be k_{12} and k_{13} . The above formula also includes the amplitude of the scalar power spectrum at the CMB pivot scale, which in terms of our EFT parameters (and ignoring their scale dependence) is $A_s \simeq \frac{\alpha^2}{2\pi^2} e^{2x}$.

The trispectrum receives contributions from two types of diagrams: a contact 4-point diagram coming from the quartic interactions of the theory and a scalar exchange diagram involving two insertions of the cubic Hamiltonian in Eq. (18). The full calculation is of course complicated by the fact that the Hamiltonian includes several different operators, so for the sake of simplicity we will focus only on the ζ'^3 operator in (12), although we have checked that other interactions do not qualitatively modify our results. In other words, we ignore the operator $\zeta'(\vec{\nabla}\zeta)^2$ as well as the whole quartic Hamiltonian (it will be clear in a moment, however, that the latter gives a

subdominant contribution), and write

$$H^{(3)} = \int d^3x \mathcal{C} \zeta'^3, \quad \mathcal{C} \equiv -\frac{M_{\text{Pl}}^2 \epsilon}{H} \left(\frac{1}{|c_s|^2} + 1 \right) \frac{A}{|c_s|^2}, \quad (20)$$

and we take $\mathcal{C}$ to be constant to leading order in slow-roll. Inserting this in Eq. (18) and performing some standard manipulations we arrive at

$$\begin{aligned} \langle \zeta_{\vec{k}_1} \zeta_{\vec{k}_2} \zeta_{\vec{k}_3} \zeta_{\vec{k}_4} \rangle &= -144(2\pi)^3 \mathcal{C}^2 \delta(\sum_i \vec{k}_i) \int_{\tau_0}^0 \frac{d\tau_1}{H\tau_1} \int_{\tau_0}^{\tau_1} \frac{d\tau_2}{H\tau_2} \\ &\times \left(\text{Im} [\zeta'_{k_1}(\tau_2) \zeta'_{k_2}(\tau_2) \zeta'_{k_{12}}(\tau_2) \zeta'^*_{k_{12}}(\tau_1) \zeta^*_{k_1}(0) \zeta^*_{k_2}(0)] \right. \\ &\quad \left. + \text{Im} [\zeta'_{k_3}(\tau_1) \zeta'_{k_4}(\tau_1) \zeta^*_{k_3}(0) \zeta^*_{k_4}(0)] + (5 \text{ perm.}) \right). \end{aligned} \quad (21)$$

This formula includes one imaginary part of product of mode functions for each of the vertices in the exchange diagram. For this reason, the decaying mode in Eq. (11) must be taken into account in some of the ζ 's, and we isolate the leading term in the large x regime by choosing exactly one decaying mode per vertex. Substituting we obtain an expression of the form

$$\begin{aligned} \mathcal{T} &= \frac{9A^2 |c_s|^6}{32} \left(\frac{1}{|c_s|^2} + 1 \right)^2 (k_1 k_2 k_3 k_4)^{5/4} \\ &\times \left[k_{12} \sum_{\vec{k}_1, \vec{k}_2} \sigma_{\vec{k}_1, \vec{k}_2} \int_{\tau_0}^0 d\tau_1 \tau_1^2 e^{\tilde{k}_1 |c_s| \tau_1} \int_{\tau_0}^{\tau_1} d\tau_2 \tau_2^2 e^{\tilde{k}_2 |c_s| \tau_2} \right. \\ &\quad \left. + (5 \text{ perm.}) \right], \end{aligned} \quad (22)$$

where $\tilde{k}_1 = \pm k_{12} \pm k_3 \pm k_4$ and $\tilde{k}_2 = \pm k_1 \pm k_2 \pm k_{12}$, and the sum is over all choices of signs in $\vec{k}_1$ and $\vec{k}_2$, but subject to the condition that exactly one of the momenta in each imaginary part in Eq. (21) should carry a minus sign ($\sigma_{\vec{k}_1, \vec{k}_2} = \pm 1$ is an overall sign that depends on the specific permutation). From this result it is clear that the configurations of momenta that maximize the absolute value of $\mathcal{T}$ (in terms of its scaling with x) are achieved when $\tilde{k}_1 = \tilde{k}_2 = 0$, corresponding for each vertex to constructive interactions between two growing and one decaying mode. This condition notably enforces the four external momenta to be collinear, leading to a quadrilateral shape of the flattened type. Note however that this collinearity is necessary but not sufficient; not all flattened shapes lead to a maximally enhanced trispectrum. Although analyzing the full shape-dependence of the trispectrum is beyond the scope of this Letter, let us quote the result for the configuration that is the natural extension of the representative flattened configuration maximizing the bispectrum, and evaluated in (7). It corresponds to $\vec{k}_4 = -3\vec{k}_1 = -3\vec{k}_2 = -3\vec{k}_3$ (so that $k_{1,2,3} = k_m/3$, $k_4 = k_m$, $k_{12} = 2k_m/3$) and gives

$$\mathcal{T} = -\mathcal{N} A^2 \left(\frac{1}{|c_s|^2} + 1 \right)^2 x^6, \quad (23)$$

with a numerical prefactor $\mathcal{N}^{-1} = 2592 \times 3^{3/4}$.

2. Higher-point functions

Eq. (22) can be generalized to an arbitrary tree diagram with n external legs. Consider such a diagram with v vertices, each corresponding to an insertion of the Hamiltonian $H^{(m_j)}$, where $m_j \geq 3$ and $j \in \{1, \dots, v\}$. By dimensional analysis we have $H^{(m_j)} \sim \frac{M_{\text{Pl}}^2 \epsilon}{H^{m_j-2} a^{m_j-3}} \int d^3x (\zeta')^{m_j}$, where we emphasize that the numerical prefactor depends on $|c_s|$ and on various Wilson coefficients. It is convenient to change variables in the integrals in (18) with $y_j = -k_m |c_s| \tau_j$. Then the generalization of (22) is given by

$$\begin{aligned} \frac{\langle \zeta^n \rangle}{\langle \zeta^2 \rangle^{n-1}} &\sim \int_0^x dy_1 y_1^{2m_1-4} e^{-(\tilde{k}_1/k_m)y_1} \\ &\times \int_{y_1}^x dy_2 y_2^{2m_2-4} e^{-(\tilde{k}_2/k_m)y_2} \\ &\times \dots \times \int_{y_{v-1}}^x dy_v y_v^{2m_v-4} e^{-(\tilde{k}_v/k_m)y_v}, \end{aligned} \quad (24)$$

where $\tilde{k}_j = \pm k_{j,1} \pm \dots \pm k_{j,m_j}$, and by $k_{j,l}$ we denote all the momenta at the j -th vertex. Of course, due to momentum conservation, all of them can be ultimately related in terms of the n external momenta $\vec{k}_i$. The maximum enhancement of the reduced n -point function is then clearly achieved for configurations with all of the $\tilde{k}_j$ vanishing. This condition notably requires all the momenta at each vertex to be collinear, and therefore the external momenta must also be collinear. Once again, this collinearity is necessary but not sufficient. Thus the optimal enhancement is attained for the flattened shapes verifying $\vec{k}_j = 0$. We immediately get in that case

$$\frac{\langle \zeta^n \rangle}{\langle \zeta^2 \rangle^{n-1}} \sim x^{2(m_1+\dots+m_v)-3v}. \quad (25)$$

Noting that for a tree diagram one has $m_1 + \dots + m_v = n + 2v - 2$, this result thus reproduces the expression quoted in the main text.

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5.3 Revisiting non-Gaussianity in multifield inflation with curved field space

At the time when this thesis was initiated, the cubic order action of multifield inflation was only known in terms of the fields' perturbations in the flat gauge, Q_{flat}^I [57, 58]. Although all gauge-invariant quantities are equally correct to describe physical phenomena, some may be more useful than others depending on the problem at hand, and manipulating directly the observable curvature perturbation happens to be very efficient for analytical approaches. Indeed, although the Q_{flat}^I might be useful intermediate quantities, they are not observable themselves, and therefore one shall always resort to a gauge transformation, such as the following one at linear order, $\mathcal{R} = H\dot{\phi}_I Q_{\text{flat}}^I / \dot{\sigma}^2$, see Eq. (4.38), in order to find the observable bispectrum. At non-linear order, these gauge transformations may be tricky to find, in particular on sub-horizon scales, and this is why for example in `PyTransport` one can only make this gauge transformation on super-Hubble scales, therefore finding the final value of the observable bispectrum of $\mathcal{R}$ at the end of inflation when the modes of interest are all well above the horizon, but however rendering inaccessible the whole evolution of $B_{\mathcal{R}}$ on sub-horizon scales. More generally and going back to analytical approaches, although one may very well understand the physics with the fields' perturbations in the flat gauge, this understanding may be completely spoiled by the necessity to perform this non-linear gauge transformation that is mixing many effects one with the others, in order to find an observational prediction.

Moreover, the article presented in Sec. 5.2 showed that primordial non-Gaussianities in multifield inflation could be importantly impacted by the presence of a curved field space, a strongly non-geodesic notation, and multifield instabilities. These effects are best understood in the adiabatic-entropic basis, where the criteria of stability are clearly encoded in the entropic sector that is orthogonal to the background trajectory, the efficiency of the adiabatic-entropic coupling is easily parameterised by the simple number $\eta_{\perp}$ which has an obvious geometrical interpretation, and where the adiabatic perturbation can be chosen in the comoving gauge to coincide directly with the observable perturbation $\mathcal{R}$. Last but not least, the single-field effective theory used in Sec. 5.2 to compute the bispectrum of these interesting two-field models with a negatively curved field space, was initially not fully predictive. Indeed, although the speed of sound c_s^2 was importantly derived from the full two-field theory, the parameter A *a priori* encoding the two-field cubic interactions was simply chosen to be of order unity to respect the spirit of the EFToI, but was not derived from first principles. In order to find how A reads in the low-energy EFT, one should first compute the interactions in the UV completion, *i.e.* the two-field model with a curved field space, and this should be done in the adiabatic-entropic basis.

This section presents the two articles that were published during my thesis on this topic.

5.3.1 Two-field case (article)

In this section, where Ref. [2],

S. Garcia-Saenz, L. Pinol, S. Renaux-Petel. 2019,
REVISITING NON-GAUSSIANITY IN MULTIFIED INFLATION WITH CURVED FIELD SPACE,
Journal of High Energy Physics (JHEP) 2020, 73 (2020),

is reproduced, it is presented how to calculate the generic cubic order action in two-field inflation, with any potential and field-space metric, without assuming a particular background evolution, therefore generalising Maldacena's calculation to these more intricate but phenomenologically interesting two-field models. This program first necessitates the identification of the two fundamental fluctuating degrees of freedom at non-linear order, $\mathcal{R}$ (denoted ζ in the article) and $\mathcal{F}$, respectively the adiabatic comoving curvature perturbation and the entropic perturbation in the comoving gauge defined by $E_{\text{com}} = 0 = Q_{\sigma}^{\text{com}}$. The action is expanded at cubic order, but then requires careful manipulations in order to simplify operators with integrations by parts and making use of the linear EoM verified by the interacting fields $\mathcal{R}^I$ and $\mathcal{F}^I$, and to render explicit the size of interactions after eliminating their redundancies. As an important first application of our formalism, we also show how to find the single-field effective theory for $\mathcal{R}$ when the entropic perturbation $\mathcal{F}$ is heavy and can be integrated out, and we detail the regime of validity of this procedure. In particular, we find that the parameter A encoding the cubic two-field interactions as effective single-field self-interaction in the low-energy effective theory, can be expressed in terms of four independent contributions encoding: the non-trivial speed of sound c_s^2 that is induced by the quadratic mixing, the third covariant derivative of the potential in the entropic direction, $V_{;sss}$, the relative size of the field-space curvature contribution to the mass of $\mathcal{F}$, *i.e.* $\epsilon R_{\text{fs}} H^2 M_{\text{Pl}}^2 / m_s^2$, and the derivative of the field-space curvature in the entropic direction $R_{\text{fs},s}$. Because this formula is both important and elegant, it is reproduced here:

$$A = -\frac{1}{2} (1 + c_s^2) + \frac{2}{3} (1 + 2c_s^2) \frac{\epsilon H^2 M_{\text{Pl}}^2 R_{\text{fs}}}{m_s^2} - \frac{1}{6} (1 - c_s^2) \left(\frac{\kappa V_{;sss}}{m_s^2} + \frac{\kappa \epsilon H^2 M_{\text{Pl}}^2 R_{\text{fs},s}}{m_s^2} \right), \quad (5.110)$$

where $\kappa = \sqrt{2\epsilon} M_{\text{Pl}} / \eta_{\perp}$ corresponds to the bending radius of the field-space trajectory.

The original article as published in JHEP is now displayed. The notations that are used are very close to the ones of this manuscript, and only differ (again) by the fact that the comoving curvature perturbation is denoted ζ in the article, while it is $\mathcal{R}$ here.

Revisiting non-Gaussianity in multifield inflation with curved field space

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ABSTRACT: Recent studies of inflation with multiple scalar fields have highlighted the importance of non-canonical kinetic terms in novel types of inflationary solutions. This motivates a thorough analysis of non-Gaussianities in this context, which we revisit here by studying the primordial bispectrum in a general two-field model. Our main result is the complete cubic action for inflationary fluctuations written in comoving gauge, i.e. in terms of the curvature perturbation and the entropic mode. Although full expressions for the cubic action have already been derived in terms of fields fluctuations in the flat gauge, their applicability is mostly restricted to numerical evaluations. Our form of the action is instead amenable to several analytical approximations, as our calculation in terms of the directly observable quantity makes manifest the scaling of every operator in terms of the slow-roll parameters, what is essentially a generalization of Maldacena's single-field result to non-canonical two-field models. As an important application we derive the single-field effective field theory that is valid when the entropic mode is heavy and may be integrated out, underlining the observable effects that derive from a curved field space.

KEYWORDS: Cosmology of Theories beyond the SM, Effective Field Theories, Sigma Models

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1 Introduction

Primordial non-Gaussianities are arguably the most promising probe of the physics of the early universe (see [1] for the most recent observational constraints and e.g. [2–6] for reviews). In the context of inflation, they offer a unique observational window into energy scales even above the Hubble scale — very likely the highest scales that we may ever hope to indirectly probe. In this setting, non-Gaussianities are predominantly due to the three-point interactions of the scalar degrees of freedom that are active during the inflationary epoch, which in most typical scenarios correspond to (in a suitable gauge) the comoving curvature perturbation ζ , plus possibly a slew of additional heavy fields, which are expected to be present if inflation is to be realized within a more fundamental theory, for instance

as moduli arising in compactifications of string theory. If these extra fields are sufficiently heavy, with masses much larger than the Hubble scale H , it follows from the principle of decoupling that they should have had a negligible imprint on the inflationary dynamics, leading to the standard paradigm of single-field inflation.

However, over the past decade it has been realized that neglecting the effects of heavy fields beyond the inflaton may be premature (see e.g. [7–19]). This is best appreciated when one considers the effective field theory (EFT) of single-field inflation [20, 21] obtained upon integrating out all heavy fields, where one finds in particular that the remaining light degree of freedom — the curvature mode ζ in the present case — propagates with a reduced speed of sound, $c_s^2 < 1$. A subluminal speed of sound has direct observational consequences: for instance the tensor-to-scalar ratio is suppressed by a factor of c_s relative to the fully single-field expectation. More intriguing is the effect on the bispectrum, which schematically reads $B_\zeta \sim (\frac{1}{c_s^2} - 1)\mathcal{O}(1) + \mathcal{O}(\epsilon)$, with ϵ denoting some slow-roll parameter. Considering that $\epsilon \ll 1$ in slow-roll models, this result implies the striking conclusion that even a small departure from an exactly luminal dispersion relation can significantly affect the size and shape of primordial non-Gaussianities. Even more interesting however, at least from the observational viewpoint, is to entertain the possibility of a strongly reduced speed of sound, by which we mean $\frac{1}{c_s^2} - 1 \gtrsim 1$, leading to non-Gaussianities that can be probed by next-generation experiments.

Given the expectation, purely on dimensional grounds, that $\frac{1}{c_s^2} - 1 = \alpha H^2/m_h^2$, for some (time-dependent) coupling parameter α and a typical scale m_h for the heavy fields (or their perturbations to be precise), it may naively seem hard to generate a sizable bispectrum when $m_h \gg H$. However, an interesting twist in the story is provided by the coupling α , which in two-field models (with an inflaton and a single extra heavy field) is related to the degree of geodesic deviation of the inflationary trajectory in the internal field space, as we will make explicit below. Indeed, it has recently been appreciated that having a large coupling with $\alpha \gg 1$ can be easily achieved within multi-field models of inflation with a curved field space, which are characterized by non-canonical kinetic terms [22–32]. In this set-up, the interplay between the curvature of the internal space and the potential of the heavy fields can give rise to novel attractor solutions featuring a large coupling α and hence possibly $\frac{1}{c_s^2} - 1 \gtrsim 1$ even if $m_h \gg H$.

These as well as other recent developments in inflationary cosmology (see e.g. [33–47]) motivate us to revisit the problem of calculating the bispectrum in two-field models of inflation with a curved field space. Our main result is the cubic action for inflationary perturbations in comoving gauge, which allows for the direct computation of correlation functions of the mode of primary observational interest, namely the curvature perturbation ζ . It is worth remarking that the cubic action for general non-canonical multi-field models has already been derived in the flat gauge [48], and has been used in numerical implementations of the transport method [49–53]. Although it is in principle possible to translate these results, via a nonlinear gauge transformation, to deduce the cubic interactions for ζ , in practice this is of limited use as multiple operations would still be necessary to render the sizes of the interactions manifest. This fact is of course well known in the single-field context: given that the reduced bispectrum is proportional to ϵ (to leading order in slow-

roll), one expects the coefficients of the cubic action to be suppressed by ϵ^2 , and yet this is far from manifest after a direct expansion or after one switches gauge. Exhibiting the “correct” size of the cubic vertices of ζ requires non-trivial manipulations, as first shown by Maldacena in the single-field case [54]. Our primary goal is to extend this result to a generic model with two scalars and a curved field space. We emphasize that our result is completely general: it does not use any slow-roll approximation, and it is valid for any value of the mass of the entropic (or isocurvature) perturbation. Our cubic action is therefore applicable in all types of inflationary scenarios, such as models with features, ultra slow-roll behaviours, or displaying a non-trivial evolution of fluctuations on super-Hubble scales.

An important application of our result is that the single-field EFT for ζ , obtained upon integrating out the entropic mode, can be derived in a very direct way. The resulting cubic effective action provides insight into the explicit relation between the EFT of inflation and its multi-field UV completions. In particular, we have derived an explicit result for the unique Wilson coefficient that enters in the cubic action (at leading order in the derivative expansion) and that is not fixed by symmetry from the quadratic action, in terms of parameters defining the full two-field theory and the inflationary trajectory. Interestingly, in addition to an expected contribution from the third derivative of the potential, we find contributions to this coefficient that depend on the curvature of the internal field space, which to our knowledge had not been appreciated before. Our result also allows one to make contact with models of k-inflation [55–58], defined by a Lagrangian $\mathcal{L} = P(X, \phi)$ that is a generic function of a single scalar field ϕ and its kinetic term $X = -\frac{1}{2}(\partial\phi)^2$. Since the EFT of inflation at leading order in the derivative expansion falls in this class of models, we can use our results to (partially) reconstruct the function P by relating its first few derivatives to the parameters of the two-field UV completion. Lastly, as a byproduct of our derivation of the single-field EFT, we clarify various aspects concerning the assumptions behind the validity of integrating out the entropic perturbation and the truncation of the effective action to first order in derivatives.

2 Generalities

In this paper, we consider general two-field non-linear sigma models of inflation, described by the action

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{Pl}}^2}{2} R(g) - \frac{1}{2} G_{IJ}(\phi) \nabla^\mu \phi^I \nabla_\mu \phi^J - V(\phi) \right], \quad (2.1)$$

with G_{IJ} the metric of the internal field space manifold. Our convention for the Riemann tensor is

$$R^I{}_{JKL} = \Gamma^I_{JL,K} - \Gamma^I_{KL,J} + \Gamma^M_{KM} \Gamma^M_{JL} - (K \leftrightarrow L), \quad (2.2)$$

where we denote by Γ^I_{JK} the corresponding Levi-Civita connection. The fact that the field space is two-dimensional allows us to write

$$R_{IJKL} = \frac{R_{\text{fs}}}{2} (G_{IK} G_{JL} - G_{IL} G_{JK}) \quad (2.3)$$

in terms of the field space Ricci scalar R_{fs} .

Before considering cubic interactions in the next two sections, here we set-up our notations, describe the gauge choice and covariant parameterization of the fluctuations that we employ, and briefly review the dynamics of the background and of linear fluctuations, that will be extensively used in the rest of the paper.

2.1 Background

The inflationary background is characterized by a spatially flat Friedmann-Lemaître-Robertson-Walker (FLRW) metric with scale factor $a(t)$ and Hubble parameter $H(t) = \dot{a}/a$, and by homogeneous scalar fields $\bar{\phi}^I(t)$. The equations of motion of the latter read $\mathcal{D}_t \dot{\bar{\phi}}^I + 3H\dot{\bar{\phi}}^I + G^{IJ}V_{,J} = 0$, where the time field-space covariant derivative of any field space vector A^I is defined as $\mathcal{D}_t A^I = \dot{A}^I + \Gamma_{JK}^I \dot{\bar{\phi}}^J A^K$. As for the Einstein equations, they can be cast in the form

$$\dot{\sigma}^2 = 2M_{\text{Pl}}^2 H^2 \epsilon, \quad V = M_P^2 H^2 (3 - \epsilon), \quad (2.4)$$

where $\epsilon \equiv -\frac{\dot{H}}{H^2}$ and we define $\dot{\sigma} \equiv \sqrt{G_{IJ}\dot{\bar{\phi}}^I\dot{\bar{\phi}}^J}$. It is useful to introduce a particular set of vielbeins along the background trajectory, the adiabatic-entropic basis defined by $e_\sigma^I \equiv \dot{\bar{\phi}}^I/\dot{\sigma}$ and e_s^I , which is orthogonal to e_σ^I ; the ambiguity in the direction of the latter can be fixed by requiring the basis (e_σ^I, e_s^I) to have a definite orientation. The metric in this basis is just the identity, since by definition $G_{IJ}e_\sigma^I e_s^J = \delta_{\hat{I}\hat{J}}$ with $\hat{I} = \sigma, s$. The derivatives of these orthonormal vectors can be expressed as

$$\mathcal{D}_t e_\sigma^I = H\eta_\perp e_s^I, \quad \mathcal{D}_t e_s^I = -H\eta_\perp e_\sigma^I, \quad (2.5)$$

and we take these relations to define the bending parameter $\eta_\perp$ [59, 60]. This dimensionless parameter quantifies the acceleration of the scalar fields perpendicular to their velocities, and it is a measure of the deviation of the background trajectory from a geodesic. With these variables, the adiabatic and entropic components of the scalar eq. of motion simply read

$$\ddot{\sigma} + 3H\dot{\sigma} + V_{,\sigma} = 0, \quad H\dot{\sigma}\eta_\perp + V_{,s} = 0. \quad (2.6)$$

2.2 Covariant field fluctuations and gauge choice

Covariance. When going beyond the study of linear fluctuations, one should be careful to use variables that are covariant under field space redefinitions. Although not a requirement *per se*, as predictions for observable quantities do not depend on particular choices of variables, it is useful and conceptually clearer to deal with covariant objects. The concern and its resolution have been first described in ref. [61] for generic multifield models. In any given gauge, the idea is to use, not the field fluctuations $\delta\phi^I = \phi^I - \bar{\phi}^I$, which do not transform covariantly, but the vector Q^I living in the tangent space at $\bar{\phi}^I$ and that corresponds to the ‘initial velocity’ of the geodesic connecting the two points labelled by $\bar{\phi}^I$ and ϕ^I (this geodesic is unique if the separation between the two points is sufficiently small). Up to third order in fluctuations, one finds the following relationship between the

covariant perturbation Q^I and the coordinate perturbation $\delta\phi^I$.¹

$$\delta\phi^I = Q^I - \frac{1}{2}\Gamma_{JK}^I Q^J Q^K + \frac{1}{6}(2\Gamma_{LM}^I \Gamma_{JK}^M - \Gamma_{JK,L}^I) Q^J Q^K Q^L + \mathcal{O}(Q^4). \quad (2.7)$$

Gauge choice and constraints. The description of the mixing between the fluctuations of the scalar fields and the ones of the metric is simplified by using the ADM form of the metric [62, 63]:

$$ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt), \quad (2.8)$$

where N is the lapse function and N^i the shift vector, and in terms of which the action (2.1) reads²

$$S = \frac{1}{2} \int dt d^3x \sqrt{h} \left(NR^{(3)} + \frac{1}{N}(E_{ij}E^{ij} - E^2) \right) + \frac{1}{2} \int dt d^3x \sqrt{h} N \left(\frac{1}{N^2} G_{IJ} v^I v^J - G_{IJ} h^{ij} \partial_i \phi^I \partial_j \phi^J - 2V \right), \quad (2.9)$$

where $h = \det(h_{ij})$ and $R^{(3)}$ is the Ricci curvature calculated with h_{ij} . The symmetric tensor E_{ij} is defined by $E_{ij} = \frac{1}{2}\dot{h}_{ij} - N_{(i|j)}$, where the symbol $|$ denotes the spatial covariant derivative associated with the spatial metric h_{ij} , and $v^I = \dot{\phi}^I - N^j \partial_j \phi^I$. The lapse and shift appear without time derivatives in the action and can thus be solved from their eqs. of motion in terms of the genuine degrees of freedom.

Throughout the paper, we neglect tensor and vector perturbations, for the usual reasons that they are decoupled from the scalar fluctuations at linear order, and they only contribute to higher-order correlation functions of the latter by loops, which are suppressed compared to the tree-level interactions we will take into account. For scalar fluctuations, a usual gauge choice when studying multifield inflation is the spatially flat gauge, such that $h_{ij}^{\text{flat}} = a^2(t)\delta_{ij}$, and in which all physical degrees of freedom are the field fluctuations Q^I . This choice is made in many studies (see e.g. [48, 64–68] for general formalisms) and has a number of advantages. However, as we discussed in the introduction, here we consider the comoving gauge in which the adiabatic field fluctuation $e_{\sigma I} Q^I$ is set to zero — but not the entropic fluctuation³ $e_s Q^I \equiv \mathcal{F}$ — and the spatial part of the metric reads $h_{ij}^{\text{comoving}} = a^2 e^{2\zeta} \delta_{ij}$. We note that referring to this gauge as comoving is a slight abuse of terminology as there is strictly speaking no comoving gauge in multifield models beyond linear perturbation theory [69–72]. However, as shown in these works, setting $e_{\sigma I} Q^I = 0$ defines an approximate comoving gauge on super-Hubble scales in expanding universes, so we decided to keep the terminology ‘comoving gauge’ for simplicity.

¹The results looks superficially different from eq. (8) in [61] as they are using the covariant derivative $\Gamma_{JK,L}^I$ and not the simple derivative $\Gamma_{JK,L}^I$ as we do. The equivalent eq. (2.4) in [48] has typos and should read as ours.

²As we will pay attention to boundary terms, which contribute to higher-order correlation functions in general, we note that this result actually corresponds to the full action of General Relativity, composed of the Einstein-Hilbert term supplemented by the Gibbons-Hawking-York boundary term that makes the initial problem well defined, and that we omitted for simplicity in eq. (2.1).

³We prefer not to call this variable Q_s as the latter is usually employed in the literature to refer to $e_s Q^I$ in the flat gauge.

To compute the action up to cubic order, it is sufficient to plug back in the action the expressions of the lapse and the shift at linear order in terms of the physical degrees of freedom ζ and $\mathcal{F}$. Writing $N = 1 + \alpha$ and $N^i = \delta^{ij}\partial_j\theta/a^2$, one obtains

$$\alpha^{(1)} = \frac{\dot{\zeta}}{H}, \quad \theta^{(1)} = -\frac{\zeta}{H} + \chi, \quad (2.10)$$

where the function χ is defined by

$$\frac{1}{a^2}\partial^2\chi = \epsilon\dot{\zeta} + \frac{\dot{\sigma}\eta_\perp}{M_{\text{Pl}}^2}\mathcal{F}. \quad (2.11)$$

Let us note that χ is not merely a useful quantity in intermediate calculations. Rather, χ defined at linear order by $\theta + \zeta/H$ in the comoving gauge that we employ coincides with $-\Psi/H$, where Ψ is the gauge-invariant Bardeen potential (see e.g. ref. [65]). Relatedly, the solution (2.11) to the constraint equations corresponds in our gauge with the gauge-invariant relativistic generalization of the Poisson equation $\partial^2\Psi/a^2 = \delta\rho_m/(2M_{\text{Pl}}^2)$, with $\delta\rho_m$ the linear comoving energy density perturbation. When $\partial^2\chi/a^2$ is negligible on super-Hubble scales, one recovers from eq. (2.11) the familiar feeding of the (comoving) curvature perturbation by the entropic fluctuation $\mathcal{F}$ when the background trajectory differs from a geodesic ($\eta_\perp \neq 0$).

2.3 Quadratic action and linear equations of motion

At second order in the fluctuations, after substituting $\alpha = \alpha^{(1)}$ in the action (2.9) (the contributions from $\theta^{(1)}$ cancel out at this order), and using the background eq. of motion, ones arrives at (writing $S = \int dt d^3x \mathcal{L}$)

$$\mathcal{L}^{(2)} = a^3 \left[M_{\text{Pl}}^2 \epsilon \left(\dot{\zeta}^2 - \frac{(\partial\zeta)^2}{a^2} \right) + 2\dot{\sigma}\eta_\perp \dot{\zeta}\mathcal{F} + \frac{1}{2} \left(\dot{\mathcal{F}}^2 - \frac{(\partial\mathcal{F})^2}{a^2} - m_s^2 \mathcal{F}^2 \right) \right], \quad (2.12)$$

where one finds the familiar expression for the entropic mass:

$$m_s^2 \equiv V_{;ss} - H^2\eta_\perp^2 + \epsilon H^2 M_{\text{Pl}}^2 R_{\text{fs}}, \quad (2.13)$$

with $V_{;ss} = e_s^I e_s^J V_{;IJ}$ the projection of the covariant Hessian of the potential along the entropic direction. For future use we write the linear eqs. of motion deduced from $\mathcal{L}^{(2)}$:

$$\begin{aligned} \mathcal{E}_\zeta &\equiv -\frac{1}{a^3} \frac{\delta S^{(2)}}{\delta \zeta} = 2M_{\text{Pl}}^2 \left[\frac{1}{a^3} \left(a^3 \epsilon \dot{\zeta} \right)' - \frac{\epsilon}{a^2} \partial^2 \zeta \right] + \frac{2}{a^3} (a^3 \dot{\sigma} \eta_\perp \mathcal{F})' \\ \mathcal{E}_\mathcal{F} &\equiv -\frac{1}{a^3} \frac{\delta S^{(2)}}{\delta \mathcal{F}} = \frac{1}{a^3} \left(a^3 \dot{\mathcal{F}} \right)' - \frac{1}{a^2} \partial^2 \mathcal{F} + m_s^2 \mathcal{F} - 2\dot{\sigma} \eta_\perp \dot{\zeta}, \end{aligned} \quad (2.14)$$

and we note that the eq. of motion of ζ can also be compactly rewritten as

$$\mathcal{E}_\zeta = \frac{2M_{\text{Pl}}^2}{a^2} \partial^2 (\dot{\chi} + H\chi - \epsilon\zeta) \quad (2.15)$$

in terms of χ defined in eq. (2.11). As the formal appearance of (2.15) is the same as in the single-field case, it will be particularly useful in order to extend the single-field computation

of the cubic action to the two-field situation. Note eventually that the conjugate momenta of the fields read (at linear order)

$$p_\zeta = 2a^3 M_{\text{Pl}}^2 \left(\epsilon \dot{\zeta} + \frac{\dot{\sigma} \eta_\perp}{M_{\text{Pl}}^2} \mathcal{F} \right) = 2a M_{\text{Pl}}^2 \partial^2 \chi, \quad (2.16)$$

$$p_{\mathcal{F}} = a^3 \dot{\mathcal{F}}. \quad (2.17)$$

3 Multifield cubic action

Expanding the full action (2.9) to cubic order and substituting the linear solution (2.10) for α and θ , it is straightforward to obtain a first form of the cubic action. Details about this computation can be found in appendix A.1. We add the three contributions (A.1)–(A.3) and use the background equations to replace $\dot{\sigma}^2$, V , $V_{,s}$ and $V_{,ss}$ in favor of H , ϵ , $\eta_\perp$ and m_s^2 (but single powers of $\dot{\sigma}$ are kept as is for now), finding:

$$\begin{aligned} \mathcal{L}^{(3)} = a^3 \Big\{ & M_{\text{Pl}}^2 \left[\epsilon \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\zeta}^2 - \frac{\epsilon}{a^2} \zeta (\partial\zeta)^2 + \frac{1}{2a^4} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) (\partial_i \partial_j \theta \partial_i \partial_j \theta - (\partial^2 \theta)^2) \right. \\ & - \frac{2}{a^4} \partial_i \zeta \partial_i \theta \partial^2 \theta \Big] + \dot{\sigma} \eta_\perp \left(6\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\mathcal{F}} + \frac{1}{2} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\mathcal{F}}^2 - \frac{1}{2a^2} \left(\zeta + \frac{\dot{\zeta}}{H} \right) (\partial\mathcal{F})^2 \\ & - \frac{1}{a^2} \dot{\mathcal{F}} \partial\mathcal{F} \partial\theta - \frac{1}{2H} \left(m_s^2 + 2H^2 \eta_\perp^2 - 2\epsilon M_P^2 H^2 R_{\text{fs}} \right) \dot{\mathcal{F}} \mathcal{F}^2 - \frac{3}{2} m_s^2 \zeta \mathcal{F}^2 \\ & \left. - \frac{1}{6} (V_{,sss} - 2\dot{\sigma} H \eta_\perp R_{\text{fs}} + \epsilon M_{\text{Pl}}^2 H^2 R_{\text{fs},s}) \mathcal{F}^3 \right\} + \mathcal{D}_0, \end{aligned} \quad (3.1)$$

where $\theta = -\frac{\zeta}{H} + \chi$, $V_{,sss} \equiv e_s^I e_s^J e_s^K V_{,IJK}$, $R_{\text{fs},s} = e_s^I R_{\text{fs},I}$ and

$$\mathcal{D}_0 = \frac{M_{\text{Pl}}^2}{2} \partial_t \left\{ 2a^3 \left[-9H\zeta^3 + \frac{1}{a^2 H} \zeta (\partial\zeta)^2 \right] \right\} \quad (3.2)$$

is a total derivative term. When setting $\mathcal{F}$ to zero, this results boils down to eq. (3.7) in Maldacena's classic paper [54], as it should. However, for the same reason as there, the form (3.1) of the cubic action is not particularly useful, and even misleading for estimating the amplitude of non-Gaussianities. In the pure adiabatic sector for instance (the ζ^3 terms in brackets), there appear cubic interactions of order ϵ^0 and ϵ , whereas it is known, by comparing to the cubic action computed in the flat gauge, that interactions terms in this sector are genuinely suppressed by ϵ^2 (where ϵ is a generic slow-varying parameter). In the single-field case, a lot of work is required to render explicit the true size of the cubic interactions, by performing multiple integrations by parts and making use of the linear equation of motion. Our task here is similar but more complicated as we have to deal with the two coupled fluctuations ζ and $\mathcal{F}$. However, by generalizing it to the two-field case, we actually simplified the computation compared to the existing literature for the single-field framework (to our knowledge, this is only presented in ref. [73]). We explain in detail the different steps of this long computation in appendix A.2, which is a central part of our work. Before giving our result, we would like to emphasize conceptual points related to it.

3.1 Principles of the computation

Let us recall generally that after having quantized the linear Gaussian theory, and identified the interacting action, one can determine higher-order correlation functions by using the *in-in* (also called Schwinger-Keldysh) formalism [74–76]. Starting from first principles in quantum field theory, this shows that the expectation value of an observable $O(t)$ (an hermitian operator) can be computed perturbatively as

$$\begin{aligned} \langle in|O(t)|in \rangle = \langle 0| \left[\bar{T} \exp \left(i \int_{-\infty(1-i\epsilon)}^t H_I(t') dt' \right) \right] \\ \times O^I(t) \left[T \exp \left(-i \int_{-\infty(1+i\epsilon)}^t H_I(t'') dt'' \right) \right] |0 \rangle \end{aligned} \quad (3.3)$$

where we omit the hat on all operators for simplicity, $|in\rangle$ is the vacuum of the interacting theory at some moment t_i in the far past, T denotes the time-ordered product, the I 's indicate the use of the interaction picture, the $i\epsilon$ prescription projects onto the true vacuum and turns off the interactions in the far past, and H_I is the interacting Hamiltonian. At first-order in the latter, as relevant for the calculation of tree-level three-point correlation functions, one finds

$$\langle O(t) \rangle^{(1)} = i \int_{-\infty(1-i\epsilon)}^t dt' \langle 0| [H_I(t'), O^I(t)] |0 \rangle. \quad (3.4)$$

The form (3.1) of the cubic action makes the use of this formalism transparent as it contains only the fields ζ and $\mathcal{F}$ and their first-order time derivatives. Hence, it is straightforward to determine their conjugate momenta and the interacting Hamiltonian at cubic order, which turn out to simply read $H^{(3)} = - \int d^3x \mathcal{L}^{(3)}$, where $\dot{\zeta}$ and $\dot{\mathcal{F}}$ in the right-hand side should be expressed in terms of the (linear) momenta (2.16)–(2.17). However, as explained above, we will manipulate the cubic action, performing integrations by parts that will make appear second-order time derivatives of the fields. While this is classically allowed, what is the status of these manipulations in the quantum theory?

There are two ways to address this question. The first is conceptually the clearest. It says that the *in-in* formalism should be applied to the form (3.1) of the cubic action and the corresponding Hamiltonian. After using the expansion of the fields into creation and annihilation operators in (3.4) (remember that all fields here are in the interaction scheme and hence are free fields), the computation of say, the tree-level bispectrum, amounts to performing time integrals of products of mode functions, which are *c*-numbers. Doing so, one is perfectly allowed to employ integrations by parts and use that the mode functions obey $\mathcal{E}_\zeta = 0$ and $\mathcal{E}_\mathcal{F} = 0$. The second practical point of view, justified by the previous reasoning, is that one can readily perform integrations by parts at the level of the classical interacting action: all second-order time derivatives generated in this process should be thought of, in the quantum theory, as operators defined in terms of the original fields and linear momenta by imposing that the linear equations of motion are satisfied. In other words, there is no independent quantum operator associated to $\ddot{\zeta}$ or $\ddot{\mathcal{F}}$, which would wrongly signal the existence of additional degrees of freedom beyond ζ and $\mathcal{F}$, and $\mathcal{E}_\zeta$ and $\mathcal{E}_\mathcal{F}$ can be, and should be taken to be identically zero.

A last important subtlety concerns temporal boundary terms in the action. While they do not contribute to the equations of motion, they do in general contribute to correlation functions in the *in-in* formalism [77–79] (contrary to computations of in-out scattering amplitudes in particle physics). From eq. (3.4), one indeed deduces that a total derivative term in $\mathcal{L}^{(3)}$ gives a local contribution (in time):

$$\mathcal{L}^{(3)} \supset \frac{d}{dt} B \quad \Rightarrow \quad \langle O(t) \rangle^{(1)} \supset -i \int d^3x \langle 0 | [B(t), O(t)] | 0 \rangle. \quad (3.5)$$

This shows for instance that boundary operators which do not involve time derivatives do not contribute to the correlation function of an operator involving fields only (as field operators commute with themselves), like the primordial bispectrum, in agreement with a similar argument in [78]. On the contrary, boundary operators involving momenta are relevant in general, and to keep the possibility to compute more general correlation functions, we will keep all temporal boundary terms. However, we will discard the spatial boundary terms generated by the numerous spatial integrations by parts, as they do not contribute to any correlation function.

3.2 Result

Referring the interested reader to the appendix A.2 for the derivation, we quote here our final result for the cubic action:

$$\begin{aligned} \mathcal{L}^{(3)} = & M_{\text{Pl}}^2 a^3 \left[\epsilon(\epsilon - \eta) \dot{\zeta}^2 \zeta + \epsilon(\epsilon + \eta) \zeta \frac{(\partial \zeta)^2}{a^2} + \left(\frac{\epsilon}{2} - 2 \right) \frac{1}{a^4} (\partial \zeta) (\partial \chi) \partial^2 \chi + \frac{\epsilon}{4a^4} \partial^2 \zeta (\partial \chi)^2 \right] \\ & + a^3 \left[\frac{1}{2} m_s^2 (\epsilon + \mu_s) \zeta \mathcal{F}^2 + (2\epsilon - \eta - 2\lambda_\perp) \dot{\sigma} \eta_\perp \zeta \dot{\zeta} \mathcal{F} + \frac{\dot{\sigma} \eta_\perp}{a^2 H} \mathcal{F} (\partial \zeta)^2 \right. \\ & - \frac{\dot{\sigma} \eta_\perp}{H} \dot{\zeta}^2 \mathcal{F} - \frac{1}{H} (H^2 \eta_\perp^2 - \epsilon M_{\text{Pl}}^2 H^2 R_{\text{fs}}) \dot{\zeta} \mathcal{F}^2 \\ & - \frac{1}{6} (V_{;sss} - 2\dot{\sigma} H \eta_\perp R_{\text{fs}} + \epsilon M_{\text{Pl}}^2 H^2 R_{\text{fs},s}) \mathcal{F}^3 \\ & \left. + \frac{1}{2} \epsilon \zeta \left(\dot{\mathcal{F}}^2 + \frac{(\partial \mathcal{F})^2}{a^2} \right) - \frac{1}{a^2} \dot{\mathcal{F}} \partial \mathcal{F} \partial \chi \right] + \mathcal{D} + \mathcal{E} \end{aligned} \quad (3.6)$$

with

$$\begin{aligned} \mathcal{D} = & \frac{d}{dt} \left\{ -\frac{a}{2H} \zeta (\partial \mathcal{F})^2 + \frac{a M_{\text{Pl}}^2}{H} (1 - \epsilon) \zeta (\partial \zeta)^2 - 9H M_{\text{Pl}}^2 a^3 \zeta^3 - \frac{a^3}{2H} (m_s^2 + 4H^2 \eta_\perp^2) \zeta \mathcal{F}^2 \right. \\ & - \frac{M_{\text{Pl}}^2}{4aH^3} (\partial \zeta)^2 \partial^2 \zeta - \frac{\zeta p_\zeta^2}{4\epsilon H a^3 M_{\text{Pl}}^2} + \frac{\dot{\sigma} \eta_\perp}{\epsilon H M_{\text{Pl}}^2} \mathcal{F} \zeta p_\zeta - \frac{\zeta}{8a^3 H M_{\text{Pl}}^2} (\partial^{-2} p_{\zeta,ij} \partial^{-2} p_{\zeta,ij} - p_\zeta^2) \\ & \left. + \frac{\zeta}{4aH^2} (\zeta_{,ij} \partial^{-2} p_{\zeta,ij} - \partial^2 \zeta p_\zeta) - \frac{1}{2Ha^3} \zeta p_{\mathcal{F}}^2 \right\}. \end{aligned} \quad (3.7)$$

and

$$\begin{aligned} \mathcal{E} = & \frac{a^3}{H} \mathcal{E}_\zeta \left[\dot{\zeta} \zeta - \frac{1}{4a^2 H} ((\partial \zeta)^2 - \partial^{-2} \partial_i \partial_j (\partial_i \zeta \partial_j \zeta) - 2H (\partial \zeta \partial \chi - \partial^{-2} \partial_i \partial_j (\partial_i \zeta \partial_j \chi))) \right] \\ & + \frac{a^3}{H} \mathcal{E}_{\mathcal{F}} \zeta \dot{\mathcal{F}}, \end{aligned} \quad (3.8)$$

and where it will prove convenient to use the (linear) conjugate momenta (2.16)–(2.17) in the boundary term (3.7). Employing integrations by parts and making appear the linear equations of motion, the cubic action may appear in very different forms. We now argue why the result (3.6) is in some sense the best form one can achieve, and emphasise a couple of points regarding it.

- First, we stress that this compact result is exact. In particular, the various parameters $\epsilon = -\dot{H}/H^2$, $\eta = \dot{\epsilon}/(H\epsilon)$, $\lambda_\perp = \dot{\eta}_\perp/(H\eta_\perp)$, $\mu_s = (m_s^2)'/(Hm_s^2)$ are just short-hand notations, and no slow-varying approximation has been employed. It can hence be used in any model, whatever the dynamics of the background and the related mass scales dictating the physics of entropic fluctuations and their couplings to the adiabatic fluctuation.
- Contrary to the intermediate result (3.1), the genuine size of interactions is made manifest in (3.6). Concerning the pure adiabatic sector, the interactions in $\mathcal{O}(\zeta^3)$ are explicitly of order $\mathcal{O}(\epsilon, \eta)^2$ or higher, like in the single-field case. In a similar way, besides the intrinsic multifield effects encoded in operators proportional to $\eta_\perp, m_s^2, R_{\text{fs}}, R_{\text{fs},s}$ and $V_{;sss}$, the interactions in $\mathcal{O}(\zeta\mathcal{F}^2)$ in the last line are proportional to ϵ .
- As we will demonstrate in the next section, this form is particularly convenient to discuss the limit of a heavy entropic fluctuation that can be integrated out, resulting in a single-field effective field theory for the adiabatic mode ζ .
- How to dispatch interactions between the bulk Lagrangian and the boundary term $\mathcal{D}$ has been chosen to minimize the influence of the latter and to easily deduce their effects. In this respect, note that in the single-field case where $\mathcal{F} = 0$ and only the first line of the bulk action is present, our result matches the form of the cubic action given in ref. [78]. In particular, no operator in $\zeta^2\dot{\zeta}$ is present in the bulk action, contrary to refs. [54, 57, 58]. As argued in [78], nothing is gained by having one additional operator in the bulk action, all the more as it would come with an extra operator in the boundary term that would contribute to the primordial bispectrum. Below, we discuss the contributions of the boundary term to the primordial bispectrum in a general multifield situation.

3.3 Contribution of boundary terms

It is common practice to evaluate the contributions of boundary terms by performing field redefinitions [54, 57, 58]. The idea is that by carefully choosing the field redefinition $\zeta = \tilde{\zeta} + f[\tilde{\zeta}, \tilde{\mathcal{F}}]$ the second and cubic action written in terms of $\tilde{\zeta}$ may not contain contributing boundary terms. One can then simply evaluate the difference between the 3-point correlation functions of ζ and $\tilde{\zeta}$ by applying Wick theorem. However, as we explain in more details in appendix B, this procedure can be ambiguous as different field redefinitions may be chosen to cancel boundary terms, giving different answers for $\langle \zeta^3 \rangle$ in general.

In what follows, we evaluate the contribution of boundary terms following first principles. Concentrating for definiteness on the main observable of interest, the three-point

correlation function of the curvature perturbation

$$\langle \zeta_{\mathbf{k}_1} \zeta_{\mathbf{k}_2} \zeta_{\mathbf{k}_3} \rangle \equiv (2\pi)^3 \delta\left(\sum_i \mathbf{k}_i\right) B_\zeta(k_1, k_2, k_3), \quad (3.9)$$

the relevant boundary terms, that involve the conjugate momentum p_ζ and hence contribute to the bispectrum, read

$$S_{\mathcal{D}} \supset (2\pi)^3 \int \prod_i \frac{d^3 \mathbf{k}_i}{(2\pi)^3} \delta\left(\sum_i \mathbf{k}_i\right) \left[a(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \mathcal{F}(\mathbf{k}_1) \zeta(\mathbf{k}_2) p_\zeta(\mathbf{k}_3) \right. \\ \left. + b(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \zeta(\mathbf{k}_1) \zeta(\mathbf{k}_2) p_\zeta(\mathbf{k}_3) + c(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) p_\zeta(\mathbf{k}_1) p_\zeta(\mathbf{k}_2) \zeta(\mathbf{k}_3) \right], \quad (3.10)$$

where b and c are taken symmetric under $\mathbf{k}_1 \leftrightarrow \mathbf{k}_2$ without loss of generality, with

$$a(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \frac{\dot{\sigma} \eta_\perp}{\epsilon H M_{\text{Pl}}^2} \quad (3.11)$$

$$b(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \frac{1}{8a^2 H^2} \left(k_1^2 + k_2^2 - (\mathbf{k}_1 \cdot \hat{\mathbf{k}}_3)^2 - (\mathbf{k}_2 \cdot \hat{\mathbf{k}}_3)^2 \right) \quad (3.12)$$

$$c(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \frac{1}{8a^3 \epsilon H M_{\text{Pl}}^2} \left(-2 + \epsilon (1 - (\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)^2) \right), \quad (3.13)$$

and where $\hat{\mathbf{k}}_i$ is the unit vector $\mathbf{k}_i/k_i$. Using eqs. (3.4)–(3.5) and (the quantum) Wick theorem, these various interactions contribute to the bispectrum as products of three two-point correlation functions. For instance, the second term gives

$$B_\zeta \supset i \langle \zeta(\mathbf{k}_1) \zeta(-\mathbf{k}_1) \rangle' \langle \zeta(\mathbf{k}_2) \zeta(-\mathbf{k}_2) \rangle' \langle \zeta(\mathbf{k}_3) p_\zeta(-\mathbf{k}_3) \rangle' b(-\mathbf{k}_1, -\mathbf{k}_2, -\mathbf{k}_3) + \text{cc} + 5 \text{ perms.} \quad (3.14)$$

where we omit hats on all operators, and use the notation $\langle A(\mathbf{k}_1) B(\mathbf{k}_2) \rangle = (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \langle A(\mathbf{k}_1) B(-\mathbf{k}_1) \rangle'$. While $\langle \zeta(\mathbf{k}_1) \zeta(-\mathbf{k}_1) \rangle'$ is simply the real power spectrum $P_\zeta(k_1)$, one has

$$\langle \zeta(\mathbf{k}) p_\zeta(-\mathbf{k}) \rangle' = P_{\zeta p_\zeta}(k) + \frac{i}{2} \quad (3.15)$$

where $P_{\zeta p_\zeta}(k) = \frac{1}{2} \left(\langle \zeta(\mathbf{k}) p_\zeta(-\mathbf{k}) \rangle' + \langle p_\zeta(\mathbf{k}) \zeta(-\mathbf{k}) \rangle' \right)$ is the real cross-spectrum, and where we used the commutation relation $\langle \zeta(\mathbf{k}) p_\zeta(-\mathbf{k}) \rangle' - \langle p_\zeta(\mathbf{k}) \zeta(-\mathbf{k}) \rangle' = i$. Using (3.15), it is straightforward to deduce that boundary terms of the type (3.10) contribute to the bispectrum as

$$B_\zeta(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) - B_{\zeta, \text{bulk}}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = -a(-\mathbf{k}_1, -\mathbf{k}_2, -\mathbf{k}_3) P_{\zeta \mathcal{F}}(k_1) P_\zeta(k_2) + 5 \text{ perms.} \\ -2 b(-\mathbf{k}_1, -\mathbf{k}_2, -\mathbf{k}_3) P_\zeta(k_1) P_\zeta(k_2) + 2 \text{ perms.} \\ -2 c(-\mathbf{k}_1, -\mathbf{k}_2, -\mathbf{k}_3) P_\zeta(k_3) P_{\zeta p_\zeta}(k_2) + 5 \text{ perms.,} \quad (3.16)$$

where $B_{\zeta, \text{bulk}}$, generated by bulk interactions in (3.6), can be calculated using standard methods, numerically or with analytical approximations. The form (3.16) has the advantage of rendering manifest that various rewritings of the boundary terms that differ by total

spatial derivatives contribute in the same way to the bispectrum, as, taking into account total momentum conservation, they all define unambiguously the same functions b and c symmetric in their first two arguments. As we discuss in appendix B, this independence of the bispectrum on the precise form of the action and on spatial boundary terms is not shared by the method of field redefinitions, which is ambiguous in general.

We stress that no approximation has been used and that eq. (3.16) can be used at any time. However, it is particularly convenient to discuss the late-time super-Hubble behaviour. In particular, it is useful not to split $P_{\zeta p_\zeta}$ into $2a^3 M_{\text{Pl}}^2 (\epsilon P_{\zeta\dot{\zeta}} + \dot{\sigma} \eta_\perp M_{\text{Pl}}^{-2} P_{\zeta\mathcal{F}})$. Indeed, as discussed after eq. (2.11), $p_\zeta / (2a^3 M_{\text{Pl}}^2) = \partial^2 \chi / a^2$ is suppressed on super-Hubble scales. In this limit, the third term in (3.16) therefore gives negligible contributions, while the second one is manifestly negligible, and we are left with only the first term, that make explicitly appear $P_{\zeta\mathcal{F}}$. The result (3.16) thus enables one to treat the single and multifield situation in a unified manner: independently of whether ζ approaches a constant or not on super-Hubble scales, only the first term contributes. In the single-field situation, it is simply absent and the boundary terms do not contribute at late times. In a multifield setup, if entropic fluctuations get exhausted by the end of inflation (and hence an adiabatic limit is reached where ζ becomes constant), the first term eventually becomes negligible, but this need not be the case in general. In these circumstances in which correlation functions have to be followed through (p)reheating, equation (3.16), with the first term in particular, would provide correct initial conditions.

4 Single-field effective theories

In sections 4.1 and 4.2, as a first application of our general result (3.6), we discuss the particularly interesting limit of a heavy entropic fluctuation, and the single-field effective theory that results up to cubic order when the former is integrated out at leading order in derivatives. This subject has been extensively studied in the literature (see e.g. [8–11, 26, 28, 80–90]). However, it is the first time that a general formalism is derived: away from any decoupling limit, keeping all interactions and in a generic curved field space. Our result will thus unify and generalise previous partial results. In section 4.3, we consider a large class of two-field models where one may integrate out a heavy field at the level of the full action, resulting in an effective $P(X, \phi)$ Lagrangian. From this, we derive explicit expression for the parameters governing the cubic interactions of fluctuations, and show their consistency with our previous general result where heavy *fluctuations* are integrated out.

4.1 Generalities and regime of validity

Before moving to the actual computation in the next section, here we discuss the conditions of validity and of predictivity of the EFT we will derive. Let us recall that the linear equation of motion for $\mathcal{F}$, $\mathcal{E}_{\mathcal{F}} = 0$, reads

$$(m_s^2 - \square) \mathcal{F} = 2\dot{\sigma} \eta_\perp \dot{\zeta} \quad \text{with} \quad \square = -\frac{\partial^2}{\partial t^2} - 3H \frac{\partial}{\partial t} + \frac{\partial^2}{a^2}. \quad (4.1)$$

As a first assumption that will be made more precise below, we consider situations with $m_s^2 \gg H^2$, and work out the effective action by substituting in the second and cubic order

actions (2.12) and (3.6) the expression for $\mathcal{F}$ that results from solving its eq. of motion at leading order in the derivative expansion, that is

$$\mathcal{F} = \mathcal{F}_{\text{LO}} \equiv \frac{2\dot{\sigma}\eta_{\perp}}{m_s^2} \dot{\zeta}. \quad (4.2)$$

Independently of any derivative expansion, let us recall that for our purpose, it is sufficient to plug back in the action the solution to the *linear* eq. of motion for $\mathcal{F}$, like for the lapse and shift: the quadratic correction to $\mathcal{F}$ coming from cubic interactions could be kept, but its total contribution to the action identically vanishes up to cubic order.

Inserting (4.2) into the quadratic action (2.12), and consistently neglecting the kinetic and gradient terms of $\mathcal{F}$, one readily obtains the effective quadratic Lagrangian

$$\mathcal{L}_{\text{LO}}^{(2)} = a^3 M_{\text{Pl}}^2 \frac{\epsilon}{c_s^2} \left(\dot{\zeta}^2 - c_s^2 \frac{(\partial\zeta)^2}{a^2} \right), \quad (4.3)$$

where c_s^2 such that

$$\frac{1}{c_s^2} - 1 \equiv \frac{4H^2\eta_{\perp}^2}{m_s^2} \quad (4.4)$$

is the so-called speed of sound (squared) of fluctuations. Note that the linear eq. of motion obtained by varying (4.3) consistently coincides with the “effective” eq. of motion of ζ , i.e. the expression for $\mathcal{E}_{\zeta}$ (2.14) obtained after replacing $\mathcal{F} = \mathcal{F}_{\text{LO}}$:

$$\mathcal{E}_{\zeta,\text{LO}} = 2M_{\text{Pl}}^2 \left[\frac{1}{a^3} \left(a^3 \frac{\epsilon}{c_s^2} \dot{\zeta} \right)' - \frac{\epsilon}{a^2} \partial^2 \zeta \right]. \quad (4.5)$$

In a related manner, the expression of χ (2.11) in the two-field theory simply boils down to $\partial^2 \chi_{\text{LO}}/a^2 = \epsilon \dot{\zeta}/c_s^2$ in the single-field EFT.

We note that models giving rise to $c_s^2 < 0$ — an imaginary sound speed — have been recently studied, as well as the implications of such a non-standard framework [26, 28, 90]. These models, corresponding to a large negative m_s^2/H^2 , can be compatible with a stable background when the background trajectory strongly deviates from a geodesic. However, in these models, entropic fluctuations experience a transient tachyonic instability, which generates large primordial non-Gaussianities [28]. Hence, although our results in this paper formally hold in situations with $c_s^2 < 0$, and may be used to analyse some of these models, in the following, we implicitly and conservatively assume that m_s^2 and c_s^2 are positive.

Obviously, neglecting the gradient term $(\partial\mathcal{F})^2/a^2$ compared to the mass term $m_s^2 \mathcal{F}^2$ in the action requires that the relevant k -mode enters the low-energy regime $k^2/a^2 \ll m_s^2$. However, there also exist adiabaticity conditions bounding the time scale of variations of background quantities, owing to the fact that we also neglected the kinetic term of $\mathcal{F}$. Formally inverting the equation of motion for $\mathcal{F}$ as:

$$\mathcal{F} = (m_s^2 - \square)^{-1} 2\dot{\sigma}\eta_{\perp} \dot{\zeta} = \frac{1}{m_s^2} \sum_{i=0}^{\infty} \left(\frac{\square}{m_s^2} \right)^i 2\dot{\sigma}\eta_{\perp} \dot{\zeta}, \quad (4.6)$$

this shows that the dynamics of $\mathcal{F}$ is reliably described by the first term in the expansion $\mathcal{F}_{\text{LO}}$ (4.2) only if $\square/m_s^2 \ll 1$. In particular it requires that background quantities (and the

mode function of ζ that inherits any time variation of the background) evolve on time scales much larger than m_s^{-1} , so as not to excite high-frequency modes that are not captured by the low-energy effective field theory (4.3). More precisely, let us consider for definiteness the next-to-leading order correction to $\mathcal{F}$ ($i = 1$ in (4.6)). Using (4.5), one obtains

$$\begin{aligned} \square(\dot{\sigma}\eta_\perp\dot{\zeta}) &= (1 - c_s^2)\dot{\sigma}\eta_\perp\frac{\partial^2\dot{\zeta}}{a^2} + c_s^2(2 + 2\epsilon - 2\lambda_\perp - 4s)\dot{\sigma}H\eta_\perp\frac{\partial^2\dot{\zeta}}{a^2} \\ &\quad - \dot{\sigma}H^2\eta_\perp\dot{\zeta}\left[\left(-3 - \epsilon - \frac{\eta}{2} + \lambda_\perp + 2s\right)\left(-2\epsilon - \frac{\eta}{2} + \lambda_\perp + 2s\right)\right. \\ &\quad \left. - \eta\epsilon - \frac{\dot{\eta}}{2H} + \frac{\dot{\lambda}_\perp}{H} + 2\frac{\dot{s}}{H}\right] \end{aligned} \quad (4.7)$$

where $s = (c_s^2)/(2Hc_s^2)$.⁴ Requiring that it is consistently negligible compared to the leading-order term, i.e. $\square(\dot{\sigma}\eta_\perp\dot{\zeta}) \ll m_s^2\dot{\sigma}\eta_\perp\dot{\zeta}$ imposes some restrictions. The first term in the right hand side of (4.7) is readily negligible, being suppressed by $(1 - c_s^2)k^2/(a^2m_s^2)$. However, the third term is safely negligible only if H^2/m_s^2 multiplied by the expression between brackets in (4.7) is much smaller than unity. Barring cancellations, this requires

$$\left(\frac{\dot{X}}{m_s X}\right)^2 \ll 1 \quad \text{and} \quad \frac{\ddot{X}}{m_s^2 X} \ll 1 \quad (4.9)$$

for the various parameters $X = (H, \epsilon, c_s, \eta_\perp)$. As a prolonged phase of inflation requires ϵ and $\eta \ll 1$, these conditions are usually taken for granted for the first two parameters, but should be kept in mind in case of transient features. More interesting is the fact that the speed of sound c_s and the bending parameter $\eta_\perp$ are allowed to vary significantly on a Hubble time scale, although not on scales m_s^{-1} [82]. Note that considering higher-order terms in the expansion (4.6) would have bounded any $X^{(n)}/(m_s^n X)$, so that it is really the time scale of variation of the various quantities that are bounded, and not specific time-derivatives. Eventually, as c_s^2 (4.4) not only depends on the bending parameter but also on the entropic mass (2.13), which may vary on different time scales, the validity of the EFT can not be judged simply by inspecting the time variations of c_s , but should be verified at the level of the various entropic quantities. While we considered so far the first and last terms in (4.7), the second one in $\partial^2\zeta$ can not be straightforwardly compared to $\dot{\zeta}$ without some knowledge about the time-dependence of the mode function, which is not known analytically in a general time-dependent background. However, when the adiabaticity conditions above are satisfied, one expects the standard behaviours $\dot{\zeta} \sim \frac{kc_s}{a}\zeta$ inside the sound horizon and $\dot{\zeta} \sim \frac{k^2c_s^2}{a^2H}\zeta$ outside. This enables one to deduce that the second term is also well negligible under these circumstances.

Besides the adiabaticity conditions, we have seen that higher-derivative corrections to the leading-order EFT are in $k^2/(a^2m_s^2)$. To express this in terms of energy scales ω , let

⁴Of course s is not independent of other parameters already introduced. Explicitly,

$$s = (1 - c_s^2)\left(\epsilon - \lambda_\perp + \frac{\mu_s}{2}\right). \quad (4.8)$$

us use the dispersion relation $\omega^2 = c_s^2 k^2 / a^2$ deduced from the EFT (4.3). This shows that corrections to the EFT action are in $\omega^2 / \omega_{\text{new}}^2$, where

$$\omega_{\text{new}}^2 = m_s^2 c_s^2 \quad (4.10)$$

has been indeed identified as the energy scale of new physics above which higher-order derivative terms should be taken into account [9, 80].

In retrospect, using the expression (4.2), one can compute $\dot{\mathcal{F}}$:

$$\dot{\mathcal{F}}_{\text{LO}} = \frac{2\dot{\sigma}\eta_{\perp}}{m_s^2} \left[\frac{c_s^2}{a^2} \partial^2 \zeta - H\dot{\zeta} \left(3 + \epsilon + \frac{\eta}{2} - \lambda_{\perp} + \mu_s - 2s \right) \right], \quad (4.11)$$

omitting $\mathcal{E}_{\zeta, \text{LO}}$ on the right-hand side, and deduce that under the conditions of validity of the EFT, we were indeed allowed to neglect the kinetic term of $\mathcal{F}$ in the action compared to the mass term, the former being suppressed by the hierarchies H^2/m_s^2 , $c_s^2 \omega^2 / \omega_{\text{new}}^2$ and combinations thereof. This shows however that any appearance of $\dot{\mathcal{F}}$ in the higher-order action may not be neglected, in particular if it is multiplied by possibly large factors like m_s^2/H^2 or $\eta_{\perp}$. We have taken this into account to choose the ‘best form’ of the cubic action we displayed in (3.6) (see appendix A.2.2).

Eventually, let us consider a situation in which $H^2/c_s^2 \gg m_s^2$. Then modes described by the EFT, such that $k^2/a^2 \ll m_s^2$, are outside the sound horizon and already constant, hence the EFT can not predict the final observable values of their correlation functions. To be able to impose proper initial conditions from the EFT alone (for instance and typically Bunch-Davies), without knowledge from its two-field UV completion, there should exist an intermediate regime in which modes are both of sufficiently low-energy that they can be described by the EFT, and sufficiently under the sound horizon, i.e. they should verify $m_s^2 \gg k^2/a^2 \gg H^2/c_s^2$. Hence, one deduces that in addition to the conditions of validity that we delineated above, one should require

$$\frac{H^2}{m_s^2 c_s^2} \ll 1 \quad (4.12)$$

for the EFT to have predictive power, which is more constraining than simply having a massive field: $H^2/m_s^2 \ll 1$. This is of course consistent with higher-order derivative corrections to the EFT action being in $\omega^2 / \omega_{\text{new}}^2$: as modes become constant around $\omega \sim H$, describing this process with our low-energy EFT requires $H^2 \ll \omega_{\text{new}}^2$, i.e. eq. (4.12).

4.2 Single-field effective theory of fluctuations

To deduce the effective cubic action, we should substitute $\mathcal{F}$ by $\mathcal{F}_{\text{LO}}$ (4.2) in the cubic action. As we mentioned, the form (3.6) is particularly convenient for that purpose. Indeed, the last line of the bulk action should be consistently discarded, as it involves either gradient terms suppressed by $k^2/(a^2 m_s^2)$, or interactions in $\dot{\mathcal{F}}$ that are suppressed by H^2/m_s^2 . The other bulk interactions involve $\mathcal{F}$ only, and their contributions to the effective action for ζ are straightforward to deduce, with $\partial^2 \chi / a^2 \rightarrow \epsilon \dot{\zeta} / c_s^2$ for the first line, the first two terms of the second line giving $\dot{\zeta}^2 \zeta$ interactions, the last term of the second line giving a vertex

in $\dot{\zeta}(\partial\zeta)^2$, and the whole third line giving rise to interactions in $\dot{\zeta}^3$. As for the boundary terms, the general expression (3.16) in the multifield situation shows that their contribution on super-Hubble scales are negligible in the single-field effective theory where ζ becomes constant on super-Hubble scales. Hence quoting the bulk action only for simplicity, one arrives at

$$\mathcal{L}_{\text{EFT,bulk}}^{(3)} = M_{\text{Pl}}^2 a^3 \frac{\epsilon}{c_s^2} \left[f_0 c_s^2 \frac{\dot{\zeta}}{H} \frac{(\partial\zeta)^2}{a^2} + \frac{f_1}{H} \dot{\zeta}^3 + f_2 \dot{\zeta}^2 \zeta + f_3 c_s^2 \zeta \frac{(\partial\zeta)^2}{a^2} + f_4 \dot{\zeta} \partial_i \partial^{-2} \dot{\zeta} \partial_i \zeta + f_5 \partial^2 \zeta (\partial_i \partial^{-2} \dot{\zeta})^2 \right] \quad (4.13)$$

with

$$\begin{aligned} f_0 &= \left(\frac{1}{c_s^2} - 1 \right) & f_1 &= \left(\frac{1}{c_s^2} - 1 \right) A & f_2 &= \epsilon - \eta + 2s \\ f_3 &= \epsilon + \eta & f_4 &= \frac{\epsilon}{2c_s^2} (\epsilon - 4) & f_5 &= \frac{\epsilon^2}{4c_s^2} \end{aligned} \quad (4.14)$$

and

$$A = -\frac{1}{2}(1 + c_s^2) + \frac{2}{3}(1 + 2c_s^2) \frac{\epsilon H^2 M_{\text{Pl}}^2 R_{\text{fs}}}{m_s^2} - \frac{1}{6}(1 - c_s^2) \left(\frac{\kappa V_{;sss}}{m_s^2} + \frac{\kappa \epsilon H^2 M_{\text{Pl}}^2 R_{\text{fs},s}}{m_s^2} \right), \quad (4.15)$$

and where we introduced the so-called bending radius of the trajectory $\kappa = \sqrt{2\epsilon} M_{\text{Pl}} / \eta_\perp$. The cubic action (4.13)–(4.15) constitutes the second main result of this paper. It incorporates without approximations all the interactions in the effective field theory that results from integrating out heavy entropic fluctuations at leading-order in a derivative expansion. The normalisation of operators in (4.13) have been chosen such that the coupling constants f_i 's in (4.14) represent the genuine typical contributions of each interaction to the dimensionless shape function of the bispectrum, i.e. the f_i 's represent the typical contributions to f_{NL} in featureless models. As we explain below, the set of six operators in (4.13) are redundant. However, this form of the cubic action has the appealing physical advantage to make transparent the link with the single-field effective field theory of fluctuations [20, 21].

Dominant interactions and EFT of inflationary fluctuations. As we have discussed in section 4.1, the EFT is perfectly valid in situations with $(\epsilon, \eta, s) = \mathcal{O}(1)$, as motivated by transient features and sharp turns in field space in the multifield theory, and in which case all interactions in (4.13) should be kept a priori. Here however, we concentrate on smooth models in which a slow-varying approximation $(\epsilon, \eta, s) \ll 1$ is verified. In this context, a particularly interesting regime, theoretically and observationally, corresponds to situations in which the sound speed (4.4) differs substantially from unity, i.e. $\left(\frac{1}{c_s^2} - 1 \right) \gtrsim \mathcal{O}(1)$. Considering A of order one (we will come back to this below and discuss the various contributions to A), one deduces from (4.14) that the first two operators in (4.13) are dominant. Hence, not writing explicitly boundary terms, which do not play a role for observational predictions in this context, one can effectively write

$$S_{\text{EFT,main}}^{(3)} = \int dt d^3x a^3 M_{\text{Pl}}^2 \frac{\epsilon}{H} \left(\frac{1}{c_s^2} - 1 \right) \left[\dot{\zeta} \frac{(\partial\zeta)^2}{a^2} + \frac{A}{c_s^2} \dot{\zeta}^3 \right]. \quad (4.16)$$

These two operators are precisely the ones encountered in the decoupling limit of the effective field theory of single-clock inflationary fluctuations at leading-order in derivatives [21]: $\dot{\zeta}(\partial\zeta)^2$ interactions, whose size is fixed by symmetry in terms of the sound speed appearing in the second-order action (4.3), and $\dot{\zeta}^3$ interactions, whose overall contribution is not fixed. To be more precise, although the EFT of single-clock inflationary fluctuations can be in principle formulated exactly in terms of the comoving curvature perturbation ζ , in practice computations in this context are often performed in terms of the Goldstone boson of spontaneously broken time translations π , in the decoupling limit in which its mixing with gravity can be neglected, at leading-order in a slow-varying approximation, and with the linear approximate relation $\zeta \simeq -H\pi$. Under these hypotheses and approximations, it agrees with eq. (4.16). However, we stress that our general result (4.13), of which (4.16) is a particular limit, holds without these approximations: it encompasses the usual formulation of the single-clock EFT of inflation, but goes beyond it. To our knowledge, this is the first time that the dominant operators expected in the EFT of single-clock fluctuations are derived from first principles from a UV completion (here two-field models with a background trajectory deviating from a geodesic motion), away from the decoupling limit, and readily in terms of the observable comoving curvature perturbation.

Under the slow-varying approximation used above, the observational predictions corresponding to the EFT (4.3)–(4.16) are very well known, for the power spectrum and bispectrum. We reproduce these results for completeness. The primordial power spectrum reads

$$\frac{k^3}{2\pi^2} P_\zeta(k) = \left(\frac{H^2}{8\pi^2 \epsilon c_s} \right)_\star, \quad (4.17)$$

with a mild scale dependence given by the slight dependence of H, ϵ and c_s on the time of evaluation $\star$ such that $kc_s = aH$, i.e. $n_s - 1 = -(2\epsilon + \eta + s)_\star$. As for the bispectrum (3.9), its shape S , such that

$$B_\zeta = (2\pi)^4 \frac{S(k_1, k_2, k_3)}{(k_1 k_2 k_3)^2} A_s^2, \quad (4.18)$$

with A_s the power spectrum (4.17) evaluated at a pivot scale, reads, in a scale-invariant approximation:

$$S = S_{\dot{\zeta}(\partial\zeta)^2} + S_{\dot{\zeta}^3}, \quad \text{with} \quad (4.19)$$

$$S_{\dot{\zeta}(\partial\zeta)^2} = \left(\frac{1}{c_s^2} - 1 \right) \frac{1}{k_1 k_2 k_3} \left[-\frac{1}{K} \sum_{i>j} k_i^2 k_j^2 + \frac{1}{2K^2} \sum_{i \neq j} k_i^2 k_j^3 + \frac{3}{2K^3} \prod_i k_i^2 + \frac{1}{8} \sum_i k_i^3 \right] \quad (4.20)$$

$$S_{\dot{\zeta}^3} = A \left(\frac{1}{c_s^2} - 1 \right) \frac{3k_1 k_2 k_3}{2K^3}, \quad (4.21)$$

and were $K = k_1 + k_2 + k_3$. These two individual shapes are similar, peak on equilateral triangles, and can be represented in a first approximation by the well known equilateral template [91]. However, their linear combination assumes a very different shape in the range $3.1 \lesssim A \lesssim 4.3$, peaking near flattened configurations $k_2 + k_3 \simeq k_1$, and is more accurately described by the orthogonal template [92]. In this respect, it is instructive to

quote the amplitude of the total shape function (4.19) in the representative equilateral and squashed configurations

$$S(1, 1, 1) = -\frac{17}{72} \left(\frac{1}{c_s^2} - 1 \right) \left(1 - \frac{4A}{17} \right) \quad (4.22)$$

$$S(1, 1/2, 1/2) = -\frac{3}{64} \left(\frac{1}{c_s^2} - 1 \right) (1 - A) , \quad (4.23)$$

where (4.22) indicates in a simple manner that for values of A around $17/4 = 4.25$, one can not expect indeed the equilateral template to faithfully represent the bispectrum.

Full result and comparison with $P(X)$ models. We derived the low energy EFT (4.3)–(4.13) at lowest order in derivatives in terms of the single fluctuating degree of freedom ζ . Hence, it should correspond to a particular case of the EFT of single-clock inflation at lowest-order in derivatives, and indeed we have seen above that our result encompasses the decoupling limit result of this formulation. There exist another interesting class of models, single-field inflationary models of Lagrangian $P(X = -\frac{1}{2}(\partial\phi)^2, \phi)$, also-called k -inflation or $P(X)$ theories, whose fluctuations can be exactly described by the single-clock EFT at lowest order in derivatives (this is readily visible in the uniform inflaton gauge). Hence, our full result (4.3)–(4.13) should agree with the well known full quadratic and cubic action of k -inflation [57, 58], upon identification of the multifield background quantities c_s^2 and f_i 's (4.14) with suitable combination of the derivatives $P^{(n)}(X)$.

As discussed in 3.2, given the way we organised the splitting between bulk and boundary terms in (3.6) and in the resulting EFT, i.e. without a bulk operator in $\zeta^2 \dot{\zeta}$, it is convenient to compare our result to the one of ref. [78], where the same choice is made and boundary terms are innocuous. Concentrating on bulk terms, their result contains the five last operators in (4.13), but with different coupling constants, and without the first operator in $\dot{\zeta}(\partial\zeta)^2$. However, the latter can be manipulated as (see e.g. [93])

$$\begin{aligned} \frac{a\epsilon}{H} \left(\frac{1}{c_s^2} - 1 \right) \dot{\zeta}(\partial\zeta)^2 &= \frac{a\epsilon}{c_s^2} \left((1 - c_s^2)(1 + \epsilon + \eta) - 2s \right) \zeta(\partial\zeta)^2 + \frac{a^3\epsilon(1 - c_s^2)}{c_s^4} \frac{\dot{\zeta}^3}{H} \\ &+ \frac{a^3\epsilon}{c_s^4} \left((1 - c_s^2)(-3 + \epsilon - \eta) - 2c_s^2 s \right) \dot{\zeta}^2 \zeta \\ &- \partial_t \left[\frac{a\epsilon}{H} \left(\frac{1}{c_s^2} - 1 \right) \zeta(\partial\zeta)^2 + \frac{a^3\epsilon(1 - c_s^2)}{H c_s^4} \dot{\zeta}^2 \zeta \right] \\ &+ \frac{a^3(1 - c_s^2)}{M_{\text{Pl}}^2 H c_s^2} \dot{\zeta} \zeta \mathcal{E}_{\zeta, \text{LO}} , \end{aligned} \quad (4.24)$$

where the generated boundary terms are also innocuous on large scales. Using this redundancy between operators, the coupling constants in the bulk action may be reshuffled as

$$\begin{aligned} \tilde{f}_0 &= 0 & \tilde{f}_1 &= \left(\frac{1}{c_s^2} - 1 \right) (1 + A) & \tilde{f}_2 &= -3 \left(\frac{1}{c_s^2} - 1 \right) + \frac{\epsilon - \eta}{c_s^2} \\ \tilde{f}_3 &= \frac{1}{c_s^2} - 1 + \frac{\epsilon + \eta - 2s}{c_s^2} & \tilde{f}_4 &= \frac{\epsilon}{2c_s^2} (\epsilon - 4) & \tilde{f}_5 &= \frac{\epsilon^2}{4c_s^2} , \end{aligned} \quad (4.25)$$

which indeed exactly matches the k -inflationary result of ref. [78] (eqs. 3.10-3.11 there with slightly different notations), upon the identifications:

$$\left(\frac{1}{c_s^2} - 1\right)^{P(X)} = \frac{2XP_{,XX}}{P_{,X}} \leftrightarrow \left(\frac{1}{c_s^2} - 1\right)^{\text{two-field}} = \frac{4H^2\eta_\perp^2}{m_s^2} \quad (4.26)$$

$$2\frac{\lambda}{\Sigma} = \frac{2X^2P_{,XX} + 4/3X^3P_{,XXX}}{XP_{,X} + 2X^2P_{,XX}} \leftrightarrow -\left(\frac{1}{c_s^2} - 1\right)A. \quad (4.27)$$

While (4.26) is obvious from the identifications of the sound speed in the two different class of models already at the level of the quadratic action, eq. (4.27) is new and non-trivial, and we will perform an additional consistency check of it in 4.3.

Eventually, we verified that not only the bulk terms but the whole cubic actions agree between our EFT result and the k -inflationary one in ref. [78], as it should. Also, note that one can readily integrate out the heavy fluctuation $\mathcal{F}$ at the level of eq. (3.1). The subsequent manipulations required to display the genuine size of interactions are similar to the ones performed in appendix A.2 and we have checked that the result obtained in this way agrees with our computation.

Ultraviolet sensitivity and observable effects of curved field space. As we have just seen, at the level of the effective action for the fluctuations, beyond the well known appearance of a reduced sound speed, related to the deviation of a background trajectory from a geodesic (4.4), the precise multifield origin of the EFT is encapsulated in the dimensionless coefficient A (4.15), which enters into the cubic action and hence in the non-Gaussian signal, together with c_s^2 (see i.e. (2.1)-(4.23)). The first contribution to A , fixed by c_s^2 , has already been identified in a decoupling limit analysis in ref. [11]. The three other contributions have not been taken into account so far in a generic context. The third term, proportional to $V_{,sss}$, agrees with the decoupling limit analysis of a specific two-field model in flat field space in [87]. The two others, proportional to the Ricci curvature of the two-dimensional field space, as well as to its derivative along the entropic direction, are specific to models with curved field space and are newly derived. Although these geometrical quantities affect observables only through the global combination A , and hence their effects may be hard to disentangle from other effects like the one of the potential, we find it very interesting that the non-Gaussian signal carries such information about the field space geometry. In this respect, note that all terms in (4.15) are important in general, despite the fact that we integrated out heavy fluctuations and that some may naively appear suppressed by $1/m_s^2$: just like c_s^2 in (4.4) may differ significantly from unity when $H^2\eta_\perp^2 \gg m_s^2$, the last three contributions involve ratios between m_s^2 and other physical scales than H^2 , and hence can contribute to A as importantly as, or larger than, the first term of order one. This is clearly visible for the second contribution for instance, whose size is set by the relative contribution of the geometrical term to the entropic mass (2.13). Eventually, we pointed out in section 4.1 that, within the regime of predictivity of the EFT, relative corrections to its predictions are of order $\mathcal{O}(H^2/(m_s^2c_s^2))$. Hence, contributions to A of that order should be self consistently neglected.

4.3 When full fields can be integrated out

In some two-field models of the type we consider, one may be able to integrate out a *heavy field* at the level of the full action, resulting at lowest order in derivatives in an effective EFT for a single scalar field which is of $P(X, \phi)$ type [8]. In their common domain of validity, the action governing the fluctuations in these theories should agree with our general result (4.25)–(4.27) where the background is studied at the two-field level and *heavy fluctuations* about it are integrated out. We perform this consistency check in a large class of models, deriving useful explicit results for observables readily in terms of the functions defining the two-field Lagrangian.

We consider the general class of Lagrangians

$$\mathcal{L} = -\frac{1}{2}e^{2b(\chi)}(\partial\phi)^2 - \frac{1}{2}(\partial\chi)^2 - V(\phi, \chi), \quad (4.28)$$

which has been used in the past by many authors to study the effects of non-trivial kinetic terms and field space curvature (see, e.g. [8, 94–98]). Following ref. [8], one considers situations in which the effective mass of χ (called the gelaton in this reference) is much larger than the Hubble scale H , so that it adiabatically follows the minimum of its effective potential, at the value $\chi_\star(\phi, X)$ that depends on the inflaton field ϕ and its kinetic energy $X = -\frac{1}{2}(\partial\phi)^2$. With the equation of motion of χ reading $\square\chi - 2b'e^{2b}X + V_{,\chi} = 0$, one deduces that $\chi_\star(\phi, X)$ verifies

$$V_{,\chi}(\phi, \chi_\star) - 2b'(\chi_\star)e^{2b(\chi_\star)}X = 0. \quad (4.29)$$

Substituting this back into the action, and consistently neglecting the kinetic term of χ , one obtains

$$\mathcal{L}^{\text{EFT}} = e^{2b(\chi_\star(\phi, X))}X - V(\phi, \chi_\star(\phi, X)) = \frac{V_{,\chi}(\phi, \chi_\star(\phi, X))}{2b'(\chi_\star(\phi, X))} - V(\phi, \chi_\star(\phi, X)), \quad (4.30)$$

and hence a low-energy effective theory which is equivalent, at leading order, to a $P(X, \phi)$ theory. Like in any inflationary setup, model-dependent quantum corrections to this classical picture may be important in general. Additionally, the requirement that the mass of the gelaton be both much larger than H and smaller than the cutoff of the $P(X)$ theory, so that perturbation theory remains weakly coupled, imposes constraints on the parameter space of viable and observationally interesting models [8, 53]. Here however, we only want to check the formal consistency between predictions derived from (4.30) and the ones from our two-field reasoning, hence we keep $b(\chi)$ and $V(\phi, \chi)$ general.

In order to determine the explicit expressions of the various multifield quantities used in this paper in terms of b, V and their derivatives, one only needs to know the background velocities of fields. From (4.29), one finds $V_{,\chi} = b'e^{2b}\dot{\phi}^2$ while one should consider $\dot{\chi} \simeq 0$ for consistency. Hence, in the coordinate basis (ϕ, χ) , the adiabatic and entropic vectors simply read

$$e_\sigma^I = (e^{-b}, 0), \quad e_s^I = (0, -1), \quad (4.31)$$

where we took $\dot{\phi} > 0$ without loss of generality. Using $V_{;ss} = V_{,\chi\chi}$, $H^2\eta_\perp^2 = V_{,\chi}b'$, $R_{\text{fs}} = -2(b'^2 + b'')$, $V_{;sss} = -V_{,\chi\chi\chi}$, one obtains

$$m_s^2 = V'' - \frac{V'}{b'}(2b'^2 + b'') \quad (4.32)$$

and the expressions (4.34)–(4.35) below for c_s^2 and A , where here in and in the following, all derivatives of the potential are with respect to χ so that there is no source of confusion.

In the $P(X)$ perspective, the explicit expression of $\chi_\star(\phi, X)$ solution of (4.29) is not known in general, and hence neither is the expression of $P(X, \phi)$ in (4.30). However, taking the derivative of (4.29) with respect to X , one obtains

$$\frac{\partial \chi_\star(\phi, X)}{\partial X} = \frac{2e^{2b}b'}{V'' - \frac{V'}{b'}(2b'^2 + b'')}, \quad (4.33)$$

which can be used to compute from (4.30) all successive derivatives $\partial P^{(n)}/\partial X^n$, and hence the expressions of c_s^2 and λ/Σ as defined in the left-hand sides of (4.26)–(4.27). Working this out, one obtains

$$\left(\frac{1}{c_s^2} - 1\right)^{P(X)} = \left(\frac{1}{c_s^2} - 1\right)^{\text{two-field}} = \frac{4b'V'}{V'' - \frac{V'}{b'}(2b'^2 + b'')} \quad (4.34)$$

and

$$2\frac{\lambda}{\Sigma} = -\left(\frac{1}{c_s^2} - 1\right)A = -\frac{2b'^2V'(3b''^2V'^2 + 4b'^4V'^2 + b'^2(2V''''V' - 3V''^2)) - 2b''b'V'^2}{3(2b'^2V' + b''V' - b'V'')^2(2b'^2V' - b''V' + b'V'')}, \quad (4.35)$$

where we have stressed the agreement with the derivation in the two-field language, and the equivalence (4.26)–(4.27). In ref. [8], the expression (4.34) of the sound speed was derived from the two-field picture, and its equivalence with the k -inflationary result was shown for the special case of an hyperbolic field space with $b(\chi) = g\chi/M_{\text{Pl}}$. Here, the equivalence is shown in generic models. More importantly, eq. (4.35) provides a non-trivial consistency check of the more general expression (4.15) of A in terms of multifield quantities.

5 Conclusions

In this work we have presented the complete cubic action for fluctuations in a general two-field non-linear sigma model of inflation, written in comoving gauge in terms of the curvature perturbation ζ and the entropic mode $\mathcal{F}$, and expressed in a way that makes manifest the size of the contribution of each operator to the three-point correlation functions. The outcome is therefore essentially the generalization of Maldacena's result to two scalar fields with non-canonical kinetic terms. Our form of the action is interesting as it highlights the role of the various parameters that are unique to the multi-field context, such as the bending $\eta_\perp$ and the curvature of the internal field space, which have been recognized to be crucial in several novel inflationary scenarios. Along the way, we also identified and clarified some potential issues related to the contributions to correlation

functions of boundary terms in the action, and we explained in particular that the usual approach of performing a field redefinition to remove such terms can be ambiguous. Given their generality, we expect our results to open the door to a wide range of applications. In particular, we believe that the action written in the form we have derived is very well suited to analytical approximations, for instance under a slow-varying approximation that is manifest in our result, or to study transient violations of it in models with features. It would also be interesting to use our form of the action in terms of the curvature perturbation to complement existing numerical methods to compute the primordial bispectrum.

A first important application that we have studied in detail is the effective single-field description that is valid when the entropic mode is heavy and may be integrated out. We showed how the EFT for the curvature mode can be very directly derived, at leading order in the derivative expansion, from our general two-field action. The resulting effective action includes all contributions from slow-roll parameters as well as all the other background coefficients of the UV completion. In particular, we have derived a general expression for the cubic Wilson coefficient A that includes contributions that had not been taken into account in full generality so far in the literature, namely the third derivative of the potential and terms proportional to the field space curvature. As a non-trivial check of these results, we showed explicitly how the single-field EFT can be recast as a model of k -inflation, which we further verified by comparing with a general class of two-field models for which the EFT can be derived in terms of the full inflaton field (as opposed to only its fluctuation). Our calculations in this context can be extended in various directions, some of which we plan to tackle in future work. For instance, it would be interesting to work out the effective action to higher orders in the derivative expansion. This would provide an EFT with a wider range of validity, which may be of potential use in the analysis of multi-field theories featuring non-trivial dynamics of perturbations around the time of horizon crossing. A higher derivative EFT could also be useful to better understand the relation between more general single-field models, such as galileon inflation [99], and multi-field UV completions. Another case worth exploring is when the entropic fluctuation is light but may nevertheless be integrated out due to a large bending, giving rise to a different type of EFT characterized by a modified dispersion relation [9, 80, 85, 88]. Our general two-field cubic action would then provide a straightforward way to compute the relevant Wilson coefficients in such a set-up.

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A Two-field cubic action

A.1 First building blocks

We first calculate separately the three contributions to the action (2.9): the GR action in the first line, as well as for the scalar sector in the second line, the kinetic term and the potential. Writing $S = \int dt d^3x \mathcal{L}$, and after substituting the linear solution (2.10), i.e. $\alpha = \frac{\dot{\zeta}}{H}, \theta = -\frac{\dot{\zeta}}{H} + \chi$ where $\frac{1}{a^2} \partial^2 \chi = \epsilon \dot{\zeta} + \frac{\dot{\sigma} \eta_\perp}{M_{\text{Pl}}^2} \mathcal{F}$, they read:

$$\mathcal{L}_{\text{GR}}^{(3)} = \frac{M_{\text{Pl}}^2}{2} a^3 \left[-9H^2 \epsilon \dot{\zeta}^3 - \frac{2\epsilon}{a^2} \zeta (\partial \zeta)^2 + \frac{1}{a^4} \left(3\dot{\zeta} - \frac{\dot{\zeta}}{H} \right) (\partial_i \partial_j \theta \partial_i \partial_j \theta - (\partial^2 \theta)^2) - \frac{4}{a^4} \partial_i \zeta \partial_i \theta \partial^2 \theta \right], \quad (\text{A.1})$$

$$\mathcal{L}_{\text{pot}}^{(3)} = -a^3 \left[\frac{V_{;sss}}{6} \mathcal{F}^3 + \frac{V_{;ss}}{2} \left(\frac{\dot{\zeta}}{H} + 3\zeta \right) \mathcal{F}^2 + V_{;s} \left(\frac{3\zeta \dot{\zeta}}{H} + \frac{9}{2} \zeta^2 \right) \mathcal{F} + \frac{9}{2} V \left(\frac{\zeta^2 \dot{\zeta}}{H} + \zeta^3 \right) \right] \quad (\text{A.2})$$

$$\mathcal{L}_{\text{kin}}^{(3)} = a^3 \left\{ \left[\frac{1}{3} \dot{\sigma} H \eta_\perp R_{\text{fs}} - \frac{\dot{\sigma}^2}{12} R_{\text{fs},s} \right] \mathcal{F}^3 - \frac{1}{2} \left(\frac{\dot{\zeta}}{H} - 3\zeta \right) \left[\dot{\mathcal{F}}^2 + \left(H^2 \eta_\perp^2 - \frac{\dot{\sigma}^2}{2} R_{\text{fs}} \right) \mathcal{F}^2 \right] - \frac{1}{2a^2} \left(\frac{\dot{\zeta}}{H} + \zeta \right) (\partial \mathcal{F})^2 - \frac{1}{a^2} \dot{\mathcal{F}} \partial \mathcal{F} \partial \theta - \dot{\sigma} H \eta_\perp \left(\frac{\dot{\zeta}^2}{H^2} - \frac{3\zeta \dot{\zeta}}{H} + \frac{9}{2} \zeta^2 \right) \mathcal{F} - \frac{\dot{\sigma}^2}{2} \left(\frac{\dot{\zeta}^3}{H^3} - \frac{3\zeta \dot{\zeta}^2}{H^2} + \frac{9\zeta^2 \dot{\zeta}}{2H} - \frac{9}{2} \zeta^3 \right) \right\}, \quad (\text{A.3})$$

supplemented by the boundary term (3.2), and where for the kinetic term it may be useful to first expand the tensor $\mathcal{G}_{\mu\nu} \equiv G_{IJ}(\phi) \partial_\mu \phi^I \partial_\nu \phi^J$ to cubic order in perturbations:

$$\begin{aligned} \mathcal{G}_{00} &= \dot{\sigma}^2 - 2\dot{\sigma} H \eta_\perp \mathcal{F} + \dot{\mathcal{F}}^2 + H^2 \eta_\perp^2 \mathcal{F}^2 - \frac{\dot{\sigma}^2}{2} R_{\text{fs}} \mathcal{F}^2 + \frac{2}{3} \dot{\sigma} H \eta_\perp R_{\text{fs}} \mathcal{F}^3 - \frac{\dot{\sigma}^2}{6} R_{\text{fs},s} \mathcal{F}^3, \\ \mathcal{G}_{0i} &= \dot{\mathcal{F}} \partial_i \mathcal{F}, \quad \mathcal{G}_{ij} = \partial_i \mathcal{F} \partial_j \mathcal{F}. \end{aligned} \quad (\text{A.4})$$

Summing the three contributions (A.1)–(A.3) and using the background equations, one arrives at the simple form (3.1) of the cubic action. As explained in the main text, many manipulations should be performed in order to render explicit the true size of the cubic couplings. These are presented in the next subsection.

A.2 Manipulations of the cubic action

To structure the computation, we split the initial form (3.1) of the cubic action into

$$\mathcal{L}^{(3)} = \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta) + \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \mathcal{F}) + \mathcal{D}_0 \quad (\text{A.5})$$

with $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta)$ the part coming (mostly) from the GR action, whose dependence on $\mathcal{F}$ only comes through solving the constraint equations and hence the $\mathcal{F}$ -dependence of θ , i.e.

$$\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta) = a^3 M_{\text{Pl}}^2 \left[\epsilon \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\zeta}^2 - \frac{\epsilon}{a^2} \zeta (\partial\zeta)^2 + \frac{1}{2a^4} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) (\partial_i \partial_j \theta \partial_i \partial_j \theta - (\partial^2 \theta)^2) - \frac{2}{a^4} \partial_i \zeta \partial_i \theta \partial^2 \theta \right], \quad (\text{A.6})$$

and $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \mathcal{F})$ that has no single-field counterpart and originates (mostly) from the scalar kinetic and potential terms of the action, i.e.

$$\begin{aligned} \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \mathcal{F}) = a^3 \Big\{ & -\frac{1}{a^2} \dot{\mathcal{F}} \partial \mathcal{F} \partial \theta + \frac{1}{2} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\mathcal{F}}^2 - \frac{1}{2a^2} \left(\zeta + \frac{\dot{\zeta}}{H} \right) (\partial \mathcal{F})^2 \\ & + \dot{\sigma} \eta_{\perp} \left(6\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\zeta} \mathcal{F} - \frac{1}{2H} \left(m_s^2 + 2H^2 \eta_{\perp}^2 - 2\epsilon M_{\text{Pl}}^2 H^2 R_{\text{fs}} \right) \dot{\zeta} \mathcal{F}^2 - \frac{3}{2} m_s^2 \zeta \mathcal{F}^2 \\ & - \frac{1}{6} (V_{;sss} - 2\dot{\sigma} H \eta_{\perp} R_{\text{fs}} + \epsilon M_{\text{Pl}}^2 H^2 R_{\text{fs},s}) \mathcal{F}^3 \Big\}. \end{aligned} \quad (\text{A.7})$$

A.2.1 Manipulations of $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta)$

Similarly to ref. [73], we consider separately terms in (A.6) with different powers of a . Our computation is different in practice, as we treat on equal footing the two contributions to $\theta = -\frac{\zeta}{H} + \chi$, and, as much as possible, do not split χ into its two contributions in (2.11). This simplifies the computation even in the single-field framework, and it enables one to extend it more easily to the two-field situation. We thus divide $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta)$ into four groups of terms:

$$\mathcal{L}_{\text{ini}}^{(3),\text{I}}(\zeta) = a^3 M_{\text{Pl}}^2 \epsilon \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\zeta}^2 \quad (\text{A.8})$$

$$\mathcal{L}_{\text{ini}}^{(3),\text{II}}(\zeta) = -a M_{\text{Pl}}^2 \epsilon \zeta (\partial\zeta)^2 \quad (\text{A.9})$$

$$\mathcal{L}_{\text{ini}}^{(3),\text{III.B.}}(\zeta, \theta) = \frac{M_{\text{Pl}}^2}{2a} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) (\partial_{ij} \theta \partial_{ij} \theta - (\partial^2 \theta)^2) \quad (\text{A.10})$$

$$\mathcal{L}_{\text{ini}}^{(3),\text{III.A.}}(\zeta, \theta) = -\frac{2}{a} M_{\text{Pl}}^2 \partial^2 \theta (\partial\theta) (\partial\zeta), \quad (\text{A.11})$$

First group. Integrating by parts, one simply writes:

$$\mathcal{L}_{\text{ini}}^{(3),\text{I}}(\zeta) = a^3 M_{\text{Pl}}^2 \epsilon (\epsilon - \eta) \dot{\zeta}^2 \zeta + \frac{2}{H} \zeta \dot{\zeta} \frac{d}{dt} \left(a^3 M_{\text{Pl}}^2 \epsilon \dot{\zeta} \right) + \mathcal{D}_1 \quad (\text{A.12})$$

$$\text{with } \mathcal{D}_1 = -\frac{d}{dt} \left[a^3 M_{\text{Pl}}^2 \frac{\epsilon}{H} \dot{\zeta}^2 \zeta \right] \quad (\text{A.13})$$

Second group. No manipulation is needed on the second group. However we will show later that it combines with other terms to give a term proportional to the equation of motion for ζ .

Third and fourth groups. More manipulations are needed here. Using $\theta = -\frac{\zeta}{H} + \chi$, the third group reads:

$$\mathcal{L}_{\text{ini}}^{(3), \text{III.B.}}(\zeta, \theta) = \frac{M_{\text{Pl}}^2}{2a} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \left[\frac{1}{H^2} \left(\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2 \right) - \frac{2}{H} \left(\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi \right) + \left(\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2 \right) \right] \quad (\text{A.14})$$

Performing temporal integrations by parts, and using (2.15), one can derive the useful identities, for any background functions $f_i(t)$:

$$\begin{aligned} f_1(t) \dot{\zeta} \left(\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2 \right) &= \frac{1}{3} \frac{d}{dt} \left[f_1 \dot{\zeta} \left(\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2 \right) \right] - \frac{1}{3} \dot{f}_1 \zeta \left(\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2 \right) \end{aligned} \quad (\text{A.15})$$

$$\begin{aligned} f_2(t) \dot{\zeta} \left(\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi \right) &= \frac{1}{2} \frac{d}{dt} \left[f_2 \dot{\zeta} \left(\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi \right) \right] - \frac{\epsilon}{2} f_2 \zeta \left(\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2 \right) \\ &\quad - \frac{1}{2} \left(\dot{f}_2 - f_2 H \right) \zeta \left(\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi \right) - \frac{a^2 f_2}{4M_{\text{Pl}}^2} \zeta \left(\zeta_{,ij} \partial_i \partial_j \partial^{-2} \cdot - \partial^2 \zeta \right) \mathcal{E}_\zeta \end{aligned} \quad (\text{A.16})$$

$$\begin{aligned} f_3(t) \dot{\zeta} \left(\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2 \right) &= \frac{d}{dt} \left[f_3 \dot{\zeta} \left(\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2 \right) \right] - 2\epsilon f_3 \left(\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi \right) \\ &\quad - \left(\dot{f}_3 - 2f_3 H \right) \zeta \left(\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2 \right) - \frac{a^2 f_3}{M_{\text{Pl}}^2} \zeta \left(\chi_{,ij} \partial_i \partial_j \partial^{-2} \cdot - \partial^2 \chi \right) \mathcal{E}_\zeta. \end{aligned} \quad (\text{A.17})$$

Applying these relations to (A.14), with $f_1(t) = -\frac{M_{\text{Pl}}^2}{2aH^3}$, $f_2(t) = \frac{M_{\text{Pl}}^2}{aH^2}$ and $f_3(t) = -\frac{M_{\text{Pl}}^2}{2aH}$, and using the identity

$$\zeta \left(\partial_i \partial_j g \partial_i \partial_j h - \partial^2 g \partial^2 h \right) = \frac{1}{2} \partial^2 \zeta \partial_i g \partial_i h + \frac{1}{2} \left(\partial^2 g \partial_i \zeta \partial_i h + \partial^2 h \partial_i \zeta \partial_i g \right) \quad (\text{A.18})$$

valid for any functions g and h , and where total spatial derivative are discarded, to simplify bulk terms, one obtains:

$$\mathcal{L}_{\text{ini}}^{(3), \text{III.B.}}(\zeta, \theta) = \frac{2M_{\text{Pl}}^2}{aH^2} \left[(\partial \zeta)^2 \partial^2 \zeta \right] - \frac{M_{\text{Pl}}^2}{aH} \left[(\partial \zeta)^2 \partial^2 \chi + 2(\partial \zeta)(\partial \chi) \partial^2 \zeta \right] \quad (\text{A.19})$$

$$+ \frac{\epsilon M_{\text{Pl}}^2}{4a} \left[(\partial \chi)^2 \partial^2 \zeta + 2(\partial \zeta)(\partial \chi) \partial^2 \chi \right] + \mathcal{D}_{\text{III.B.}} + \text{EoM}_{\text{III.B.}} \quad (\text{A.20})$$

with

$$\begin{aligned} \mathcal{D}_{\text{III.B.}} &= -M_{\text{Pl}}^2 \frac{d}{dt} \left[\frac{1}{6aH^3} \zeta \left(\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2 \right) - \frac{1}{2aH^2} \zeta \left(\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi \right) \right. \\ &\quad \left. + \frac{1}{2aH} \zeta \left(\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2 \right) \right] \end{aligned} \quad (\text{A.21})$$

and

$$\text{EoM}_{\text{III.B.}} = -\frac{a\zeta}{4H^2} [(\zeta_{,ij}\partial_i\partial_j\partial^{-2} - \partial^2\zeta) - 2H(\chi_{,ij}\partial_i\partial_j\partial^{-2} - \partial^2\chi)] \mathcal{E}_\zeta. \quad (\text{A.22})$$

Developing the expression of the fourth group (A.11) in terms of ζ and χ , it reads

$$\begin{aligned} \mathcal{L}_{\text{ini}}^{(3),\text{III.A.}}(\zeta, \theta) = & -\frac{2M_{\text{Pl}}^2}{aH^2} [(\partial\zeta)^2 \partial^2\zeta] + \frac{2M_{\text{Pl}}^2}{aH} [(\partial\zeta)^2 \partial^2\chi + (\partial\zeta)(\partial\chi) \partial^2\zeta] \\ & - \frac{2M_{\text{Pl}}^2}{a} [(\partial\zeta)(\partial\chi) \partial^2\chi], \end{aligned} \quad (\text{A.23})$$

from which one deduces the rather compact form

$$\begin{aligned} \mathcal{L}_{\text{ini}}^{(3),\text{III.A.}}(\zeta, \theta) + \mathcal{L}_{\text{ini}}^{(3),\text{III.B.}}(\zeta, \theta) \\ = \frac{M_{\text{Pl}}^2}{aH} (\partial\zeta)^2 \partial^2\chi + \frac{M_{\text{Pl}}^2}{a} \left[\left(\frac{\epsilon}{2} - 2 \right) (\partial\zeta)(\partial\chi) \partial^2\chi + \frac{\epsilon}{4} (\partial\chi)^2 \partial^2\zeta \right] \\ + \mathcal{D}_{\text{III.B.}} + \text{EoM}_{\text{III.B.}}, \end{aligned} \quad (\text{A.24})$$

where the expression of χ (2.11) may now be used to express all quantities explicitly in terms of ζ and $\mathcal{F}$.

Addition and manipulation of the four groups. Adding the four groups all together and using

$$\begin{aligned} \frac{2}{H} \zeta \dot{\zeta} \frac{d}{dt} (a^3 M_{\text{Pl}}^2 \epsilon \dot{\zeta}) + a \epsilon M_{\text{Pl}}^2 \left(\frac{\dot{\zeta}}{H} - \zeta \right) (\partial\zeta)^2 = & a \epsilon M_{\text{Pl}}^2 (\epsilon + \eta) \zeta (\partial\zeta)^2 - \frac{2}{H} \zeta \dot{\zeta} \frac{d}{dt} (a^3 \dot{\sigma} \eta_\perp \mathcal{F}) \\ & - \frac{d}{dt} \left[\frac{a \epsilon M_{\text{Pl}}^2}{H} \zeta (\partial\zeta)^2 \right] + \frac{a^3}{H} \dot{\zeta} \zeta \mathcal{E}_\zeta, \end{aligned} \quad (\text{A.25})$$

one eventually obtains

$$\begin{aligned} \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta) = & a^3 M_{\text{Pl}}^2 \left[\epsilon(\epsilon - \eta) \dot{\zeta}^2 \zeta + \epsilon(\epsilon + \eta) \zeta \frac{(\partial\zeta)^2}{a^2} \right. \\ & + \left(\frac{\epsilon}{2} - 2 \right) \frac{1}{a^4} (\partial\zeta)(\partial\chi) \partial^2\chi + \frac{\epsilon}{4a^4} \partial^2\zeta (\partial\chi)^2 \Big] \\ & + a \eta_\perp \frac{\dot{\sigma}}{H} \mathcal{F} (\partial\zeta)^2 - \frac{2}{H} \zeta \dot{\zeta} \frac{d}{dt} (a^3 \dot{\sigma} \eta_\perp \mathcal{F}) + \mathcal{D}_1 + \text{EoM}_1 \end{aligned} \quad (\text{A.26})$$

with

$$\begin{aligned} \mathcal{D}_1 = & -M_{\text{Pl}}^2 \frac{d}{dt} \left[a^3 \frac{\epsilon}{H} \zeta \dot{\zeta}^2 + a \frac{\epsilon}{H} \zeta (\partial\zeta)^2 + \frac{1}{6aH^3} \zeta (\zeta_{,ij}\zeta_{,ij} - (\partial^2\zeta)^2) \right. \\ & \left. - \frac{1}{2aH^2} \zeta (\zeta_{,ij}\chi_{,ij} - \partial^2\zeta \partial^2\chi) + \frac{1}{2aH} \zeta (\chi_{,ij}\chi_{,ij} - (\partial^2\chi)^2) \right] \end{aligned} \quad (\text{A.27})$$

$$\text{EoM}_1 = \left\{ \frac{a^3}{H} \dot{\zeta} \zeta - \frac{a\zeta}{4H^2} [(\zeta_{,ij}\partial_i\partial_j\partial^{-2} - \partial^2\zeta) - 2H(\chi_{,ij}\partial_i\partial_j\partial^{-2} - \partial^2\chi)] \right\} \mathcal{E}_\zeta \quad (\text{A.28})$$

The form (A.26) of the cubic action (supplemented with $\mathcal{D}_0$ (3.2)) reproduces the single-field result when $\mathcal{F}$ is absent. We chose to organize the vertices and the boundary terms in the same manner as in ref. [78] (see eqs. 3.2 and 3.10 there). As explained in detail in the main text, this form of the action is interesting because, in the single-field case where ζ becomes constant on super-Hubble scales, the displayed boundary terms do not contribute to the bispectrum, and the number of operators in the bulk action is minimized. More importantly, all manipulations have been made so that the dynamically relevant terms in (A.26) are manifestly of order $\mathcal{O}(\epsilon, \eta)^2$ or higher. In the more general two-field case of interest, similar manipulations should be performed for the terms involving $\mathcal{F}$, to which we now turn.

A.2.2 Manipulating the interactions involving entropic perturbations and total cubic action

The cubic interactions involving $\mathcal{F}$ in (A.7) and (A.26) and that do not manifestly display the right amplitude of the interactions all appear in the first line of (A.7). These terms appear without ϵ factors, nor background parameters related to the entropic sector like $\eta_\perp, m_s^2, R_{\text{fs}}$ and similar). The manipulations that remedy this are

$$\frac{a}{2} \left[\frac{2}{H} \dot{\mathcal{F}} \partial \mathcal{F} \partial \zeta - (\partial \mathcal{F})^2 \left(\zeta + \frac{\dot{\zeta}}{H} \right) \right] = \frac{a}{2} \left[\epsilon \zeta (\partial \mathcal{F})^2 - \frac{2}{H} \zeta \dot{\mathcal{F}} \partial^2 \mathcal{F} \right] - \frac{d}{dt} \left[\frac{a}{2H} (\partial \mathcal{F})^2 \zeta \right] \quad (\text{A.29})$$

and

$$\begin{aligned} \frac{a^3}{2} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\mathcal{F}}^2 &= \frac{a^3}{2} \epsilon \zeta \dot{\mathcal{F}}^2 + \frac{a}{H} \zeta \dot{\mathcal{F}} \partial^2 \mathcal{F} - \frac{a^3 m_s^2}{H} \dot{\mathcal{F}} \mathcal{F} \zeta + \frac{2a^3 \dot{\sigma} \eta_\perp}{H} \dot{\zeta} \zeta \dot{\mathcal{F}} \\ &\quad - \frac{d}{dt} \left(\frac{a^3}{2H} \zeta \dot{\mathcal{F}}^2 \right) + \frac{a^3}{H} \zeta \dot{\mathcal{F}} \mathcal{E}_{\mathcal{F}} \end{aligned} \quad (\text{A.30})$$

where the terms in $\zeta \dot{\mathcal{F}} \partial^2 \mathcal{F}$ in the right hand sides cancel in the total action. To put the action in the best form that we give in the main next, this is not enough though, notably because the generated terms proportional to $m_s^2 \dot{\mathcal{F}} \mathcal{F} \zeta$ and $\eta_\perp \dot{\zeta} \zeta \dot{\mathcal{F}}$ contribute to the cubic action at leading order in situations where $\mathcal{F}$ is integrated out (see section 4.1), and we prefer that terms involving $\dot{\mathcal{F}}$ are readily negligible, to make the derivation of the single-field EFT more transparent. For this purpose, we note that, integrating by parts the term in $m_s^2 \dot{\mathcal{F}} \mathcal{F} \zeta$, several cancellations arise amongst different terms to obtain

$$\begin{aligned} &a^3 \dot{\sigma} \eta_\perp \left(6\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\mathcal{F}} \mathcal{F} - \frac{d}{dt} (a^3 \dot{\sigma} \eta_\perp \mathcal{F}) \left(\frac{2}{H} \dot{\zeta} \zeta \right) - \frac{a^3 m_s^2}{H} \dot{\mathcal{F}} \mathcal{F} \zeta \\ &+ \frac{2a^3 \dot{\sigma} \eta_\perp}{H} \dot{\zeta} \zeta - \frac{3}{2} a^3 m_s^2 \zeta \mathcal{F}^2 \\ &= a^3 \dot{\sigma} \eta_\perp (2\epsilon - \eta - 2\lambda_\perp) \dot{\zeta} \zeta \mathcal{F} + \frac{a^3 m_s^2}{2H} \left(\mathcal{F} - \frac{2\dot{\sigma} \eta_\perp}{m_s^2} \dot{\zeta} \right) \dot{\zeta} \mathcal{F} \\ &\quad + \frac{1}{2} a^3 m_s^2 (\epsilon + \mu_s) \zeta \mathcal{F}^2 - \frac{1}{2} \frac{d}{dt} \left(a^3 \frac{m_s^2}{H} \zeta \mathcal{F}^2 \right) \end{aligned} \quad (\text{A.31})$$

where no derivative of $\mathcal{F}$ appears in the right hand side except for the boundary term, and we defined $\lambda_\perp = \dot{\eta}_\perp/(H\eta_\perp)$ and $\mu_s = (m_s^2)'/(Hm_s^2)$. Now summing all the contributions to (A.5), i.e. (3.2), (A.26), (A.7) and using eqs. (A.29)–(A.31), one finds:

$$\begin{aligned} \mathcal{L}^{(3)} = & M_{\text{Pl}}^2 a^3 \left[\epsilon(\epsilon - \eta) \dot{\zeta}^2 \zeta + \epsilon(\epsilon + \eta) \zeta \frac{(\partial \zeta)^2}{a^2} + \left(\frac{\epsilon}{2} - 2 \right) \frac{1}{a^4} (\partial \zeta) (\partial \chi) \partial^2 \chi + \frac{\epsilon}{4a^4} \partial^2 \zeta (\partial \chi)^2 \right] \\ & + a^3 \left[\frac{1}{2} m_s^2 (\epsilon + \mu_s) \zeta \mathcal{F}^2 + (2\epsilon - \eta - 2\lambda_\perp) \dot{\sigma} \eta_\perp \zeta \dot{\mathcal{F}} + \frac{\dot{\sigma} \eta_\perp}{a^2 H} \mathcal{F} (\partial \zeta)^2 \right. \\ & - \frac{\dot{\sigma} \eta_\perp}{H} \dot{\zeta}^2 \mathcal{F} - \frac{1}{H} (H^2 \eta_\perp^2 - \epsilon M_{\text{Pl}}^2 H^2 R_{\text{fs}}) \dot{\zeta} \mathcal{F}^2 \\ & - \frac{1}{6} (V_{;sss} - 2\dot{\sigma} H \eta_\perp R_{\text{fs}} + \epsilon M_{\text{Pl}}^2 H^2 R_{\text{fs},s}) \mathcal{F}^3 \\ & \left. + \frac{1}{2} \epsilon \dot{\zeta} \left(\dot{\mathcal{F}}^2 + \frac{(\partial \mathcal{F})^2}{a^2} \right) - \frac{1}{a^2} \dot{\mathcal{F}} \partial \mathcal{F} \partial \chi \right] + \mathcal{D} + \mathcal{E} \end{aligned} \quad (\text{A.32})$$

with

$$\begin{aligned} \mathcal{D} = & \frac{d}{dt} \left\{ -\frac{a}{2H} \zeta (\partial \mathcal{F})^2 + \frac{a M_{\text{Pl}}^2}{H} (1 - \epsilon) \zeta (\partial \zeta)^2 \right. \\ & + a^3 \left[-9 H M_{\text{Pl}}^2 \zeta^3 - \frac{\epsilon M_{\text{Pl}}^2}{H} \dot{\zeta}^2 \zeta - \frac{1}{2H} \zeta \dot{\mathcal{F}}^2 - \frac{m_s^2}{2H} \zeta \mathcal{F}^2 \right] \\ & \left. - \frac{M_{\text{Pl}}^2 \zeta}{6aH^3} \left((\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2) - 3H (\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi) + 3H^2 (\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2) \right) \right\}, \\ \mathcal{E} = & \frac{a^3}{H} \mathcal{E}_\zeta \left[\dot{\zeta} - \frac{1}{4a^2 H} ((\partial \zeta)^2 - \partial^{-2} \partial_i \partial_j (\partial_i \zeta \partial_j \zeta) - 2H (\partial \zeta \partial \chi - \partial^{-2} \partial_i \partial_j (\partial_i \zeta \partial_j \chi))) \right] \\ & + \frac{a^3}{H} \mathcal{E}_\mathcal{F} \dot{\mathcal{F}}. \end{aligned} \quad (\text{A.33})$$

The compact expression of the cubic action (A.32) with the boundary term (A.33) is the main result of this paper. Its usefulness and its consequences are discussed in the main text, where we simply slightly changed the appearance of the boundary term in (3.7) to make appear conjugate momenta, as this simplifies subsequent calculations.

B Boundary terms and field redefinitions

In this appendix we briefly review the method of performing non-linear field redefinitions to compute the contributions to cosmological correlators of boundary terms in the action (see e.g. [78]; see also [100] for a related discussion in the context of the wave function approach). In short, the idea of the method is to redefine field variables so that the relevant boundary terms disappear, and then to simply work out the relation between correlators of the new and old variables. Although this procedure has become standard in the single-field context, we would like to highlight some potential ambiguities that may lead to incorrect results, especially in the more complicated multi-field set-up. It is mainly for this reason that we chose the more direct method of section 3.3 to compute the contributions of boundary terms.

Consider a generic quadratic field redefinition

$$\zeta = \tilde{\zeta} + f[\tilde{\zeta}, \tilde{\mathcal{F}}], \quad \mathcal{F} = \tilde{\mathcal{F}} + g[\tilde{\zeta}, \tilde{\mathcal{F}}], \quad (\text{B.1})$$

where, by assumption, the functionals f and g are quadratic in the fields. It then follows that the quadratic part (2.12) of the action reads, in terms of the new variables:

$$S^{(2)}[\zeta, \mathcal{F}] = S^{(2)}[\tilde{\zeta}, \tilde{\mathcal{F}}] - \int d^4x a^3 [f\mathcal{E}_{\tilde{\zeta}} + g\mathcal{E}_{\tilde{\mathcal{F}}}] + \int d^4x \partial_t \left[2M_{\text{Pl}}^2 a f \partial^2 \tilde{\chi} + a^3 g \dot{\tilde{\mathcal{F}}} \right] + \dots \quad (\text{B.2})$$

where the ellipses stand for quartic terms. Recalling that terms proportional to the linear equations of motion $\mathcal{E}_{\tilde{\zeta}}$ and $\mathcal{E}_{\tilde{\mathcal{F}}}$ are irrelevant, one can see that the only impact of field redefinitions of ζ and $\mathcal{F}$ is to introduce boundary terms, proportional to $\partial^2 \chi$ and $\dot{\mathcal{F}}$ respectively.⁵ We precisely organised the boundary term (3.7) in that way, with the first line containing only operators with no time derivatives (hence which do not affect correlation functions of fields), and the last two lines containing the terms that can be removed via field redefinitions. Indeed, choosing the functions f and g as (note that at this order, writing them in terms of the original $(\zeta, \mathcal{F})$ is irrelevant)

$$\begin{aligned} f[\zeta, \mathcal{F}] &= \frac{\zeta \dot{\zeta}}{H} - \frac{1}{8a^2 H^2} \left((\partial \zeta)^2 - 2\partial_i \partial^{-2} (\partial^i \zeta \partial^2 \zeta) \right. \\ &\quad \left. - 2H \left(\partial \zeta \partial \chi - \frac{1}{2} \partial_i \partial^{-2} (\partial^i \chi \partial^2 \zeta) \right) + \frac{4H}{\epsilon} \zeta \partial^2 \chi \right), \quad (\text{B.3}) \\ g[\zeta, \mathcal{F}] &= \frac{1}{2H} \zeta \dot{\mathcal{F}}, \end{aligned}$$

the action up to cubic order in terms of the variables $(\tilde{\zeta}, \tilde{\mathcal{F}})$ contain only the bulk interactions in (3.6), whose contributions to correlation functions can be calculated using standard methods, with analytical approximations or numerically. Eventually, we just have to take into account the difference between three-point functions of the original and redefined variables (B.1), which is straightforward to do using Wick's theorem.

The tricky aspect of this method is the fact that the above field redefinition is not unique, simply because the structure of the boundary term (3.7) can be changed by doing spatial integrations by parts. To illustrate this, consider the terms of the form ζp_{ζ}^2 in (3.7), which in Fourier space will read $\mathcal{L} \supset h(k_1, k_2, k_3) \zeta(k_1) p_{\zeta}(k_2) p_{\zeta}(k_3)$ for some function h of the wave vectors. However, in order to read off the field redefinition that is supposed to handle this term, one needs to remove all spatial derivatives of one of the field momenta (say $p_{\zeta}(k_3)$) so that, when written in this form, the function h becomes independent of k_3 :

$$h(k_1, k_2, k_3) \zeta(k_1) p_{\zeta}(k_2) p_{\zeta}(k_3) = h_1(k_1, k_2) \zeta(k_1) p_{\zeta}(k_2) p_{\zeta}(k_3) + \text{t.d.} \quad (\text{B.4})$$

A field redefinition that removes this expression is given by taking $f = h_1(k_1, k_2) \zeta(k_1) p_{\zeta}(k_2)$ (with a convolution over the wave vectors being implicit when working in Fourier space).

⁵The fact that the generated terms, in $\partial^2 \chi$ and $\dot{\mathcal{F}}$, are proportional to the (linear) conjugate momenta of ζ and $\mathcal{F}$ is in agreement with the discussion below eq. (3.5), where the commutator form readily indicates that only boundary terms proportional to conjugate momenta contribute to correlation functions of fields.

However, as we have stressed, this is not unique because (B.4) is not unique: by doing an integration by parts we have

$$h_1(k_1, k_2)\zeta(k_1)p_\zeta(k_2)p_\zeta(k_3) = h_2(k_1, k_2)\zeta(k_1)p_\zeta(k_2)p_\zeta(k_3) + \text{t.d.}, \quad (\text{B.5})$$

with a new function h_2 and hence a different function f in (B.1). Since it is precisely the function f that determines the relation between the correlators of $\tilde{\zeta}$ and the correlators of ζ , we see that this procedure can lead to ambiguous results.

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5.3.2 General case with N_{field} scalars (article)

The work presented in the previous section clearly calls for a natural extension: indeed it only treats the first non-trivial case of multifield inflation, which is two-field inflation. Just like the cubic action of multifield inflation was known in the flat gauge for any number of scalar fields, I decided to work out the one in the comoving gauge. It should however be emphasized that Ref. [3],

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that is reproduced below, is not merely a technical generalisation of the two-field case.

First, parameterising the perturbations in the adiabatic-entropic basis with N_{field} scalars requires a new geometrical understanding of the background trajectory in a multi-dimensional space. In a two-dimensional field space, the trajectory can simply be parameterised by its curvilinear velocity $\dot{\sigma}$ and its bending $\eta_{\perp}$, but for higher dimensions one needs to specify the whole set of *curvatures* of the trajectory, which are the multi-dimensional generalisations of the bending. For example in three dimensions, the first curvature ω_1 is simply the dimensionfull bending, *i.e.* $\omega_1 = H\eta_{\perp}$, while the second curvature ω_2 , is sometimes called the torsion and corresponds to the degree of deviation of the background trajectory from a plane: the bending measures the deviation from a straight line in the so-called osculating plane that is instantaneously tangent to the velocity vector and its derivative, while the torsion measures the rate of change of orientation of this osculating plane. The direction parallel to the background trajectory is still called the adiabatic direction, the one that is perpendicular to it but parallel to its acceleration as parameterised by the bending is the first entropic direction, the one that is perpendicular to both the adiabatic and the first entropic direction as parameterised by the torsion is the second entropic direction, etc. By asking that this local basis is orthonormal and with a definite orientation, one defines uniquely a generalised adiabatic-entropic basis that may be used to describe inflationary perturbations.

Second, the physics of multifield inflation in a higher-dimensional field space has been somewhat overlooked in the past, and there seems to remain interesting effects to be uncovered. Already at the level of linear fluctuations, I found that the entropic sector can be described by both a symmetric mass matrix $m_{\alpha\beta}^2$ that generalises the scalar quantity m_s^2 , and an anti-symmetric operator $\Omega_{\alpha\beta}$ that further mixes entropic fluctuations. In particular, geometrical effects coming from the field-space metric G seem ubiquitous, as for example the mass matrix $m_{\alpha\beta}^2$ contains a projection of the Riemann tensor on the various adiabatic and entropic directions, $R_{\alpha\sigma\beta\sigma}$ where α and β are two entropic directions with $\alpha, \beta \in \{1, \dots, N_{\text{field}} - 1\}$ and σ denoting the unique adiabatic direction. And this projection contains much more geometrical information than in the two-field case where it simply reduces to the Ricci scalar curvature, as indeed

for a higher-dimensional field space one can show that:

$$R_{\alpha\sigma\beta\sigma} = \underbrace{\frac{R_{\text{fs}}}{N_{\text{field}}(N_{\text{field}} - 1)}\delta_{\alpha\beta}}_{N_{\text{field}}=2} + \underbrace{\frac{1}{N_{\text{field}} - 2} (Z_{\alpha\beta} + \delta_{\alpha\beta}Z_{\sigma\sigma}) + C_{\alpha\sigma\beta\sigma}}_{N_{\text{field}} \geq 4}, \quad (5.111)$$

where Z is the traceless Ricci tensor (vanishing for $N_{\text{field}} \leq 2$) of the field space and C is its Weyl tensor (vanishing for $N_{\text{field}} \leq 3$). These findings can for example call into question the stability of linear fluctuations in multifield inflation with a higher-dimensional field space and a traceless Ricci tensor or Weyl tensor with negative eigenvalues, in the spirit of the geometrical destabilisation of inflation [68] that has been so far studied in the two-field case, or the study of the non-trivial anti-symmetric mixing coming from the matrix $\Omega_{\alpha\beta}$ (just like $\eta_{\perp}$ can induce a transient instability, maybe those can too?).

At the level of primordial non-Gaussianities, I have extended Maldacena's calculation of the cubic action to the most general models of multifield inflation at lowest order in derivatives, *i.e.* of non-linear signal models of inflation with any potential, field-space metric, number of fields, and without assuming a particular background dynamics. I think that this very general result, encoding both tensorial generalisations of the two-field interactions and genuinely many-field ones that are absent from the two-field case, will be useful for further analytical and numerical works. As an example I derived the single-field effective theory that is found when the entropic sector is heavy and the linear EoM for entropic fluctuations can be solved simply by inverting the mass matrix $m_{\alpha\beta}^2$ and expressing the result in terms of $\hat{\mathcal{R}}$. Doing so, I found that the resulting speed of sound c_s^2 is non-trivial if and only if the first bending is non-vanishing, but that then it depends on the whole entropic sector via the inverse mass matrix element $(m^{-2})_{11}$. Moreover, the parameter A of the EFToI is also found from this more generic multifield UV completion, and corresponds to various projections of potential derivatives of geometrical contributions along the first column of the inverse mass matrix $(m^{-2})_1^\alpha$, including some that are absent from the two-field case. Last but not least, I am already using the general multifield cubic interactions that I found to generalise the setup of Quasi-Single-Field Inflation to the case of several entropic fluctuations, possibly leading to many-field effects in the squeezed limit of the bispectrum and hopefully generalising the cosmological collider program that aims at probing the masses and spins of extra particles in the early universe, to the determination of the internal geometry of inflation.

The original article as published in JCAP is now displayed. The notations that are used are very close to the ones of this manuscript, and only differ (again) by the fact that the comoving curvature perturbation is denoted ζ in the article, while it is $\mathcal{R}$ here.

Multifield inflation beyond $N_{\text{field}} = 2$: non-Gaussianities and single-field effective theory

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Abstract. In this article, we study in detail the linear dynamics and cubic interactions for any number N_{field} of scalar fields during inflation, directly in terms of the observable curvature perturbation ζ and $N_{\text{field}} - 1$ entropic fluctuations, a choice that is more suitable for analytical works. In the linear equations of motion for the perturbations, we uncover rich geometrical effects beyond terms involving just the scalar curvature of the field space, and that come from the non-canonical kinetic structure of the scalar fields when the dimension of the field space is larger than two. Moreover, we show that a fast rotation of the local entropic basis can result in negative eigenvalues for the entropic mass matrix, potentially destabilising the background dynamics when $N_{\text{field}} \geq 3$. We also explain how to render manifest the sizes of cubic interactions between the adiabatic and the entropic fluctuations, extending a previous work of ours to any number of interacting fields. As a first analytical application of our generic formalism, we derive the effective single-field theory for perturbations up to cubic order when all entropic fluctuations are heavy enough to be integrated out. In a slow-varying limit, we recover the cubic action expected from the effective field theory of inflation, but with a prediction for the usual Wilson coefficients in terms of the multifield parameters, thus proposing a new interpretation of the bispectrum in this generic N_{field} context.

Keywords: inflation, physics of the early universe, cosmological perturbation theory, non-gaussianity

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1 Introduction

Inflation, an era of almost-exponential expansion of spacetime, constitutes our paradigm for the early universe. Not only does it explain the observed spatial flatness and large-scale homogeneity of the universe at the time of recombination and photon decoupling, but it also predicts with a high accuracy the Gaussian statistics of the tiny anisotropies in the Cosmic Microwave Background (see [1, 2] for recent observational constraints). Despite these successes, the exact mechanism behind inflation is yet to be understood. Indeed, the simplest class of models, the framework of so-called single-field slow-roll inflation with canonical kinetic terms, suffers from a number of theoretical limitations as it relies on the existence of a unique degree of freedom in the early universe, the inflaton, which must have a very flat potential. First, realistic UV completions of inflation that are needed to describe phenomena at higher energies and from which inflation must be inferred (top-down approach), typically predict the presence of not only one, but several scalar fields, and they often come with non-canonical kinetic terms (for a review see, e.g., [3]). Secondly, even just as a low-energy Effective Field Theory (EFT), the single-field slow-roll picture (bottom-up approach) is not satisfactory neither as Planck-suppressed operators renormalize the potential in a way that it can not remain flat in Planck mass units (see [4, 5] for the historical papers and [6, 7] for pedagogical reviews on the so-called η -problem). In this regard, understanding the physics of inflation provides us with a formidable opportunity to test and investigate physics Beyond the Standard Model.

Amongst the possible ways to evade the aforementioned theoretical limitations, and motivated by top-down constructions, we shall consider here multifield models of inflation with non-canonical kinetic terms, i.e. with a curved field space. Multifield inflationary dynamics present striking characteristic observational signatures, such as correlated adiabatic and isocurvature perturbations, features in the primordial power spectrum and order one non-Gaussianities with specific patterns (see, e.g., [8–20]). More exotic features can also be found, such as a large flattened shape for the bispectrum and higher-order correlation

functions [21–24], a production of Primordial Black Holes (PBH) [25, 26] and of small-scale Primordial Gravitational Waves (PGW) [27]. Actually, most multifield studies focus on the simplest non-trivial setup with $N_{\text{field}} = 2$ scalar fields, and a few look at $\mathcal{O}(N_{\text{field}})$ models in the $N_{\text{field}} \rightarrow \infty$ limit (see, e.g., [28–30]), whereas here we will work in full generality with N_{field} being any positive integer. Of course, this generic setup has already been investigated, with the computation of the second-order and third-order actions for multifield inflation in the flat gauge [31–36], and even used in the numerical implementation of the transport approach [37–41]. However, the comoving gauge in which the observable adiabatic perturbation ζ naturally appears is best suited for analytical works, such as Quasi-Single-Field (QSF) calculations of the adiabatic power spectrum and bispectrum [15, 16, 42], or integrating out heavy fluctuations [43–47] (see [48, 49] for consistency checks between the two approaches in a regime of common validity, and [50] for integrating out the whole extra heavy field and not just its fluctuations). In our previous article [47], we revisited in detail the bispectrum produced in generic models of inflation with $N_{\text{field}} = 2$ scalar fields, by computing the cubic action in the comoving gauge. In particular, we unveiled the effect of the Ricci scalar of the field space on the inflationary bispectrum.

In the present article, we combine and extend previous studies by studying N_{field} -inflation with curved field space, directly in the comoving gauge and in terms of ζ and $N_{\text{field}} - 1$ entropic perturbations, highlighting the special features due to the dimension of the field space. We begin in section 2 by reviewing some notations as well as the background dynamics of multifield inflation. We explain the decomposition along adiabatic and entropic directions and define the rate of turn of the local entropic basis with the matrix Ω . Covariant perturbations beyond linear order are carefully chosen, and the ADM formalism applied to cosmology is reviewed with particular attention afforded to the boundary terms. Next, we decompose perturbations in the comoving gauge and along the unit vectors of the local orthonormal basis, identifying our fundamental degrees of freedom; ζ and $\mathcal{F}^\alpha$ for $\alpha \in \{1, \dots, N_{\text{field}} - 1\}$. We present the quadratic Lagrangian, eq. (2.15), which incorporates the mixing of the massless adiabatic perturbation with the entropic sector, as well as self-mixings of the massive entropic perturbations, together with the corresponding equations of motion (EoM) in eqs. (2.20)–(2.21). We pinpoint the role of the field-space geometry beyond its scalar curvature whenever $N_{\text{field}} \geq 3$ and comment about a conceivable destabilisation of background trajectories due to a fast rotation of the entropic basis, a possibility that was overlooked so far to our knowledge. Lastly, we derive for completeness the corresponding quadratic Hamiltonian that we use to define our free theory.

Section 3 is devoted to the computation of the cubic action in the comoving gauge, for our general setup of N_{field} scalar fields with non-canonical kinetic terms, without assuming special features for the background dynamics such as slow-varying approximations. This corresponds essentially to the N_{field} -generalisation of the famous Maldacena’s calculation of the bispectrum in canonical single-field inflation [51] and of our previous work in the two-field case [47]. We explain that the brute-force expansion of the action up to cubic order is not sufficient to unveil the true sizes of the interactions, and show how to render them manifest with uses of integrations by parts and of the linear EoM, carefully keeping the time-boundary terms that are needed for a full computation of the bispectrum. The final result (3.10)–(3.11) is one of the main achievements of this article: it presents the genuine sizes of cubic interactions between adiabatic and entropic perturbations without any approximation.

This form of the cubic action is particularly suited for analytical works, and we show in section 4 a first application of it. There, we derive the effectively single-field theory for

fluctuations that is found by integrating out heavy entropic perturbations, a procedure that is justified when the entropic mass matrix dominates over the other contributions in the EoM for $\mathcal{F}^\alpha$. We comment on the more precise conditions of validity for this single-field regime, and infer a reduced speed of sound, $c_s^2 < 1$, for the free propagation of ζ whenever the background trajectory is bending. At the level of cubic interactions, the single-field effective theory matches the one of a truly single degree of freedom ϕ with a $P(X, \phi)$ Lagrangian [52–55], provided some matching between the multifield setup and the derivatives of the function P . In a slow-varying approximation, we recover the leading-order operators expected from the EFT of inflation [56, 57], with a prediction for the Wilson coefficient A in terms of the multifield potential and the field-space geometry.

Section 5 is devoted to conclusive remarks and an outlook.

2 N_{field} -inflation in curved field space

In this section, we first review standard notations for multifield inflationary setups and choose a decomposition of the background fields and perturbations in a local orthonormal basis consisting of an adiabatic direction (instantaneously following the background trajectory) and $N_{\text{field}} - 1$ entropic (perpendicular) directions. Field-space covariant and perturbatively spacetime-gauge-invariant fluctuations are identified, and constraint equations needed to remove non-dynamical degrees of freedom, are shown. We comment on the necessity of the Gibbons-Hawking-York boundary term in the action, in order to have a well-defined variational principle. A first interesting point in this generic N_{field} setup is the quadratic action displayed in eqs. (2.15)–(2.17) and that matches the only explicit reference in the literature after a few changes of variables [58]. We outline geometrical effects beyond the scalar curvature of the field space depending on the number of fields, and identify potential background instabilities from the large-scale limit of the linear equations of motion (2.20)–(2.21) that we found. Eventually, we show the corresponding quadratic Hamiltonian that we use to define our free theory for this work, and that could be used in future works to compute analytically the power spectrum in a perturbative scheme in terms of the mixing parameters ω_α with $\alpha \in \{1, \dots, N_{\text{field}} - 1\}$, or numerically with the transport approach.

2.1 Generalities

Setup. In this paper, we consider general multifield non-linear sigma models of inflation, described by the action

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{Pl}}^2}{2} R(g) - \frac{1}{2} G_{IJ}(\phi) \nabla^\mu \phi^I \nabla_\mu \phi^J - V(\phi) \right], \quad (2.1)$$

with G_{IJ} the metric of the internal field space manifold. The latin index I runs from 1 to N_{field} the total number of scalars. Our convention for the Riemann tensor is

$$R^I{}_{JKL} = \Gamma^I_{JL,K} + \Gamma^I_{KM} \Gamma^M_{JL} - (K \leftrightarrow L), \quad (2.2)$$

where we denote by Γ^I_{JK} the corresponding Levi-Civita connection. We also use the summation convention for repeated indices.

Background. The space-time background is assumed to be of the Friedmann-Lemaître-Robertson-Walker (FLRW) type, with a scale factor $a(t)$ and related Hubble parameter $H(t) = \dot{a}(t)/a(t)$, a dot representing a derivative with respect to cosmic time. This background and its dynamics are ruled by the presence of the homogeneous parts of the N_{field} scalar fields, $\phi^I(t)$. Their evolution is given by

$$\mathcal{D}_t \dot{\phi}^I + 3H \dot{\phi}^I + G^{IJ} V_{,J} = 0, \quad (2.3)$$

where the time field-space covariant derivative action on a field-space vector A^I is given by $\mathcal{D}_t A^I = \dot{A}^I + \Gamma_{JK}^I \dot{\phi}^J A^K$, and where a comma denotes a field-space derivative: $V_{,J} = \partial V / \partial \phi^J$. The Friedmann equations can be written as

$$\dot{\sigma}^2 = 2M_{\text{Pl}}^2 H^2 \epsilon, \quad V = M_P^2 H^2 (3 - \epsilon), \quad (2.4)$$

where we have introduced the first Hubble slow-roll parameter, $\epsilon = -\dot{H}/H^2$ as well as the total background field velocity $\dot{\sigma} = \sqrt{G_{IJ} \dot{\phi}^I \dot{\phi}^J}$. Note that although what one can have in mind is a sufficiently long period of inflation for which both ϵ and $\eta = \dot{\epsilon}/(H\epsilon)$ must be small, all the results presented in this paper are exact in the sense that they are not expansions in those parameters, except if explicitly mentioned. In particular, our results are perfectly applicable to the description of transient departures from slow-roll, other attractors such as ultra-slow-roll, or even multi-scalar dynamics beyond inflation (see [59] for a recent application of our previous work [47] in the case of $N_{\text{field}} = 2$ to holographic theories).

Adiabatic-entropic decomposition. It is convenient to introduce vielbeins along the background trajectory to define a local orthonormal basis: $e_a^I = (e_\sigma^I, e_{s_\alpha}^I)$ with σ denoting the adiabatic direction and $s_\alpha = s_1, \dots, s_{N_{\text{field}}-1}$ the $N_{\text{field}} - 1$ entropic directions (that we shall denote $s_\alpha \rightarrow \alpha$ for simplicity in the following). One can decompose the field-space metric as $G^{IJ} = \delta^{ab} e_a^I e_b^J = e_\sigma^I e_\sigma^J + e_\alpha^I e_\alpha^J$. Note that in this kind of expressions there is a sum over the $N_{\text{field}} - 1$ values for α but that σ denotes only one direction: the adiabatic one. Of course, such local orthonormal basis is not unique and any orthonormal rotation conserves its properties. In particular, although the adiabatic direction has the physical interpretation of pointing towards the instantaneous direction of the background trajectory, there is no preferred frame for the entropic sector. Therefore we fix this ambiguity by defining the first entropic direction as the covariant rate of turn of the adiabatic direction (that vanishes if the background trajectory coincides with a geodesic of the field space), and all other vectors can be defined as the wedge product of the two previous ones¹ (see [58, 60] for similar constructions in the inflationary context). This results in a particular form for the covariant rate of turn of the local orthonormal basis:

$$\mathcal{D}_t \begin{pmatrix} e_\sigma^I \\ e_1^I \\ e_2^I \\ \vdots \\ e_{N_{\text{field}}-1}^I \end{pmatrix} = \begin{pmatrix} 0 & \omega_1 & 0 & \dots & 0 \\ -\omega_1 & 0 & \omega_2 & \dots & 0 \\ 0 & -\omega_2 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & -\omega_{N_{\text{field}}-1} & 0 \end{pmatrix} \begin{pmatrix} e_\sigma^I \\ e_1^I \\ e_2^I \\ \vdots \\ e_{N_{\text{field}}-1}^I \end{pmatrix}, \quad (2.5)$$

¹Note that, strictly speaking, when the bending ω_1 of the background trajectory vanishes exactly, the individual entropic directions can not be defined in an unambiguous way. However this has no practical implication as in that fine-tuned case the evolution of ζ , the observable curvature perturbation, is linearly decoupled from the dynamics of the entropic sector as we shall find soon.

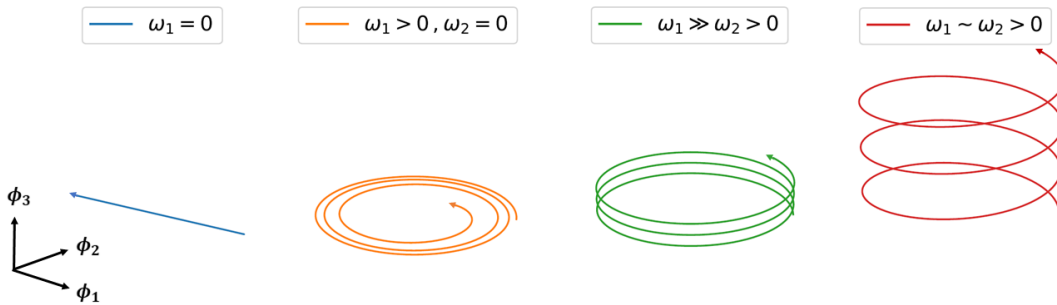


Figure 1. Examples of trajectories in a flat field-space manifold with $N_{\text{field}} = 3$, and for different values of the curvature ω_1 and of the torsion ω_2 .

where the turning rates ω_α have the dimension of a mass. One clearly sees that the first entropic direction plays a special role because it bridges together the adiabatic and purely entropic sectors. It will prove useful to use the coordinate expression of this matrix equation, separating the adiabatic direction from the entropic sector:

$$\begin{aligned}\mathcal{D}_t e_\sigma^I &= \omega_1 e_1^I \\ \mathcal{D}_t e_\alpha^I &= -\delta_{1\alpha} \omega_1 e_\sigma^I + \Omega_\alpha{}^\beta e_\beta^I,\end{aligned}\tag{2.6}$$

Ω being the anti-symmetric square matrix of size $(N_{\text{field}} - 1) \times (N_{\text{field}} - 1)$ in the lower right corner of the rotation matrix in (2.5). This decomposition is equivalent to a Cartan frame decomposition and one can interpret each of the $N_{\text{field}} - 1$ mixing parameters ω_α as the turning rates of the local basis. In mathematical studies of parametric curves in N_{field} dimensions, the parameters ω_α are called “generalized curvatures” of the trajectory (in the special case $N_{\text{field}} = 3$, ω_1 is called the curvature and ω_2 the torsion, see figure 1 for a geometrical interpretation of these parameters), but here we will name them “bendings” or “mixing parameters” not to be confused with statements about the geometry of the curved field-space manifold that are independent of a given trajectory. Note also that by definition the local metric in the adiabatic-entropic basis is flat, $G_{IJ} e_a^I e_b^J = \delta_{ab}$, this implying in particular that “entropic indices” α can be up or down for convenience without making any difference.

It is then possible to decompose the EoM of inflation along those directions. Using that by definition $\dot{\phi}^I = e_\sigma^I \dot{\sigma}$, one can rewrite the background equations of motion for the scalar fields (2.3) as

$$\ddot{\sigma} + 3H\dot{\sigma} + V_{,\sigma} = 0, \quad \sqrt{2\epsilon} H M_{\text{Pl}} \omega_1 \delta_{\alpha,1} + V_{,\alpha} = 0.\tag{2.7}$$

where we defined projections of the potential gradients along the adiabatic and entropic directions, $V_{,\sigma} = e_\sigma^I V_{,I}$ and $V_{,\alpha} = e_\alpha^I V_{,I}$. Note in particular that this last quantity is non-zero only when projected along the first entropic direction, according to (2.7). This is a convenient feature from our choice for the entropic frame.

2.2 Covariant, gauge-invariant perturbations

Covariance. When going beyond the study of linear fluctuations, one should be careful to use variables that are covariant under field-space redefinitions. Although not a requirement

per se, as predictions for observable quantities do not depend on particular choices of variables, it is useful and conceptually clearer to deal with covariant objects. The concern and its resolution have been first described in ref. [34] for generic multifield models. In any given gauge, the idea is to use, not the field fluctuations $\delta\phi^I = \phi^I - \bar{\phi}^I$, which do not transform covariantly beyond linear order, but the vectors Q^I living in the tangent space at $\bar{\phi}^I$ and that correspond to the “initial velocity” of the geodesic connecting the two points labelled by $\bar{\phi}^I$ and ϕ^I (this geodesic is unique if the separation between the two points is sufficiently small). Up to third order in fluctuations, one finds:

$$\delta\phi^I = Q^I - \frac{1}{2}\Gamma_{JK}^I Q^J Q^K + \frac{1}{6}(2\Gamma_{LM}^I \Gamma_{JK}^M - \Gamma_{JK,L}^I) Q^J Q^K Q^L + \mathcal{O}(Q^4). \quad (2.8)$$

Note that although Q is sometimes used to denote inflationary fluctuations in the flat gauge, here they denote non-linearly covariant inflatons’ fluctuations in any gauge. We shall return soon to this matter of gauge choice.

ADM formalism and genuine degrees of freedom. Let us quickly review the ADM formalism applied to the cosmological context, paying particular attention to the boundary terms. Regular cosmological spacetimes’ manifolds $\mathcal{M}$ equipped with a metric g can be foliated by Cauchy surfaces Σ_t parameterized by a global time function t . One can then define the unit normal vector n^μ to the hypersurface Σ_t , and an induced spatial 3-metric h_{ij} on each of those hypersurfaces by $h_{ij} = g_{ij} + n_i n_j$, as well as a lapse N and shift N^i such that the spacetime metric takes the following form [61, 62]:

$$ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt). \quad (2.9)$$

The idea of the ADM formalism is to interpret the spatial 3-metric h_{ij} as the dynamical quantity that evolves on a manifold Σ when moving forward in time, while the lapse N and the shift N^i only describe how to move forward in time. This intuition shall be confirmed soon by the appearance of the constraint equations that enable one to express the lapse and the shift as linear combinations of the true dynamical perturbations. Then, it is possible to decompose the 4-dimensional Ricci scalar R according to this foliation using the Gauss-Codazzi relation (see, e.g., [63]):

$$\begin{aligned} R &= 2(G_{\mu\nu} - R_{\mu\nu})n^\mu n^\nu \text{ with} \\ G_{\mu\nu}n^\mu n^\nu &= \frac{1}{2}\left(R^{(3)} + K^2 - K_{ij}K^{ij}\right), \\ R_{\mu\nu}n^\mu n^\nu &= K^2 - K_{ij}K^{ij} - \nabla_\mu(n^\mu \nabla_\nu n^\nu) + \nabla_\mu(n^\nu \nabla_\nu n^\mu), \end{aligned} \quad (2.10)$$

where K_{ij} denotes the extrinsic curvature of the spacelike hypersurfaces Σ_t , and reads $K_{ij} = \frac{1}{2N}(\dot{h}_{ij} - 2N_{(i|j)})$, with the symbol $|$ used for the spatial covariant derivative associated with the 3-metric h_{ij} and parentheses denoting symmetrization: $N_{(i|j)} = (N_{i|j} + N_{j|i})/2$, and with $K = h^{ij}K_{ij}$ its trace.

Usually, one does not care about the total derivatives in the third line of (2.10), although they do not vanish in general (note that they come from the derivatives of the Christoffel symbols in the Riemann tensor), because boundary terms in the action do not affect equations of motion. But in cosmology in particular, the equations of motion do not contain all the relevant information to derive observational predictions; to compute the meaningful equal-time correlation functions one needs to use the “in-in” formalism that requires the knowledge

of the whole Hamiltonian and not just its bulk terms. More precisely, only the total-time derivatives are important in cosmology since one is not provided with any boundary in the spatial directions, and one can check that the second of the total-derivative terms in the third line of (2.10) vanishes in the cosmological context since it is orthogonal to the spacelike hypersurfaces Σ_t . However the first one remains, and it can be rewritten in terms of the scalar extrinsic curvature which indeed reads $K = \nabla_\nu n^\nu$ at this boundary. Eventually, the resulting action can be rewritten:

$$\begin{aligned}
S &= S_{\text{EH}} + S_{\text{matter}} \text{ with} \\
S_{\text{EH}} &= \int_{\mathcal{M}} dt d^3\vec{x} \left[\frac{1}{2} \sqrt{h} N \left(R^{(3)} + (K_{ij} K^{ij} - K^2) \right) - \partial_t \left(2\sqrt{h} N K \right) \right] \\
S_{\text{matter}} &= \frac{1}{2} \int_{\mathcal{M}} dt d^3\vec{x} \sqrt{h} N \left(\frac{1}{N^2} G_{IJ} v^I v^J - G_{IJ} h^{ij} \partial_i \phi^I \partial_j \phi^J - 2V \right),
\end{aligned} \tag{2.11}$$

where $h = \det(h_{ij})$, $R^{(3)}$ is the Ricci curvature of the spatial hypersurfaces calculated with h_{ij} and $v^I = \dot{\phi}^I - N^j \partial_j \phi^I$. The total time-derivative in the Einstein-Hilbert action written in the ADM formalism is known to be potentially problematic because it contains second-order time derivatives of the spatial metric, which could wrongly point towards new spurious degrees of freedom. Interestingly, this term is exactly canceled if the bulk Einstein-Hilbert action is supplemented by the Gibbons-Hawking-York boundary term $S_{\text{GHY}} = 2 \int_{\partial\mathcal{M}} dV K$ with appropriate measure dV on the spatial boundary $\partial\mathcal{M}$, which is known to be necessary to have a well-defined variational principle for general relativity [63–65], or to define the notion of black hole entropy and for the path integral formulation of quantum gravity [66, 67]. In the following, we shall consider implicitly that the description of spacetime incorporates this boundary term, and thus that our resulting action, $S = S_{\text{EH}} + S_{\text{GHY}} + S_{\text{matter}}$, yields a well-defined variational principle with no extra degree of freedom in the metric, and that our starting point for further computations does not contain any relevant boundary term.

Also, the lapse N and the shift N^i appear without time derivatives in the action, and only linearly once expressed in a Hamiltonian language in terms of the right degrees of freedom and their canonically conjugated momenta. This means as announced that they are non-dynamical and can be perturbatively solved from constraints equations in terms of the genuine degrees of freedom: $\delta S / \delta N = 0 = \delta S / \delta N^i$.

Gauge choice. Throughout the paper, we neglect tensor and vector perturbations, for the usual reason that they are decoupled from the scalar fluctuations at linear order, so they can only contribute to two-point and three-point correlation functions of the latter by loops, such effects being usually suppressed compared to the tree-level interactions that we take here into account. As is well known in cosmological perturbation theory, there is an ambiguity in identifying quantities defined on the full spacetime manifold $\mathcal{M}$ and on the unperturbed, FLRW one $\bar{\mathcal{M}}$. This problem is tackled with an explicit choice of scalar functions T, L for the gauge $\xi^\mu = (T, \partial^i L)$ that relates $\mathcal{M}$ to $\bar{\mathcal{M}}$, which eliminates two spurious degrees of freedom. While N and N^i contain both a single scalar non-dynamical degree of freedom as we have just seen, the spatial part of the metric $h_{ij} = a^2 \left(e^{2\psi} \delta_{ij} + \partial_i \partial_j E \right)$ contains two dynamical ones. Thus, a popular gauge choice when studying multifield inflation is the spatially flat gauge, $\psi^{\text{flat}} = 0 = E^{\text{flat}}$, such that $h_{ij}^{\text{flat}} = a^2 \delta_{ij}$, and in which all physical degrees of freedom are the field fluctuations Q_{flat}^I . This choice is made in many studies (see e.g. [36, 68–72] for general formalisms) and has a number of advantages. However, as we discussed in the

introduction, here we use the “comoving gauge”² that we define by the following conditions: the adiabatic field fluctuation is set to zero, $e_I^\sigma Q_{\text{com}}^I = 0$, and $E_{\text{com}} = 0$, such that the only surviving fluctuations are

$$\begin{aligned} \text{the } N_{\text{field}} - 1 \text{ entropic field perturbations} & \quad e_I^\alpha Q_{\text{com}}^I \equiv \mathcal{F}^\alpha, \\ \text{the adiabatic curvature perturbation} & \quad \psi_{\text{com}} \equiv \zeta, \end{aligned} \quad (2.12)$$

hence the spatial part of the metric reads $h_{ij}^{\text{com}} = a^2 e^{2\zeta} \delta_{ij}$.

To compute the action up to cubic order, it is sufficient to plug back in the action the expressions of the lapse and the shift at linear order only, in terms of the physical degrees of freedom: $N = 1 + \alpha$ and $N^i = \delta^{ij} \partial_j \theta / a^2$. The linear constraint equations in our gauge read

$$\alpha^{(1)} = \frac{\dot{\zeta}}{H}, \quad \theta^{(1)} = -\frac{\zeta}{H} + \chi, \quad (2.13)$$

where the function χ , defined by

$$\frac{1}{a^2} \partial^2 \chi = \epsilon \dot{\zeta} + \sqrt{2\epsilon} \frac{\omega_1}{M_{\text{Pl}}} \mathcal{F}^1, \quad (2.14)$$

only depends on the comoving curvature perturbation ζ and the first entropic field fluctuation $\mathcal{F}^1$. Actually, χ is proportional in Fourier space to the linear canonical momentum associated with ζ as we shall see soon. It also coincides with $-\Psi/H$ where Ψ is the gauge-invariant Bardeen potential, and since $\partial^2 \chi / a^2$ is negligible on large scales, one finds from eq. (2.14) the super-Hubble feeding of ζ by the first entropic fluctuation $\mathcal{F}^1$ when the background trajectory bends in the adiabatic direction ($\omega_1 \neq 0$).

2.3 Quadratic action

The second order Lagrangian dictating the linear dynamics of the perturbations, after substitution of the constraint for $\alpha^{(1)}$ (contributions from $\theta^{(1)}$ cancel one another), is found to be:

$$\begin{aligned} \mathcal{L}^{(2)}(\zeta, \mathcal{F}^\alpha) = & a^3 \left\{ \epsilon M_p^2 \left(\dot{\zeta}^2 - \frac{(\partial \zeta)^2}{a^2} \right) + 2\sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \delta_{\alpha 1} \mathcal{F}^\alpha \dot{\zeta} \right. \\ & \left. + \frac{1}{2} \left[(\dot{\mathcal{F}}^\alpha)^2 - \frac{(\partial \mathcal{F}^\alpha)^2}{a^2} - m_{\alpha\beta}^2 \mathcal{F}^\alpha \mathcal{F}^\beta + 2\Omega_{\alpha\beta} \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \right] \right\}, \end{aligned} \quad (2.15)$$

with

$$m_{\alpha\beta}^2 = V_{;\alpha\beta} + \Omega_\alpha{}^\gamma \Omega_{\gamma\beta} - \delta_{\alpha 1} \delta_{\beta 1} \omega_1^2 + 2\epsilon H^2 M_{\text{Pl}}^2 R_{\alpha\sigma\beta\sigma}, \quad (2.16)$$

the symmetric mass-matrix elements for the entropic sector. An index σ represents a contraction with the adiabatic direction and indices α correspond to contractions with entropic directions: $V_{;\alpha\beta} = e_\alpha^I e_\beta^J V_{;IJ}$ with a semicolon denoting a covariant derivative in field space

²Strictly speaking, the comoving gauge is defined upon the vanishing of the $0-i$ component of the stress-energy tensor. We note that referring to our gauge as “comoving” is a slight abuse of terminology, as it was shown that this condition could not be matched in multifield models beyond linear perturbation theory [73–76]. However, as shown in these works, setting $e_I^\sigma Q^I = 0$ defines an approximate comoving gauge on super-Hubble scales in expanding universes, so we decided to keep the terminology “comoving gauge” for simplicity.

and $R_{\alpha\sigma\beta\sigma} = e_\alpha^I e_\sigma^J e_\beta^K e_\sigma^L R_{IJKL}$. Note also that $\Omega_\alpha{}^\gamma \Omega_{\gamma\beta}$ is nothing but the (α, β) component of the square of the $(N_{\text{field}} - 1) \times (N_{\text{field}} - 1)$ matrix Ω , which reads

$$\Omega^2 = \begin{pmatrix} -\omega_2^2 & 0 & \omega_2\omega_3 & \dots & 0 \\ 0 & -\omega_2^2 - \omega_3^2 & 0 & \dots & 0 \\ \omega_2\omega_3 & 0 & -\omega_3^2 - \omega_4^2 & \dots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \dots & \omega_{N_{\text{field}}-2}\omega_{N_{\text{field}}-1} & 0 & -\omega_{N_{\text{field}}-1}^2 \end{pmatrix}, \quad (2.17)$$

and has only negative (or vanishing) eigenvalues. Some useful notations are $(\partial X)(\partial Y) = \partial_i X \partial_i Y$ and $\partial^2 = \partial_i \partial_i$. Let us also introduce formally ∂^{-2} the inverse Laplacian operator: $\partial^{-2} \partial^2 = \partial^2 \partial^{-2} = 1$, which shall be used in the following. The quadratic Lagrangian (2.15) matches ref. [58] in the more particular context of holographic multifield inflation, once appropriate changes of variables are made.

Geometrical effects. Before proceeding, let us understand better the geometrical effects in the mass matrix of entropic modes, $m_{\alpha\beta}^2$. For this purpose, it will prove useful for $N_{\text{field}} \geq 3$ to decompose the Riemann tensor as

$$R_{IJKL} = \frac{2R_{\text{fs}}}{N_{\text{field}}(N_{\text{field}} - 1)} G_{I[J} G_{L]K} + \frac{2}{N_{\text{field}} - 2} (G_{I[K} Z_{L]J} - G_{J[K} Z_{L]I}) + C_{IJKL}, \quad (2.18)$$

where R_{fs} is the Ricci scalar curvature of the field space, obtained as the trace of the Ricci tensor R_{IJ} , $Z_{IJ} = R_{IJ} - \frac{1}{N_{\text{field}}} R_{\text{fs}} G_{IJ}$ is the traceless Ricci tensor and C_{IJKL} is the Weyl tensor of the field space. The brackets denote anti-symmetrization over two indices, for example $G_{I[J} G_{L]K} = (G_{IJ} G_{LK} - G_{IL} G_{JK})/2$. In the two-field case, $N_{\text{field}} = 2$, both the traceless Ricci tensor Z and the Weyl tensor C vanish, hence only the first term in (2.18) remains and we recover the standard result that the geometry of two-dimensional manifolds is completely defined by the Ricci scalar only. Contracting indices of the Riemann tensor with the adiabatic and entropic directions, one finds for the mass contribution:

$$R_{\alpha\sigma\beta\sigma} = \underbrace{\frac{R_{\text{fs}}}{N_{\text{field}}(N_{\text{field}} - 1)} \delta_{\alpha\beta}}_{N_{\text{field}}=2} + \underbrace{\frac{1}{N_{\text{field}} - 2} (Z_{\alpha\beta} + \delta_{\alpha\beta} Z_{\sigma\sigma}) + C_{\alpha\sigma\beta\sigma}}_{N_{\text{field}} \geq 4}. \quad (2.19)$$

Let us study the effects of the dimension of the field space. When $N_{\text{field}} = 2$, we recover the usual geometrical contribution to the entropic mass $m_s^2 \ni \epsilon R_{\text{fs}} H^2 M_{\text{Pl}}^2$ [33, 69, 77]. For $N_{\text{field}} = 3$, the Weyl tensor still vanishes but the traceless Ricci tensor is non-zero *a priori* and $m_{\alpha\beta}^2 \ni 2\epsilon H^2 M_{\text{Pl}}^2 [\delta_{\alpha\beta} (R_{\text{fs}}/6 + Z_{\sigma\sigma}) + Z_{\alpha\beta}]$. The non-diagonal piece of this quantity constitutes a non-trivial geometry-dependent mixing term between different entropic perturbations. Lastly, for $N_{\text{field}} \geq 4$ one should take into account the Weyl contribution to the Riemann tensor which contains all the geometrical information that is not in the Ricci tensor.

Linear equations of motion. The linear equations of motion for the system read:

$$\mathcal{E}_\zeta = -\frac{1}{2a^3\epsilon M_{\text{Pl}}^2} \frac{\delta S^{(2)}}{\delta \zeta} = 0 \quad (2.20)$$

$$= \frac{1}{a^3\epsilon M_{\text{Pl}}^2} \frac{d}{dt} \left(a^3\epsilon M_{\text{Pl}}^2 \dot{\zeta} + a^3\sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \mathcal{F}^1 \right) - \frac{\partial^2 \zeta}{a^2} = \frac{\partial^2}{a^2 \epsilon} (\dot{\chi} + H\chi - \epsilon\zeta) ,$$

$$\mathcal{E}_\alpha = -\frac{1}{a^3} \frac{\delta S^{(2)}}{\delta \mathcal{F}^\alpha} = 0 \quad (2.21)$$

$$= \ddot{\mathcal{F}}_\alpha + (3H\delta_{\alpha\beta} + 2\Omega_{\alpha\beta}) \dot{\mathcal{F}}^\beta + \left(m_{\alpha\beta}^2 - \delta_{\alpha\beta} \frac{\partial^2}{a^2} + 3H\Omega_{\alpha\beta} + \dot{\Omega}_{\alpha\beta} \right) \mathcal{F}^\beta \\ - 2\delta_{\alpha 1} \sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \dot{\zeta} .$$

These quantities vanish for on-shell linear perturbations, as well as for perturbations in the interaction picture which are evolved with the quadratic action exactly, even when cubic interactions are perturbatively included. Our linear equations of motion (2.20)–(2.21) also match the ones that were already derived in the special case of $N_{\text{field}} - 1 = 2$ entropic fields in [78]. Strikingly, only the first entropic perturbation couples linearly to the adiabatic curvature perturbation through the mixing parameter ω_1 , while the entropic sector mixes when $N_{\text{field}} \geq 3$ both due to the rotation of the entropic frame described by the matrix Ω , and the non-diagonal pieces of the entropic mass matrix (which themselves can come either from the potential, the rotation of the entropic frame or the geometry of the field space). It is worth noting that attempts to diagonalise the entropic mass matrix and use its eigenvectors to define another entropic frame, must be considered with care as this would necessarily result in more mixing terms between this new entropic sector and ζ .

Linear stability of the background trajectory. In the two-field context, it is known that even with a positive Hessian of the potential, the background trajectory can be unstable due to the negative geometrical contribution to the mass of entropic perturbations on large scales, for hyperbolic-like field spaces [79]. Here we explain which effects could similarly destabilise a seemingly stable background trajectory (i.e. with a covariant Hessian of the potential $V_{;\alpha\beta}$ with only positive eigenvalues) in a more general N_{field} context. For this purpose, it is necessary to look at the super-Hubble behaviour of linear perturbations. Actually, the adiabatic curvature perturbation is fed only by the first entropic perturbation as one finds $\dot{\zeta} = -\sqrt{\frac{2}{\epsilon}} \frac{\omega_1}{M_{\text{Pl}}} \mathcal{F}^1 + \mathcal{O}\left(\frac{k^2}{a^2}\right)$, which results in an effective mass matrix for the entropic sector on large scales: $m_{\text{eff},\alpha\beta}^2 = m_{\alpha\beta}^2 + 4\delta_{\alpha 1}\delta_{\beta 1}\omega_1^2$. Thus, as in the $N_{\text{field}} = 2$ case, the bending of the trajectory parameterized by ω_1 eventually has a positive contribution to the effective mass matrix in the first entropic direction, and stabilises the trajectory. However the rotation of the entropic orthonormal basis, parameterized by Ω , can have a destabilising effect when $N_{\text{field}} \geq 3$. First, the effective mass matrix has a contribution $\Omega_\alpha{}^\gamma \Omega_{\gamma\beta}$ which, as we saw from (2.17) only has negative eigenvalues, and that could overcome the other terms in $m_{\text{eff},\alpha\beta}^2$.³ Secondly, as can be seen from the large-scale EoM for the

³Note that it was argued that in the limit dubbed “extreme turning”, roughly consisting of a very large turning rate ω_1 (see ref. [80] for a more precise statement), the accelerations perpendicular to both the adiabatic and the first entropic directions should be negligible, thus bounding the possible values for the matrix elements $\Omega_{\alpha\beta}$.

entropic perturbations,

$$\ddot{\mathcal{F}}_\alpha + (3H\delta_{\alpha\beta} + 2\Omega_{\alpha\beta})\dot{\mathcal{F}}^\beta + \left(m_{\text{eff},\alpha\beta}^2 + 3H\Omega_{\alpha\beta} + \dot{\Omega}_{\alpha\beta}\right)\mathcal{F}^\beta = \mathcal{O}\left(\frac{k^2}{a^2}\right), \quad (2.22)$$

the effective mass matrix is not the only relevant parameter that determines the stability of the background trajectory: the mixing of entropic perturbations via the rotation matrix Ω (defined in eq. (2.5)) could result in complicated dynamics worth investigating⁴. Last but not least, it would be interesting to study under which conditions the geometrical term $\propto R_{\alpha\sigma\beta\sigma}$ in $m_{\text{eff},\alpha\beta}^2$ is negative beyond the contribution from the Ricci scalar: how do the traceless Ricci tensor and the Weyl tensor affect the sign of the effective mass matrix of entropic perturbations when $N_{\text{field}} \geq 3$? We leave this interesting questions for future works.

Hamiltonian formalism. For completeness, we also show the expressions for the linear canonical momenta of our N_{field} variables,

$$p_\zeta = \frac{\delta S}{\delta \dot{\zeta}} = 2a^3 M_{\text{Pl}}^2 \left(\epsilon \dot{\zeta} + \sqrt{2\epsilon} \frac{\omega_1}{M_{\text{Pl}}} \mathcal{F}^1 \right) = 2a M_{\text{Pl}} \partial^2 \chi, \quad (2.23)$$

$$p_\alpha = \frac{\delta S}{\delta \dot{\mathcal{F}}^\alpha} = a^3 \left(\dot{\mathcal{F}}_\alpha + \Omega_{\alpha\beta} \mathcal{F}^\beta \right), \quad (2.24)$$

as well as the corresponding second-order Hamiltonian:

$$\begin{aligned} \mathcal{H}^{(2)} = & a^3 \left\{ \frac{1}{4\epsilon M_{\text{Pl}}^2} \tilde{p}_\zeta^2 + \epsilon M_{\text{Pl}}^2 \frac{(\partial\zeta)^2}{a^2} - \sqrt{\frac{2}{\epsilon}} \frac{\omega_1}{M_{\text{Pl}}} \delta_{\alpha 1} \mathcal{F}^\alpha \tilde{p}_\zeta \right. \\ & \left. + \frac{1}{2} \left[\tilde{p}_\alpha^2 - 2\Omega^\alpha{}_\beta \tilde{p}_\alpha \mathcal{F}^\beta + \frac{(\partial\mathcal{F}^\alpha)^2}{a^2} + \left(m_{\alpha\beta}^2 - \Omega_\alpha{}^\gamma \Omega_{\gamma\beta} + 4\delta_{\alpha 1} \delta_{\beta 1} \omega_1^2 \right) \mathcal{F}^\alpha \mathcal{F}^\beta \right] \right\}, \end{aligned} \quad (2.25)$$

where we rescaled momenta, $p_\zeta \rightarrow \tilde{p}_\zeta = p_\zeta/a^3$ and $p_\alpha \rightarrow \tilde{p}_\alpha = p_\alpha/a^3$. Note that an interesting choice of free Hamiltonian to define interaction picture fields, could be this second-order Hamiltonian but without the mixing terms $\propto \omega_1$ and $\propto \Omega_{\alpha\beta}$. These mixing terms could then be treated as (quadratic) interactions in a perturbative treatment and in the spirit of Quasi-Single-Field (QSF) inflation [15, 16, 42], but we leave this interesting application for future work, and rather consider the full quadratic Hamiltonian as the free one, so that the interaction picture fields verify the EoM (2.20)–(2.21) that include mixings non-perturbatively.

3 Genuine sizes of cubic interactions

We now turn to the computation of the third-order action in the comoving gauge, for any number of scalar fields with kinetic and potential interactions, including the backreaction of the metric and without assuming special features of the background dynamics such as slow-roll. This corresponds essentially to the N_{field} -generalisation of the famous Maldacena's calculation of the bispectrum in canonical single-field inflation [51] and of our previous work in the two-field case [47]. Indeed, as we explained at length in this article, the naive cubic action

⁴In this spirit, note that refs. [81, 82] casted a doubt on the only use of the sign of the effective mass matrix of entropic perturbations on large scales in time-dependent setups, to conclude about the stability of a given background trajectory even when $N_{\text{field}} = 2$. It would be interesting to extend this analysis to the present case of any number of fields.

obtained from expanding the total action, does not render manifest the sizes of interactions and should be manipulated with uses of integrations by parts and linear equations of motion to remove second-order time derivatives. These manipulations are allowed even in the cubic action, since the fields' perturbations are in the interaction picture and evolve according to the full quadratic Hamiltonian only. We will thus discard all contributions proportional to the linear EoM, $\mathcal{E}_\zeta$ and $\mathcal{E}_\alpha$. However, due to the special feature of the “in-in” formalism that consists in computing cosmological correlators at a given time-boundary of interest, and contrary to “in-out” amplitudes in particle physics, total time derivatives in the cubic action play a role in the general computation of three-point functions and should be kept for consistency throughout the calculation. The reader that is not interested in the derivation can directly jump to the final result (3.10)–(3.11).

3.1 Brute-force expansion

First, one expands all contributions to the full action (2.11) (supplemented by the GHY boundary term) to cubic order in perturbations, and obtains after uses of the background EoM (2.7) and of the Friedmann constraints (2.4):

$$\mathcal{L}^{(3)} = \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta) + \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \mathcal{F}^\alpha) + \mathcal{D}_0. \quad (3.1)$$

The first part, $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta)$, comes (mostly) from the gravity sector described by the EH action in the comoving gauge and depends on the entropic sector only through the constraint equation relating θ to $\mathcal{F}^1$. It reads

$$\begin{aligned} \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta) = a^3 M_{\text{Pl}}^2 \left[\epsilon \left(3\zeta - \frac{\dot{\zeta}}{H} \right) \dot{\zeta}^2 - \frac{\epsilon}{a^2} \zeta (\partial\zeta)^2 + \frac{1}{2a^4} \left(3\zeta - \frac{\dot{\zeta}}{H} \right) (\partial_{ij}\theta\partial_{ij}\theta - (\partial^2\theta)^2) \right. \\ \left. - \frac{2}{a^4} \partial^2\theta (\partial\theta) (\partial\zeta) \right], \end{aligned} \quad (3.2)$$

exactly like in the two-field case [47]. The second part, $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \mathcal{F}^\alpha)$, originates from the matter action in the comoving gauge and has no single-field counterpart by definition:

$$\begin{aligned} \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \mathcal{F}^\alpha) = \frac{a^3}{2} \left[\left(3\zeta - \frac{\dot{\zeta}}{H} \right) (\dot{\mathcal{F}}^\alpha)^2 + 2\sqrt{2}\epsilon\omega_1 M_{\text{Pl}} \mathcal{F}^1 \dot{\zeta} \left(6\zeta - \frac{\dot{\zeta}}{H} \right) - 3m_{\alpha\beta}^2 \mathcal{F}^\alpha \mathcal{F}^\beta \zeta \right. \\ + 2\Omega_{\alpha\beta} \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \left(3\zeta - \frac{\dot{\zeta}}{H} \right) - \mathcal{F}^\alpha \mathcal{F}^\beta \frac{\dot{\zeta}}{H} (m_{\alpha\beta}^2 - 2\Omega_\alpha{}^\gamma \Omega_{\gamma\beta} + 2\delta_{\alpha 1} \delta_{\beta 1} \omega_1^2 \\ - 4\epsilon H^2 M_{\text{Pl}}^2 R_{\alpha\sigma\beta\sigma}) + \frac{4}{3} \sqrt{2}\epsilon H M_{\text{Pl}} R_{\alpha\beta\gamma\sigma} \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \mathcal{F}^\gamma \\ - \frac{\mathcal{F}^\alpha \mathcal{F}^\beta \mathcal{F}^\gamma}{3} (V_{;\alpha\beta\gamma} - 4\sqrt{2}\epsilon H M_{\text{Pl}} (\omega_1 \delta_{\alpha 1} R_{\beta\sigma\gamma\sigma} + \Omega_\alpha{}^\delta R_{\delta\beta\gamma\sigma}) + 2\epsilon H^2 M_{\text{Pl}}^2 R_{\alpha\sigma\beta\sigma;\gamma}) \\ \left. - 2\dot{\mathcal{F}}^\alpha \frac{\partial_i \mathcal{F}^\alpha \partial_i \theta}{a^2} - \frac{(\partial \mathcal{F}^\alpha)^2}{a^2} \left(\zeta + \frac{\dot{\zeta}}{H} \right) - 2 \frac{\partial_i \mathcal{F}^\alpha \partial_i \theta}{a^2} \Omega_{\alpha\beta} \mathcal{F}^\beta \right]. \end{aligned} \quad (3.3)$$

Note that it obviously contains additional multifield interactions compared to our previous work [47], which are proportional to the purely entropic anti-symmetric matrix Ω or to three contractions of the field-space Riemann tensor along entropic directions. Indeed, this last quantity is vanishing in the two-field case where there is only one entropic direction, as can be seen from the symmetries of the Riemann tensor, or equivalently by the observation that

$R_{\alpha\beta\gamma\sigma} = \frac{1}{N_{\text{field}}-2} (\delta_{\alpha\gamma} Z_{\beta\sigma} - \delta_{\beta\gamma} Z_{\alpha\sigma}) + C_{\alpha\beta\gamma\sigma}$ contains geometrical information beyond R_{fs} only. Eventually, at this stage the time-boundary term simply reads:

$$\mathcal{D}_0 = -M_{\text{Pl}}^2 \partial_t \left[9Ha^3 \zeta^3 - \frac{a}{H} \zeta (\partial \zeta)^2 \right], \quad (3.4)$$

and comes from a few manipulations to get the form of $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta)$ that is displayed in (3.2).

3.2 Rendering the sizes of interactions manifest

Using integrations by parts and the linear EoM (2.20)–(2.21) to remove second-order time derivatives, but keeping time-boundary terms, it is possible to simplify and render explicit the sizes of cubic interactions. We split this calculation in two steps, one for each of the cubic order Lagrangians showed in (3.2) and (3.3).

Lagrangian $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta)$. This part of the computation is exactly the same as in the $N_{\text{field}} = 2$ case, with the formal replacements $\mathcal{F} \rightarrow \mathcal{F}^1$ and $\eta_{\perp} \rightarrow \omega_1/H$ in the various steps of [47], coming from the constraint equation for θ and the linear EoM for ζ . We refer the interested reader to this article and only quote the final result:

$$\begin{aligned} \mathcal{L}_{\text{ini}}^{(3)}(\zeta, \theta) = & a^3 M_{\text{Pl}}^2 \left[\epsilon(\epsilon - \eta) \dot{\zeta}^2 \zeta + \epsilon(\epsilon + \eta) \zeta \frac{(\partial \zeta)^2}{a^2} + \left(\frac{\epsilon}{2} - 2 \right) \frac{1}{a^4} (\partial \zeta) (\partial \chi) \partial^2 \chi + \frac{\epsilon}{4a^4} \partial^2 \zeta (\partial \chi)^2 \right] \\ & + a\sqrt{2\epsilon} \frac{\omega_1}{H} M_{\text{Pl}} \mathcal{F}^1 (\partial \zeta)^2 - \frac{2}{H} \dot{\zeta} \zeta \partial_t \left(a^3 \sqrt{2\epsilon} \omega_1 M_{\text{Pl}} \mathcal{F}^1 \right) + \mathcal{D}_1, \end{aligned} \quad (3.5)$$

with

$$\begin{aligned} \mathcal{D}_1 = & -M_{\text{Pl}}^2 \partial_t \left[a^3 \frac{\epsilon}{H} \zeta \dot{\zeta}^2 + a \frac{\epsilon}{H} \zeta (\partial \zeta)^2 + \frac{1}{6aH^3} \zeta \left(\zeta_{,ij} \zeta_{,ij} - (\partial^2 \zeta)^2 \right) - \frac{1}{2aH^2} \zeta \left(\zeta_{,ij} \chi_{,ij} - \partial^2 \zeta \partial^2 \chi \right) \right. \\ & \left. + \frac{1}{2aH} \zeta \left(\chi_{,ij} \chi_{,ij} - (\partial^2 \chi)^2 \right) \right], \end{aligned} \quad (3.6)$$

and we recall that χ is given by (2.14).

Lagrangian $\mathcal{L}_{\text{ini}}^{(3)}(\zeta, \mathcal{F}^\alpha)$. Let us manipulate three building blocks of this purely multifield Lagrangian, which will eventually combine to simplify interactions and render their sizes more explicit. First, combining the first term in the first line with the three terms of the last line of (3.3), using integrations by parts and the linear EoM for ζ and $\mathcal{F}^\alpha$, one finds

$$\begin{aligned} & \frac{a^3}{2} (\dot{\mathcal{F}}^\alpha)^2 \left(3\zeta - \frac{\dot{\zeta}}{H} \right) - a \dot{\mathcal{F}}^\alpha \partial_i \mathcal{F}^\alpha \partial_i \theta - \frac{a}{2} (\partial \mathcal{F}^\alpha)^2 \left(\zeta + \frac{\dot{\zeta}}{H} \right) - a \partial_i \mathcal{F}^\alpha \partial_i \theta \Omega_{\alpha\beta} \mathcal{F}^\beta \\ & = a^3 \left[\frac{\epsilon}{2} \zeta (\dot{\mathcal{F}}^\alpha)^2 - \frac{\dot{\zeta}}{H} \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta (m_{\alpha\beta}^2 + 3H\Omega_{\alpha\beta} + \dot{\Omega}_{\alpha\beta}) + \frac{2}{H} \sqrt{2\epsilon} \omega_1 M_{\text{Pl}} \zeta \dot{\mathcal{F}}^1 \right] \\ & + a \left[\frac{\epsilon}{2} \zeta (\partial \mathcal{F}^\alpha)^2 - (\partial \mathcal{F}^\alpha) (\partial \chi) (\dot{\mathcal{F}}^\alpha + \Omega_{\alpha\beta} \mathcal{F}^\beta) + \frac{1}{H} (\partial \mathcal{F}^\alpha) (\partial \zeta) \Omega_{\alpha\beta} \mathcal{F}^\beta \right] \\ & - \partial_t \left[\frac{a^3}{2H} \zeta \left((\dot{\mathcal{F}}^\alpha)^2 + \frac{(\partial \mathcal{F}^\alpha)^2}{a^2} \right) \right]. \end{aligned} \quad (3.7)$$

It is clear from this result that, for example, the right size of the $\zeta - (\partial_\mu \mathcal{F}^\alpha)^2$ interactions is more suppressed (by a factor of ϵ in this case) than what it seems when looking at the

brute-force initial cubic Lagrangian. Let us proceed and look at a second block, made of the second and third terms of the first line in (3.3), to which one adds the first term in the second line of the result coming from (3.5) as well as two terms in the first line of the previous equality (3.7):

$$\begin{aligned}
 & a^3 \sqrt{2\epsilon\omega_1} M_{\text{Pl}} \mathcal{F}^1 \dot{\zeta} \left(6\zeta - \frac{\dot{\zeta}}{H} \right) - \frac{3}{2} a^3 m_{\alpha\beta}^2 \zeta \mathcal{F}^\alpha \mathcal{F}^\beta - \frac{2}{H} \dot{\zeta} \zeta \partial_t \left(a^3 \sqrt{2\epsilon\omega_1} M_{\text{Pl}} \mathcal{F}^1 \right) \\
 & + a^3 \frac{2}{H} \sqrt{2\epsilon\omega_1} M_{\text{Pl}} \zeta \dot{\mathcal{F}}^1 - \frac{a^3}{H} m_{\alpha\beta}^2 \zeta \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \\
 & = a^3 \left[\frac{1}{2} m_{\alpha\beta}^2 \frac{\dot{\zeta}}{H} \mathcal{F}^\alpha \mathcal{F}^\beta + \frac{1}{2} \left(\epsilon m_{\alpha\beta}^2 + \frac{\partial_t(m_{\alpha\beta}^2)}{H} \right) \zeta \mathcal{F}^\alpha \mathcal{F}^\beta - \sqrt{2\epsilon\omega_1} M_{\text{Pl}} \left(\frac{\dot{\zeta}^2}{H} \mathcal{F}^1 + 2\dot{\zeta} \zeta \mathcal{F}^1 \left(\frac{\eta}{2} + u_1 \right) \right) \right] \\
 & - \partial_t \left(m_{\alpha\beta}^2 \frac{a^3}{2H} \zeta \mathcal{F}^\alpha \mathcal{F}^\beta \right). \tag{3.8}
 \end{aligned}$$

Next, we use

$$\begin{aligned}
 & - \frac{a^3}{H} \Omega^\gamma{}_\alpha \Omega_{\gamma\beta} \dot{\zeta} \mathcal{F}^\alpha \mathcal{F}^\beta + a^3 \Omega_{\alpha\beta} \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \left(3\zeta - \frac{\dot{\zeta}}{H} \right) = a^3 \left[\left((3 + \epsilon) \Omega_{\alpha\beta} + \frac{\dot{\Omega}_{\alpha\beta}}{H} \right) \zeta \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \right. \\
 & + \left(\epsilon \Omega^\gamma{}_\alpha + \frac{\dot{\Omega}^\gamma{}_\alpha}{H} - \frac{m_{\gamma\alpha}^2}{H} \right) \Omega_{\gamma\beta} \zeta \mathcal{F}^\alpha \mathcal{F}^\beta + \frac{2}{H} \sqrt{2\epsilon\omega_1} M_{\text{Pl}} \Omega_{1\alpha} \dot{\zeta} \zeta \mathcal{F}^\alpha \left. \right] + \frac{a}{H} \Omega_{\alpha\beta} \zeta \partial^2 \mathcal{F}^\alpha \mathcal{F}^\beta \\
 & - \partial_t \left(\frac{a^3}{H} \Omega_{\alpha\beta} \zeta \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta + \frac{a^3}{H} \Omega^\gamma{}_\alpha \Omega_{\gamma\beta} \zeta \mathcal{F}^\alpha \mathcal{F}^\beta \right). \tag{3.9}
 \end{aligned}$$

Collecting these three blocks, being careful not to double count some terms, and adding them to the rest of the Lagrangian that has not been manipulated, one finds many cancellations and arrives at the final result:

$$\begin{aligned}
 \mathcal{L}^{(3)} = & M_{\text{Pl}}^2 a^3 \left[\epsilon(\epsilon - \eta) \dot{\zeta}^2 \zeta + \epsilon(\epsilon + \eta) \zeta \frac{(\partial\zeta)^2}{a^2} + \left(\frac{\epsilon}{2} - 2 \right) \frac{1}{a^4} (\partial\zeta)(\partial\chi) \partial^2 \chi + \frac{\epsilon}{4a^4} \partial^2 \zeta (\partial\chi)^2 \right] \\
 & + a^3 \left\{ \sqrt{2\epsilon\omega_1} M_{\text{Pl}} \left[\frac{\mathcal{F}^1}{H} \left(\frac{(\partial\zeta)^2}{a^2} - \dot{\zeta}^2 - \dot{\zeta} \zeta H (\eta + 2u_1) \right) + 2 \frac{\Omega_{1\alpha}}{H} \dot{\zeta} \zeta \mathcal{F}^\alpha \right] \right. \\
 & + \left[\frac{\epsilon}{2} m_{\alpha\beta}^2 + \frac{(\dot{m}_{\alpha\beta}^2)}{2H} + \Omega_{\gamma\beta} \left(\epsilon \Omega^\gamma{}_\alpha + \frac{\dot{\Omega}^\gamma{}_\alpha}{H} - \frac{m_{\gamma\alpha}^2}{H} \right) \right] \zeta \mathcal{F}^\alpha \mathcal{F}^\beta + \epsilon \Omega_{\alpha\beta} \zeta \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \\
 & + \left(2\epsilon H^2 M_{\text{Pl}}^2 R_{\alpha\sigma\beta\sigma} - \omega_1^2 \delta_{\alpha 1} \delta_{\beta 1} \right) \frac{\dot{\zeta}}{H} \mathcal{F}^\alpha \mathcal{F}^\beta + \frac{1}{2} \epsilon \zeta \left(\left(\dot{\mathcal{F}}^\alpha \right)^2 + \frac{(\partial\mathcal{F}^\alpha)^2}{a^2} \right) \\
 & - \frac{1}{a^2} (\partial\mathcal{F}^\alpha) (\partial\chi) \left(\dot{\mathcal{F}}^\alpha + \Omega_{\alpha\beta} \mathcal{F}^\beta \right) + \frac{2}{3} \sqrt{2\epsilon} H M_{\text{Pl}} R_{\alpha\beta\gamma\sigma} \dot{\mathcal{F}}^\alpha \mathcal{F}^\beta \mathcal{F}^\gamma \\
 & - \frac{1}{6} \left(V_{;\alpha\beta\gamma} - 4\sqrt{2\epsilon} H M_{\text{Pl}} \left(\omega_1 \delta_{\alpha 1} R_{\beta\sigma\gamma\sigma} + \Omega^\delta{}_\alpha R_{\delta\beta\gamma\sigma} \right) + 2\epsilon H^2 M_{\text{Pl}}^2 R_{\alpha\sigma\beta\sigma;\gamma} \right) \mathcal{F}^\alpha \mathcal{F}^\beta \mathcal{F}^\gamma \left. \right\} \\
 & + \mathcal{D}, \tag{3.10}
 \end{aligned}$$

where we defined the logarithmic derivative of the first bending as $u_1 = \dot{\omega}_1 / (H\omega_1)$, and with the final boundary term

$$\begin{aligned} \mathcal{D} = & -\partial_t \left\{ M_{\text{Pl}}^2 \left[9Ha^3\zeta^3 - \frac{a}{H}\zeta(\partial\zeta)^2 a^3 \frac{\epsilon}{H}\zeta\dot{\zeta}^2 + a\frac{\epsilon}{H}\zeta(\partial\zeta)^2 + \frac{1}{6aH^3}\zeta(\zeta_{,ij}\zeta_{,ij} - (\partial^2\zeta)^2) \right. \right. \\ & \left. \left. - \frac{1}{2aH^2}\zeta(\zeta_{,ij}\chi_{,ij} - \partial^2\zeta\partial^2\chi) + \frac{1}{2aH}\zeta(\chi_{,ij}\chi_{,ij} - (\partial^2\chi)^2) \right] \right. \\ & \left. + \frac{a^3}{2H}\zeta \left[(\dot{\mathcal{F}}^\alpha)^2 + \frac{(\partial\mathcal{F}^\alpha)^2}{a^2} \right] + m_{\alpha\beta}^2 \frac{a^3}{2H}\zeta\mathcal{F}^\alpha\mathcal{F}^\beta + \frac{a^3}{H}\Omega_{\alpha\beta}\zeta\dot{\mathcal{F}}^\alpha\mathcal{F}^\beta + \frac{a^3}{H}\Omega^\gamma{}_\alpha\Omega_{\gamma\beta}\zeta\mathcal{F}^\alpha\mathcal{F}^\beta \right\}, \end{aligned} \quad (3.11)$$

whose local (in time) contribution to the three-point functions can be easily computed.

4 Single-field effective theory of fluctuations

Even when the background inflationary trajectory is genuinely multifield, it may be possible to describe perturbations as a single-field system only. This so-called effective single-field theory of fluctuations is justified when entropic perturbations $\mathcal{F}^\alpha$ are heavy enough to be adiabatically expressed in terms of the adiabatic perturbation ζ to which they are mixing, and thus integrated out of the multifield theory. Within its regime of validity, this tool is extremely powerful to compute efficiently the statistics of the observable curvature perturbation as in single-field inflation. The multifield dynamics is however encoded in the parameters setting the free propagation (through c_s^2 the speed of sound) and the interactions of ζ (the to-be-found parameter A for cubic interactions, and others for higher-order ones), thus obviously affecting the theoretical predictions for cosmological observables [43–47, 50]. In this section, we remind that the first bending ω_1 plays a special role: if vanishing, the entropic sector entirely decouples from the adiabatic perturbation and the resulting single-field effective theory is unaffected by multifield effects, both at the level of linear fluctuations and Non-Gaussianities. However, as soon as $\omega_1 \neq 0$, the speed of sound is reduced, $c_s^2 < 1$, and cubic interactions are enhanced compared to the purely single-field case. As expected, we show that the resulting single-field cubic action can always be recast in the form of $P(X, \phi)$ cubic interactions. In the slow-varying limit, we recover the two leading-order cubic operators known from the decoupling limit of the Effective Field Theory of Inflation (EFToI) [56, 57], with a prediction for the Wilson coefficient A coming from the multifield UV completion. Importantly, A contains contributions from the non-trivial speed of sound c_s^2 , from third derivatives of the scalar potential, but also from the geometry of the field-space even beyond the scalar curvature: the traceless Ricci tensor and the Weyl tensor matter too.

4.1 Generalities

Integrating out $N_{\text{field}} - 1$ heavy entropic perturbations. Let us recall that the EoM (2.21) for entropic perturbations $\mathcal{F}^\alpha$ can be written:

$$\begin{aligned} (m_{\alpha\beta}^2 + \mathcal{O}_{\alpha\beta}^\Omega - \square_{\alpha\beta})\mathcal{F}^\beta &= 2\sqrt{2\epsilon}\delta_{\alpha 1}M_{\text{Pl}}\omega_1\dot{\zeta}, \\ \text{with } \square_{\alpha\beta} &= \delta_{\alpha\beta} \left[-\frac{\partial^2}{\partial t^2} - 3H\frac{\partial}{\partial t} + \frac{\partial^2}{a^2} \right] \text{ the d'Alembertian operator} \\ \text{and } \mathcal{O}_{\alpha\beta}^\Omega &= 2\Omega_{\alpha\beta}\frac{\partial}{\partial t} + (3H\Omega_{\alpha\beta} + \dot{\Omega}_{\alpha\beta}) \text{ the entropic-mixing operator.} \end{aligned} \quad (4.1)$$

In the limit $m_{\alpha\beta}^2 \mathcal{F}^\beta \gg (\mathcal{O}_{\alpha\beta}^\Omega - \square_{\alpha\beta}) \mathcal{F}^\beta$ that we shall call “heavy entropic perturbations” and whose regime of validity will soon be specified precisely, the equation of motion for $\mathcal{F}^\alpha$ can be solved at leading order (LO) by

$$\mathcal{F}_{\text{LO}}^\alpha = (m^{-2})^\alpha{}_1 2\sqrt{2}\epsilon M_{\text{Pl}} \omega_1 \dot{\zeta}, \quad (4.2)$$

where m^{-2} is the inverse matrix of m^2 . Interestingly, only the first column of this inverse matrix is needed, and one can use a famous linear algebra formula applied to the symmetric matrix m^2 , to rewrite:

$$(m^{-2})^\alpha{}_1 = \frac{(\text{Adj}(m^2))^\alpha{}_1}{\text{Det}(m^2)}, \quad (4.3)$$

where $\text{Adj}(m^2) = {}^t\text{Com}(m^2)$ is the adjugate of the entropic mass matrix, or equivalently its cofactor matrix $\text{Com}(m^2)$ since it is symmetric. Now, plugging into the N_{field} action the expression for $\mathcal{F}_{\text{LO}}^\alpha$ in (4.2), one can find the effective single-field theory for ζ when heavy entropic perturbations have been integrated out.

Linear dynamics. Consistently neglecting kinetic terms of $\mathcal{F}^\alpha$ and its mixings to other entropic modes through Ω , one finds the quadratic effective Lagrangian in terms of ζ only,

$$\mathcal{L}_{\text{EFT}}^{(2)}(\zeta) = a^3 \frac{\epsilon M_{\text{Pl}}^2}{c_s^2} \left(\dot{\zeta}^2 - \frac{(\partial\zeta)^2}{a^2} \right) \text{ with } \frac{1}{c_s^2} - 1 = 4\omega_1^2 (m^{-2})_{11}, \quad (4.4)$$

which results in the effective EoM for ζ :

$$\mathcal{E}_{\zeta, \text{EFT}}^{\text{LO}} = \frac{1}{a^3 \epsilon} \frac{d}{dt} \left(a^3 \frac{\epsilon}{c_s^2} \dot{\zeta} \right) - \frac{\partial^2 \zeta}{a^2} = 0, \quad (4.5)$$

showing that a deviation from a speed of sound $c_s^2 = 1$ is possible only if the first bending parameter ω_1 is non-zero. Indeed, ω_1 is the single parameter that controls the mixing of the whole entropic sector (which has its own mixings and interactions) with the adiabatic curvature perturbation. Note however that $(m^{-2})_{11}$ can be approximated by $1/(m^2)_{11}$ only if the matrix m^2 is mostly diagonal, and that otherwise the whole N_{field} system contributes to the effectively single-field linear dynamics through $(m^{-2})_{11}$ whenever $\omega_1 \neq 0$. Before turning to the computation of the effective single-field interactions in the cubic action, let us make more precise the conditions under which the procedure of integrating out entropic fluctuations is justified.

Regime of validity. Assuming that $\mathcal{F}^\alpha$ can be simply expressed as $\mathcal{F}_{\text{LO}}^\alpha$ displayed in eq. (4.2) amounts to neglecting higher-order corrections. Indeed, the full “non-perturbative” result for $\mathcal{F}^\alpha$ is rather

$$\mathcal{F}^\alpha = \left\{ (m^{-2}) \sum_{i=0} \left[m^{-2} (\square - \mathcal{O}^\Omega) \right]^i \right\}_{\alpha 1} 2\sqrt{2}\epsilon M_{\text{Pl}} \omega_1 \dot{\zeta}, \quad (4.6)$$

where higher powers of i are expected to be more suppressed in the regime of validity of the single-field EFT. As a consistency check, we must require that the next-to-leading-order (NLO) term $\mathcal{F}_{\text{NLO}}^\alpha$ ($i = 1$) is smaller than the leading-order one $\mathcal{F}_{\text{LO}}^\alpha$ ($i = 0$). Computing

the NLO term $\mathcal{F}_{\text{NLO}}^\alpha = \left\{ (m^{-2}) \left[m^{-2} (\Box - \mathcal{O}^\Omega) \right] \right\}_{\alpha 1} 2\sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \dot{\zeta}$ requires in particular to compute

$$\begin{aligned} \Box_{\alpha\beta} \left(2\sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \dot{\zeta} \right) &= \delta_{\alpha\beta} 2\sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \left\{ \left(1 - c_s^2 \right) \frac{\partial^2 \dot{\zeta}}{a^2} + c_s^2 (2 - 2u_1 - 4s) H \frac{\partial^2 \dot{\zeta}}{a^2} \right. \\ &\quad \left. + H^2 \dot{\zeta} \left[\left(-3 - \frac{\eta}{2} + u_1 + 2s \right) \left(\epsilon + \frac{\eta}{2} - u_1 - 2s \right) + \frac{\dot{\eta}}{2H} - \frac{\dot{u}_1}{H} - 2 \frac{\dot{s}}{H} \right] \right\}, \\ \mathcal{O}_{\alpha\beta}^\Omega \left(2\sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \dot{\zeta} \right) &= 2\sqrt{2\epsilon} M_{\text{Pl}} \omega_1 \left\{ 2\Omega_{\alpha\beta} c_s^2 \frac{\partial^2 \dot{\zeta}}{a^2} + H \dot{\zeta} \left[\Omega_{\alpha\beta} (2u_1 + 2s) + \frac{\dot{\Omega}_{\alpha\beta}}{H} \right] \right\}, \end{aligned} \quad (4.7)$$

where $s = (\dot{c}_s^2)/(2Hc_s^2) = (c_s^2 - 1) \left\{ u_1 + \frac{1}{2H} \frac{d}{dt} [(m^{-2})_{11}] / (m^{-2})_{11} \right\}$ is the logarithmic time derivative of the speed of sound c_s , and from which we infer more precise conditions on the multifield parameters for the single-field theory to be valid:

$$\text{for } X \in (H, \epsilon, \omega_1, c_s), \quad \mathcal{O} \left[\begin{aligned} &\left(\frac{\dot{X}}{X} \right)^2, \frac{\ddot{X}}{X} \left(m^{-4} \right)^\alpha{}_1 \\ &\frac{k^2 (1 - c_s^2)}{a^2} \left(m^{-4} \right)^\alpha{}_1 \\ &\left(m^{-4} \dot{\Omega} \right)^\alpha{}_1 \\ &(u_1 + s) H \left(m^{-4} \Omega \right)^\alpha{}_1 \end{aligned} \right] \ll \left(m^{-2} \right)^\alpha{}_1, \quad (4.8)$$

as well as less clear “operators” inequalities: $c_s^2 \left[H \left(m^{-4} \right)^\alpha{}_1 + \left(m^{-4} \Omega \right)^\alpha{}_1 \right] \partial^2 \dot{\zeta} / a^2 \ll \left(m^{-2} \right)^\alpha{}_1 \dot{\zeta}$. The first line of (4.8) means that the first and second derivatives of background quantities must be slowly evolving in units of the entropic squared mass matrix. Had we considered higher terms in the i -expansion, we would have found that even higher derivatives should be small in those units. Eventually, this means that the whole functions describing the background, and not just their first derivatives, should be slowly evolving during a time scale set by the mass matrix m^2 . These adiabaticity conditions are the same as the ones previously found in the case of $N_{\text{field}} = 2$ scalar fields [47] and that were first proposed in [83], but generalized to a system of any number of entropic fields. The second line in (4.8) is important as it sets the UV cutoff of the single-field EFT in terms of wavenumbers. It states that only wavenumbers below the scale set by the entropic mass are incorporated in the EFT, higher momenta being excluded from this description as they are affected by new physics [84, 85]. This makes sense because for higher values of the momenta, the spatial derivatives of the entropic perturbations are becoming larger than the mass terms and the scalar fields should behave as in Bunch-Davies vacuum. The third and fourth lines in (4.8) are new requirements coming from the fact that several entropic perturbations were integrated out, and constrain the maximal amount of rotation (and its derivative) of the local entropic basis. Although the vectorial structure of this equation is such that only the second bending ω_2 seems to be constrained, again it can be shown that for higher values of i we would get constraints on a larger set of bendings and their multiple derivatives. Thus, from the third line we understand that it is actually the whole matrix Ω which is constrained to be slowly evolving in units of the entropic mass matrix, and not just the first or the two first bendings and their first derivatives. The fourth line is more intricate to understand as it mixes derivatives of ω_1 and c_s with the matrix Ω but it roughly states that the bendings in Ω

can not be too large, a necessary requirement to neglect $\mathcal{O}_{\alpha\beta}^\Omega$ in the EoM for $\mathcal{F}^\alpha$, at leading order.

In the regime where those conditions are satisfied, time derivatives of entropic perturbations, $\dot{\mathcal{F}}_{\text{LO}}^\alpha$, which although generically suppressed at the linear level will be needed in the cubic action, read:

$$\dot{\mathcal{F}}_{\text{LO}}^\alpha = 2\sqrt{2\epsilon}M_{\text{Pl}}\omega_1 \left\{ \left(m^{-2}\right)^\alpha{}_1 \left[\left(-3 - \frac{\eta}{2} + u_1 + 2s\right) H\dot{\zeta} + c_s^2 \frac{\partial^2 \zeta}{a^2} \right] + \frac{d}{dt} \left[\left(m^{-2}\right)^\alpha{}_1 \dot{\zeta} \right] \right\}. \quad (4.9)$$

4.2 Effective cubic interactions

We begin by recalling that, in order to derive the effectively single-field cubic interactions, it is sufficient to plug into the full N_{field} action the linear constraints of $\mathcal{F}^\alpha$ and its derivative as a function of ζ , i.e. quadratic corrections are irrelevant. Indeed, let us write formally $\mathcal{F}^\alpha[\zeta] = \mathcal{F}_{(1)}^\alpha[\zeta] + \mathcal{F}_{(2)}^\alpha[\zeta]$ where $\mathcal{F}_{(1)}^\alpha$ is linear in ζ and comes from the second action only, and $\mathcal{F}_{(2)}^\alpha$ is quadratic and comes from the correction due to the cubic action. Then, up to cubic order in perturbations, one gets

$$\begin{aligned} S_{\text{EFT}}[\zeta] &= S^{(2)}[\zeta, \mathcal{F}_{(1)}^\alpha[\zeta] + \mathcal{F}_{(2)}^\alpha[\zeta]] + S^{(3)}[\zeta, \mathcal{F}_{(1)}^\alpha[\zeta]] \\ &= S^{(2)}[\zeta, \mathcal{F}_{(1)}^\alpha[\zeta]] + \underbrace{\frac{\delta S^{(2)}}{\delta \mathcal{F}^\alpha} \Big|_{\zeta, \mathcal{F}_{(1)}^\alpha[\zeta]}}_{=0} \times \mathcal{F}_{(2)}^\alpha[\zeta] + S^{(3)}[\zeta, \mathcal{F}_{(1)}^\alpha[\zeta]], \end{aligned} \quad (4.10)$$

where the second term in the second line vanishes by virtue of the linear EoM, in a way that only $\mathcal{F}_{(1)}^\alpha$ is relevant. Of course this is true only up to cubic order, and for higher-order interactions, one would need to take into account non-linear corrections to $\mathcal{F}_{(1)}^\alpha$.

General result. Performing the integrating-out procedure at the level of the full multifield cubic action (3.10) (but disregarding the single-field boundary terms that give a vanishing contribution to the adiabatic power spectrum on super-Hubble scales), consistently neglecting terms that are not encapsulated by the leading-order expressions (4.2) and (4.9), yields the following result:

$$\begin{aligned} \mathcal{L}_{\text{EFT,bulk}}^{(3)} &= M_{\text{Pl}}^2 a^3 \frac{\epsilon}{c_s^2} \left[f_0 c_s^2 \frac{\dot{\zeta}}{H} \frac{(\partial\zeta)^2}{a^2} + \frac{f_1}{H} \dot{\zeta}^3 + f_2 \dot{\zeta}^2 \zeta + f_3 c_s^2 \zeta \frac{(\partial\zeta)^2}{a^2} + f_4 \dot{\zeta} \partial_i \partial^{-2} \dot{\zeta} \partial_i \zeta \right. \\ &\quad \left. + f_5 \partial^2 \zeta (\partial_i \partial^{-2} \dot{\zeta})^2 \right], \end{aligned} \quad (4.11)$$

with

$$\begin{aligned} f_0 &= \left(\frac{1}{c_s^2} - 1 \right) & f_1 &= \left(\frac{1}{c_s^2} - 1 \right) A & f_2 &= \epsilon - \eta + 2s \\ f_3 &= \epsilon + \eta & f_4 &= \frac{\epsilon}{2c_s^2} (\epsilon - 4) & f_5 &= \frac{\epsilon^2}{4c_s^2}. \end{aligned} \quad (4.12)$$

The parameter A encoding multifield effects reads

$$\begin{aligned}
 A = & -\frac{1}{2}(1+c_s^2) + \frac{4}{3}(1+2c_s^2)\epsilon H^2 M_p^2 (m^{-2})_{11} R_{m\sigma m\sigma} \\
 & - \frac{\kappa}{6}(1-c_s^2) (m^{-2})_{11} \left[V_{,mmm} + 2\epsilon H^2 M_p^2 R_{m\sigma m\sigma;m} \right. \\
 & \left. + 4\sqrt{2}\epsilon H M_p \left(\Omega^\alpha_m + \frac{1}{(m^{-2})_{11}} \frac{d(m^{-2})^\alpha_1}{dt} \right) R_{m\alpha m\sigma} \right],
 \end{aligned} \tag{4.13}$$

with $\kappa = \sqrt{2\epsilon} M_{\text{Pl}} H / \omega_1$ the bending radius of the background trajectory in field space, and where an index m means a contraction of a generic entropic index α with the projection vector $(m^{-2})^\alpha_1 / (m^{-2})_{11}$; for example $R_{m\sigma m\sigma} = (m^{-2})^\alpha_1 (m^{-2})^\beta_1 / [(m^{-2})_{11}]^2 R_{\alpha\sigma\beta\sigma}$ and there is no sum left on m nor σ . The first two lines in (4.13) generalise the result of the $N_{\text{field}} = 2$ case in [47], and genuinely new contributions for $N_{\text{field}} \geq 3$ are displayed in the third line. Note however that even the quantities in the first two lines are affected by the whole multifield setup, for example through the projection vectors that sum over all entropic directions. In particular, the geometrical contribution to the bispectrum is more complex than in the single-field case since not only the scalar curvature of the field space, R_{fs} , enters in the final result: Ricci scalar, contractions of the traceless Ricci tensor and of the Weyl tensor as well as their derivatives in entropic directions, are all relevant in the general case. Eventually, note that eqs. (4.11)–(4.12) correspond to the cubic interactions of higher-derivatives, single-field theories with a $P(X, \phi)$ Lagrangian [86], where X is the standard kinetic term, $X = -1/2 g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi$, provided a matching between our parameters (c_s^2, A) and the derivatives of the function P , $\Sigma = X P_{,X} + 2X^2 P_{,XX}$ and $\lambda = X^2 P_{,XX} + 2/3 X^3 P_{,XXX}$, which reads $c_s^2 = X P_{,X} / \Sigma$ and $(c_s^{-2} - 1) A = -2\lambda / \Sigma$ (see [47] for the simple manipulation of (4.11) needed to explicitly find the corresponding $P(X, \phi)$ cubic Lagrangian).

Slow-varying limit. Until now, our results were independent of any assumption regarding the background dynamics (except that it must be such that the integrating-out procedure at leading order is justified), and in particular we have not required the slow-roll parameters to be small. In a slow-varying approximation, the whole background dynamics is assumed to be smooth, which implies in particular that $\epsilon, \eta, s \ll 1$. In this limit, the leading-order operators are the ones predicted by the decoupling limit of the EFToI [56, 57], i.e. $\zeta (\partial\zeta)^2$ and ζ^3 , and the single-field effective action for ζ reads:

$$\mathcal{L}_{\text{EFT, slow-varying}}^{(3)} = M_{\text{Pl}}^2 a^3 \frac{\epsilon}{H} \left(\frac{1}{c_s^2} - 1 \right) \left[\zeta \frac{(\partial\zeta)^2}{a^2} + \frac{A}{c_s^2} \zeta^3 \right], \tag{4.14}$$

where all parameters should be considered as constants for consistency. Clearly, the interesting point of starting from the multifield setup and integrating out heavy perturbations, is that we end up with a prediction for the EFT parameters c_s^2 and A depending on the multifield UV completion. In the usual approach of the EFT of Inflation, those parameters are free and should be measured or constrained through cosmological observations (for the most recent constraints in the (c_s^2, A) -plane, see [2]). Also, let us insist on the fact that we derived a single-field effective action for the perturbations, but that nothing forbids the homogeneous background dynamics to be genuinely multifield. Thus, this tool is useful to compute the observable bispectrum of multifield models that have a non-trivial multifield dynamics at the level of the background, but with heavy entropic perturbations. Lastly, if

the background is not slowly-varying, or if c_s^2 is not much smaller than unity, one should expect all operators in (4.11) to be relevant, a situation that is not encapsulated by the decoupling limit of the EFToI.

Limitations of this approach. The effective single-field theory for adiabatic perturbations during inflation that we uncovered relies on several assumptions. More precisely, we neglected both the kinetic terms $\square$ and the entropic mixing terms $\mathcal{O}^\Omega$ in the linear EoM of $\mathcal{F}^\alpha$, for all entropic perturbations. Although this is justified when all perturbations in the entropic sector are very heavy, different regimes would be interesting to study. First, it is possible that there is a hierarchy between the eigenstates of the mass matrix m^2 , and that only some of the directions are heavy and can be integrated out, while the other ones should be kept dynamical. We conjecture that the resulting theories should drastically differ depending on whether the first entropic direction, $\mathcal{F}^1$, which mixes with the adiabatic one, is heavy or not. If $\mathcal{F}^1$ is heavy, the resulting theory should be the one of several light entropic perturbations coupled to an adiabatic perturbation that has a non-canonical kinetic term spontaneously breaking boosts symmetries, i.e. with $c_s^2 < 1$. If $\mathcal{F}^1$ remains light and dynamical, then ζ should keep the canonical structure with $c_s^2 = 1$. A very different regime is also reached when there is a hierarchy between the kinetic terms and the entropic mixing terms, for example if the latter are larger than the former. It would be interesting to study this other kind of “integrating-out” procedure that incorporates non-trivial effects coming from a fast rotation of the local entropic basis, and that were not taken into account in the present single-field effective theory analysis (although contained in the full multifield description of course). Lastly, we assumed that both the time and the spatial derivatives (that we called “kinetic terms”) of the entropic perturbations were equally negligible. However there is a sub-Hubble regime where gradients are much larger than time derivatives, in which case one can have the hierarchy $\frac{1}{a^3} \frac{d}{dt} (a^3 \dot{\mathcal{F}}^\alpha) \ll \left(\frac{k^2}{a^2} \delta_{\alpha\beta} + m_{\alpha\beta}^2 \right) \mathcal{F}^\beta$ that would result in a single-field effective theory for ζ with a modified dispersion relation, i.e. a scale-dependent speed of sound $c_s^2(k)$ [45, 83, 87], as found also in genuinely single-field models at higher-order in derivatives like ghost inflation (see, e.g. [57, 88, 89]).

5 Conclusion

In this article, we have studied the background and linear dynamics, as well as non-Gaussianities, in multifield inflation with any number N_{field} of scalar fields. We parameterized the multifield dynamics by defining the adiabatic direction as the one instantaneously parallel to the background trajectory, and the entropic directions as the ones perpendicular (in a field-space covariant manner) to it and to one another. Then, we identified covariant perturbations in the comoving gauge; ζ along the adiabatic direction and $\mathcal{F}^\alpha$ for $\alpha \in \{1, \dots, N_{\text{field}} - 1\}$ along the entropic ones, see eq. (2.12). Because we keep the boundary terms in the cubic action as they can play a role in the final observable bispectrum, we recalled the crucial role of the GHY boundary term in cosmology to have a well-defined variational principle. We computed the quadratic Lagrangian, eqs. (2.15)–(2.16), which contains the massless adiabatic perturbation and the $N_{\text{field}} - 1$ massive entropic ones. We found that the entropic sector mixes within itself via the non-diagonal elements of the mass matrix $m_{\alpha\beta}^2$ and the rotation of the local entropic basis $\Omega_{\alpha\beta}$, and mixes also with the adiabatic perturbation through the first entropic fluctuation $\mathcal{F}^1$ due to the bending of the background trajectory parameterized by ω_1 . We showed in eq. (2.19) that the geometrical contribution to the entropic mass matrix is

richer than in the two-field case as not only the scalar curvature of the field space is relevant but its whole Ricci tensor should be taken into account for $N_{\text{field}} = 3$, and even its Weyl tensor for $N_{\text{field}} \geq 4$. Moreover, we explained that Ω contributes to the linear dynamics in two different ways: first squared in the effective mass matrix for large-scale fluctuations m_{eff}^2 , where it comes only with negative eigenvalues, but also as a linear coupling between $\mathcal{F}^\alpha$ and $\dot{\mathcal{F}}^\beta$ with $|\alpha - \beta| = 1$, where its role is more complicated to analyse. This can be seen in eqs. (2.15)–(2.16) at the level of the quadratic Lagrangian or eq. (2.22) at the level of the effective linear equations of motion on large scales. Although the goal of the present article was not to address in detail the question of the linear stability of background trajectories in N_{field} -inflation, we think that those findings motivate a thorough reanalysis of it. For completeness, we also showed the quadratic Hamiltonian that may be used for in-in computations of the power spectrum in a perturbative scheme.

Next, we investigated in full generality non-Gaussianities in the form of cubic interactions, for any number of scalar fields with non-canonical kinetic terms and any potential, during inflation and without assuming particular features of the background dynamics. For this, we computed the cubic action in terms of the adiabatic perturbation and the entropic ones, a work that required many non-trivial manipulations: integrations by parts, uses of linear equations of motion. We kept the boundary terms that are needed for a careful computation of the bispectrum with the in-in formalism and identified new interactions within the entropic sector that vanish for a single isocurvature perturbation, as well as more complex geometrical interactions amongst the entropic sector and with the adiabatic perturbation. Again, we stress that the only assumption behind the general result (3.10)–(3.11) is that of small perturbations, and that otherwise it is fully generic and could be used in a large number of cases.

As a first analytical application of our general result, we explained how models that feature heavy entropic perturbations can lead to a single-field effective theory for fluctuations by integrating them out. This procedure assumes that both the kinetic terms and the entropic mixing terms via the rotation of the entropic basis, are negligible compared to the mass matrix (that needs not be diagonal, hence entropic perturbations can mix through it). At the quadratic level, this resulted in a single-field theory for ζ with a reduced speed of sound when $\omega_1 \neq 0$, see eq. (4.4). Interestingly, the ratio of mass scales setting the deviations of c_s^2 from 1 is given by $(m^{-2})_{11} \omega_1^2$, where the inverse mass matrix m^{-2} incorporates effects from the whole multifield setup, and can be large when the bending is strong. Next, after explaining that only the linear equations of motion relating the entropic fluctuations to the adiabatic perturbation were needed to compute the effectively single-field cubic interactions, we proceeded to the integrating-out procedure at that level. As in the case of $N_{\text{field}} = 2$ scalar fields treated in our previous article [47], we found without further approximation a $P(X, \phi)$ -like cubic Lagrangian with a direct mapping between the derivatives of P and the multifield parameters, in eq. (4.11). We show that in a slow-varying approximation we recover the decoupling limit of the Effective Field Theory of Inflation, but with a prediction for the otherwise unknown Wilson coefficients $(c_s^{-2} - 1)$ and A . The latter incorporates effects from the potential as well as from the geometry of the field space, where again not only the scalar curvature matters contrary to the case $N_{\text{field}} = 2$.

We think that this work can lead to various interesting applications, both analytical and numerical. First, we showed that the analysis of the linear stability of background trajectories has to be further questioned as soon as more than one entropic perturbation is considered. Indeed, even the effective mass matrix on large scales may become negative due to strong

turning rates of the local entropic basis, parameterized by the matrix Ω which also enters in the dynamics independently of the mass matrix. It would be worth investigating for the first non-trivial case of $N_{\text{field}} = 3$ the effect of the torsion parameter ω_2 , and we conjecture about the possibility of a “torsion destabilisation of inflation”, provided the two effects do not cancel one another. Moreover, the geometrical contribution to the entropic mass matrix is more complex than in the case of a two-dimensional field space for which only the scalar curvature is relevant, hence it would be worth investigating in more detail its effects on the linear dynamics of perturbations and thereby possible instabilities. We also showed the full quadratic Hamiltonian that we chose in order to define our free theory for the computation of the cubic action. But different choices could be made in order to enable an analytical computation of the mode functions in the interaction picture: the mixing parameters (all or only some) could be considered small and the corresponding terms in the Hamiltonian treated as quadratic interactions in an in-in formulation. With this quasi-single-field picture, one could perturbatively compute corrections to the adiabatic power spectrum due to the presence of extra scalar fields (the entropic perturbations), in the spirit of the cosmological collider program [17]. And since we computed the multifield cubic action in the present article, one could apply the same treatment to cubic interactions and check the effect of several extra scalar fields on the bispectrum. More precisely, it would be extremely interesting to understand if adding several extra fields with $m \simeq H$ either strengthens the oscillatory pattern of the squeezed limit of the bispectrum [15], or completely blurs it. For these applications, a particular regime of interest would be the one of $N_{\text{field}} \rightarrow \infty$ for which one can hope to find universal results. Apart from these analytical works, one could also extend the transport approach for multifield inflationary correlation functions to the comoving gauge, a numerical study that would rely on the full cubic action that we displayed in this article, and would enable to probe numerically the regime of cosmological collider physics. Eventually, we explained in this work how to derive a single-field theory for ζ when all entropic fluctuations are heavy enough to neglect both their kinetic terms and their self-mixings. We expect different regimes to be interesting as well, for example if the mixings are not negligible one would have to define a different integrating out procedure. Moreover, it could happen that only some of the entropic fluctuations are heavy and others are light, in which case a partial integration of entropic modes could be relevant. We leave these exciting prospects for future works.

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Part III

Stochastic inflation: a non-perturbative treatment of large-scale fluctuations

Chapter 6

Single-field, slow-roll stochastic inflation

This chapter aims at introducing the stochastic formalism for single-field inflation in a technical way. Indeed, a more conceptual introduction containing the many relevant references on the topic, is presented in the introduction of the research article [5] presented in Sec. 7.2, and indeed in the following references shall be sparse. The main physical features of stochastic inflation are explained: effects of a time-dependent coarse-graining scale, the stochastic differential equation for the scalar field ϕ , called a Langevin equation, and how it translates into a partial differential equation for its Probability Density Function (PDF) $P(\phi; N)$, then how it enables one to compute observables like the power spectrum of the comoving curvature perturbation, as well as formal results of Quantum Field Theory (QFT) in curved spacetimes. The chapter finishes with an extension of the formalism in phase space, where not only the scalar field ϕ is dynamical, but also its canonically conjugate momentum π , and shows that one can still write Langevin equations for both of them, as well as a Fokker-Planck equation for their joint PDF $P(\phi, \pi; N)$.

6.1 Coarse-graining and the emergence of stochasticity

Roughly speaking, stochasticity can be understood as an effective description of a complex physical phenomenon whose details have been washed out. For example, the Brownian motion of the many molecules in a room accurately describes the statistics of these molecules, even though their actual positions and velocities are unknown, and even though the deterministic micro-physical interactions (they depend on the positions and velocities of all molecules so they can in principle be predicted) are treated as random forces. Of course, it is the aim of statistical physics to bridge the gap between these two descriptions, and to provide a micro-physical interpretation of the room temperature. More technically, the emergence of stochasticity is a consequence of coarse-graining a physical theory, *i.e.* of integrating out the small-scale physics and describing the large ones in an effective way. This is exactly the spirit of stochastic inflation: once the details

of the so-called UV modes are forgotten, and only their effects on the long-wavelength IR ones are taken into account, the description of the IR sector contains a random component whose statistical properties should depend on the small-scale physics. In the following, one shall focus entirely on the single-field stochastic description of inflation, and, once more, the reader willing to get a broader view on coarse-graining in statistical physics and in cosmology is referred to the introduction of Ref. [5] presented in Sec. 7.2.

6.1.1 A separation of scales

First, one shall try to get some intuition about the physics at hand in stochastic inflation. For this, one can look at Fig. 6.1, where relevant scales are represented. Actually, there is a single physical distance during inflation, which is the comoving Hubble radius $(aH)^{-1}$ and therefore must be used to define small and large scales. The idea being to describe the largest scales, called the IR sector of the theory, in a stochastic but classical way, the cut-off separating the UV from the IR sector should be chosen such that the IR fluctuations have well lost their quantum nature. And indeed, it is generally expected that when being stretched on super-horizon scales, cosmological fluctuations “classicalise” in the sense that their quantum description becomes irrelevant (this can be measured *e.g.* by the exponential decay of the ratio between the commutator and anti-commutator of the quantum operators at hand, on super-horizon scales). Therefore, the modes that are well above the horizon constitute the

$$\boxed{\text{(IR sector): } k \leq k_\sigma(N) = \sigma \times (aH)(N)}, \quad (6.1)$$

for which $k_\sigma(N)$ is a *time-dependent* UV cut-off. Note that the parameter $\sigma \ll 1$ is arbitrary and simply supposed to be small, so that the IR sector is composed only of modes that are well above the horizon. The time-dependence $(dk_\sigma/dN) \sim k_\sigma$ at first order in a slow-varying approximation is crucial because it results in the only UV-IR interactions of stochastic inflation: as time passes, more and more modes from the UV sector join the IR one, therefore making the set of large scales an open system, see Fig. 6.1. As one shall see soon, this continuous flow can indeed be interpreted as stochastic kicks that the IR sector receives, and whose statistical properties are set by the dynamics of the sub-Hubble perturbations during inflation.

6.1.2 Langevin equation: a stochastic differential equation

Now, one shall derive the stochastic differential equation verified by the IR part of the scalar field under the slow-roll approximation for which the usual background field verifies:

$$\frac{d\bar{\phi}}{dN} = -\frac{V_{,\phi}(\bar{\phi})}{3H^2}. \quad (6.2)$$

In this heuristic approach, the full field $\phi(N, \vec{x})$ with Fourier components $\tilde{\phi}_{\vec{k}}(N)$ (in the following, one omits the tilde) is simply split into an IR part $\varphi(N, \vec{x})$ and an UV one

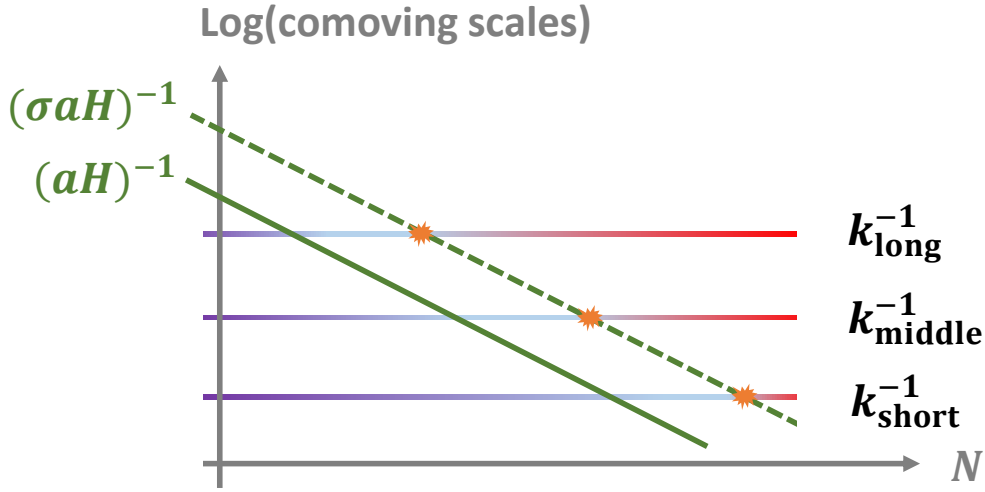


Figure 6.1: Relevant comoving scales for stochastic inflation: the comoving Hubble radius $(aH)^{-1}$ is decreasing because of the accelerated expansion of space, and therefore so is the comoving cut-off between UV and IR modes in real space, sometimes called the comoving σ -Hubble radius or σ -horizon, $k_{\sigma}^{-1} = (\sigma aH)^{-1} \gg (aH)^{-1}$ since $\sigma \ll 1$. Each given mode with comoving scale k^{-1} first begins its history deep in the horizon and in its Bunch-Davies vacuum as in the usual treatment of inflation, but after it has been stretched to super-horizon scales by the expansion of space, it joins the IR sector at a time $N_{\sigma}(k)$ such that $k_{\sigma}[N_{\sigma}(k)] = k$. The color gradient represents this evolution from UV (purple) to IR (red) and the orange dots denote the events at $[N_{\sigma}(k), k^{-1}]$ signaling that the corresponding mode is now considered as an IR one. Clearly in this picture, the IR sector is an open system receiving contributions from the UV one, but note that on the contrary the UV sector is not corrected by the IR dynamics.

$Q(N, \vec{x})$, as:

$$\begin{aligned}\phi(N, \vec{x}) &= \int \frac{d^3 \vec{k}}{(2\pi)^3} e^{i\vec{k} \cdot \vec{x}} \phi_{\vec{k}}(N) \\ &= \varphi(N, \vec{x}) + Q(N, \vec{x}) \quad \text{with} \quad \varphi(N, \vec{x}) = \int \frac{d^3 \vec{k}}{(2\pi)^3} e^{i\vec{k} \cdot \vec{x}} W\left(\frac{k}{k_\sigma(N)}\right) \phi_{\vec{k}}(N),\end{aligned}\tag{6.3}$$

where $W(\theta)$ is a window function such that:

$$W(u) \sim \begin{cases} 1 & \text{if } u \ll 1 \\ 0 & \text{if } u \gg 1 \end{cases}, \tag{6.4}$$

therefore effectively smearing out the short-wavelength modes. In practice, it is a common choice to take $W(u) = \theta(1 - u)$, where θ is the Heaviside step function, as it then results in a simple white noise as one shall see in the following. Note however, that a smoother window function would seem more reasonable and physically motivated, although therefore leading to a more complicated coloured noise [258]. Clearly, this approach is shaky and this IR/UV splitting is more carefully investigated in Sec. 7.2 in a path integral formalism. Equipped with these definitions, one notes that the derivative of φ contains two terms:

$$\frac{d\varphi}{dN} = \int \frac{d^3 \vec{k}}{(2\pi)^3} e^{i\vec{k} \cdot \vec{x}} \left\{ \frac{d}{dN} \left[W\left(\frac{k}{k_\sigma(N)}\right) \right] \phi_{\vec{k}}(N) + W\left(\frac{k}{k_\sigma(N)}\right) \frac{d\phi_{\vec{k}}(N)}{dN} \right\}, \tag{6.5}$$

where for W that is a step function,

$$\frac{d}{dN} \left[W\left(\frac{k}{k_\sigma(N)}\right) \right] = \frac{k}{k_\sigma} \delta[1 - k/k_\sigma(N)], \tag{6.6}$$

therefore showing that for such choice only the mode $k_\sigma(N)$ plays a new role at the time N compared to the usual case where σ is formally pushed to 0.

The stochastic formalism is mixing perturbative and non-perturbative statements, as in the following one treats φ as a fluctuation with possibly large amplitude but negligible spatial dependence, *i.e.* one neglects gradients of φ , while Q is supposed to be a small perturbation: the idea behind this scheme is that although the UV perturbations are small, their effects on the IR sector may accumulate over time to produce large inhomogeneities on cosmological scales. Therefore expanding the full field $\phi = \varphi + Q$ according to this scheme and replacing the derivatives of φ by Eq. (6.5), one finds in the slow-roll approximation:

$$\frac{d\varphi}{dN} = -\frac{V_{,\varphi}(\varphi)}{3H^2} + \int \frac{d^3 \vec{k}}{(2\pi)^3} e^{i\vec{k} \cdot \vec{x}} \left\{ \frac{d}{dN} \left[W\left(\frac{k}{k_\sigma(N)}\right) \right] \phi_{\vec{k}}(N) + \left[1 - W\left(\frac{k}{k_\sigma(N)}\right) \right] E_{Q,\vec{k}}^{\text{sr}}(N) \right\}, \tag{6.7}$$

where $E_{Q,\vec{k}}^{\text{sr}}(N)$ is the linear equation of motion verified by the Fourier space, first-order perturbation $\phi_{\vec{k}}(N)$ in slow-roll single-field inflation. In the following, it is simply

assumed to be identically vanishing in this heuristic approach: $E_{Q,\vec{k}}^{\text{sr}}(N) = 0$, meaning that the stochastic formalism does not affect the behaviour of the UV sector which behaves as the usual linear perturbations of the canonical approach. Again, this shall be better justified in the path integral approach of Sec. 7.2. The effective equation for the coarse-grained fluctuation φ may therefore be simplified to:

$$\frac{d\varphi}{dN} = -\frac{V_{,\varphi}(\varphi)}{3H^2} + \xi_Q. \quad (6.8)$$

This equation is called a Langevin equation because it contains both a deterministic drift derived from the potential, $-V_{,\varphi}(\varphi)/(3H^2)$, in a similar way as the background EoM, as well as a random diffusion ξ_Q defined as:

$$\xi_Q(x) = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}} \frac{d}{dN} \left[W \left(\frac{k}{k_\sigma(N)} \right) \right] \phi_{\vec{k}}(N). \quad (6.9)$$

As one shall see now, this second contribution may be interpreted as a random noise. Indeed, the mode function $\phi_{\vec{k}}(N)$ in its definition should rather be the quantum operator $\hat{\phi}_{\vec{k}}(N)$, evaluated at the wavenumber $|\vec{k}| = k_\sigma(N)$ due to the $\delta[1 - k/k_\sigma(N)]$ from the derivative of the step function that selects this mode only. Strictly speaking, ξ_Q should therefore be a quantum operator, and indeed one shall find that it is actually only defined at the level of its statistics. Decomposing $\hat{\phi}_{\vec{k}}(N)$ in the fundamental quantum oscillator and the corresponding mode function,

$$\hat{\phi}_{\vec{k}}(N) = \phi_{k_\sigma}(N) \hat{a}_{\vec{k}} + \phi_{k_\sigma}^*(N) \hat{a}_{-\vec{k}}^\dagger \quad (6.10)$$

and remembering that the mode function $\phi_k(N)$ converges, up to an irrelevant constant phase, to real values on super-horizon scales (and it is the case at the time N for the mode $k_\sigma(N)$ of interest here), one may actually write

$$\hat{\phi}_{\vec{k}}(N) = \phi_{k_\sigma}(N) \underbrace{\left(\hat{a}_{\vec{k}} + \hat{a}_{-\vec{k}}^\dagger \right)}_{b_{\vec{k}}} \quad (6.11)$$

where one forgot on purpose the hat on the “operator” $b_{\vec{k}}$ since it is then the only relevant one on super-horizon scales, and its quantum nature can be understood as lost: it commutes with all other operators, which are actually only itself.¹ But $b_{\vec{k}}$ inherits the statistical properties of the fundamental quantum oscillator described by the annihilation and creation operators, since it follows Gaussian statistics: $\langle b_{\vec{k}} \rangle = 0$, $\langle b_{\vec{k}} b_{\vec{k}'} \rangle = (2\pi)^3 \delta^{(3)}(\vec{k} + \vec{k}')$.

¹Of course, the quantum nature of the perturbations is not completely lost: the Heisenberg uncertainty principle should always hold and therefore the canonical commutations should be true even on super-horizon scales. And indeed, this information is encoded in the non-real dynamical part of the scalar field that was neglected in this treatment; it is actually exponentially decaying on super-horizon scales, but strictly speaking never vanishing. This can also be seen in the non-zero but quickly decreasing imaginary part of the field-momentum power spectrum $\mathcal{P}_{QP}$ where P is the linear canonical conjugate momentum of Q .

From this, a more accurate definition of the noise term ξ_Q can be given:

$$\xi_Q(x) = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}} \delta[1 - k/k_\sigma(N)] \phi_{k_\sigma}(N) b_{\vec{k}}, \quad (6.12)$$

which enables one to show that ξ_Q follows centered Gaussian statistics with

$$\begin{aligned} \langle \xi_Q(N, \vec{x}) \rangle &= 0, \\ \langle \xi_Q(N, \vec{x}) \xi_Q(N', \vec{x}') \rangle &= \delta(N - N') \text{sinc}(k_\sigma r) \mathcal{P}_Q(N, k_\sigma(N)), \end{aligned} \quad (6.13)$$

where $\text{sinc}(u) = \sin(u)/u$, $r = |\vec{x} - \vec{x}'|$ and $\mathcal{P}_Q$ is the dimensionless (in units of k but not of energy in general) power spectrum of the UV perturbations Q , evaluated at the common time $N = N'$ and for the mode $k_\sigma(N)$ associated with this particular time. The presence of the temporal delta function, $\delta(N - N')$, shows that the noise in this stochastic formalism is white, but remember that this is a consequence of the choice for the window function. Another consequence of this particular choice is the exact form of the spatial correlation $\text{sinc}(k_\sigma r)$, which may simply be understood as a function taking the value ~ 1 inside a sphere of radius $\sim k_\sigma^{-1}$ and vanishing outside of it. In practice, one wants first to know the time evolution of a given σ -Hubble patch, and then recollect the statistics of the various patches making up the observable universe, as shall be explained in Sec. 6.2, and therefore one may as a first approximation neglect the spatial dependence of the noises and simply look at the one-point (one-patch) statistics of φ in this patch p (after this equation, one will drop the index p for simplicity):

(Langevin equation for single-field, slow-roll, stochastic inflation):

$$\frac{d\varphi_p}{dN} = -\frac{V_{,\varphi}(\varphi_p)}{3H_p^2} + \sqrt{\mathcal{P}_Q^p(N, k_\sigma(N))} \times \xi_p, \quad \text{with} \quad \langle \xi_p(N) \xi_q(N') \rangle = \delta(N - N') \delta_{pq}.$$

(6.14)

Now an important question to address is the time and field dependence of the power spectrum at the coarse-graining scale, $\mathcal{P}_Q(N, k_\sigma(N))$. Indeed, qualitatively different regimes are reached depending on the physical assumptions that one makes about the value of the noise amplitude. Strictly speaking, and this is explained in further details in Sec. 7.2, the stochastic process at play during inflation is *non-Markovian*, meaning that the statistics of the noise at a given time N_0 when the field value is $\varphi_0 = \varphi(N_0)$ can not be expressed as a function of (N_0, φ_0) , but actually depends on the whole path that the stochastic process has followed for $N < N_0$, and therefore of the previous realisations of the random draws of the noise. Indeed, $\mathcal{P}_Q(N, k_\sigma(N))$ is found with the mode functions $Q(N, k)$ that are solutions of the usual linear equations of motion for perturbations at first order in single-field inflation, but in which the background functions such as H and φ are rigorously stochastic variables that must be computed at each time step depending on the actual realisation of the noise: thus, to compute the noise at the time N_0 , you first

need to give the realisations of the noise for $N < N_0$. In slow-roll, single-field inflation with a very flat potential such that quantum diffusion may eventually dominate over the classical drift and therefore make the stochastic formalism relevant, the power spectrum of the linear perturbations a few e -folds after horizon crossing (roughly $-\ln\sigma$ e -folds after horizon crossing for the mode $k = k_\sigma(N)$), at $N_\sigma(k)$, is known approximately and reads $\mathcal{P}_Q(N, k_\sigma(N)) = [H_{*(k_\sigma(N))}/(2\pi)]^2$ where $*(k_\sigma(N))$ means evaluated at horizon crossing for the mode $k_\sigma(N)$. From this expression, it is clear that the process is non-Markovian: the noise amplitude at the time N depends on the past value of H at a time roughly $N + \ln(\sigma)$.

To overcome this difficulty (non-Markovian processes are harder to handle analytically than Markovian ones, for example as one shall see a Markovian process can be studied with the analysis of its corresponding Fokker-Planck equation, while a non-Markovian one cannot), it is customary to take $H_* \rightarrow H(\varphi(N))$ as may be justified in a slow-varying approximation (remember that only $-\ln(\sigma)$ separate these two times). Then the process is Markovian because the noise amplitude at a time N_0 , $H(\varphi(N_0))$ only depends on the value of the stochastic process $\varphi_0 = \varphi(N_0)$ *at the same time*, as can be seen from the Friedmann equation. Therefore in each patch p , one may write

$$\begin{array}{c} \text{(Stochastic inflation with multiplicative noise):} \\ \frac{d\varphi_p}{dN} = -\frac{V_{,\varphi}(\varphi_p)}{3H(\varphi_p)^2} + \frac{H(\varphi_p)}{2\pi}\xi_p, \text{ with } \langle \xi_p(N)\xi_q(N') \rangle = \delta(N - N')\delta_{pq}, \end{array} \quad (6.15)$$

where the explicit field-dependent noise amplitude is called *multiplicative*. This is the most common setup of stochastic inflation, for which the details of the discretisation scheme (at which time $N_i^\alpha = N_i + \alpha\Delta N$ exactly should be evaluated the stochastic variable φ in the noise amplitude, when evolving φ from the time step N_i to $N_{i+1} = N_i + \Delta N$? this choice of $\alpha \in [0, 1]$ does not matter for ordinary differential equations, but it does for stochastic differential equations with multiplicative noise) are crucial as explained in the following, Chap. 7.

But this formalism can also be applied for a massless test scalar field in a de Sitter spacetime (such as a sub-dominant fluctuating field during inflation), which simplifies the description since then the noise amplitude $H(\varphi(N)) \rightarrow H(N)$ is a given function of time and does not depend on the field amplitude φ at all, a case described as *additive* noise and for which the details of the discretisation scheme do not matter:

$$\begin{array}{c} \text{(Stochastic inflation with additive noise):} \\ \frac{d\varphi_p}{dN} = -\frac{V_{,\varphi}(\varphi_p)}{3H(N)^2} + \frac{H(N)}{2\pi}\xi_p, \text{ with } \langle \xi_p(N)\xi_q(N') \rangle = \delta(N - N')\delta_{pq}. \end{array} \quad (6.16)$$

To go even further in the simplification, one may consider the particular case of a test scalar field in a perfect de Sitter spacetime, provided the replacement $H(N) \rightarrow H_0$

that renders the noise amplitude constant,

(Stochastic formalism for a test scalar field in de Sitter):

$$\frac{d\varphi_p}{dN} = -\frac{V_{,\varphi}(\varphi_p)}{3H_0^2} + \frac{H_0}{2\pi}\xi_p, \text{ with } \langle \xi_p(N)\xi_q(N') \rangle = \delta(N - N')\delta_{pq}. \quad (6.17)$$

Next, it shall be extended to a phase-space dynamics which may be relevant away from the slow-roll limit, as well as to the multifield case with non-canonical kinetic terms and in phase space, in Chapter 7. But first, one shall turn to the physical outputs of this simplest stochastic formalism.

6.2 Correlation functions

Stochastic inflation is interesting because it enables one to derive quite straightforwardly relevant statistical information about the IR fluctuation φ which may be large and therefore may encode non-perturbative results. In the following, one shall see how the Langevin equation corresponds to a so-called Fokker-Planck equation for the PDF of φ , which itself enables one to compute the correlation functions of φ as well as the statistics of the comoving curvature perturbation.

6.2.1 Fokker-Planck equation and test scalar fields in de Sitter

The Langevin Eq. (6.15) describes the random evolution of φ when the process can be considered as Markovian. In order to find the statistical properties of φ , one may therefore simply solve it many times and compute these statistics with ensemble averages (this actually seems to be the only possibility in the non-Markovian case). However, there is a way to possibly push further the analytical treatment. One first defines $P(\varphi; N)$ the one-point PDF of φ , which may be interpreted as the transition probability from a given point $(\varphi_{\text{ini}}; N_{\text{ini}})$ to the other one $(\varphi; N)$: $P(\varphi; N | \varphi_{\text{ini}}; N_{\text{ini}})$. It is then standard to show (see *e.g.* Ref. [259]) from the Langevin equation (6.14) that:

$$\frac{\partial P}{\partial N} = \frac{\partial}{\partial \varphi} \left[\left(\frac{V_{,\varphi}(\varphi)}{3H(\varphi)^2} - \alpha \frac{H(\varphi)}{2\pi} \frac{\partial}{\partial \varphi} \frac{H(\varphi)}{2\pi} \right) P \right] + \frac{1}{2} \frac{\partial^2}{\partial \varphi^2} \left[\left(\frac{H(\varphi)}{2\pi} \right)^2 P \right], \quad (6.18)$$

which is a well-known partial differential equation: the convection-diffusion equation for the PDF P , where convection is due to the deterministic drift derived from the potential (plus a noise-induced drift for $\alpha \neq 0$), and where diffusion is the consequence of the random noise.

Although it has been claimed that the choice of discretisation α was irrelevant in stochastic inflation, it has been shown in this thesis that it was not the case, see Refs. [4, 5] and Chap. 7. First, note the presence of the *noise-induced drift* $\propto \alpha$ for any time discretisation that is different from the Itô, $\alpha = 0$, one, and that necessitates to find a square-root of the noise amplitude. Here in the single-field case it was trivial (and

unique) to find the square-root of $[H/(2\pi)]^2$, but in more complex multifield situations, there is an infinite number of possible square-roots for the noise amplitude matrix $\langle \xi_Q^I \xi_Q^J \rangle$, and the noise-induced drift depends on the choice of such square root. This argument seems to indicate that the Itô prescription, the only one avoiding the need to define a square-root of the noise amplitude, should be used, but actually as it is presented, the stochastic formalism for inflation is not covariant under field redefinitions $\varphi \rightarrow \tilde{\varphi}(\varphi)$, *even in the single-field case*, except if the discretisation scheme is chosen to be the Stratonovich, $\alpha = 1/2$, one. Indeed, Itô calculus shows that the standard rule for the derivative of composite function does not hold any more, hence general covariance is lost if no extra ingredients are added in order to define Itô-covariant derivatives [5]. However, we showed [4] that the two prescriptions, provided one does not make a field redefinition in the Itô one, were leading to the same predictions in the single-field case to a high level of accuracy (the difference between the two being $\propto v = V/M_{\text{Pl}}^4 \ll 1$ by consistency of the semi-classical approach), although crucially this is not the case in multifield inflation.

Famously, the convection-diffusion equation cannot be solved exactly (and even proves to be quite challenging to solve numerically), but the Fokker-Planck equation (6.18) can still be used to derive results that are either perturbative, or only valid in given regimes. In the following, one focuses on the simpler, maybe formal but still interesting, case of a test scalar field in de Sitter spacetime, $H(\varphi) \rightarrow H_0$. As a warm-up, the final equilibrium distribution may be inferred by setting $\partial_N P = 0$ and therefore reducing the problem to an ordinary differential equation for $P_{\text{eq}}(\varphi) = \lim_{N \rightarrow \infty} P(\varphi, N)$ which can be solved and gives [94]:²

$$P_{\text{eq}}(\varphi) = P_0 \times \exp \left[-\frac{8\pi^2 V(\varphi)}{3H_0^4} \right], \quad (6.19)$$

where P_0 is simply a normalisation constant such that $\int d\varphi P_{\text{eq}}(\varphi) = 1$. This is a result which is clearly non-perturbative and that could not have been predicted from the

²Although requiring slightly more work, the equilibrium PDF $P_{\text{eq}}(\varphi)$ for the inflaton, in which case the Hubble parameter is a function of φ , can still be found. Indeed, one should now replace $H(\varphi)$ by its value according to the Friedmann equation, that is $H^2(\varphi) \approx V(\varphi)/(3H^2 M_{\text{Pl}}^2)$ at zeroth order in slow-roll, which then yields a new differential equation for the variable VP_{eq} :

$$\frac{1}{VP_{\text{eq}}} \frac{\partial (VP_{\text{eq}})}{\partial \varphi} = \left(\alpha \frac{V_{,\varphi}}{V} - 24\pi^2 M_{\text{Pl}}^4 \frac{V_{,\varphi}}{V^2} \right),$$

where the noise-induced drift was kept. Defining a dimensionless potential shape function $v(\varphi) = V(\varphi)/(24\pi^2 M_{\text{Pl}}^4)$, one finds the equilibrium solution, with $P_{0,\alpha}$ a scheme-dependent constant enforcing normalisation of the PDF:

$$P_{\text{eq}}(\varphi) = \frac{P_{0,\alpha}}{[v(\varphi)]^{1-\alpha}} e^{\frac{1}{v(\varphi)}}.$$

Note that the $1/v(\varphi)$ behaviour of the argument of the exponential for the inflaton PDF is very different from the one of a test scalar field in de Sitter, moreover it does not seem possible to retrieve the former from the latter, as even taking formally $3H_0^4 \rightarrow V^2/(3M_{\text{Pl}}^4)$ would give a PDF $\propto \exp[-1/v(\varphi)]$ with a wrong sign in the argument of the exponential and without the field-dependent pre-exponential factor (without even talking about the α -dependence).

canonical treatment of inflation where the scalar field is divided into a homogeneous background and small perturbations. If the scalar potential is quadratic, $V(\varphi) = m^2\varphi^2/2$, then the equilibrium PDF of φ is simply a Gaussian with zero mean and standard deviation $\sigma = \sqrt{3/2 H_0^2/(2\pi m)}$, but otherwise it is not the case (at all). But the time necessary to reach equilibrium may be very large, and in the idea that de Sitter space-time could approximate the inflationary universe with a very light dynamical scalar field, inflation may stop well before equilibrium is reached, and therefore the equilibrium solution may actually be irrelevant for cosmological purposes.

In order to find time-dependent statements, one can first derive the following transport equations for the correlation functions of φ , since $\langle\varphi^n\rangle(N) = \int d\varphi \varphi^n P(\varphi; N)$:

$$\forall n \in \mathbb{N}, \quad \frac{d\langle\varphi^n\rangle}{dN} = -\frac{n}{3H_0^2} \langle\varphi^{n-1} V_{,\varphi}(\varphi)\rangle + \frac{H_0^2}{8\pi^2} n(n-1) \langle\varphi^{n-2}\rangle, \quad (6.20)$$

which are now ordinary differential equations again, and where one can assume the simple initial conditions $\langle\varphi^n\rangle(N_{\text{ini}} = 0) = 0$. The situation is then different depending on the form of the scalar potential. Indeed, for a potential that is a quadratic polynomial, the set of differential equations is closed: to solve for $\langle\varphi^n\rangle$ it is sufficient to know the lower order correlations $\langle\varphi^k\rangle$ with $k \leq n-1$. In the example of a free massive field, $V(\varphi) = m^2\varphi^2/2$, one simply finds:

$$\langle\varphi\rangle(N) = 0, \quad \langle\varphi^2\rangle(N) = \underbrace{\frac{3H_0^4}{8\pi^2 m^2}}_{\sigma^2} \left[1 - \exp\left(-\frac{2m^2}{3H_0^2} N\right) \right], \quad \langle\varphi^3\rangle(N) = 0, \quad \dots, \quad (6.21)$$

from which it is clear that a typical time scale to reach the Gaussian distribution is $N_c = 3H_0^2/(2m^2)$ (corresponding in cosmic time t with $dN = H_0 dt$, to a time scale $t_c = 3H_0/(2m^2)$), which is indeed large in the regime of validity of the stochastic formalism that applies for very light fields: $m \ll H_0$ and therefore $N_c \gg 1$, meaning that equilibrium takes a long time to be reached. Some results may also be derived in interacting theories, but they are harder to get and intrinsically perturbative: for concreteness, one assumes in the following a simple but interacting theory: $V(\varphi) = \lambda\varphi^4$. Then it is easy to show that the differential equation verified by $\langle\varphi^n\rangle$ depends on higher-order correlations $\langle\varphi^k\rangle$ for $k > n$, and therefore the set of transport equations is not closed. A possible perturbative analysis consists in developing each correlation function in series of N , as $\langle\varphi^n\rangle = \sum_{m=0}^{\infty} A_m^n N^m$ which enables one to close the set of equations at finite but arbitrary order m and therefore to find the correlation functions at this arbitrary order [95, 97]. Unfortunately, the series are typically divergent, and only the first terms may be trusted in a perturbative way. For example, one can show in the $\lambda\varphi^4$ -case that:

$$\langle\varphi\rangle(N) = 0, \quad \langle\varphi^2\rangle(N) = \frac{H_0^2 N}{4\pi^2} \left[1 - \frac{\lambda N^2}{6\pi^2} + \dots \right], \quad \langle\varphi^3\rangle(N) = 0, \quad \dots, \quad (6.22)$$

where the first non-trivial correction of $\langle\varphi^2\rangle$ in λ indeed matches much more involved perturbative computations of Quantum Field Theory in de Sitter spacetime [260].

6.2.2 Cosmological observables in stochastic inflation

After these interesting but rather formal results, one shall focus in the following on the derivation of statistical properties of the observable comoving curvature perturbation at the end of inflation in a quasi-de Sitter spacetime.

The stochastic δN -formalism

The δN -formalism was already presented in Sec. 5.1.1 in the context of perturbation theory, in order to compute the evolution of the statistics of the comoving curvature perturbation on large scales. This is precisely what is required for the stochastic formalism to become predictive, as indeed so far one has only studied the statistics of φ which are not observable *per se*. The stochastic picture of the δN -formalism is very similar to the classical one: it appeals to the separate universe approach in order to treat each causally disconnected patch independently. But now, even with identical initial conditions, the value of N between an initial time slice defined with spatially flat hypersurfaces, and a final time slice using constant energy density hypersurfaces, depends upon the sample path *i.e.* the random draws of the noise, and becomes itself a stochastic variable. Hence, one can not compare *the* value of δN_p in different patches p , but only their statistics. From given initial conditions, *i.e.* for a given patch, at the time N_{ini} corresponding to horizon exit for the mode k of interest, the mean number of required e -folds to reach the final slice is $\langle N(k) \rangle$, a time at which the wavenumber exiting the horizon is k_{end} , therefore with $\langle N(k) \rangle \approx \ln(k_{\text{end}}/k)$ at zeroth order in slow-roll. An important point is that $N(k)$ depends on the patch under consideration, and therefore its statistics encode the large-scale fluctuations in the universe. More precisely, its higher-order cumulants measure the dispersion of the PDF for $N(k)$ and can be used to compute the observable power spectrum and local bispectrum of $\mathcal{R} \simeq \delta N$ on large scales [261, 262]:

$$P_{\mathcal{R}}(k) = \left. \frac{d \langle \delta N^2 \rangle}{d \langle N \rangle} \right|_{\langle N \rangle = \ln(k_{\text{end}}/k)} \quad \text{and} \quad B_{\mathcal{R}}^{\text{loc}}(k) = \frac{1}{2} \left. \frac{d^2 \langle \delta N^3 \rangle}{d \langle N \rangle^2} \right|_{\langle N \rangle = \ln(k_{\text{end}}/k)}, \quad (6.23)$$

where the different averaged histories for each patch p should be compared in order to calculate the variation with respect to $\langle N \rangle$ that depends on the initial conditions of the corresponding patch. This provides one with a program to numerically solve for the power spectrum and local bispectrum:

- The universe is separated in different patches p that each have different initial conditions, like $\varphi_p(N_{\text{ini}})$ in the single-field, slow-roll picture.
- For each patch, solve many times the Langevin equations until the final time slice is attained, thus enabling to compute the statistics of N_p in this patch: $\langle N_p \rangle$, $\langle \delta N_p^2 \rangle$, $\langle \delta N_p^3 \rangle$.
- Compute (still numerically) how $\langle \delta N_p^2 \rangle$ and $\langle \delta N_p^3 \rangle$ vary depending on the initial conditions (encoded in $\langle N_p \rangle$).

Note that the initial conditions φ_p can be chosen at will but such that they faithfully represent the $\langle N \rangle$ line around the point $\ln(k_{\text{end}}/k)$ for the mode k of interest.

But fortunately, it is also possible to derive analytical predictions for the observable comoving curvature perturbation with the stochastic formalism, although it requires slightly more elaborate tools borrowed from studies of the Brownian motion.

First passage time and the adjoint Fokker-Planck equation

The idea is the following: the Fokker-Planck equation dictates the evolution of the transition probability $P(\varphi; N | \varphi_{\text{ini}}; N_{\text{ini}})$ from an initial state $(\varphi_{\text{ini}}; N_{\text{ini}})$ to a final one $(\varphi; N)$, but to compute the statistics of $\mathcal{R} \sim \delta N$ it seems that one is rather interested in the variation of this transition probability reaching a fixed final slice $(\varphi; N)$ with respect to the initial conditions $(\varphi_{\text{ini}}; N_{\text{ini}})$ [86, 262]. This question is in some sense *dual* to the previous one and indeed one can define an adjoint Fokker-Planck operator $\mathcal{L}_{\text{FP}}^\dagger$ acting on the initial conditions rather than on the final ones, and finds in the context of single-field slow-roll inflation:

$$\begin{aligned} \frac{\partial P}{\partial N_{\text{ini}}} &= -\mathcal{L}_{\text{FP}}^\dagger(\varphi_{\text{ini}}) \cdot P, \text{ with} \\ \mathcal{L}_{\text{FP}}^\dagger(\varphi_{\text{ini}}) &= M_{\text{Pl}}^2 \left[- \left(\frac{v_{,\varphi}(\varphi_{\text{ini}})}{v(\varphi_{\text{ini}})} - \alpha v_{,\varphi}(\varphi_{\text{ini}}) \right) \frac{\partial(\cdot)}{\partial \varphi_{\text{ini}}} + v(\varphi_{\text{ini}}) \frac{\partial^2(\cdot)}{\partial \varphi_{\text{ini}}^2} \right], \end{aligned} \quad (6.24)$$

and where we defined the dimensionless potential shape function

$$v(\varphi) = \frac{V(\varphi)}{24\pi^2 M_{\text{Pl}}^4}, \quad (6.25)$$

which must be much smaller than unity in order to remain in the regime of validity of the semi-classical approach to quantum gravity. This equation can be used to find transport equations for the moments of the variable N (and therefore for its characteristic function), in a way that is very analogous to the one that was used to derive transport equations for the moments of φ with the Fokker-Planck operator:

$$\mathcal{L}_{\text{FP}}^\dagger(\varphi_{\text{ini}}) \cdot \langle N^n \rangle(\varphi_{\text{ini}}) = -n \langle N^{n-1} \rangle(\varphi_{\text{ini}}). \quad (6.26)$$

These ordinary differential equations may now be solved.

The first moments of N were first computed in Ref. [262] in the Itô scheme, and later extended for any prescription α in Ref. [4], see Sec. 7.1. Note that analytical results may be derived in a perturbative manner that shall be defined in the following, but that numerical ones can be found non-perturbatively. First, a generic recurrence formula for any n can be shown:

$$\langle N^n \rangle(\varphi_{\text{ini}}) = \frac{n}{M_{\text{Pl}}^2} \int_{\varphi_{\text{end}}}^{\varphi_{\text{ini}}} d\varphi \int_{\varphi}^{\tilde{\varphi}_n} d\tilde{\varphi} \frac{\langle N^{n-1} \rangle(\tilde{\varphi})}{v^\alpha(\varphi) v^{1-\alpha}(\tilde{\varphi})} \mathcal{K}(\varphi, \tilde{\varphi}), \quad (6.27)$$

with the kernel $\mathcal{K}(\varphi, \tilde{\varphi}) = \exp[v^{-1}(\tilde{\varphi}) - v^{-1}(\varphi)]$ that is very peaked on $\tilde{\varphi} \sim \varphi$ because the dummy variables are ordered such that $v(\varphi) < v(\tilde{\varphi}) \ll 1$, and with $\tilde{\varphi}_n$ boundary conditions that should in principle be carefully defined and studied [262], but will however disappear in practice in the following.

Perturbative expansion of the first moments: duration of inflation, power spectrum and bispectrum

It is then straightforward to compute the average duration between N_{ini} and the final time slice provided the initial conditions φ_{ini} :

$$\begin{aligned}\langle N \rangle (\varphi_{\text{ini}}) &= \frac{1}{M_{\text{Pl}}^2} \int_{\varphi_{\text{end}}}^{\varphi_{\text{ini}}} d\varphi \int_{\varphi}^{\tilde{\varphi}^1} d\tilde{\varphi} \frac{1}{v^\alpha(\varphi) v^{1-\alpha}(\tilde{\varphi})} \mathcal{K}(\varphi, \tilde{\varphi}) \\ &\simeq \frac{1}{M_{\text{Pl}}^2} \int_{\varphi_{\text{end}}}^{\varphi_{\text{ini}}} d\varphi \frac{v}{v_{,\varphi}} [1 + (1 + \alpha)v - \eta_{\text{cl}} + \dots],\end{aligned}\quad (6.28)$$

with $\eta_{\text{cl}} = v^2 v_{,\varphi\varphi}/v_{,\varphi}^2$ (note the small, $\propto v^2$, difference of notation compared to Ref. [262] where this quantity is rather $|v^2 - \eta_{\text{cl}}|$ in the notations of this thesis) being a dimensionless measure of the expected size of stochastic effects that have been supposed to be small in order to find the second line: the dots stand for corrections that are higher-order in v or η_{cl} as well as in similar parameters measuring the strength of the stochastic effects. The slow-roll approximation at leading order has also been used. Note that the first term in the brackets, 1, gives the same duration of inflation as the one computed with the usual perturbation theory at the level of a homogeneous background and assuming slow-roll, see Sec. 3.2.1 and Eq. (3.19). The second term in the brackets, $(1 + \alpha)v$ is always negligible as one should remember from the requirement to work in the perturbative regime of quantum gravity, *i.e.* that $V(\varphi)/M_{\text{Pl}}^4 \ll 1$: this shows explicitly that the choice of discretisation scheme does not affect the average duration of inflation in the single-field case. The third term was supposed to be small and provides a first non-trivial stochastic correction to the duration of inflation: interestingly, even though the random noise has zero mean, it leaves an imprint even in the mean number of e -folds of inflation. This is a well-known non-linear effect: diffusion eventually results in a drift (independently of the noise-induced drift from a non-zero value of α).

Moreover, the second moment of δN is found as [4]:

$$\begin{aligned}\langle \delta N^2 \rangle (\varphi_{\text{ini}}) &= 2 \int_{\varphi_{\text{end}}}^{\varphi_{\text{ini}}} d\varphi \int_{\varphi}^{\tilde{\varphi}^2} d\tilde{\varphi} \left(\frac{v(\tilde{\varphi})}{v(\varphi)} \right)^\alpha \left[\frac{\partial \langle N \rangle (\tilde{\varphi})}{\partial \tilde{\varphi}} \right]^2 \mathcal{K}(\varphi, \tilde{\varphi}) \\ &\simeq \frac{1}{M_{\text{Pl}}^4} \int_{\varphi_{\text{end}}}^{\varphi_{\text{ini}}} d\varphi \frac{v^4}{v_{,\varphi}^3} [1 + (6 + 3\alpha)v - 5\eta_{\text{cl}} + \dots],\end{aligned}\quad (6.29)$$

where again a slow-roll, small-stochastic-effects, approximation has been used to find the second line. Now the power spectrum may be computed from $\langle N \rangle$ and $\langle \delta N^2 \rangle$, and reads:

$$\mathcal{P}_{\mathcal{R}} = \frac{2}{M_{\text{Pl}}^2} \frac{v^3}{v_{,\varphi}^2} [1 + (5 + 2\alpha)v - 4\eta_{\text{cl}} + \dots] \quad (6.30)$$

Once more, one can see that the first term corresponds to the slow-roll power spectrum in the classical picture, $\mathcal{P}_{\mathcal{R}}^{\text{cl}} = v/\epsilon_V \approx H^2/(8\pi^2 \epsilon M_{\text{Pl}}^2)$, see Sec. 3.2.2 and Eq. (3.61), while the second term $\propto v$ is always negligible independently of the discretisation scheme α , and the third term is the first non-trivial stochastic correction. The same scheme

is found for the scalar spectral index n_s that can be derived from the power spectrum: classical result n_s^{cl} , plus negligible corrections $\propto v$ with an α -dependent coefficient, plus the first stochastic correction:

$$n_s = n_s^{\text{cl}} - [2(2 + \alpha)\epsilon_V - 3\eta_V]v - 6\eta_V\eta_{\text{cl}} + 8\epsilon_V\xi_{\text{cl}} + \dots, \quad (6.31)$$

where $\xi_{\text{cl}} = v^3 v_{,\varphi\varphi\varphi}/v_{,\varphi}^3$ is one of the other dimensionless parameters measuring the size of the stochastic effects, again supposed to be small here, and ϵ_V, η_V are the slow-roll potential parameters.

For completeness, one simply quotes the result of Ref. [262] for the local bispectrum parameter (in the Itô, $\alpha = 0$ scheme):

$$f_{\text{NL}}^{\text{loc}} \simeq \frac{5}{12} [6\epsilon_V - 2\eta_V + v(25\epsilon_V - 17\eta_V) + 12\eta_V\eta_{\text{cl}} - 10\epsilon_V\xi_{\text{cl}} + \dots], \quad (6.32)$$

which again displays the same structure: one recognizes the classical result $f_{\text{NL,cl}}^{\text{loc}} \simeq 5/12(1 - n_s^{\text{cl}})$, see Sec. 5.1.2 and Eq. (5.65), plus small $\mathcal{O}(v)$ corrections as well as the first non-trivial stochastic corrections in η_{cl} and ξ_{cl} . It is interesting to notice that, even when taking the $v \rightarrow 0$ limit, the stochastic corrections $\eta_{\text{cl}}, \xi_{\text{cl}}$ seem to violate this single-field consistency condition between $f_{\text{NL}}^{\text{loc}}$ and $(1 - n_s)$, as one finds:

$$f_{\text{NL}}^{\text{loc}} \simeq \frac{5}{12} (1 - n_s + 6\eta_V\eta_{\text{cl}} - 2\epsilon_V\xi_{\text{cl}}), \quad (6.33)$$

showing that potentially large local non-Gaussianities may arise in single-field contexts away from the classical regime, where stochastic effects are largely dominant and either η_{cl} or ξ_{cl} is very large. However, from the definition of η_{cl} one finds that

$$\eta_{\text{cl}} \simeq \mathcal{P}_{\mathcal{R}}^{\text{cl}} \left(\epsilon - \frac{\eta}{4} \right), \quad (6.34)$$

thus showing that it must be small for the cosmological scales in the CMB, since one has there $\mathcal{P}_{\mathcal{R}}(k_{\text{pivot}}) = A_s = 2.10 \times 10^{-9}$. A similar reasoning stands for ξ_{cl} and stochastic effects in general must be small for the largest observable scales. However, there could be large stochastic effects (and therefore large local non-Gaussianities) for smaller scales of astrophysical relevance, such as the ones that may collapse to form Primordial Black Holes, but this is a whole other topic of research since then the whole PDF of $\mathcal{R}$, and not just the first moments, should be computed in real space.

Note that in this thesis, see Sec. 7.1 and Ref. [4], the first moments $\langle N \rangle$ and $\langle \delta N^2 \rangle$ have been computed numerically for a benchmark model (hilltop) of single-field stochastic inflation, enabling to extend the analysis beyond a perturbative stochastic regime, where $\eta_{\text{cl}}, \xi_{\text{cl}}$ may be much larger than unity. One of the interesting findings there was that even when stochastic effects are large, the effect of choosing different α prescriptions was small.

In the next chapter, Chapter 7, one shall see how to extend the simplest stochastic formalism for single-field, slow-roll inflation, used here to explain the concepts and main tools of stochastic inflation, to a full phase-space dynamics beyond the slow-roll approximation, and to multifield models of inflation including the ones with non-canonical kinetic interactions.

Chapter 7

Multifield stochastic inflation: a path to the discretisation ambiguity and its resolution

This chapter proposes an extension of the stochastic formalism to the more general case of multifield inflation with non-canonical kinetic terms, therefore enabling to investigate the effects of kinetic interactions in a non-perturbative way. Despite its technical appearance, this program has not merely consisted in writing the Langevin equations of single-field stochastic inflation with more field-space indices. Indeed, by working in a higher-dimensional field space where field reparameterisations are ubiquitous, we have uncovered a generic ambiguity in the stochastic formalism for inflation, that is even present in the single-field case and that stems from the very discrete nature of stochastic differential equations. This is explained in Sec. 7.1 with the article where we first understood the presence of these inflationary stochastic anomalies after having derived in the usual way the Langevin equations in phase space, though for the first time in the context of multifield inflation and curved internal space. This article was selected by the committee of the peer-reviewed journal *Classical and Quantum Gravity* as one of its 2019-2020 Highlights. But at that time, the ambiguity remained, and it is only after a long and difficult work of two years that we eventually understood how to solve it, and it is the purpose of Sec. 7.2 to explain this. The article that is reproduced there first contains a long introduction to stochastic inflation in general and a pedagogical review of the inflationary stochastic anomalies, then shows how to avoid any ambiguity by investigating the very quantum nature of the sub-Hubble perturbations that uniquely fixes the frame in which equations should be phrased, and proposes a derivation of the multifield Langevin equations with the use of the Schwinger-Keldysh formalism as well as a new multifield approximation for the noise statistics in the curved field-space case.

7.1 Inflationary stochastic anomalies, or the discretisation ambiguity (article)

In this section, Ref. [4],

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INFLATIONARY STOCHASTIC ANOMALIES,
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is reproduced.

We begin by explaining the fundamental discrete nature of Stochastic Differential Equations (SDE), and the fact that the choice of time discretisation, amongst which the pre-point, Itô one, and the mid-point, Stratonovich one, are most popular, must come from a different physical input than the Langevin equations themselves, and that the solution of these equations explicitly depends on such a choice, in striking contrast to ordinary differential equations. This is a well-known fact in statistical physics, that we revisited in the context of multifield stochastic inflation since it brings a few conceptual issues.

We indeed remind that if the Itô prescription is used, the standard chain rule for the derivative of composite functions must be corrected, which therefore results in a breaking of the covariance of the Langevin equations in the context of stochastic inflation, under a reparameterisation of the fields' coordinates. This conceptual issue is exemplified both at the level of the Langevin equations themselves, but also at the one of the corresponding Fokker-Planck equation that may be derived under the Markovian assumption and that explicitly depends on the choice of time discretisation. On the other hand, it is shown that the Stratonovich prescription, although being the only choice leading to a covariant description of the physics, which is clearly a desirable property of any physical theory, results in an ambiguity in the choice of the basis in which diagonalising of the noise matrix; an issue that is shared by all prescriptions... but the Itô one! It therefore seems that all stochastic inflationary formalisms are plagued by this same conceptual ambiguity, and we show that the numerical difference between the Itô and the Stratonovich choices can be arbitrarily large in multifield inflation, although always remaining negligible for single-field inflation in the regime of validity of stochastic inflation.

Assuming that the Stratonovich is correct and that the ambiguity in the choice of a basis for diagonalising the noise matrix has been resolved, we also infer important new results from this stochastic formalism, such as the phase-space multifield Fokker-Planck equation or its slow-roll version that enables us to compute the time evolution of correlation functions in two-field models with kinetic interactions in de Sitter spacetime, therefore extending previously known perturbative and non-perturbative Quantum Field Theory results, to a curved field space. As an example of such interesting results, I chose to reproduce here the first terms of a perturbative double expansion in λN^2 and $(H_0/M)^2 \times N$, of the one-point and two-point functions of a scalar field ϕ in de Sitter spacetime with Hubble constant H_0 , that is both self-interacting with a potential

$V(\phi) = \lambda\phi^4$ and has kinetic interactions with a second scalar field ψ , as described by the hyperbolic field-space metric $G_{\phi\phi} = 1$, $G_{\phi\psi} = G_{\psi\phi} = 0$, $G_{\psi\psi} = e^{-2\phi/M}$:

$$\langle\phi(N)\rangle = -\frac{H_0^2 N}{8\pi^2 M} \left[1 - \frac{\lambda N^2}{12\pi^2} - \frac{\lambda H_0^2 N^3}{768\pi^4 M^2} + \dots \right], \quad (7.1)$$

$$\langle\phi^2(N)\rangle = \frac{H_0^2 N}{4\pi^2} \left[1 + \frac{H_0^2 N}{16\pi^2 M^2} - \frac{\lambda N^2}{6\pi^2} - \frac{7\lambda H_0^2 N^3}{384\pi^4 M^2} + \dots \right], \quad (7.2)$$

which therefore generalises the single-field result shown in Eq. 6.22 to the two-field case with non-trivial kinetic interactions. Note interestingly that the one-point function is non-vanishing only if the field space has a finite curvature M , since in the flat-space limit, $M \rightarrow \infty$, it gives zero. Moreover, the secular divergence of these perturbative expansions is clearly affected by these kinetic interactions with another scalar field. It would be exciting to compare them to exact QFT computations in de Sitter space, which have not been done yet in this kind of models with derivative couplings. The equilibrium distribution of ϕ is also shown in the article and deviations from the single-field case are explicated.

The original article as published in CQG is now displayed. Regarding notation, they should be easy to understand, ϕ^I are the scalar fields and π_I are their linear canonical conjugate momenta rescaled by a^3 , but the reader's attention is drawn to the diverse definitions of covariant derivatives, both in field space and in phase space.

Letter

Inflationary stochastic anomalies

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Abstract

The stochastic approach aims at describing the long-wavelength part of quantum fields during inflation by a classical stochastic theory. It is usually formulated in terms of Langevin equations, giving rise to a Fokker–Planck equation for the probability distribution function of the fields, and possibly their momenta. The link between these two descriptions is ambiguous in general, as it depends on an implicit discretisation procedure, the two prominent ones being the Itô and Stratonovich prescriptions. Here we show that the requirement of general covariance under field redefinitions is verified only in the latter case, however at the expense of introducing spurious ‘frame’ dependences. This stochastic anomaly disappears when there is only one source of stochasticity, like in slow-roll single-field inflation, but manifests itself when taking into account the full phase space, or in the presence of multiple fields. Despite these difficulties, we use physical arguments to write down a covariant Fokker–Planck equation that describes the diffusion of light scalar fields in non-linear sigma models in the overdamped limit. We apply it to test scalar fields in de Sitter space and show that some statistical properties of a class of two-field models with derivative interactions can be reproduced by using a correspondence with a single-field model endowed with an effective potential. We also present explicit results in a simple extension of the single-field $\lambda\phi^4$ theory to a hyperbolic field space geometry. The difficulties we describe seem to be the stochastic counterparts of the notoriously difficult problem of maintaining general covariance in quantum theories, and the related choices of operator ordering and path-integral constructions. Our work thus opens new avenues of research at the crossroad between cosmology, statistical physics, and quantum field theory.

Keywords: inflation, quantum fields in curved spacetime, anomalies, stochastic processes, nonlinear sigma model

(Some figures may appear in colour only in the online journal)

Introduction

The theory of cosmological inflation can boast from a spectacular success to explain the patterns observed in the cosmic microwave background anisotropies [1, 2]. According to it, cosmological fluctuations originate from microscopic quantum fluctuations stretched to cosmological scales. This paradigm is therefore deeply rooted both in quantum field theory (QFT) and in general relativity. However, in its conventional formulation, the geometry of spacetime and the fields active during inflation are split between an homogeneous background, obeying classical equations of motion, and spatial fluctuations, which are treated quantum-mechanically [3, 4]. In the absence of a full theory of quantum gravity, this practical approximation scheme is justified in situations in which the classical behaviour dominates the dynamics. Conceptually, it is not entirely satisfactory though, and moreover, it is expected to break down in the presence of very light scalar fields. The stochastic formalism aims at addressing this issue by deriving a classical effective theory for the coarse-grained super-Hubble part of the quantum fields driving inflation [5, 6]. The expansion of the universe results in a continuous flow of initially sub-Hubble modes joining the super-Hubble sector, which gives rises in this framework to a stochastic dynamics. Stochastic inflation is at the heart of the concepts of eternal chaotic inflation and the multiverse [7–9], with possibly far-reaching consequences. Moreover, as the production of primordial black holes during inflation necessitates very flat potentials, in which quantum diffusion effects are non-negligible, it is also necessary to take it into account in the context of the identification of the nature and origin of dark matter [10–13]. Scrutinising the theoretical grounds of stochastic inflation is therefore conceptually and practically very important, and it has recently received a renewed attention [14–25]. In this Letter, we summarize the salient features of a detailed investigation [26], highlighting in particular the hitherto unnoticed conceptual issue of formulating a generally covariant theory of stochastic inflation. This difficulty is related to the Itô versus Stratonovich dilemma in statistical physics [27, 28], and ultimately to the notoriously difficult problem of studying path integral and quantum anomalies in curved target spaces [29–32].

Itô versus Stratonovich

It is well known that stochastic differential equations (SDE) are not completely defined in general unless they are accompanied with a prescription to make sense of their stochasticity. Different types of consistent stochastic calculus have been defined by mathematicians, chief amongst them Itô and Stratonovich calculus [33, 34], that physically correspond to different discretisation procedures for stochastic processes⁴ (see e.g. [35, 36]). It will prove useful to present them in a rather general way. For this, let us consider an arbitrary number of random variables X^a , which depend on time N , and that obey the generic Langevin equations

$$\frac{dX^a}{dN} = h^a + g_\alpha^a \xi^\alpha, \quad (1)$$

⁴ We concentrate on these two well known discretisations, but one can easily consider more general α -discretisations [26], where $0 \leq \alpha \leq 1$, recovering Itô calculus for $\alpha = 0$ and the Stratonovich one for $\alpha = 1/2$.

where ξ^α are independent normalised Gaussian white noises, verifying $\langle \xi^\alpha(N) \xi^\beta(N') \rangle = \delta^{\alpha\beta} \delta(N - N')$, and whose numbers need not be the same as the number of X^a 's. Both the deterministic and stochastic parts h^a and g_α^a are in general functions of the fields X^a and of N , although we will omit to mention the time-dependence for simplicity. In a discretised version, the physical ambiguity comes from whether the strengths of the random kicks are determined by the amplitudes of the noises g_α^a at a time immediately before the kicks—this is the Itô choice—or, motivated by the fact that white noises are idealisations of random processes with finite correlation time, whether they are determined by the average of the noises amplitudes over the duration of the kick—this is the Stratonovich choice. The two procedures are physically distinct, and the corresponding probability distribution functions $P(\mathbf{X}, N)$ (PDF) verify the distinct Fokker–Planck (FP) equation

$$\frac{\partial P}{\partial N} = \mathcal{L}_{\text{FP}}(\mathbf{X}) \cdot P$$

$$\text{with } \mathcal{L}_{\text{FP}}(\mathbf{X}) = -\frac{\partial}{\partial X^a} D^a + \frac{1}{2} \frac{\partial^2}{\partial X^a \partial X^b} D^{ab}, \quad (2)$$

where the so-called drift D^a is given by $D_I^a = h^a$ in the Itô prescription, and by $D_S^a = h^a + \frac{1}{2} g_\alpha^b \partial g_\alpha^a / \partial X^b$ in the Stratonovich one, and where the diffusion coefficient reads $D^{ab} = g_\alpha^a g_\alpha^b$ in both cases. The two frameworks differ in the presence of multiplicative noises, i.e. when the g_α^a depend on the random variables X^a , which results in the noise-induced drift in the Stratonovich prescription, in addition to the deterministic drift. The Stratonovich FP operator can be rewritten as $\mathcal{L}_{\text{FP},S} \cdot P = -\partial_a (h^a P) + \frac{1}{2} \partial_a (g_\alpha^a \partial_b (g_\alpha^b P))$, so that the choice between the two prescriptions is reminiscent of the factor ordering problem in QFT. Mathematically, a given set of SDE can always be rewritten in either of the two prescriptions by changing the expression of h^a in the Langevin equation (1), but physically the deterministic part of the evolution is often specified, so that other physical considerations should be taken into account to fix the ambiguity.

In the context of inflation, it has been argued that the Itô prescription should be preferred to respect causality [23, 37], although the Stratonovich choice is in no way problematic in this respect. On the other hand, the Stratonovich prescription has been advocated by the fact that the white noises should be treated as a limit of colored noises when the smooth decomposition between short and long-wavelength modes becomes sharp [38]. It has been also argued that the choice between the two prescriptions exceeds the accuracy of the stochastic approach [15, 39]. We will show that while this latter point is indeed true in a certain sense for slow-roll single-field inflation, the Itô versus Stratonovich dilemma strikes back in a non-trivial manner as soon as more than one degree of freedom is involved, in the full phase space or when multiple fields are taken into account.

Slow-roll single-field inflation

We begin by considering the simple framework of slow-roll single-field inflation, with the corresponding Langevin equation [5]

$$\frac{d\phi}{dN} = -\frac{V_{,\phi}}{3H^2(\phi)} + \frac{H(\phi)}{2\pi} \xi \quad (3)$$

where $3H^2(\phi) M_{\text{Pl}}^2 = V(\phi)$. Here, ϕ is the coarse-grained scalar field, $V(\phi)$ denotes its potential, the deterministic drift describes the overdamped, slow-roll, behaviour, and the amplitude of the noise term is given by the size of super-Hubble fluctuations of a light scalar

field (we will discuss below the origin and regime of validity of equation (3) and consider more general situations). It is now well understood that the number of e -folds of expansion $N \propto \ln a$, where a is the scale factor, should be used as the time variable in stochastic inflation, in order to agree with cosmological perturbation theory and to warrant the agreement with perturbative quantum field theory [15, 40, 41]. Note that there is a considerable conceptual and technical difference between test and non-test scalar fields. If a test scalar field in a fixed spacetime geometry is considered, the instances of $H(\phi)$ in (3) should be replaced by the deterministically determined Hubble scale $H(N)$, which is constant in the most studied case of de Sitter spacetime. The stochastic formalism can then be seen as a powerful method to resum infrared divergences of a light quantum scalar field in de Sitter spacetime. In addition, in the case of a scalar field driving inflation, the Langevin equation (3) has been used to compute various observable quantities like the power spectrum of the curvature perturbation, using the techniques of first passage time analysis, recovering results of conventional cosmological perturbation theory in a suitable classical limit [15]. Using the same techniques, we show that the Itô or Stratonovich prescriptions lead in this context to the same results to an excellent accuracy. Let $\mathcal{N}(\phi)$ be the number of e -folds of inflation that is realised by starting from the initial value ϕ , from which the distribution of primordial density perturbations can be easily computed with the stochastic- δN formalism [15, 37, 42, 43]. The PDF of this stochastic variable is equivalently defined by its Fourier transform, the characteristic function $\chi_{\mathcal{N}}(\omega, \phi) \equiv \langle e^{i\omega \mathcal{N}(\phi)} \rangle$. From the FP equation, one can show that $\chi_{\mathcal{N}}$ satisfies $\mathcal{L}_{\text{FP}}^\dagger(\phi) \chi_{\mathcal{N}}(\omega, \phi) = -i\omega \chi_{\mathcal{N}}(\omega, \phi)$, where $\dagger$ indicates the adjoint operator. Whereas $\mathcal{L}_{\text{FP},I}^\dagger/M_{\text{Pl}}^2 = v \frac{\partial^2}{\partial \phi^2} - \frac{v'}{v} \frac{\partial}{\partial \phi}$, one has $\mathcal{L}_{\text{FP},S}^\dagger/M_{\text{Pl}}^2 = v \frac{\partial^2}{\partial \phi^2} - \frac{v'}{v} \left(1 - \frac{v}{2}\right) \frac{\partial}{\partial \phi}$, with the same boundary conditions, and where $v \equiv V/(24\pi^2 M_{\text{Pl}}^4)$ is the dimensionless potential in Planck units. As $v \ll 1$ for consistently working in the classical gravity regime, one can see that in the regime of validity of stochastic inflation, the Itô or Stratonovich prescriptions for slow-roll single-field inflation lead to the same results, both when the classical result of standard perturbation theory is recovered, and when stochastic effects are large. This can be confirmed by deriving recursive differential equations between the moments of $\mathcal{N}$, and computing numerically all related observables like the power spectrum and the scalar spectral index (see appendix A).

General covariance

The physical criterion that we use to shed new light on the conceptual issues of stochastic inflation is the one of its covariance under general coordinate transformations. The conundrum can be stated rather concisely: on one hand, Itô calculus does not verify the standard chain rule, and the corresponding Fokker–Planck equation does not respect general covariance under field redefinitions. On the other hand, Stratonovich calculus does respect general covariance, but at the expense of introducing spurious ‘frame’ dependences⁵. In both cases, a classical symmetry is broken by the inclusion of stochastic effects, a phenomenon we refer to as a stochastic anomaly.

To present the issue in a simple but rather general form, let us consider the generalisation of (3) to non-linear sigma models (NLSM), with Lagrangian $\mathcal{L} = -\frac{1}{2} G_{IJ} \partial_\mu \phi^I \partial^\mu \phi^J - V$, assuming for simplicity that all properly normalised fields are effectively light. If one uses the slow-roll classical equation of motion to determine the drift, such a generalisation reads

⁵ Itô calculus has nothing particular in this respect, as only Stratonovich calculus respects general covariance in the general class of α -discretisations.

$$\frac{d\phi^I}{dN} = -\frac{G^{IJ}V_{,J}}{3H^2(\phi)} + \Xi^I, \quad (4)$$

where Ξ^I are stochastic noises, $3H^2(\phi)M_{\text{Pl}}^2 = V(\phi)$, and ϕ denotes the set of fields. A crucial point is that any derivation of this equation or generalisations thereof—be it from a heuristic approach at the level of the equations of motion, or from the more elaborate perspective of deriving a coarse-grained action within the Schwinger–Keldysh formalism [26]—does not result in Langevin equations of the form (1), but only determines the correlation functions of the noises, i.e. determines the diffusion matrix D^{ab} , and not a set of ‘square-roots’ g_α^a , which can differ by arbitrary field-dependent rotations $g_\alpha^a \rightarrow \Omega_\alpha^\beta(\mathbf{X})g_\beta^a$. For instance, in a generalised slow-roll approximation, one obtains

$$\langle \Xi^I(N) \Xi^J(N') \rangle = \left(\frac{H}{2\pi} \right)^2 G^{IJ} \delta(N - N'), \quad (5)$$

but no prescription to write down Ξ^I as a weighted sum of independent white noises. The correlations (5) can be realised by writing $\Xi^I = g_\alpha^I \xi^\alpha$ with $g_\alpha^I = \frac{H}{2\pi} e_\alpha^I$, for *any* set of vielbeins of the field space metric. This arbitrariness is innocuous in Itô calculus, as the precise expression of g_α^a does not alter the FP equation (2), which depends only on the deterministic drift and on the diffusion matrix. It does matter in the Stratonovich interpretation however, as the field space derivatives of g_α^a enter into the FP equation.

Now comes the issue of general covariance: physical quantities should not depend on arbitrary field redefinitions that one can perform at the level of the action. For NLSM studied here, the fields ϕ^I are indeed merely coordinates on the field space manifold of metric G_{IJ} . To discuss the covariance of the FP equation, it is convenient to express it in terms of the rescaled PDF $P_s = P(\phi)/\sqrt{\det(G_{IJ})}$, which is a scalar under general field redefinitions $\phi \rightarrow \tilde{\phi}(\phi)$, and in terms of which any sensible stochastic theory should be manifestly covariant. Using the above equations, one obtains that this required property is not satisfied in the Itô interpretation. One way to understand this is to note that in Itô calculus, the drift h^a in the Langevin equation (1) does not transform as a vector under redefinitions $X^a \rightarrow \tilde{X}^a$, whereas the drift in equation (4) does classically transform as a vector under field space redefinitions (see [26] for details). If one uses the Stratonovich interpretation however, one obtains the manifestly covariant result

$$\begin{aligned} \frac{\partial P_s}{\partial N} = & \nabla_I \left(\frac{V^I}{3H^2} P_s \right) + \frac{1}{2} \nabla_I \left(\frac{H}{2\pi} \nabla^I \left(\frac{H}{2\pi} P_s \right) \right) \\ & + \frac{1}{2} \nabla_I \left(\left(\frac{H}{2\pi} \right)^2 e_\alpha^I (\nabla_J e_\alpha^J) P_s \right) \end{aligned} \quad (6)$$

where field space indices are raised with the inverse metric, and ∇_I denotes the covariant derivative with respect to the field space metric. As announced, through their covariant derivatives in the second line, this comes however at the expense of a spurious dependence on the arbitrary choice of vielbeins, which can result in qualitatively very different results (see appendix B). Note also that for a general metric, no privileged frame exists that would make this effect disappear. More generally, had we considered a more general situation in which the right-hand side of equation (5) is different, this would not have changed the fact that the sub-Hubble physics dictates only $\langle \Xi^I(N) \Xi^J(N') \rangle$, and that the Stratonovich interpretation, necessary to maintain general covariance, forces us to introduce an artificial structure that does not drop out from physical observables without further modifications, be it in a curved or

flat field space. It is also interesting to use this general point of view to shed different light on our discussion of single-field slow-roll inflation. If one allows field redefinition in that case, at the somewhat artificial expense of not having a standard kinetic term, different ‘coordinates’ would yield different results in the Itô interpretation, because of its lack of general covariance. Such a difficulty disappears in the Stratonovich one however, as in one dimension, there is no ambiguity in defining the square-root g_α^a up to an irrelevant sign.

First principle ‘derivation’ in phase space

An attempt to derive the stochastic theory from first principles in a general setup enables us to spell out various assumptions behind such a description, which is important in order to delineate its regime of validity, and shows that the difficulties described above hold true in more complete descriptions. Leaving details to [26], using the Schwinger–Keldysh formalism, one derives there a coarse-grained action for the long-wavelength part of fields in NLSM, taking into account the full phase space using the Hamiltonian language, as well as the coupling to gravity, unifying and generalising previous works [18, 20, 23, 25, 44]. Assuming that an effective classical description emerges, this gives rise to the following set of equations:

$$\phi'^I = \frac{G^{IJ}\pi_J}{H} + \xi_Q^I, \quad D_N\pi_I = -3\pi_I - \frac{V_I}{H} + \xi_{\bar{P}I} \quad (7)$$

where π_I represent the conjugate momentum of ϕ^I (divided by a^3), $' = d/dN$, $D_N\pi_I = \pi'_I - \Gamma_{IJ}^K\phi'^J\pi_K$, $3H^2M_{\text{Pl}}^2 = V(\phi) + \frac{1}{2}G^{IJ}\pi_I\pi_J$, and where the two-point correlation functions of the stochastic noises $(\xi_Q^I, \xi_{\bar{P}I})$ can be computed in principle [26]. This system of equations is not of the type (1), for several reasons. The dynamics is strictly speaking non-Markovian [45], as the statistical properties of the noises do not depend only on the current location (ϕ^I, π_I) in phase space, but on the entire past history for each realisation. Indeed, the physics of the small scale fluctuations is dictated by the coarse-grained dynamics, which itself depends on all the stochastic kicks it has received. The stochastic noises are also in general non-Gaussian—a feature that would give rise not to a FP but to a more general Kramers–Moyal equation [35, 46]—and colored, owing to the smooth splitting between the long wavelength modes and the short ones that are integrated out [47–49]. Even when the assumptions of a Markovian dynamics sourced by Gaussian white noises are adequate, the subtlety pointed out above is still present: one needs to introduce by hand ‘square-roots’ of the correlation matrix of the noises, $g_{Q\alpha}^I$ and $g_{\bar{P}I\alpha}$, which transform as field-space vectors and covectors under field redefinitions [26]. They do not appear in the Itô FP equation, which however does not respect the criterion of general covariance, but explicitly appear in the covariant Stratonovich FP equation:

$$\begin{aligned} \frac{\partial P}{\partial N} = & -\frac{\pi^I}{H}D_{\phi^I}P + \left(\frac{V_I}{H} + 3\pi_I\right)\partial_{\pi_I}P + 3nP \\ & + \frac{1}{2}\left(D_{\phi^I}[g_{Q\alpha}^I\cdot] + \partial_{\pi_I}[g_{\bar{P}I\alpha}\cdot]\right) \\ & (D_{\phi^I}(g_{Q\alpha}^JP) + \partial_{\pi_I}(g_{\bar{P}I\alpha}P)), \end{aligned} \quad (8)$$

where the phase space PDF $P(\phi^I, \pi_I)$ is a proper scalar under field redefinitions, n is the number of fields, and $D_{\phi^I} = \nabla_I + \Gamma_{IJ}^K\pi_K\partial_{\pi_J}$ and ∂_{π_I} are covariant derivatives in phase space. In addition to the arbitrariness that we point out in the diffusion term, note that the first line of (8) provides a neat reformulation of the deterministic evolution in non-linear sigma-models.

It has a similar formal structure as a covariant Boltzmann equation in curved spacetime [50], and can be useful beyond stochastic inflation, for instance to study attractor behaviour and the sensitivity to initial conditions. In [26], we also discuss the relationship between the full phase space description here and the overdamped limit in the previous section, and in particular how the latter can be approximately derived from the former in a suitable limit.

Stochastic diffusion in curved field space

The various limitations of stochastic inflation that we have described should not diminish its successes, notably to reproduce non-trivial results from QFT in curved spacetime [40, 51–53]. In the current lack of a more fundamental understanding, we assume that the covariant anomaly, manifested by the dependence on the arbitrary choice of vielbeins in (6), is a limitation of the stochastic description, and does not hold in the full quantum theory. Hence, we dismiss the last term in (6), which is technically equivalent to adding a suitable noise-induced term to the deterministic drift in (4). Considering test scalar fields in de Sitter space for simplicity in the following, we thus take

$$\frac{\partial P_s}{\partial N} = \frac{1}{3H_0^2} \nabla_I (V^I P_s) + \frac{1}{2} \left(\frac{H_0}{2\pi} \right)^2 \nabla_I \nabla^I P_s \quad (9)$$

as our covariant equation that describes the corresponding diffusion of light scalar fields in a curved field space in the overdamped limit. Given that equation (9) is the simplest multi-field covariantisation of the corresponding single-field equation, one can wonder whether field space curvature invariants can also enter into this equation [54]. To answer this question, one can use our knowledge of the relevant microphysics, i.e. of quantum fluctuations of fields in NLSM. The Riemann curvature of the field space does enter at quadratic order in the action, however only in the effective mass matrix of the fluctuations. While in general this can have important consequences like the geometrical destabilisation of inflation [55–58], we deduce that no curvature invariant should enter into the description of effectively *light* fields, i.e. with all the eigenvalues of the effective mass matrix much smaller than H^2 , and that equation (9) is thus sufficient for this purpose.

Let us now apply it to two-field models with field space metric $(\partial\phi)^2 + e^{2b(\phi)}(\partial\psi)^2$. For a generic potential, one can easily derive from (9) evolution equations for arbitrary correlation functions, including for $n \geq 0$:

$$\begin{aligned} \langle \phi^n \rangle' &= -\frac{n}{3H_0^2} \langle \phi^{n-1} V_{,\phi} \rangle \\ &+ \frac{1}{2} \left(\frac{H_0}{2\pi} \right)^2 [n(n-1) \langle \phi^{n-2} \rangle + n \langle \phi^{n-1} b_{,\phi} \rangle]. \end{aligned} \quad (10)$$

For sum separable potentials, this system of equations has the interesting feature of involving only ϕ . When $V_{,\phi}$ and the non-canonical function $b(\phi)$ are polynomials in ϕ , it can thus be solved iteratively, starting from any initial distribution of ϕ , and independently of the one of ψ . Let us concentrate on the interesting and simple case of an hyperbolic geometry, with $b(\phi) = -\phi/M$, and a quartic potential $\lambda\phi^4/4$. Formally Taylor-expanding the correlation functions as a function of the number of e -folds, $\langle \phi^n \rangle = \sum_{m=0}^{\infty} A_m^n N^m$, one obtains the recursive relations $(m+1)A_{m+1}^n = -\frac{n\lambda}{3H_0^2} A_m^{n+2} + n(n-1) \frac{H_0^2}{8\pi^2} A_m^{n-2} - \frac{n}{M} \frac{H_0^2}{8\pi^2} A_m^{n-1}$, from which all the correlation functions can be deduced to arbitrary order m . With initial conditions $\langle \phi^n(0) \rangle = 0$ for $n > 0$, one finds for instance (see [26] for more results)

$$\langle \phi(N) \rangle = -\frac{H_0^2 N}{8\pi^2 M} \left[1 - \frac{\lambda N^2}{12\pi^2} - \frac{\lambda H_0^2 N^3}{768\pi^4 M^2} + \dots \right]$$

$$\langle \phi^2(N) \rangle = \frac{H_0^2 N}{4\pi^2} \left[1 + \frac{H_0^2 N}{16\pi^2 M^2} - \frac{\lambda N^2}{6\pi^2} - \frac{7\lambda H_0^2 N^3}{384\pi^4 M^2} + \dots \right].$$

Compared to the single-field case, the field space geometry breaks the Z_2 symmetry of ϕ , hence the appearance of non-zero correlations of odd powers of ϕ . Note also the interplay between the effects of the potential and the field space curvature, coming with series expansion in $\lambda N^2/\pi^2$ and $H_0^2 N/(\pi^2 M^2)$ respectively. This model, as a simple generalisation of the well studied $\lambda\phi^4$ single-field case, offers an interesting playground for studying stochastic effects in curved field space, and it would be interesting to confront these predictions to quantum field theory computations, which are comparably much more involved. Like in the single-field case, at late time, truncating the series to any finite order is misleading, but equations (9) and (10) enable one to understand the asymptotic behaviour of the system. For a generic $b(\phi)$ and for sum-separable potentials, one can see from equation (10) that the statistical properties of ϕ can indeed be computed as in a single-field model with an effective potential $V_{\text{eff}}(\phi) = V(\phi) - 3H_0^4/(8\pi^2) b(\phi)$, with equilibrium distribution $P_{\text{eq}} \propto e^{-8\pi^2/(3H_0^4)V_{\text{eff}}(\phi)}$. Of course, this stationary distribution need not exist in general, i.e. when it is not normalisable, for instance in the previous example with $\lambda = 0$, which describes a simple Brownian motion around the linearly evolving shifted value $-H_0^2 N/(8\pi^2 M)$. Eventually note that the consistency of our approach requires that its results should be such that all canonically normalised field fluctuations are light around the mean trajectory, which depends on the precise choice of potential $V(\phi, \psi)$ and the initial distribution of both fields.

Conclusions

The stochastic approach aims at describing the long-wavelength part of quantum fields, in inflationary or de Sitter spacetimes, by a classical stochastic theory. As any effective theory, it comes with its regime of validity and its limitations, several of which have already been emphasised in the literature. Here we highlighted an important conceptual issue of the stochastic approach that has not been previously pointed out, although similar difficulties are well identified in statistical physics (see e.g. [59–62]): the Itô interpretation of the Langevin equations does not respect general covariance under field redefinitions, while the Stratonovich one does, but at the expense of introducing spurious ‘frame’ dependences. This feature holds in the overdamped description in terms of fields only (a description of the Einstein–Smoluchowski’s type in the statistical physics’ language), but also in a more complete phase space (Kramers) description. Despite these limitations, we used physical arguments to write down a manifestly covariant and physically motivated Fokker–Planck equation, with the aim of describing the quantum diffusion and the late-time behaviour of effectively light fields in a curved field space. We applied it to test scalar fields in de Sitter space and showed that for a certain class of two-field models with derivative interactions, some statistical properties can be derived using a correspondence with a single-field model endowed with an effective potential. We also studied a simple extension of the single-field $\lambda\phi^4$ theory to a hyperbolic field space geometry, making predictions that would be interesting to compare to first principles quantum field theory computations.

We stress that the difficulties we have described to formulate a generally covariant stochastic formalism seems to be the stochastic counterparts of the notoriously difficult problem

of maintaining general covariance in quantum theories [29–32]. In particular, the way the Stratonovich prescription maintains formal general field space covariance at the expense of introducing local frame dependencies is reminiscent of the fact that the gravitational anomaly can be shifted from the general coordinate symmetry to the local Lorentz symmetry [63]. It would be very interesting to further investigate these links, and to determine whether the stochastic anomalies that we have described can be circumvented by using techniques like the covariant background field expansion and the nonperturbative renormalisation group (see e.g. [22, 64, 65]), path-integral discretisation schemes that are more complex than simple α -discretisations [66], or by using the tools of open quantum systems and directly working with the quantum density matrix (see e.g. [14, 16, 21]).

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Appendix A. Stochastic observables in slow-roll single-field inflation

The observable impact of stochastic effects on the curvature perturbation can be computed with the stochastic- δN formalism [37, 42] and its formulation in terms of the adjoint Fokker–Planck operator [11, 15, 43]. From a generic Fokker–Planck equation (2), one can deduce the statistical properties of the first passage time $\mathcal{N}(\mathbf{X})$ from some point $\mathbf{X}$ to a given boundary. Indeed its characteristic (generating) function $\chi_{\mathcal{N}}(\omega, \mathbf{X}) = \langle e^{i\omega\mathcal{N}(\mathbf{X})} \rangle$ can be shown to obey the adjoint FP equation [67]

$$\begin{aligned} \mathcal{L}_{\text{FP}}^{\dagger}(\mathbf{X})\chi_{\mathcal{N}}(\omega, \mathbf{X}) &= -i\omega\chi_{\mathcal{N}}(\omega, \mathbf{X}) \\ \text{with } \mathcal{L}_{\text{FP}}^{\dagger}(\mathbf{X}) &= D^a \frac{\partial}{\partial X^a} + \frac{1}{2} D^{ab} \frac{\partial^2}{\partial X^a \partial X^b}. \end{aligned} \quad (\text{A.1})$$

This can be readily applied to inflation, in which the δN approach [68] indicates that the observable curvature fluctuation coincides with the fluctuation of the number of e -folds elapsed until the system reaches the end-of-inflation surface. In particular, at leading order in slow-roll, its power spectrum $\mathcal{P}_{\zeta}$ can be expressed in terms of the moments of $\mathcal{N}$ as [42]

$$\mathcal{P}_{\zeta}(k) = \frac{d\langle \delta\mathcal{N}^2 \rangle}{d\langle \mathcal{N} \rangle} \Big|_{\langle \mathcal{N} \rangle = \ln(k_{\text{f}}/k)}, \quad (\text{A.2})$$

whereas the moments $\mathcal{M}_n = \langle \mathcal{N}^n \rangle$ obey the recursive partial differential equations (PDE)

$$\mathcal{L}_{\text{FP}}^{\dagger} \mathcal{M}_n = -n\mathcal{M}_{n-1}, \quad (\text{A.3})$$

from which the variance itself $\mathcal{C}_2 = \langle \delta\mathcal{N}^2 \rangle = \langle \mathcal{N}^2 \rangle - \langle \mathcal{N} \rangle^2$ can be deduced to verify $\mathcal{L}_{\text{FP}}^{\dagger} \mathcal{C}_2 = -D^{ab} \frac{\partial \mathcal{M}_1}{\partial X^a} \frac{\partial \mathcal{M}_1}{\partial X^b}$.

When applied to the canonical slow-roll single-field description in terms of the Langevin equation (3), the equation (A.3) reduce to the simple set of ordinary differential equations

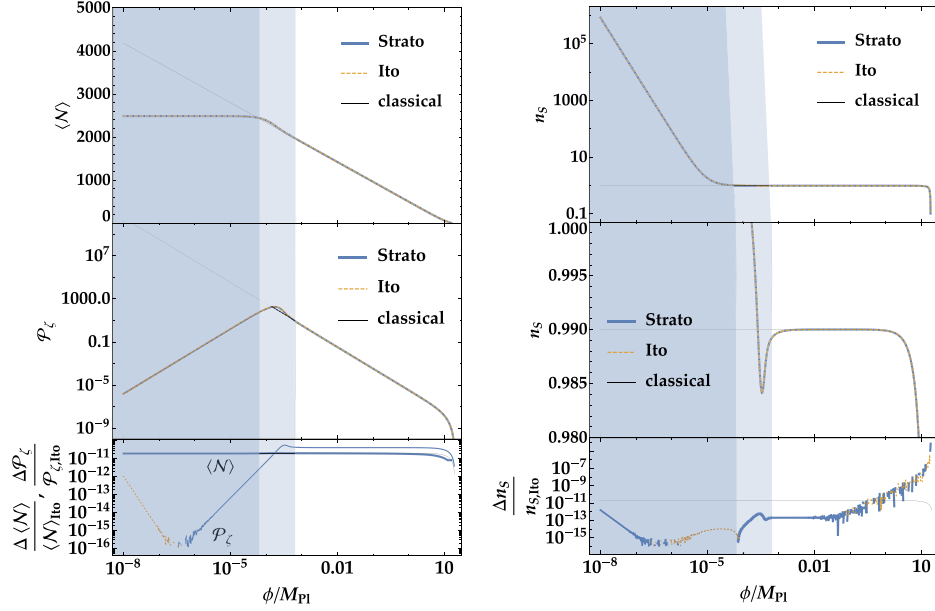


Figure A1. Numerical results for the mean number of e -folds $\langle \mathcal{N} \rangle$ (top left), power spectrum $\mathcal{P}_\zeta$ (bottom left), and spectral index n_s (right), computed with the full stochastic formulae (A.5)–(A.7) in the Stratonovich (‘Strato’) and Itô (‘Ito’) interpretation, as well as the standard textbook ones (‘classical’), in the hilltop model (A.12) with $\bar{\phi}_1 = \bar{\phi}_2 = 0$. Stochastic effects are non-negligible in the light blue region where $10^{-2} < |\eta_{\text{cl}}| < 1$ and very large in the dark blue region where $|\eta_{\text{cl}}| > 1$. The lower plots enable one to see the very small fractional differences between the Itô and Stratonovich results, which are expected to scale like $v(\phi)/2$, indicated by the thin black line. Blue plain lines represent positive values while orange dotted lines represent negative values.

$$\begin{cases} v\mathcal{M}_n'' - \frac{v'}{v}(1 - \alpha v)\mathcal{M}_n' = -n\frac{\mathcal{M}_{n-1}}{M_{\text{Pl}}^2}, \\ v\mathcal{C}_2'' - \frac{v'}{v}(1 - \alpha v)\mathcal{C}_2' = -2v\mathcal{M}_1'^2, \end{cases} \quad (\text{A.4})$$

where $v \equiv V/(24\pi^2 M_{\text{Pl}}^4)$ is the dimensionless potential in Planck units, $\alpha = 0$ or $1/2$ in the Itô or Stratonovich interpretation respectively, and $' = d/d\phi$ here. Its formal solution is given by

$$\mathcal{M}_n(\phi) = n \int_{\phi_f}^{\phi} \frac{dx}{M_{\text{Pl}}} \int_x^{\bar{\phi}_n} \frac{dy}{M_{\text{Pl}}} \frac{\mathcal{M}_{n-1}(y)}{v^\alpha(x)v^{1-\alpha}(y)} \mathcal{K}(x, y) \quad (\text{A.5})$$

$$\mathcal{C}_2(\phi) = 2 \int_{\phi_f}^{\phi} dx \int_x^{\bar{\phi}_2} dy \left(\frac{v(y)}{v(x)} \right)^\alpha \mathcal{M}_1'^2(y) \mathcal{K}(x, y), \quad (\text{A.6})$$

with the kernel $\mathcal{K}(x, y) = \exp\left[\frac{1}{v(y)} - \frac{1}{v(x)}\right]$, ϕ_f represents the end of inflation and $\bar{\phi}_n$ and $\bar{\phi}_2$ are constants of integration so that $v(y) > v(x)$. At leading order in slow-roll, where $\partial/\partial \log k \simeq -\partial\phi/\partial\langle \mathcal{N} \rangle \times \partial/\partial\phi$, one thus obtains

$$\mathcal{P}_\zeta = \mathcal{C}'_2/\mathcal{M}'_1, \quad n_s - 1 = -\frac{\mathcal{C}''_2}{\mathcal{M}'_1 \mathcal{C}'_2} + \frac{\mathcal{M}''_1}{\mathcal{M}'_1{}^2}, \quad (\text{A.7})$$

where the right-hand sides are evaluated at ϕ , the mean inflaton value when the scale k crosses the Hubble radius.

In the classical gravity regime where the inflationary energy scale is much smaller than the Planck scale, i.e. $v(x) < v(y) \ll 1$, the exponential suppression in $\exp\left[\frac{1}{v(y)} - \frac{1}{v(x)}\right]$ implies that, under certain conditions delineated below, the integrands in (A.5) and (A.6) acquire their main contributions from the region $y \sim x$. In this saddle-point limit, one obtains⁶

$$\mathcal{M}_1(\phi) \simeq \int_{\phi_f}^{\phi} \frac{dx}{M_{\text{Pl}}^2} \frac{v}{v'} (1 + (1 + \alpha)v - \eta_{\text{cl}}), \quad (\text{A.8})$$

$$\mathcal{C}_2(\phi) \simeq 2 \int_{\phi_f}^{\phi} \frac{dx}{M_{\text{Pl}}^4} \frac{v^4}{v'^3} (1 + (6 + 3\alpha)v - 5\eta_{\text{cl}}), \quad (\text{A.9})$$

$$\mathcal{P}_\zeta \simeq \mathcal{P}_{\zeta, \text{cl}} (1 + (5 + 2\alpha)v - 4\eta_{\text{cl}}), \quad (\text{A.10})$$

$$n_s - 1 \simeq n_{s, \text{cl}} - 1 + (-2(2 + \alpha)\epsilon_V + 3\eta_V)v - 6\eta_V\eta_{\text{cl}} + 8\epsilon_V\xi_{\text{cl}}, \quad (\text{A.11})$$

where the expansion is reliable under the condition that the stochasticity parameters $\eta_{\text{cl}} = v^2 v''/v'^2$ and $\xi_{\text{cl}} = v^3 v'''/v'^3$ are small. In this regime, stochastic effects entail small corrections to the classical results $\mathcal{P}_{\zeta, \text{cl}} = \frac{2}{M_{\text{Pl}}^2} \frac{v^3}{v'^2}$ and $n_{s, \text{cl}} = 1 - 6\epsilon_V - \eta_V$, where $\epsilon_V = \frac{M_{\text{Pl}}^2}{2} \frac{v'^2}{v^2}$ and $\eta_V = M_{\text{Pl}}^2 \frac{v''}{v}$ are the standard slow-roll parameters.

Note that the α -dependence of the above results, resulting from the choice between the Itô or Stratonovich interpretation, is suppressed by $v \ll 1$, and not by the stochasticity parameters η_{cl} and ξ_{cl} . This suggests that this choice hardly affects observables, even when stochastic effects are large, i.e. away from the saddle-point limit. We have checked this by resorting to numerical calculations for several choices of inflationary models. In figure A1 we present the results for the mean number of e -folds, the curvature power spectrum and the spectral index, for the hilltop model employed in [15] to exemplify stochastic effects:

$$V(\phi) = \Lambda^4 \left(1 - \frac{\phi^2}{\mu^2}\right), \quad \Lambda = 10^{-2} M_{\text{Pl}}, \quad \mu = 20 M_{\text{Pl}}, \quad (\text{A.12})$$

with the same parameters $\bar{\phi}_1 = \bar{\phi}_2 = 0$ (one can check that observables away from the boundary conditions are insensitive to their precise choices). One can see there that the stochastic results substantially differ from the classical ones when the inflaton field traverses regions where $|\eta_{\text{cl}}| \gtrsim 10^{-2}$, and even more so in regions with $|\eta_{\text{cl}}| > 1$ (note that $\xi_{\text{cl}} = 0$ for this potential). More importantly, results derived from the Itô or Stratonovich interpretations coincide to an excellent approximation, in the classical regime as well as when stochastic effects are large.

⁶ These results consistently reduce to those of [15] when $\alpha = 0$, i.e. for the Itô interpretation.

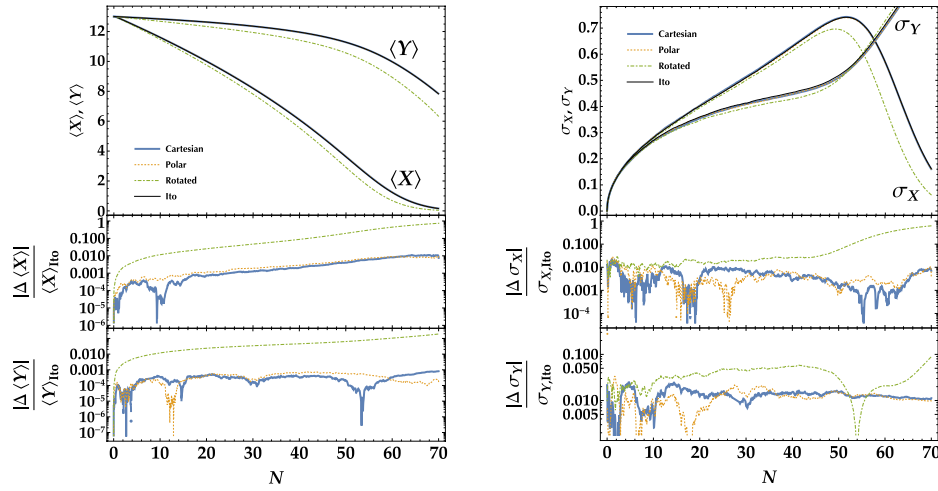


Figure B1. Time evolution of the averages (left) and standard deviations (right) of X and Y in the simple two-field model (B.1) with initial conditions $X^{\text{ini}} = Y^{\text{ini}} = 13M_{\text{Pl}}$. Averages are made out of 10^4 realizations of the Langevin equation (4) with $\Xi^I = \frac{H}{2\pi} e^I_\alpha \xi^\alpha$, and several choices of vielbeins e^I_α : ‘Cartesian’ (B.2), ‘Polar’ and ‘Rotated’ (respectively $m = 1$ and $m = 100$ in (B.3)). We also included the result of the Itô interpretation in the Cartesian coordinates. The lower plots enable one to visualise more easily the differences between the different curves, by displaying the fractional differences (in absolute value) with the Itô result.

Appendix B. Spurious frame-dependence in multifield situations

In this appendix, we show the concrete effects of different choices of vielbeins in the Stratonovich interpretation of the Langevin equation (4). We consider the simple example of a two-field model with flat field space, whose Lagrangian reads

$$\mathcal{L} = -\frac{1}{2}\partial_\mu X \partial^\mu X - \frac{1}{2}\partial_\mu Y \partial^\mu Y - \frac{1}{2}M_X^2 X^2 - \frac{1}{2}M_Y^2 Y^2. \quad (\text{B.1})$$

To make the effects of the noise easily visible, we choose unnaturally large masses $M_X = 3M_Y = 0.1M_{\text{Pl}}$, but the effects we discuss also apply to more realistic cases. We numerically solve 10^4 realizations of the Langevin equation (4) with $\Xi^I = \frac{H}{2\pi} e^I_\alpha \xi^\alpha$, in the Stratonovich interpretation, with initial conditions $X^{\text{ini}} = Y^{\text{ini}} = 13M_{\text{Pl}}$, and for three different sets of vielbeins e^I_α . We use the ‘Cartesian’ fields (X, Y) in the resolution but the results do not depend on this choice due to the general covariance of that interpretation. The first set of vielbeins that we choose is the natural ones in Cartesian coordinates:

$$(e^X_1 = 1, e^Y_1 = 0), (e^X_2 = 0, e^Y_2 = 1). \quad (\text{B.2})$$

The two other sets belong to the family of vielbeins defined by $(e^m)_\alpha^a = (\Omega^m)_\alpha^\beta e^a_\beta$, where the field-dependent rotation matrix is

$$(\Omega^m)_\alpha^\beta = \begin{pmatrix} \cos(m\Theta) & \sin(m\Theta) \\ -\sin(m\Theta) & \cos(m\Theta) \end{pmatrix}, \quad (\text{B.3})$$

and where $\Theta = \tan^{-1} \frac{Y}{X}$ is the angle of the polar field space coordinates. We use $m = 1$, which simply corresponds to the natural vielbeins used in polar coordinates (hence denoted as ‘Polar’), and $m = 100$ (denoted as ‘Rotated’), in addition to the original Cartesian vielbeins (B.2) ($m = 0$). The three corresponding results are shown in figure B1, for the time-dependence of the average fields and of their standard deviations. One can see that, while the Cartesian and polar choices do not lead to appreciable differences for these variables, the choice $m = 100$ significantly affects even the average dynamics. This is naturally expected from the corresponding FP equation (6), whose second-line contains a noise-induced drift $-\frac{1}{2} \left(\frac{H}{2\pi}\right)^2 e_\alpha^I (\nabla_J e_\alpha^I)$, with $e_\alpha^I (\nabla_J e_\alpha^I) = m(X, Y)/(X^2 + Y^2)$ in that case. For completeness, we also solved the corresponding Langevin equations with the Itô interpretation in the Cartesian coordinates, whose results are almost indistinguishable from the Stratonovich results with Cartesian vielbeins.

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7.2 A manifestly covariant, anomaly-free theory of multi-field stochastic inflation (article)

This section proposes the resolution of the aforementioned inflationary stochastic anomalies, and a more rigorous derivation of the multifield Langevin equations in stochastic inflation with curved field space, see Ref. [5],

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that is reproduced below.

This article is rather long because it not only presents new results but also reviews quite exhaustively the stochastic formalism for inflation and its micro-physical roots. Reading its introduction is particularly recommended for the stochastic-illiterates, since a general effort has been put on pedagogy and on explaining the general context. After reminding how the Hamiltonian formalism is related to the more usual Lagrangian one, having defined the canonically conjugate momenta and found the constraint equations, we spend some time explicating the intricate gauge issue in stochastic inflation that treats differently the fluctuations depending on if they are on small or large scales. Then, the multifield, phase-space Langevin equations of stochastic inflation with curved field space are first derived in a “heuristic way”, in the sense that the separation between the UV and IR sectors is abruptly made at the level of the mode functions and of the linear equations of motion that they must verify, by the introduction of a time-dependent coarse-graining scale $k_\sigma(N)$. The UV part is then supposed to behave as in the standard canonical treatment of inflation, *i.e.* they are assumed to still follow the linear EoM, while the IR part has a background dynamics corrected by a noise term whose statistical properties are set by the time-dependent power spectra of the UV modes. Although this procedure is qualitatively justified, we explain that it relies on a few assumptions that cannot be verified, and that it inconsistently leads to noise statistics that have a non-vanishing imaginary part, which is clearly impossible for the real scalar fields ϕ^I under investigation. We also comment on the *a priori* non-Markovian nature of the Langevin equations, since the noise statistics is set by the UV modes whose EoM depend on the values of the stochastic IR modes under consideration, and therefore may vary upon the integrated cosmic history: the noise statistic is rather a functional than a function of the IR modes. Only in some approximation can the dynamics be considered Markovian, and a corresponding Fokker-Planck equation may then be derived.

Then, we show how the stochastic anomalies are solved. After reviewing them, we explain that the canonical quantisation of the scalar fields on sub-Hubble scales comes with the prescription of a particular frame, which is the one of the independent quantum oscillators on which they must project, remember indeed that one has $\hat{Q}_k^I(\tau) = Q_A^I(\tau, k)\hat{a}_k^A + \text{h.c.}$, where the letter A labels the N_{field} independent quantum oscillators.

One is thus *given* a specific frame (actually this frame is not unique, but it can be entirely fixed after the specification of a constant unitary matrix which does not affect any observable quantity like the power spectra) which has a physical interpretation, and in which the noise statistics *must be* reduced, since for example the field-field noise amplitude reads symbolically

$$A^{QQIJ} \propto \left\langle \hat{Q}_{k_\sigma \vec{i}}^I \times \hat{Q}_{k_\sigma \vec{j}}^J \right\rangle' \propto Q_A^I(N, k_\sigma(N)) [Q_A^J(N, k_\sigma(N))]^* ,$$

with $\vec{i}, \vec{j}$ two unit vectors and a prime denoting that the $(2\pi)^3 \delta^{(3)}(\dots)$ factor has been removed, and therefore a natural “square-root” of it is simply the mode function Q_A^I itself. This treatment shows that there is actually no ambiguity in the choice of a frame in which to reduce the noise statistics, which was the issue that was spoiling the use of the Stratonovich prescription for concrete numerical resolutions or in order to write the associated Fokker-Planck equation. Since it is the only one that provides a covariant formalism to describe stochastic inflation, we therefore conclude that it must be the one to be used in the Langevin equations of the stochastic formalism for inflation, hence solving the discretisation ambiguity. But once the initial Langevin equations are understood as being defined the Stratonovich description, they may be instead written in the $\hat{\text{Ito}}$ way, upon the introduction of appropriate corrections to the Langevin equations in order to compensate this change. Thus we also show how to write the multifield stochastic formalism in $\hat{\text{Ito}}$, which requires the introduction of unusual $\hat{\text{Ito}}$ -covariant derivatives thanks to the correction terms mentioned above, and such that they compensate the breaking of the standard chain rule, therefore making the resulting equations as explicitly covariant as the ones written in Stratonovich, but better suited for numerical calculations for example.

Next, we show how to derive the multifield Langevin equations in phase space using the Schwinger-Keldysh, or *in-in* formalism, together with well-defined covariant perturbations of the fields and their momenta. This elaborate technique, borrowed from out-of-equilibrium statistical physics, enables us to identify “classical” and “quantum components” for each of the IR and UV fields and momenta, after having doubled the number of degrees of freedom in order to avoid the path integral to be defined on a closed trajectory in the complex time domain, from the in vacuum to the time of interest, and then back to the in vacuum. Still working at the level of the action and of the path integral, we show the procedure to integrate out the UV sector at each instant of time (remember its very definition is a time-dependent concept), and how this results in an effective action for the IR modes. We compute the second-order correction to the effective action in terms of quantum components, which enables us to derive the stochastic Langevin equations as a kind of “semi-classical” approximation, but we also explain that in principle this formalism could be used to derive corrections to the stochastic theory itself. We check that the resulting noise statistics is purely real contrary to the “heuristic” derivation, thanks to a careful investigation of the boundary between UV and IR sectors at the scale $k_\sigma(N)$, and also free from extra friction terms as could be expected from the fluctuation-dissipation theorem: indeed we explain that in this setup, the UV

fluctuations can not backreact on themselves since they only affect the IR dynamics at the precise time when they leave the UV sector.

Eventually, we show the Fokker-Planck equation for the Probability Density Function $P(\varphi^I, \varpi_J; N)$ of fields and momenta, for multifield stochastic inflation in phase space and with kinetic interactions, when a Markovian assumption is made, and this is the physical result that I would like to highlight:

$$\begin{aligned} \partial_N P = & -D_{\varphi^I} \left[\frac{G^{IJ}}{H} \varpi_J P \right] + \partial_{\varpi_I} \left[\left(3\varpi_I + \frac{V_I}{H} \right) P \right] \\ & + \frac{1}{2} D_{\varphi^I} D_{\varphi^J} (A^{QQIJ} P) + D_{\varphi^I} \partial_{\varpi_J} (A^{Q\tilde{P}I}{}_J P) + \frac{1}{2} \partial_{\varpi_I} \partial_{\varpi_J} (A^{\tilde{P}\tilde{P}}{}_{IJ} P), \end{aligned} \quad (7.3)$$

where we have defined the covariant derivative D_{φ^I} with respect to the IR fields φ^I , the phase-space one, whose action on a rank-1 tensor is $D_{\varphi^I} U^J = \nabla_I U^J + \Gamma_{IL}^K \varpi_K \partial_{\varpi_L} U^J$ and generalisation to rank- n tensors is straightforward, and ∂_{ϖ_I} is a simple derivative with respect to IR momenta ϖ_I . As for the $A^{\tilde{X}\tilde{Y}IJ}$'s, these are the noises' auto-correlations at coincident points:

$$A^{\tilde{X}\tilde{Y}IJ}(N) \delta(N - N') = \langle \xi^{\tilde{X}I}(N) \xi^{\tilde{Y}J}(N') \rangle = \frac{k'_\sigma}{k_\sigma} \text{Re}[\mathcal{P}^{\tilde{X}\tilde{Y}IJ}(N, k_\sigma(N))] \delta(N - N'), \quad (7.4)$$

where $\tilde{X} = (Q, \tilde{P})$ are the covariant perturbations of the fields and momenta and $\mathcal{P}^{\tilde{X}\tilde{Y}IJ}$ are their power spectra (note the real part that makes the noise's statistics explicitly real).

The original article as published in JCAP is now displayed. Notations can be heavy, and that is why they are summarised in one of the appendices of the paper. The reader is advised to ream them once before digging into technical details.

A manifestly covariant theory of multifield stochastic inflation in phase space: solving the discretisation ambiguity in stochastic inflation

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Abstract. Stochastic inflation is an effective theory describing the super-Hubble, coarse-grained, scalar fields driving inflation, by a set of Langevin equations. We previously highlighted the difficulty of deriving a theory of stochastic inflation that is invariant under field redefinitions, and the link with the ambiguity of discretisation schemes defining stochastic differential equations. In this paper, we solve the issue of these “inflationary stochastic anomalies” by using the Stratonovich discretisation satisfying general covariance, and identifying that the quantum nature of the fluctuating fields entails the existence of a preferred frame defining independent stochastic noises. Moreover, we derive physically equivalent Itô-Langevin equations that are manifestly covariant and well suited for numerical computations. These equations are formulated in the general context of multifield inflation with curved field space, taking into account the coupling to gravity as well as the full phase space in the Hamiltonian language, but this resolution is also relevant in simpler single-field setups. We also develop a path-integral derivation of these equations, which solves conceptual issues of the heuristic approach made at the level of the classical equations of motion, and allows in principle to compute corrections to the stochastic formalism. Using the Schwinger-Keldysh

formalism, we integrate out small-scale fluctuations, derive the influence action that describes their effects on the coarse-grained fields, and show how the resulting coarse-grained effective Hamiltonian action can be interpreted to derive Langevin equations with manifestly real noises. Although the corresponding dynamics is not rigorously Markovian, we show the covariant, phase-space Fokker-Planck equation for the Probability Density Function of fields and momenta when the Markovian approximation is relevant, and we give analytical approximations for the noises' amplitudes in multifield scenarios.

Keywords: inflation, physics of the early universe, cosmological perturbation theory, quantum field theory on curved space

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1 Introduction

Inflation and high-energy physics. Inflation, an era of accelerated expansion of the early universe, currently provides us with the best understanding of the initial conditions for the subsequent cosmological eras. The simplest mechanism to explain this quasi-exponential, de Sitter like expansion, is to assume that the energy density of the universe was then dominated by the one of a scalar field, the inflaton, endowed with a very flat potential in Planck units, so that it slowly rolls down its potential. This results in a homogeneous, isotropic and spatially flat Universe on cosmological scales, as required by observations of the cosmic microwave background (CMB). Moreover, it naturally comes with a mechanism by which the quantum fluctuations of the inflaton are stretched to cosmological scales to give rise to primordial density fluctuations at the origin of the CMB anisotropies and of the large scale structure of the universe that we observe nowadays, a scenario in perfect agreement with the latest CMB data from the Planck satellite [1, 2].

Despite its success at explaining data in a simple manner, single-field slow-roll inflation is usually seen only as a phenomenological description that emerges from a more realistic physical framework to be determined (see, e.g., ref. [3]). One of the main reasons behind this is the peculiar ultraviolet (UV) sensitivity of inflation: order-one changes in the strengths of the interactions of the field(s) responsible for inflation with Planck-scale degrees of freedom generically have significant effects on the inflationary dynamics, to the point sometimes of ruining inflation itself. Addressing this UV sensitivity implies justifying in a controllable setup that high-energy interactions are innocuous, which can be done either by specifying the physics at the Planck scale, typically in string theory constructions, or at least by taking it into account using the methods of effective field theory (EFT). Either way, this naturally leads one to consider the impact of the existence of several degrees of freedom during inflation, and indeed the UV sensitivity of inflation provides us with a formidable opportunity to use the early universe as a giant particle detector. In this respect, looking for new physics in cosmological data, for instance through non-Gaussianities or/and features of the primordial fluctuations, can be seen as looking for multifield effects (see, e.g., refs. [4–8] for reviews). Typical UV embeddings of inflation include several scalar fields interacting through their potential as well as through their kinetic terms, with a Lagrangian of the type

$$\mathcal{L} = -\frac{1}{2}g^{\mu\nu}G_{IJ}(\phi)\partial_\mu\phi^I\partial_\nu\phi^J - V(\phi). \quad (1.1)$$

This general class of so-called non-linear sigma models have been studied for a long time (see, e.g., the review [9]), but recent years have seen a flurry of activity concerning them (see, e.g., refs. [10–47]), in particular about geometrical aspects related to the curved field space described by the metric G_{IJ} , the possibility to inflate along trajectories characterised by a strongly non-geodesic motion in field space, and the corresponding distinct observational signatures.

Stochastic inflation. Standard Perturbation Theory (SPT) during inflation treats perturbatively quantum fluctuations around supposedly homogeneous classical background fields. This distinct treatment is not only conceptually unsatisfactory, but it is also expected to break down in the presence of very light scalar fields whose large-scale evolutions are dominated, not by their classical dynamics, but instead by quantum diffusion effects. The stochastic approach aims at dealing directly with the super-Hubble parts of the quantum fields driving inflation (see refs. [48–57] for the first papers on the subject). The corresponding theory, resulting from a *coarse-graining* procedure, can be thought of as an EFT for long-wavelength modes during

inflation. More precisely, and concentrating for definiteness on test scalar fields evolving in de Sitter space, the scalar fields are divided into infrared (IR) and UV parts delineated by a constant physical scale, the first one corresponding to the “coarse grained” super-Hubble parts of the quantum fields, with comoving momenta smaller than the time-dependent cutoff $k_\sigma(N) = \sigma a(N)H$, with a small positive parameter $\sigma \ll 1$ and where $N = \ln a$ is the number of e -folds. The IR sector of the theory can be understood as an open system receiving a continuous flow of UV modes as they cross the growing coarse-graining scale k_σ . Strikingly, the effect of this flow can be understood as classical random kicks added to the deterministic dynamics of the IR fields. More technically, the IR fields verify stochastic, so-called *Langevin* equations, rather than the deterministic equations verified by the background fields in SPT.

An excellent agreement between the stochastic formalism and usual quantum field theory techniques has been found in a number of studies, mostly in the paradigmatic setup of the $\lambda\phi^4$ theory in de Sitter space, but also including backreaction in the single-field slow-roll regime [58–65]. This agreement is noteworthy because the computations of correlation functions are almost immediate in the stochastic theory, at least in the simplest contexts: it enables one to determine without effort what would be the results of intricate loop calculations in renormalised perturbative quantum field theory. Moreover, and importantly, the stochastic formalism enables one to resum the IR divergences of perturbative QFT, and derive fully non-perturbative results (such as equilibrium distributions in de Sitter space), a subject that has attracted a lot of attention and has been investigated using a variety of methods (see, e.g., refs. [66–80]).

The stochastic formalism is not only useful for such formal investigations, as well as to tackle the issues related to eternal inflation [81–83], but it can also be used to compute observationally relevant quantities such as the power spectrum, higher n -point functions and other statistical properties of the adiabatic curvature perturbation ζ generated during inflation. This is achieved with the help of the separate universe approach, which states that each region of the universe slightly larger than the Hubble radius evolves like a separate FLRW universe that is locally homogeneous and evolves independently from its neighbours [84]. Then, patching these regions enables one to deduce the curvature perturbation on even larger scales, identified as the fluctuation of the local number of e -folds of expansion $N(\mathbf{x})$, a method known as the δN formalism [85–88]. Its generalisation to stochastic inflation was called the *stochastic- δN formalism* [89–95], and it enables one to compute the statistical properties of ζ in a non-perturbative manner (see also refs. [96–100] for a related approach), reducing to SPT in a suitable classical limit, while being able to treat the regime where quantum diffusion effects dominate. This has notably proved useful recently to compute the abundance of primordial black holes (PBH) resulting from the collapse of local overdensities generated during inflation [92, 101–105] (see, e.g., refs. [106–109] for early applications of the stochastic formalism in this context), a field that regained attention as PBHs are considered as candidates for LIGO/Virgo gravitational wave sources [110–112], a possibly important component of dark matter (see, e.g., refs. [113, 114]), as well as possible explanations of the microlensing events found by OGLE [115] and even of the hypothetical Planet 9 [116, 117].

Despite many achievements, and the fact that stochastic inflation with multiple fields has already been studied (see [118–120] for first works at the early stage of stochastic inflation), we stress that it has never been formulated in a manner that is generally covariant under field redefinitions, nor derived from first principles in this context. This, together with the many recent developments concerning the geometrical aspects of nonlinear sigma models, constitute the main motivations of this work.

Path integrals and Hamiltonian action. In the present paper, we begin by showing a “heuristic” derivation of the phase-space Langevin equations of stochastic inflation in the general context of multifield inflation with curved field space, by working at the level of the classical equations of motion, but we also propose a rigorous path-integral derivation solving the ambiguities of this heuristic approach. Path integrals are ubiquitous in physics, from statistical physics and quantum mechanics to field theories. In the context of stochastic inflation, they appear in a manner quite similar to the path-integral representation of the Brownian motion of a system linearly coupled to a thermal bath that is integrated out [121], the role of the system and the bath being respectively replaced by the IR and UV sectors [122–132] (see also refs. [133–136] for the use of similar tools in other gravitational contexts).

Path integrals are first constructed on a discrete time (and space for field theories that we shall focus on from now on) grid as the integral over all possible discrete *jumps* from a field’s value to any other one, with fixed initial and final values. In the continuous limit, it corresponds to an integral over all the possible *paths* to go from a fixed initial point to a fixed final one, thus justifying its name as “integration over possible histories”. Microscopically, the law governing the probability of a given jump between times N_{j-1} and N_j is dictated by the unitary operator $\hat{U}_j = e^{-i\hat{H}(\phi,\pi;N_j)(N_j-N_{j-1})}$, where $\hat{H}$ is the Hamiltonian operator of the system, and ϕ and π denote the corresponding fields and momenta. In this fundamental phase-space approach, the action entering in the final expression for the path integral over the values of the fields and momenta is called the *Hamiltonian action* and reads $S = \int d^4x [\pi\dot{\phi} - \mathcal{H}(\phi, \pi)]$ where $\mathcal{H}$ is the Hamiltonian density associated with H . Note that when the Hamiltonian (density) is at most quadratic in momenta, it is possible to perform exactly the path integration over them, and express the theory as a path integral over fields only. However one would recover the standard Lagrangian action only when the terms quadratic in momenta are field-independent [137], which is neither the case in general, nor in our situation of interest.

Partition function, “in-in” formalism and doubling of the degrees of freedom.

In particle physics, transition amplitudes between asymptotic “in” and “out” states can be deduced from time-ordered correlation functions. The latter can themselves be derived from the generating functional $Z[J]$, i.e. the partition function with sources, which has a convenient path-integral representation. In cosmology, one rather looks for the expectation values of operators in some “in” state defined in the far past (typically the Bunch-Davies vacuum), as well as the corresponding causal equations of motion that they verify. However these can also be deduced from a generating functional expressed as a path integral, with the important peculiarity, for this “in-in” partition function, that the path integral turns out to be performed on a Closed-Time-Path (CTP) of integration in the time domain, as represented in figure 1 in the main body of this paper. Working with this CTP amounts to considering a “doubling of the histories”: one along the forward branch, and one along the reverse one, and with doubled degrees of freedom, one version for each of the two paths. Naturally, there is no doubling of the genuine physical degrees of freedom in the theory, but only as dummy variables inside the path integral: the two copies of the degrees of freedom are treated independently at any time *but* the final one, at which the two branches of the CTP close, and boundary conditions must be imposed. Of course, the “in-in” formalism was not intended for cosmology in the first place, but rather developed in the field of non-equilibrium statistical and quantum field theories, in which it is also known as the *Schwinger-Keldysh formalism* [138, 139], proving extremely useful to describe quantum and thermal fluctuations, dissipation, decoherence and many other effects in various areas of physics (see, e.g., refs. [140–142]).

Coarse-graining. Stochastic inflation corresponds to a low-energy effective version of the full theory that can be described by the “in-in” path integral as explained above. To derive it, one must thus identify the relevant degrees of freedom (the super-Hubble modes in our case), and integrate out of the theory the other ones (the sub-Hubble modes). After splitting the full system into our subsystem of interest composed of IR fields, plus a bath of UV fluctuations, one can perturbatively integrate out explicitly the UV modes of the description. However, remembering that “integrating out is different from truncating”, the UV fluctuations will leave an imprint on the IR dynamics, and this will be the source of the explicit noise and randomness in the equations of motion for the long-wavelength fields. This concept of *coarse-grained effective action* is widely used in physics, from the study of Brownian processes in statistical physics, to the applications of renormalisation in field theories and decoherence in quantum mechanics, but was also applied to the cosmological context [123, 126, 130, 132, 133]. The coarse-graining procedure can also be understood at the level of the density matrix, which for a bipartite system (IR and UV sectors) can give the EFT for an open system (the IR modes) by tracing out the environment (the UV modes) and obtaining the *reduced density matrix*. Be it at the level of the partition function or the density matrix, the coarse-graining approach within the in-in formalism is powerful because it enables one to control the approximations that are made and possibly derive next-order corrections [143–146].

Langevin equations, multiplicative noise and ambiguity of the discretisation scheme. As we explain in the body of this paper, the effect of the UV modes on the IR dynamics is encapsulated in the *influence action*. After careful investigation and introduction of auxiliary variables, it can be shown that this results in an explicit noise term in the equations of motion for the IR fields, with a covariance dictated by the (real part of the) power spectrum of the UV modes. The long-wavelength fields thus verify Langevin equations, with a deterministic drift coming from the ordinary background dynamics, but supplemented by a diffusion term due to the random kicks. Crucially, the effect of the small-scale, quantum fluctuations on the long-wavelength, classicalised IR fields, can be interpreted as a classical noise. Hence, the resulting theory describes genuinely quantum effects, albeit in a classically-looking stochastic manner.

Langevin equations have been studied for a long time in the context of Brownian processes, signal theory, etc. They constitute Stochastic Differential Equations (SDE) rather than Ordinary Differential Equations (ODE), and this difference is crucial. Indeed, consider the simplest example of the Brownian motion of a particle, due to shocks with its environment at a given temperature; its position is a random quantity whose statistical properties may be determined. However for a given realisation, the position of the particle, although being a continuous function of time, is not a differentiable function of time due to the properties of the white noise that affects its dynamics. Thus, the mathematical understanding of trajectories and in particular time derivatives of the position of the particle, is intricate and leads to interesting subtleties. Of course, a discrete-time interpretation of the dynamics is always possible and may even be clearer, and complications arise when going to the continuous-time limit of the description. A famous example (for statistical physicists) of possible difficulties is met when the noise is *multiplicative*, that is when its amplitude (or covariance) is itself a function of the random variable that verifies the Langevin equations. Then, there is an ambiguity when going from the discrete-time representation to the continuous one: at which time exactly should the random variable that enters the noise amplitude be evaluated? When dealing with ODEs, we are used to forget about these subtleties because any choice of a discrete

scheme leads to the same physical result. However, this is not the case any more for SDEs with multiplicative noise, for which different scheme choices, usually parameterised by a number α between 0 and 1, lead to different values for physical quantities like statistical averages, Probability Density Functions (PDF), etc. Amongst the infinite number of possible choices for α , two have been particularly investigated for their interesting properties, the prepoint, $\alpha = 0$ Itô discretisation [147], and the midpoint, $\alpha = 1/2$ Stratonovich [148] one. Indeed, while Itô is widely used in applied and computational mathematics for its appealing mathematical properties (the covariance matrix can be arbitrarily reduced in any frame to identify independent noises, the noise at a given time step only depends on the values of the random variables at previous time steps, etc.), Stratonovich may be preferred in theoretical physics, where changes of variable are ubiquitous, because the standard chain rule for the derivative of composite functions is only verified in that case. In particular, this last property simplifies discussions about general covariance of the equations. In this respect, it is important to highlight that, while a given SDE, interpreted with different schemes, defines different physical theories, it is always possible to describe the same physics by using different discretisation schemes. Indeed, one knows how to go from one continuous form of a SDE understood in a given discretisation scheme, to another form with a different scheme, while leaving the physics unaffected.

Keeping this in mind, whether the conventional form of the Langevin equations of stochastic inflation should be interpreted according to Itô or Stratonovich schemes has already been discussed in the literature. On one hand, the Stratonovich scheme has been advocated by the fact that white noises should be treated as the limit of colored noises when the smooth decomposition between short and long-wavelength modes becomes sharp [149]. On the other hand, it has been suggested that only the Itô scheme could be invariant under reparameterisation of the time variable [150], and consistently reproduce one-loop QFT computations in the $\lambda\phi^4$ theory [130]. Eventually, it has also been argued that the choice between the two prescriptions exceeds the accuracy of the stochastic approach [91]. In our previous paper [95], we tackled for the first time the issue of the discretisation ambiguity of the Langevin equations of stochastic inflation in the multifield context, and we discovered various conceptual issues with the stochastic description of IR fields during inflation, that we called “inflationary stochastic anomalies”.

Inflationary stochastic anomalies. In stochastic inflation, the covariance matrix of the noises entering the Langevin equation is proportional to the (real part of the) power spectra of the UV modes. However the UV modes themselves evolve according to linear equations of motion (at first order in perturbation theory for the UV modes) whose “coefficients” are set by the values of the IR fields that constitute the random variables of interest. Thus, the noise amplitude for the IR fields clearly depends on their own values, which corresponds to a multiplicative noise. Actually, the situation is even more intricate since rigorously the power spectra of UV modes (and thus the noise amplitude) cannot be simply expressed as functions of the IR fields at the current time, but rather are solutions of differential equations that involve them. This situation is called *non-Markovian*, in contrast to Markov processes where the noise amplitude only depends on the random variables at the time step of evaluation, and not at previous times.

However even letting aside the non-Markovian difficulty, the multiplicative noise results in the discretisation scheme ambiguity discussed above, and since the derivation of the Langevin equations does not *a priori* come with any prescription regarding their discrete-time version, one should choose how to interpret them (i.e. prescribe a value for the parameter α)

based on physical criteria. However, in our previous paper [95], we found that no choice was satisfactory because of the following. The standard chain rule for the derivative of composite functions is only verified in the Stratonovich $\alpha = 1/2$ case. Thus, for any other choice, the Langevin equations as they are usually shown do not respect general covariance under field redefinitions. However at that time we thought the Stratonovich choice was not satisfactory neither, even if for a different reason: only in the Itô case is the frame of reduction of the noise matrix (necessary to identify independent Gaussian white noises and solve the Langevin equations numerically or proceed further analytically) irrelevant to the final result, as already known in statistical physics contexts (see e.g. refs. [151–155]). So we were left with a dilemma: breaking of general covariance following the Itô interpretation or spurious frame-dependence in the Stratonovich one? It is important to note that, although more striking in the multifield context, this ambiguity is also present in single-field models of stochastic inflation. Although we showed that, for such a single scalar field in the overdamped limit, the difference between the two prescriptions is numerically small in the final correlation functions, the conceptual issue was still remaining. By including a tadpole diagram cancelling the frame dependence in the Stratonovich scheme, a covariant and frame-independent formulation was proposed in ref. [156], considering the overdamped limit (i.e. in field space and not in phase space) of test scalar fields in de Sitter space and in a Markovian approximation. In this paper, we will show how inflationary stochastic anomalies are solved in full generality from first principles.

Structure of the paper. The structure of the paper is as follows. We begin by introducing in section 2 the definitions and the concepts behind stochastic inflation in phase space with several scalar fields and a general field-space metric, and developing an intuitive approach to derive “heuristically” the Langevin equations for the coarse-grained fields and their momenta. We also highlight the conceptual issues behind these equations and their derivation using the classical equations of motion. Notably, we review in section 3 why these equations suffer from “inflationary stochastic anomalies”, an issue that we solve by using the Stratonovich discretisation satisfying general covariance, and identifying that the quantum nature of the fluctuating fields entails the existence of a preferred noise frame. The corresponding covariant Itô SDE, which can readily be used in numerical and analytical computations, are also derived as one of our main results. In section 4, we turn to the rigorous derivation of stochastic inflation using a path-integral approach. This enables one to solve the other conceptual issues of the heuristic approach and to keep a better control over the approximations made throughout, paying a particular attention to the doubling of the degrees of freedom and the necessary boundary conditions imposed at the UV/IR transition by the Closed-Time-Path of integration. We also show how the identification of covariant Vilkovisky-DeWitt variables in phase space, is crucial to maintain general covariance. We derive the influence action for the long-wavelength fields and momenta, resulting from integrating out the UV modes, and we show how the coarse-grained effective action can be interpreted to derive Langevin equations with manifestly real noises. We finish in section 5 by showing, in the Markovian limit, the phase-space, covariant Fokker-Planck equation corresponding to our multifield Langevin equations, as well as some analytical approximations for the noises’ amplitudes. These results can be used in practical applications of our covariant multifield stochastic inflation framework. Section 6 is then devoted to conclusions and future prospects. Eventually, we gathered in appendices some technical details as well as a summary of our notations. We adopt natural units, $c = \hbar = 1$ throughout this paper.

Main results. We gather here in a few lines the main results of the paper:

- “Inflationary stochastic anomalies” are solved by the observation that the quantum nature of the fluctuating fields provides one with a natural frame for reducing the noise covariance matrix: the one of the independent creation and annihilation operators. This leads to a unique set of independent Gaussian white noises in the Langevin equations (up to a constant, irrelevant, orthogonal matrix), and highlights the genuine quantum origin of their stochasticity
- The Langevin equations as they are usually derived must be interpreted with the Stratonovich discretisation scheme and the preferred frame mentioned above, but they are easier to interpret and use after transforming them to their Itô version. The corresponding noise-induced terms can then be used to define covariant time-derivatives compatible with Itô calculus, $\mathfrak{D}_N$, see eqs. (3.4)–(3.6). The resulting, Itô-covariant, phase-space, Langevin equations for multifield inflation with curved field space and including back-reaction on the metric are eventually found to be:

$$\boxed{\mathfrak{D}_N \varphi^I = \frac{\varpi^I}{H} + \xi^{QI}, \quad \mathfrak{D}_N \varpi_I = -3\varpi_I - \frac{V_I}{H} + \xi_I^{\tilde{P}}.} \quad (1.2)$$

Here, V_I denotes the gradient of the potential, H is the local Hubble scale, given in terms of the infrared fields φ^I and momenta ϖ_I by the Friedmann equation (2.26), and indices are raised with the inverse field-space metric. We also find the auto-correlation of the Gaussian white noises to be given by, for $\tilde{X} = (Q, \tilde{P})$:

$$\boxed{\langle \xi^{\tilde{X}I}(N) \xi^{\tilde{Y}J}(N') \rangle \equiv A^{\tilde{X}\tilde{Y}IJ}(N) \delta(N - N') = \text{Re} \mathcal{P}^{\tilde{X}\tilde{Y}IJ}(N; k_\sigma(N)) \delta(N - N'),} \quad (1.3)$$

with $\mathcal{P}^{\tilde{X}\tilde{Y}IJ}$ the dimensionless power spectra of the UV modes $(Q^I, \tilde{P}_I)$ that follow the EoMs (4.29) deduced from the action (4.20), and evaluated at the scale $k_\sigma(N) = \sigma a(N)H$ that joins the IR sector at the time N .

- When the dynamics can be approximated as Markovian, it is possible to derive the phase-space Fokker-Planck equation for the one-point scalar PDF $P(\varphi^I, \varpi_J; N)$ as

$$\boxed{\begin{aligned} \partial_N P = & -D_{\varphi^I} \left[\frac{G^{IJ}}{H} \varpi_J P \right] + \partial_{\varpi_I} \left[\left(3\varpi_I + \frac{V_I}{H} \right) P \right] \\ & + \frac{1}{2} D_{\varphi^I} D_{\varphi^J} (A^{QQIJ} P) + D_{\varphi^I} \partial_{\varpi_J} (A^{Q\tilde{P}I}{}_J P) + \frac{1}{2} \partial_{\varpi_I} \partial_{\varpi_J} (A^{\tilde{P}\tilde{P}}{}_{IJ} P), \end{aligned}} \quad (1.4)$$

with D_{φ^I} a phase-space covariant derivative defined by its action on field-space vectors: $D_{\varphi^I} \mathcal{U}^J = \nabla_I \mathcal{U}^J + \Gamma_{IL}^K \varpi_K \partial_{\varpi_L} \mathcal{U}^J$, where ∇_I is the usual field-space covariant derivative. Under a slow-varying approximation, we further provide some analytical estimates for the noise properties in eqs. (5.16)–(5.18).

2 Stochastic formalism: heuristic approach

In this section we introduce the concepts and definitions used throughout the paper, by showing a heuristic derivation, made at the level of the classical equations of motion, of the

Langevin equations in the general class of multifield models described by the action (1.1). Our analysis is valid beyond the test approximation, i.e. it takes into account the backreaction of the scalar fields on the spacetime metric. Moreover, we do so using a phase-space Hamiltonian language, without assuming any slow-roll regime (see, e.g., refs. [102, 129–132, 157–168] for previous works on the subject, albeit not in this general multifield context, and sometimes with different results and approaches). Eventually, we highlight the limitations of this heuristic approach, and stress the non-Markovian character of the IR dynamics.

2.1 Generalities and ADM formalism

The general action of several scalar fields minimally coupled to gravity that we consider is given by

$$S = \int d^4x \sqrt{-g} \left[\frac{1}{2} M_{\text{Pl}}^2 \mathcal{R} - \frac{1}{2} g^{\mu\nu} G_{IJ}(\phi) \partial_\mu \phi^I \partial_\nu \phi^J - V(\phi) \right]. \quad (2.1)$$

Here $\mathcal{R}$ is the Ricci scalar associated with the spacetime metric $g_{\mu\nu}$, G_{IJ} denotes the metric of the field space, curved in general, spanned by the scalar fields ϕ^I , and $V(\phi)$ denotes the scalar potential. In the ADM formalism [85, 169], the spacetime metric is written in the form

$$ds^2 = -\mathcal{N}^2 dt^2 + \gamma_{ij} (dx^i + \beta^i dt)(dx^j + \beta^j dt), \quad (2.2)$$

where $\mathcal{N}$ is the lapse function, β^i is the shift vector, and γ_{ij} is the spatial metric. The action (2.1) then reads $S = \int dt d^3x \mathcal{L}$ with the Lagrangian density

$$\mathcal{L} = \mathcal{N} \sqrt{\gamma} \left[\frac{M_{\text{Pl}}^2}{2} (\mathcal{R}^{(3)} + K_{ij} K^{ij} - K^2) + \frac{1}{2\mathcal{N}^2} G_{IJ} v^I v^J - \frac{1}{2} G_{IJ} \gamma^{ij} \partial_i \phi^I \partial_j \phi^J - V \right], \quad (2.3)$$

where $\gamma = \det(\gamma_{ij})$ and $\mathcal{R}^{(3)}$ is the Ricci curvature of the spatial hypersurfaces. Here, spatial indices are lowered and raised with γ_{ij} and its inverse γ^{ij} ,

$$K_{ij} = \frac{1}{2\mathcal{N}} \left(2\beta_{(i|j)} - \dot{\gamma}_{ij} \right), \quad (2.4)$$

is the extrinsic curvature of spatial slices (where dots denote time derivatives, the symbol $|$ denotes the spatial covariant derivative associated with the spatial metric γ_{ij} , and parentheses signal symmetrisation), and one has

$$v^I = \dot{\phi}^I - \beta^i \partial_i \phi^I. \quad (2.5)$$

The Lagrangian (2.3) does not depend upon the time derivatives of $\mathcal{N}$ and β^i . This shows that the lapse function and the shift vector are not dynamical variables, and that the only dynamical variables are ϕ^I and γ_{ij} whose canonically conjugate momenta are given by

$$\pi_I = \frac{\delta \mathcal{L}}{\delta \dot{\phi}^I} = \frac{\sqrt{\gamma}}{\mathcal{N}} G_{IJ} v^J, \quad (2.6)$$

$$\pi^{ij} = \frac{\delta \mathcal{L}}{\delta \dot{\gamma}_{ij}} = \frac{M_{\text{Pl}}^2}{2} \sqrt{\gamma} (K \gamma^{ij} - K^{ij}). \quad (2.7)$$

The Hamiltonian density is given by the Legendre transform $\mathcal{H} = \pi_I \dot{\phi}^I + \pi^{ij} \dot{\gamma}_{ij} - \mathcal{L}$, or equivalently the action can be written in a Hamiltonian form as (see e.g. ref. [170] for the single-field case)

$$S = \int d^4x \left[\pi_I \dot{\phi}^I + \pi^{ij} \dot{\gamma}_{ij} - \mathcal{H} \right], \quad (2.8)$$

where

$$\mathcal{H} = \sqrt{\gamma} \left(\mathcal{N}C + \beta^i C_i \right), \quad (2.9)$$

and the so-called constraints read

$$C \equiv \frac{2}{\gamma M_{\text{Pl}}^2} \left[\pi_{ij} \pi^{ij} - \frac{1}{2} \left(\pi_i^i \right)^2 \right] - \frac{M_{\text{Pl}}^2}{2} \mathcal{R}^{(3)} + \frac{1}{2\gamma} G^{IJ} \pi_I \pi_J + G_{IJ} \frac{\gamma^{ij}}{2} \partial_i \phi^I \partial_j \phi^J + V, \quad (2.10)$$

$$C_i \equiv -2 \left(\frac{\pi_i^j}{\sqrt{\gamma}} \right)_{|j} + \frac{1}{\sqrt{\gamma}} \pi_I \partial_i \phi^I = \frac{1}{\sqrt{\gamma}} \left(-2\partial_k \left(\gamma_{ij} \pi^{jk} \right) + \pi^{jk} \partial_i \gamma_{jk} + \pi_I \partial_i \phi^I \right). \quad (2.11)$$

The Hamilton equations $\dot{\gamma}_{ij} = \frac{\delta}{\delta \pi^{ij}} \left(\int d^3x \mathcal{H} \right)$ and $\dot{\pi}^{ij} = -\frac{\delta}{\delta \gamma_{ij}} \left(\int d^3x \mathcal{H} \right)$ give the dynamical parts of the Einstein equations, whose explicit form will not be needed in what follows, while the variation with respect to the lapse and shift enforce the energy and momentum constraints

$$C = C_i = 0. \quad (2.12)$$

Eventually, Hamilton equations in the scalar sector can be written in the compact form

$$\dot{\phi}^I = \frac{\mathcal{N}}{\sqrt{\gamma}} G^{IJ} \pi_J + \beta^i \partial_i \phi^I, \quad (2.13)$$

$$\mathcal{D}_t \pi_I = -\sqrt{\gamma} \mathcal{N} V_I + \mathcal{D}_i \left(\sqrt{\gamma} \mathcal{N} G_{IJ} \gamma^{ij} \partial_j \phi^J \right) + \mathcal{D}_i \left(\beta^i \pi_I \right). \quad (2.14)$$

Here $V_I = \partial V / \partial \phi^I$, while $\mathcal{D}_t$ and $\mathcal{D}_i$ are field-space covariant spacetime derivatives, whose actions on field-space vectors $\mathcal{U}^I$ and covectors $\mathcal{V}_I$ read

$$\mathcal{D}_\mu \mathcal{U}^I = \partial_\mu \mathcal{U}^I + \Gamma_{JK}^I \left(\partial_\mu \phi^J \right) \mathcal{U}^K, \quad \mathcal{D}_\mu \mathcal{V}_I = \partial_\mu \mathcal{V}_I - \Gamma_{IJ}^K \left(\partial_\mu \phi^J \right) \mathcal{V}_K, \quad \text{with } \mu \in \{t, i\}, \quad (2.15)$$

and where Γ_{JK}^I are the Christoffel symbols associated with the field-space metric G_{IJ} .

2.2 Gauge choice and smoothing procedure

In the stochastic framework, all fields (actual scalar fields as well as the spacetime metric) are divided into a classical IR component and a quantum UV component, which are the counterparts of respectively the background and the fluctuations in standard perturbation theory (SPT). An important difference between the two setups is that the fields' IR components have large-scale fluctuations, which is nothing else than what the stochastic theory aims at describing. Hence, gauge issues, which usually only concern the equivalent of the UV part, also apply to the IR sector. As standard in stochastic inflation, we will deal with fluctuations of scalar type only, letting aside vector and tensor perturbations for our purpose here, something that is not restrictive as we elaborate on below.

A convenient gauge to study multifield inflation in SPT is the spatially flat gauge, in which all genuine (scalar type) fluctuating degrees of freedom are in the scalar fields. The same holds true in the stochastic context, and we will use the scalar gauge freedom so that spatial slices are homogeneous, with no fluctuation, neither on small nor on large scales. In what we can call the *stochastic spatially flat gauge*, we thus have

$$\gamma_{ij}(N, \mathbf{x}) = a^2(N) \delta_{ij} \quad \text{and} \quad a(N) \propto e^N, \quad (2.16)$$

where a is spatially constant, and we choose to work with the time variable N such that $N = \ln(a)$ up to an arbitrary constant. This choice is convenient and conceptually relevant

(see refs. [86, 88, 165]). In the same manner as in SPT, in this gauge, the local number of e -folds of expansion computed in each (super)-Hubble patch is then identical [85, 88], and simply coincides with N . Saying it otherwise, neglecting any shear component that are suppressed on large scales in standard situations, the flat gauge coincides with the uniform- N gauge. This way, the stochastic formalism enables one to determine how the inhomogeneities of the scalar fields evolve in different patches, with a local clock that is deterministic and shared by all patches. We will not do this in this paper, but this implies that we can, at least in principle, easily use our results in the framework of the stochastic- δN formalism to deduce the properties of the large-scale curvature perturbation ζ (see, e.g., refs. [89–95]).¹ In the stochastic spatially flat gauge, covariant spatial derivatives reduce to usual ones, the curvature of spatial slices $\mathcal{R}^{(3)}$ vanishes, and $\sqrt{\gamma} = a^3$. To simplify equations, we also *rescale momenta*, $\pi_I \rightarrow a^3 \pi_I$, which we will use from now on and for the rest of this paper.

Let us now discuss the smoothing procedure splitting any quantity between its IR and UV components, first in the simpler context of quantum field theory in a fixed de Sitter background. For each quantity written in Fourier space as $X(N, \mathbf{x}) = \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} X(N, \mathbf{k})$, its IR component is defined by coarse-graining as

$$X_{\text{IR}}(N, \mathbf{x}) = \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} W\left(\frac{k}{k_\sigma(N)}\right) X(N, \mathbf{k}), \quad (2.17)$$

with some window function W such that $W \simeq 1$ when its argument is small, and $W \simeq 0$ when its argument is large, i.e., smearing out short-wavelength modes $k > k_\sigma(N) \equiv \sigma a(N)H$, corresponding to a constant smoothing physical scale $\lambda_s = (\sigma H)^{-1}$. In this context, $\sigma \ll 1$ is a small parameter ensuring that the smoothing scale is somewhat larger than the Hubble scale — allowing for a gradient-, i.e., a σ -expansion — and therefore that the infrared component can be considered as classicalised. As usual in physics, the details of this coarse-graining procedure should not affect physical observables, i.e. in this context, the properties of fluctuations on physical scales $\lambda \gg \lambda_s$. Like in the context of the renormalisation group, a smooth window function seems physically motivated and desirable. However, this comes in general at the expense that the resulting description involves colored noises [124, 125, 171], which are more difficult to handle analytically than white noises. In this paper, we will conservatively use the simpler choice of a sharp window function $W(x) = \theta(1 - x)$, which is largely used in the literature. This has the advantage of being intuitive, and this will enable us to use the well-developed machinery of stochastic differential equations with white noises. However, as we will see in section 4, in the path-integral approach in which short-wavelength fluctuations are integrated out, special attention has to be paid to the integration measure's split into IR and UV sectors [129, 130, 132, 161].

For notational simplicity, we will also write $k_\sigma(N) = \sigma a(N)H$ in the case of scalar fields backreacting on spacetime, although the time-dependent Hubble scale H is not defined *a priori* in such a stochastic context, but should emerge as an IR quantity itself. One will find

¹Anticipating somewhat on following elements of the paper, let us mention that this important fact holds even when taking into account the tensor and vector modes. First, at quadratic order in the action as considered in the paper, the UV parts of the tensor and vector modes are decoupled from the UV parts of the scalar ones. More importantly, the tensor degrees of freedom, properly defined non-perturbatively in a way that they do not affect the spatial volume element, are such that at leading-order in the gradient expansion, their IR parts are time-independent and locally homogeneous in each σ -Hubble patch (while the vector modes vanish). Hence, they can be transformed away by a choice of spatial coordinates. This does not affect neither the local Hubble parameter, nor the proper time [88], and thus our time variable N is a local clock that is deterministic and shared by all patches, despite the existence of large-scale tensor fluctuations.

indeed that the quantity $1/\mathcal{N}_{\text{IR}}$ plays the role of a “local Hubble parameter” (see eq. (2.26)), in agreement with the literature in SPT [88]. One can thus imagine self-consistently defining the smoothing scale such that eq. (2.17) is verified for $X = \mathcal{N}$ with $k_\sigma = \sigma a/\mathcal{N}_{\text{IR}}$. We will not consider further this slight ambiguity, that is also present in single-field inflation while not being addressed in the literature to the best of our knowledge, and simply assume that the smoothing scale can be defined at least implicitly through a procedure similar to the one suggested above.

2.3 Stochastic equations

We now decompose the scalar fields and the metric components into IR and UV parts as

$$\begin{cases} \phi^I = \varphi^I + Q^I, & \pi_I = \varpi_I + P_I = \varpi_I + \tilde{P}_I + \Gamma_{IJ}^K \varpi_K Q^J, \\ \mathcal{N} = \mathcal{N}_{\text{IR}} + \mathcal{N}_{\text{UV}}, & \beta^i = a^{-2} \delta^{ij} \partial_j \psi, \end{cases} \quad (2.18)$$

where φ^I , ϖ_I , and $\mathcal{N}_{\text{IR}}$ are IR quantities, and one can fix $\beta_{\text{IR}}^i = 0$ as it is a pure gauge choice in the long-wavelength limit. The second term in the decomposition of π_I , where Γ_{IJ}^K is evaluated at the infrared values of fields φ^I , may seem arbitrary, but it ensures that the UV quantity $\tilde{P}_I$ transforms at linear order in a covariant manner under field redefinitions, as we prove in section 4.2

In the heuristic stochastic approach, one simply substitutes the decomposition (2.18) into the original EoM (2.13) and (2.14), keeping all nonlinearities in the IR sector — albeit working at leading-order in the gradient expansion — but keeping only linear terms in UV quantities. One thus obtains

$$\varphi^{I'} = \frac{1}{H} G^{IJ} \varpi_J + \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} \left[W' \left(\frac{k}{k_\sigma} \right) \phi^I(N, \mathbf{k}) + \left(1 - W \left(\frac{k}{k_\sigma} \right) \right) E^{QI}(N, \mathbf{k}) \right], \quad (2.19)$$

and

$$\begin{aligned} \mathcal{D}_N \varpi_I = -3\varpi_I - \frac{1}{H} V_I + \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} & \left[W' \left(\frac{k}{k_\sigma} \right) \left(\pi_I(N, \mathbf{k}) - \Gamma_{IJ}^K \varpi_K \phi^J(N, \mathbf{k}) \right) \right. \\ & \left. + \left(1 - W \left(\frac{k}{k_\sigma} \right) \right) E_I^{\tilde{P}}(N, \mathbf{k}) \right], \end{aligned} \quad (2.20)$$

where a prime $'$ denotes a simple derivative with respect to N and we denote the covariant time derivative $\mathcal{D}_N \varpi_I = \partial_N \varpi_I - \Gamma_{IJ}^K \varphi^{J'} \varpi_K$ — covariant with respect to field redefinitions of the IR fields — by the same symbol $\mathcal{D}_N$ as in the fully nonlinear eq. (2.15) for simplicity. Here, E^{QI} and $E_I^{\tilde{P}}$, whose expressions are given below in eqs. (2.28) and (2.29), stand for the linearised EoM in Fourier space, and the expression of $H \equiv 1/\mathcal{N}_{\text{IR}}$ in terms of φ^I and ϖ_I will be given in eq. (2.26).

In SPT, which one formally recovers in the limit $k_\sigma \rightarrow 0$, one assumes that the dynamics of fluctuations decouples from the one of the background, in which case one has $E^{QI} = E_I^{\tilde{P}} = 0$. The terms in W' vanish in this limit and thus each of the equations (2.19) and (2.20) splits into two parts, one for the background and one for the fluctuations. In the heuristic approach to stochastic inflation, one still assumes that UV fluctuations obey the same evolution equations $E^{QI} = E_I^{\tilde{P}} = 0$ as in SPT. However, due to the time-dependence of the coarse-graining scale $k_\sigma(N)$, the IR dynamics is affected by the flow of UV modes joining

the IR sector, an effect described by the terms involving the time-derivative of the window function, W' . Thus writing

$$\xi^{QI}(x) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} W' \left(\frac{k}{k_\sigma(N)} \right) Q^I(N, \mathbf{k}), \quad \xi_I^{\tilde{P}}(x) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} W' \left(\frac{k}{k_\sigma(N)} \right) \tilde{P}_I(N, \mathbf{k}), \quad (2.21)$$

one obtains the desired effective equations of motion for infrared fields and momenta,

$$\varphi^{I'} = \frac{1}{H} G^{IJ} \varpi_J + \xi^{QI}, \quad \mathcal{D}_N \varpi_I = -3\varpi_I - \frac{1}{H} V_I + \xi_I^{\tilde{P}}, \quad (2.22)$$

the so-called Langevin equations. In this description, one assumes that the UV quantities $Q^I(N, \mathbf{k})$ and $\tilde{P}_I(N, \mathbf{k})$, which in fact are quantum operators, can be described classically as they join the IR sector at the time $N_\sigma(k)$ such that $k = k_\sigma(N_\sigma(k))$. Hence, the ξ 's can be interpreted as classical random noises, and when computing their statistical properties, one identifies ensemble averages with expectation values of the corresponding operators in the quantum vacuum state of the theory. As we treat UV fluctuations at linear order, one can consider that the ξ 's obey a Gaussian statistics, with zero mean and fully characterised by their two-points correlations. In the case of the sharp window function $W(x) = \theta(1 - x)$, the latter can be easily computed and are directly related to the power spectra of the UV fluctuations when they reach the coarse-graining scale:

$$\langle \xi^{\tilde{X}I}(x) \xi^{\tilde{Y}J}(x') \rangle = \underbrace{\mathcal{P}^{\tilde{X}\tilde{Y}IJ}(N, k_\sigma(N)) \frac{k'_\sigma}{k_\sigma} \frac{\sin k_\sigma r}{k_\sigma r}}_{A^{\tilde{X}\tilde{Y}IJ}(N)} \delta(N - N'), \quad (2.23)$$

where $r = |\mathbf{x} - \mathbf{x}'|$ is the comoving distance between the spacetime points x and x' , and with the dimensionless power spectra $\mathcal{P}$ such that

$$\langle Q^{\tilde{X}I}(N, \mathbf{k}) Q^{\tilde{Y}J}(N, \mathbf{k}') \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k} + \mathbf{k}') \frac{2\pi^2}{k^3} \mathcal{P}^{\tilde{X}\tilde{Y}IJ}(N, k). \quad (2.24)$$

Here, we used a condensed notation adapted to our phase-space description where $\tilde{X} = (Q, \tilde{P})$ refers both to UV fields and covariant momenta, i.e. $\xi^{\tilde{X}I} = (\xi^{QI}, \xi_I^{\tilde{P}} = G^{IJ}(\varphi) \xi_J^{\tilde{P}})$ and $Q^{\tilde{X}I} = (Q^I, \tilde{P}^I = G^{IJ}(\varphi) \tilde{P}_J)$. The auto-correlation of the noises $A^{\tilde{X}\tilde{Y}IJ}$ is a contravariant rank-2 tensor since it inherits the transformation properties of the UV modes $(Q^I, \tilde{P}^I)$. Because of the presence of the delta function $\delta(N - N')$ coming from the time derivative of the step window function, the ξ 's can be regarded as white noises. This property would not hold true had we chosen a smooth window function. Notice also that the noise correlations (2.23) are proportional to $k'_\sigma/k_\sigma \times \sin k_\sigma r/k_\sigma r$. First, the ratio $k'_\sigma/k_\sigma = 1 - \epsilon$ in eq. (2.23), with ϵ in eq. (2.33), may be approximated by unity. Indeed, this slow-roll correction is likely to be too precise for the accuracy of the coarse-graining procedure, and other authors also proposed considering a slightly time-dependent parameter σ such that σH is exactly constant [57]. Second, the precise form $\sin k_\sigma r/k_\sigma r$ of the apparent spatial correlation in the noises' two-point function depends on the choice of the window function W . However, since we neglected any spatial dependence of the IR fields, this oscillating and decaying term should only be understood as a step theta function $\theta(1 - k_\sigma r)$ taking values 1 inside a “ σ -Hubble patch” and 0 outside, in agreement with the separate universe approach. The ξ 's can thus be understood as k_σ -patch-independent Brownian noises, the evolution of each σ -Hubble patch

being determined only by the local physics. In this paper we will discuss only one-point statistics (one “ σ -Hubble patch” statistics to be accurate), the idea being that starting from one progenitor σ -Hubble patch, the observable universe at the end of inflation is made of many σ -Hubble patches that emerge from the same initial condition. Hence, by ergodicity, the ensemble average of the stochastic evolution of one σ -Hubble patch can also be seen as the spatial average among these σ -Hubble patches. Moreover, the study of the one-point statistics is not as restrictive as it may seem, and it is actually possible to extract detailed spatial information from it. Indeed, any two σ -Hubble patches initially share the same dynamics, until they become separated by the physical distance $(\sigma H)^{-1}$ and subsequently evolve independently. Using this time-scale correspondence, Starobinsky and Yokoyama have shown in ref. [57] how, once the Fokker-Planck operator for the one-point probability density function (PDF) is known, one can determine the evolution equation for the two-point PDF, or even any n -point PDF (at different spatial and temporal locations), and thus, at least in principle, retrieve all the statistical information (see, e.g., [172–174] for recent applications).² This logic is also put to good use in the stochastic- δN approach, with which one can compute Fourier space correlation functions of the observable large-scale curvature perturbation ζ (and not only statistics of the inflationary fields) (see, e.g., refs. [89–95]).

Eventually, note that first-principles methods to compute the power spectra will be reviewed in section 3.2, and that analytical estimates will be discussed in section 5. Before explaining in section 2.5 why this heuristic approach to stochastic inflation is not fully satisfactory, let us now fill in the gaps in the above description by characterising the dynamics of the UV fluctuations.

2.4 Dynamics of UV fluctuations

First, one needs to relate the perturbations of the non-dynamical parts of the metric, $\mathcal{N}_{\text{UV}}$ and ψ , to the genuine degrees of freedom: the UV parts of the scalar fields and momenta Q^I and $\tilde{P}_I$. For this, it is important to notice that the energy and momentum constraints (2.12) contain no time derivative. Hence, contrary to the Hamilton equations (2.19) and (2.20), no explicit noise enters in their IR/UV decomposition, and they can be straightforwardly split into independent equations on large and small scales.

The momentum constraint gives no information on large scales, in agreement with the fact that all choices of threadings are equivalent at leading-order in the gradient expansion, while the small scale component gives the expression of $\mathcal{N}_{\text{UV}}$:

$$\mathcal{N}_{\text{UV}} = \frac{\varpi_I Q^I}{2M_{\text{Pl}}^2 H^2}. \quad (2.25)$$

As for the energy constraint, its long-wavelength limit is non-trivial and is equivalent to the first Friedmann equation, while the small scale part relates ψ to $\mathcal{N}_{\text{UV}}$ and $Q^I, \tilde{P}_I$:

$$\frac{3M_{\text{Pl}}^2}{\mathcal{N}_{\text{IR}}^2} \equiv 3M_{\text{Pl}}^2 H^2 = \frac{1}{2} G^{IJ} \varpi_I \varpi_J + V, \quad (2.26)$$

$$2M_{\text{Pl}}^2 H^2 \frac{k^2}{a^2} \psi = \varpi_I \tilde{P}^I + V_I Q^I + 6M_{\text{Pl}}^2 H^3 \mathcal{N}_{\text{UV}}. \quad (2.27)$$

²Naturally, given the hard cutoff in the spatial correlations of the stochastic noises, spatial correlations can be reliably computed only when the relevant length scales are well above H^{-1} , but that is overwhelmingly the case for observationally relevant scales.

The equation (2.26) confirms that $1/\mathcal{N}_{\text{IR}}$ plays the role of a local Hubble parameter, with the usual Friedmann constraint holding in each k_σ -patch. In this respect, note that if one converts ϖ_I to φ^{II} with use of the IR EoM (2.22), the Friedmann equation would include an explicit noise term. This demonstrates the conceptual advantage of the Hamiltonian language over the Lagrangian one in the stochastic formalism.

Equipped with the constraints (2.25) and (2.27), one can express E^{QI} and $E_I^{\tilde{P}}$ in the condensed form:

$$E^{QI}(N, \mathbf{k}) = -\mathcal{D}_N Q^I(N, \mathbf{k}) + \frac{\tilde{P}^I(N, \mathbf{k})}{H} + M_{\tilde{P}Q}^2{}^I{}_J Q^J(N, \mathbf{k}), \quad (2.28)$$

$$E_I^{\tilde{P}}(N, \mathbf{k}) = -\mathcal{D}_N \tilde{P}_I(N, \mathbf{k}) - 3\tilde{P}_I(N, \mathbf{k}) - \frac{k^2}{a^2 H} Q_I(N, \mathbf{k}) - \frac{1}{H} M_{QIJ}^2 Q^J(N, \mathbf{k}) - M_{Q\tilde{P}I}^2{}^J \tilde{P}_J, \quad (2.29)$$

where indices are lowered and raised with the IR metric in field space $G_{IJ}(\varphi)$ and its inverse, and

$$M_{QQIJ}^2 = V_{;IJ} - R_I{}^{KL}{}_J \varpi_K \varpi_L + \frac{1}{2M_{\text{Pl}}^2 H} (V_I \varpi_J + \varpi_I V_J) + \frac{3\varpi_I \varpi_J}{2M_{\text{Pl}}^2}, \quad (2.30)$$

$$M_{Q\tilde{P}IJ}^2 = M_{\tilde{P}QIJ}^2 = \frac{\varpi_I \varpi_J}{2M_{\text{Pl}}^2 H^2}, \quad (2.31)$$

with $V_{;IJ} \equiv \nabla_J V_I = V_{,IJ} - \Gamma_{IJ}^K V_K$ the covariant Hessian of the potential, and $R^S{}_{IJK} \equiv \Gamma_{IK,J}^S - \Gamma_{IJ,K}^S + \Gamma_{IK}^R \Gamma_{JR}^S - \Gamma_{IJ}^R \Gamma_{KR}^S$ the Riemann tensor of the field space. To obtain the expressions (2.28)–(2.29), and in accordance with treating the UV modes linearly, we have simplified the infrared “coefficients” by neglecting the noise terms in eq. (2.22), and similarly, we used $E^{QI} = 0$ in eq. (2.29). As expected, the equations $E^{QI} = E_I^{\tilde{P}} = 0$ are equivalent to the EoM for linear perturbations in SPT [86], with background fields replaced by IR ones, i.e. their combination gives

$$\mathcal{D}_N^2 Q^I + (3 - \epsilon) \mathcal{D}_N Q^I + \left(\frac{k^2}{a^2 H^2} \delta_J^I + \frac{M^{2I}{}_J}{H^2} \right) Q^J = 0, \quad (2.32)$$

where (consistently neglecting noise terms in the second equality)

$$\epsilon \equiv -\frac{H'}{H} = \frac{\varpi_I \varpi^I}{2M_{\text{Pl}}^2 H^2}, \quad (2.33)$$

and the mass matrix reads

$$M^{2I}{}_J = V^I{}_{;J} - R^{IKL}{}_J \varpi_K \varpi_L - \frac{H}{a^3 M_{\text{Pl}}^2} \mathcal{D}_N \left(\frac{a^3}{H} \varpi^I \varpi_J \right). \quad (2.34)$$

2.5 Limitations of the heuristic approach

Although qualitatively satisfying, the above heuristic approach to stochastic inflation suffers from a number of technical and conceptual issues.

- When going from eqs. (2.19)–(2.20) to (2.21), we attributed $\phi^I(N, k_\sigma(N))$, the Fourier component of the full field at the transition time, to the UV part Q^I (and similarly for momenta), in a rather arbitrary manner.

- We assumed that the UV modes obey $E^{QI} = E_I^{\tilde{P}} = 0$, i.e. the same equations as in standard perturbation theory with background fields replaced by IR ones.
- Despite the fact that φ^I and ϖ_I are real, the noise correlation $\langle \xi^{QI} \xi^{\tilde{P}J} \rangle$ has an imaginary component, owing to the fact that the quantum operators $Q^I(N, k_\sigma(N))$ and $\tilde{P}^I(N, k_\sigma(N))$ do not commute. To interpret eq. (2.22) as proper real stochastic equations, one has to replace by hand $\langle \xi^{QI} \xi^{\tilde{P}J} \rangle \rightarrow \frac{1}{2} (\langle \xi^{QI} \xi^{\tilde{P}J} \rangle + \langle \xi^{\tilde{P}J} \xi^{QI} \rangle) = \text{Re} [\langle \xi^{QI} \xi^{\tilde{P}J} \rangle]$, i.e. to take the (real) vev of hermitian operators only (see e.g. ref. [162]).³
- In addition to these difficulties, there remains an ambiguity in the treatment of stochastic differential equations of the type (2.22) as the continuous limit of discrete processes. In a previous letter [95], we emphasised the role of such discretisations and unveiled the presence of *inflationary stochastic anomalies*, potentially inducing spurious frame dependences or breaking the covariance of the theory.

All these difficulties are related and motivates a careful treatment of quantum aspects of the problem. First, in section 3, we will discuss and solve the issue of the aforementioned stochastic anomalies. Critical to this resolution is the identification of *independent* Gaussian white noises — as required from a proper mathematical treatment of stochastic differential equations — in one-to-one correspondence with the *independent* quantum creation and annihilation operators necessary for the quantisation of the UV modes. Second, in section 4, we solve the other difficulties related to IR/UV interactions by working at the level of the action and integrating out the quantum UV modes in the closed-time-path formalism. We do so paying a particular attention to issues of covariance and, following refs. [130, 132], to the integration measure’s split into IR and UV sectors. Notably, the fact that UV modes become IR, but not the reverse, entails the existence of fluctuations without dissipation, in contrast to ordinary open systems.

2.6 To be or not to be Markovian

Here we would like to stress an ever-present subtlety, be it in the heuristic approach or in a proper quantum field theory treatment. It lies in the fact that the effective dynamics of the coarse-grained scalar fields is strictly speaking non-Markovian (see, e.g., refs. [175–183] for related discussions in various areas of physics). For the equations (2.22) to describe a Markov process, characterised by the absence of memory, one would need the statistical properties of the noises to be a function of the infrared variables (φ^I, ϖ_I) at current time N . However, the power spectra of the UV modes (2.24), or in a related manner their mode functions, are not even functions of the IR variables. They are simply solutions of the differential equations (2.28) and (2.29), whose “coefficients” depend on the IR variables, and that are evaluated at time N for the mode with wave number $k_\sigma(N)$. Moreover, this effective “background” for the UV dynamics is described by coarse-grained fields whose values were affected by previous realisations of the noises. The dynamics described by such equations is thus very rich and complex.

In this respect, we would like to stress that the bulk of this paper as well as its main result (1.2)–(1.3) do not involve any Markovian approximation, as our emphasis is on the first-

³This problem is not present for the $\xi^Q \xi^Q$ and $\xi^{\tilde{P}} \xi^{\tilde{P}}$ correlations which are real, as the (real space) Q^I (and the $\tilde{P}^I$ separately) are hermitian operators that commute with one another at equal times, see also eqs. (3.14) and (3.15).

principle derivation of these manifestly covariant equations. This means that our Langevin-type equations can be in principle solved numerically together with the dynamics of the UV modes dictating the noise properties. They can also serve as a basis for future analytical works, and in this context, it can be convenient to resort to the Markovian approximation, at the expense for instance of assuming some slow-varying regime. We discuss such analytical estimates in section 5. One of the advantage of the Markovian approximation is that one can then write a Fokker-Planck (FP) equation for the (one-point) probability density function of the IR fields and momenta, with the result (5.1). Such an equation is easier to handle numerically or analytically than the Langevin-type equations, and indeed covariance is even more manifest with such a formulation. However, we stress again that our main results hold more generally.

3 Stochastic anomalies and their solution

A generic difficulty in the description of stochastic processes is that stochastic equations like the one (2.22) are not mathematically defined unless specifying their discretisation schemes (see e.g. refs. [184, 185]). In particular, in our context, different choices of discretisations (among which Itô and Stratonovich are the most famous ones) can lead to a violation of the EoM's covariance, and/or an unphysical noise-frame dependence as we pointed out previously [95]. We first review such *stochastic anomalies* in section 3.1. To make the physics easier to grasp, we sometimes restrict ourselves to the particular case of a Markov process. Indeed, this enables one to write the so-called Fokker-Planck equation, corresponding to the Langevin equations with a no-memory noise, that dictates the deterministic evolution of the probability density function for the IR fields and their momenta. We then explain in section 3.2 why the particular framework of stochastic inflation, where the classical stochastic noise emerges from a quantum field theory description, provides us with a preferred frame for the reduction of the noise auto-correlation matrix: the one of independent creation and annihilation quantum operators. Stochastic anomalies are thus solved when interpreting the Langevin equations (2.22) with this particular choice of frame and in the Stratonovich scheme. However, this resolution is rather formal and in order to make it more explicit, we introduce *stochastically-parallel-transported vielbeins* in section 3.3. Strikingly, with the use of such vielbeins, the Langevin equations (2.22) interpreted in the Stratonovich scheme can be recast in the form (3.33) interpreted in the Itô scheme, featuring covariant derivatives adapted to Itô calculus. These equations constitute one of the main results of this paper: they are manifestly covariant, readily adapted to numerical implementations, and when supplemented with a Markovian approximation, they lead to the phase-space Fokker-Planck equation (5.1).

3.1 Ambiguity of the discretisation scheme

A stochastic differential equation (SDE), or equivalently its solution as a stochastic integral, is mathematically defined as the infinitesimal-step, continuous limit of a finite-step, discrete summation, in the same way that the Riemann integral is defined. From step i to step $i + 1$, the integrand must be evaluated at some time between times N_i and N_{i+1} , expressed as $(1 - \alpha)N_i + \alpha N_{i+1}$ with the parameter $0 \leq \alpha \leq 1$. The Riemann integral of differential functions is independent of this discretisation choice of α in the continuous limit. However, due to the non-differentiability of the stochastic noise, the stochastic integral does depend on α . Conveniently for our purpose, let us explain these subtleties in a situation where the stochastic variables $\mathcal{X}^I$ are coordinates on a manifold, endowed with a metric whose components in these

coordinates are G_{IJ} (see appendix A for generic mathematical properties independently of this specific context). Let us further assume that the stochastic process under study is described by a deterministic drift h^I as well as noises' amplitudes $g_A^{\mathcal{X}I}$ that all transform as vectors under redefinitions of the coordinates $\mathcal{X}^I$, and such that the corresponding set of Langevin equations reads

$$\frac{d\mathcal{X}^I}{dN} = h^I + g_A^{\mathcal{X}I} \circ_\alpha \xi^A, \quad \langle \xi^A(N) \xi^B(N') \rangle = \delta^{AB} \delta(N - N'), \quad \delta^{AB} g_A^{\mathcal{X}I} g_B^{\mathcal{X}J} = A^{\mathcal{X}XIJ}, \quad (3.1)$$

together with a specified discretisation scheme α represented by the symbol $\circ_\alpha$. Here $A^{\mathcal{X}XIJ}$ stands for the auto-correlation of the effective noises $\xi^I = g_A^{\mathcal{X}I} \xi^A$, i.e. $\langle \xi^I(N) \xi^J(N') \rangle = A^{\mathcal{X}XIJ} \delta(N - N')$, and transforms as a rank-2 tensor under coordinate transformations.⁴ It is important to understand that prescribing this auto-correlation is not sufficient to define the corresponding SDE, but that one needs to specify the full set of $g_A^{\mathcal{X}I}$'s, i.e. the decomposition of the ξ^I 's onto a set of independent noises ξ^A , what we may call in what follows an orthonormal frame for the noises. The setup (3.1) encapsulates the specific case of stochastic inflation when momenta are neglected (although a decomposition into independent noises ξ^A has not been identified yet), i.e., only the first of the Langevin equations (2.22) is considered here. We do so to simplify the presentation, but the discussion will be extended next to the more general setup of Langevin equations in phase space.

The simplest situation for such kind of SDE is when the noise amplitude $g_A^{\mathcal{X}I}$ is only a (deterministic) function of time, in which case the noise is called *additive*, and all discretisations have the same continuous limit. In the generic case however, the noise also depends on the stochastic variables $\mathcal{X}^I$ at time N , in which case it is called *multiplicative* and choices of discretisations matter. As we stressed in section 2.6, the stochastic equations for the coarse-grained scalar fields are even more complicated as, contrary to standard SDEs, the dependence of the noise on the stochastic variables is only indirect. This is the reason why we sometimes refer to them as Langevin-type equations. Despite this, let us begin by explaining the covariance issue in the simplest context of a Markovian description in which the $g_A^{\mathcal{X}I}$'s explicitly depend on $\mathcal{X}^I(N)$. In that case, there is a one-to-one correspondence between the Langevin equations (3.1) with a given discretisation scheme α and a Fokker-Planck partial differential equation for the transition probability from the initial state $\mathcal{X}_{\text{ini}}^I(N_{\text{ini}})$ to $\mathcal{X}^I(N)$, sometimes simply referred to as the probability density function (PDF) of the stochastic variables, $P(N; \mathcal{X}^I)$:

$$\partial_N P_s = -\nabla_I (h^I P_s) + \alpha \nabla_I \left[g_A^{\mathcal{X}I} \nabla_J (g_A^{\mathcal{X}J} P_s) \right] - \left(\alpha - \frac{1}{2} \right) \frac{1}{\sqrt{G}} \partial_I \partial_J (\sqrt{G} A^{\mathcal{X}XIJ} P_s). \quad (3.2)$$

Here, ∇_I is the usual field-space covariant derivative and we defined a rescaled PDF $P_s = P/\sqrt{G}$, with $G = \det(G_{IJ})$, where the subscript s indicates that it is a scalar under redefinition of the coordinates. From this expression, it is possible to identify two particular values of α . It is indeed possible to set to zero the second term in eq. (3.2) with the choice of a *pre-point*, $\alpha = 0$ discretisation, called the Itô scheme. Another interesting option is to keep this second term but to set to zero the third one by preferring a *midpoint*, $\alpha = 1/2$ discretisation,

⁴Notice that in this more general mathematical context, we label the noises' amplitudes $g_A^{\mathcal{X}I}$ and their auto-correlation $A^{\mathcal{X}XIJ}$ by the stochastic variables $\mathcal{X}^I$ that receive the stochastic kicks via the Langevin equation. This notation is slightly different from the one used in the specific multifield stochastic inflation context, where the noises' amplitudes $g_A^{\tilde{\mathcal{X}}I}$ and their auto-correlation $A^{\tilde{\mathcal{X}}\tilde{\mathcal{X}}IJ}$ are labeled by the UV modes $(Q^I, \tilde{P}^I)$ that are responsible for the stochastic kicks received by the IR fields (φ^I, ϖ^I) .

called the Stratonovich scheme. In the rest of this section, we will review the pros and cons of each of these two choices, keeping in mind that our derivation of the Langevin equations in the previous section did not come with any prescription for α , so at this stage one should discriminate between the possibilities of discretisation based on physical arguments.

3.1.1 Itô scheme

The Itô scheme, corresponding to $\alpha = 0$, is widely used in applied and computational mathematics because it has the advantage of expressing explicitly the stochastic variables at time N_{i+1} in terms of known values at N_i . Not only is it conceptually clear, but it is also easy to implement numerically, which explains its widespread use in various areas of science. However, this description seems to suffer from a fundamental issue in our context: in the Fokker-Planck (FP) equation (3.2), where the third term survives for $\alpha = 0$, only partial derivatives ∂_I appear, rather than covariant derivatives ∇_I . Thus, the FP equation as it is breaks covariance. More precisely, the problem is not that this equation is formulated in terms of non-covariant objects, i.e., that is not manifestly covariant, it is that it is not consistent with P_s being a scalar quantity.

Actually, this fundamental flaw can already be seen at the level of the Langevin-type equations, even when the process is not assumed to be Markovian. Indeed, the standard chain rule for the derivation of composite functions of the stochastic variables $\mathcal{X}^I$ does not hold in the Itô prescription, but gets corrected by the auto-correlation of the noise. This so-called Itô's lemma states that, under a change of variables $\mathcal{X}^I \rightarrow \bar{\mathcal{X}}^{\bar{I}} = \bar{\mathcal{X}}^{\bar{I}}(\mathcal{X}^I)$, the infinitesimal variations read [147]:

$$d\bar{\mathcal{X}}^{\bar{I}} = \frac{\partial \bar{\mathcal{X}}^{\bar{I}}}{\partial \mathcal{X}^I} d\mathcal{X}^I + \frac{1}{2} \frac{\partial^2 \bar{\mathcal{X}}^{\bar{I}}}{\partial \mathcal{X}^I \partial \mathcal{X}^J} A^{\mathcal{X}^I \mathcal{X}^J} dN. \quad (3.3)$$

We prove such kinds of exotic properties of stochastic calculus in appendix A and refer the interested reader to it. However the form of this lemma can be easily understood: a white noise is not a differentiable function because its infinitesimal variation $d\xi$ is proportional to $\sqrt{dN}$ rather than dN , thus $d\xi/dN$ diverges when $dN \rightarrow 0$. Therefore at order dN even the second derivative of $\mathcal{X}^I$ matters in the Taylor expansion (3.3). The conclusion is that the standard infinitesimal variation $d\mathcal{X}^I$ does not transform as a vector, contrary to the expectation for the infinitesimal variation of a coordinate on a manifold. Thus, although equations (3.1) and (2.22) are covariant under the standard chain rule, they are actually not if they are interpreted in the Itô sense, precisely because the standard chain rule is not verified. This fact forbids us to interpret the Langevin equations derived in the heuristic approach with the Itô scheme. However, covariance and Itô together are not doomed to fail, and it is actually possible to define covariant derivatives compatible with Itô calculus that compensate for the breaking of the standard chain rule. A possible such derivative for the coordinates $\mathcal{X}^I$ is given by

$$\mathfrak{D}\mathcal{X}^I = d\mathcal{X}^I + \frac{1}{2} \Gamma_{JK}^I A^{\mathcal{X}^J \mathcal{X}^K} dN, \quad (3.4)$$

which we show to transform as a vector in Itô calculus in appendix A.⁵ There we also derive Itô-covariant derivatives for vectors $\mathcal{U}^I$ and covectors $\mathcal{V}_I$ when they are subject to Langevin

⁵Related notions of Itô covariant derivatives have been discussed in the literature independently of the context of inflation in ref. [155].

equations with noises $g^{\mathcal{U}I}$ and $g^{\mathcal{V}}_I$:

$$\mathfrak{D}\mathcal{U}^I = \mathcal{D}\mathcal{U}^I + \frac{1}{2} \left(\Gamma^I_{JS,K} - \Gamma^M_{JS} \Gamma^I_{MK} \right) \mathcal{U}^S A^{\mathcal{X}JK} dN + \Gamma^I_{JK} A^{\mathcal{X}\tilde{U}JK} dN, \quad (3.5)$$

$$\mathfrak{D}\mathcal{V}_I = \mathcal{D}\mathcal{V}_I - \frac{1}{2} \left(\Gamma^S_{IJ,K} + \Gamma^M_{IJ} \Gamma^S_{KM} \right) \mathcal{V}_S A^{\mathcal{X}JK} dN - \Gamma^K_{IJ} A^{\mathcal{X}\tilde{V}J}_K dN, \quad (3.6)$$

where the quantities $A^{\mathcal{X}\tilde{U}IJ} = g^{\mathcal{X}I}_A g^{\tilde{U}J}_A$ and $A^{\mathcal{X}\tilde{V}I}_J = g^{\mathcal{X}I}_A g^{\tilde{V}J}_A$ are the cross-correlations between the coordinate noise $g^{\mathcal{X}I}_A$ and the covariant combinations of (co)vector noise:

$$g^{\tilde{U}I}_A = g^{\mathcal{U}I}_A + \Gamma^I_{JK} \mathcal{U}^J g^{\mathcal{X}K}_A, \quad g^{\tilde{V}I}_A = g^{\mathcal{V}I}_A - \Gamma^K_{IJ} \mathcal{V}_K g^{\mathcal{X}I}_A. \quad (3.7)$$

Note also that the difference between these Itô-covariant derivatives and usual covariant derivatives for vectors and covectors, $\mathcal{D}\mathcal{U}^I = d\mathcal{U}^I + \Gamma^I_{JK} \mathcal{U}^J d\mathcal{X}^K$ and $\mathcal{D}\mathcal{V}_I = d\mathcal{V}_I - \Gamma^J_{IK} \mathcal{V}_J d\mathcal{X}^K$, only contains terms proportional to noise amplitudes squared.

Had we obtained Langevin equations of the type (2.22) but with d and $\mathcal{D}$ replaced by $\mathfrak{D}$, then they would be covariant under field redefinitions (and induced redefinitions of momenta) if and only if, interpreted in Itô. Actually, we will see in section 3.3 that exactly these Itô-covariant derivatives emerge when interpreting our equations in the Stratonovich scheme, and reformulating them in the Itô-language. However for the moment, one should abandon the Itô scheme together with equations (2.22), as covariance would then be lost. Let us now discuss the second most popular discretisation.

3.1.2 Stratonovich scheme

The midpoint, or Stratonovich, discretisation corresponds to $\alpha = 1/2$. Physicists like it because it is intuitive to use in analytical calculations: as proved in appendix A, the standard chain rule applies, hence it is easy to check the covariance of a given equation and straightforward to perform changes of variables. Saying it more trivially: when physicists make “naive” computations by applying standard rules in a stochastic context, like what we did in section 2, they are implicitly using the Stratonovich scheme. As we can clearly see from the FP equation (3.2), it is the only choice that respects covariance. Again, this can be understood already at the level of Langevin equations, since because the standard chain rule applies, infinitesimal variations $d\varphi^I$ and $\mathcal{D}\varpi_I$ are well vectors and covectors of the field space. Nonetheless, although general covariance is respected, this description is not yet satisfactory. Indeed, when the noise is multiplicative (which it is in most interesting scenarios), the second term in eq. (3.2) depends explicitly on the identification of an orthonormal frame for the noises, through the appearance of $g^{\mathcal{X}I}_A$. However, the only outcome of our derivation for stochastic inflation so far has been the auto-correlation of the effective noises, for instance $\langle \xi^{QI}(N) \xi^{QJ}(N') \rangle = \frac{k_\sigma}{k_\sigma'} \mathcal{P}^{QQIJ}(k_\sigma) \delta(N - N')$ in a given σ -Hubble patch. Of course, it is always possible to reduce the auto-correlation matrix in a frame where it is diagonal, i.e. to find a “square-root matrix” $g^{\mathcal{X}I}_A$ verifying $\delta^{AB} g^{\mathcal{X}I}_A g^{\mathcal{X}J}_B = A^{\mathcal{X}IJ}$. However, such a frame is not unique, and an ambiguity remains: the physics described by the FP equation (3.2) depends on the choice of this frame. This is easily seen if, after a choice $g^{\mathcal{X}I}_A$, one performs a rotation to another orthonormal frame in which the noise is diagonal again, with an orthonormal matrix $R^{\tilde{B}}_A$ such that the “square-root matrix” of the noise correlations changes without affecting its auto-correlation: $g^{\mathcal{X}I}_A = R^{\tilde{B}}_A \tilde{g}^{\mathcal{X}I}_{\tilde{B}}$. Then, the second term in the FP equation transforms as $\nabla_I [g^{\mathcal{X}I}_A \nabla_J (g^{\mathcal{X}J}_A P_s)] = \nabla_I [R^{\tilde{B}}_A R^{\tilde{C}}_A \tilde{g}^{\mathcal{X}I}_{\tilde{B}} \nabla_J (\tilde{g}^{\mathcal{X}J}_{\tilde{C}} P_s)] + \nabla_I [R^{\tilde{B}}_A (\nabla_J R^{\tilde{C}}_A) \tilde{g}^{\mathcal{X}I}_{\tilde{B}} \tilde{g}^{\mathcal{X}J}_{\tilde{C}} P_s]$. Because the matrix R is orthonormal, $R^{\tilde{B}}_A R^{\tilde{C}}_A = \delta^{\tilde{B}\tilde{C}}$, the result would be frame-independent

if there was only the first of these two terms. However since R can depend on the position in field space, its (covariant) derivative is not zero and there is no reason in general for $R^{\bar{B}}_A (\nabla_J R^{\bar{C}}_A)$ to vanish, hence the frame-dependence of the result. Actually this difficulty holds for all discretisation schemes except when $\alpha = 0$, the Itô case where this second term in eq. (3.2) is killed. That also explains why the Itô scheme is often preferred in numerical implementations: it is possible to use an algorithm to reduce the noise correlation matrix in an orthonormal frame, and the result does not depend on the choice of such frame. However this apparently unsolvable ambiguity, breaking of covariance in Itô or spurious frame-dependence in Stratonovich, is solved by the understanding that in stochastic inflation there is actually a preferred frame in which the noise is diagonal, and that it is given by the basis of independent creation and annihilation operators of the quantum UV modes. This result has close links to the classicalisation of light scalar fields on super-Hubble scales as we shall see now.

3.2 Classicalisation and frame of independent creation and annihilation operators

As is well known in the context of multifield inflation (see e.g. refs. [186–189]), the quantum operators $\hat{Q}^I$ and $\hat{P}_I$ should be decomposed on a N_{fields} -dimensional set of independent creation and annihilation operators (labeled by the index A) as:

$$\begin{cases} \hat{Q}^I(N, \mathbf{k}) = Q^I_A(N, k) \hat{a}^A_{\mathbf{k}} + (Q^I_A(N, k))^* \hat{a}^{A\dagger}_{-\mathbf{k}}, \\ \hat{P}_I(N, \mathbf{k}) = \tilde{P}_{IA}(N, k) \hat{a}^A_{\mathbf{k}} + (\tilde{P}_{IA}(N, k))^* \hat{a}^{A\dagger}_{-\mathbf{k}}, \end{cases} \quad \text{with } [\hat{a}^A_{\mathbf{k}}, \hat{a}^{B\dagger}_{\mathbf{k}'}] = (2\pi)^3 \delta^{AB} \delta^{(3)}(\mathbf{k} - \mathbf{k}'), \quad (3.8)$$

where note that indices $A, B \dots$ can be raised and lowered with the symbol δ_{AB} , so that the up or down position has no particular meaning. One should therefore follow the evolution of the $2N_{\text{fields}}^2$ complex mode functions $Q^I_A(N, k)$ and $\tilde{P}_{IA}(N, k)$ verifying the first order differential equations $E^{QI} = 0 = E^{\tilde{P}}_I$ (2.28)–(2.29), or equivalently solve N_{fields} times (corresponding to the label A) the coupled N_{fields} -dimensional system of second-order differential equations (2.32) verified by each set of $Q^I_A(N, k)$, each time with different initial conditions. This stems from the fact that in order to define a vacuum state $|0\rangle$ and to quantise the fluctuations when all relevant momenta are sub-Hubble, one should identify N_{fields} independent fields, each coming with its own creation and annihilation operators. Note that in a generic system of coordinates or/and curved field space, the field fluctuations $\hat{Q}^I$ do not verify the above property, as they are kinetically coupled. However, their projections on a set of vielbeins, or even clearer, on a set of parallel-transported vielbeins (see section 3.3), naturally provide independent degrees of freedom inside the Hubble radius.

Relatedly, let us remark that even with a fixed vacuum state annihilated by the $\hat{a}^A_{\mathbf{k}}$'s, there is no unique choice of independent operators verifying the commutation relations in eq. (3.8). Indeed, once such a set is given, any other one related by a unitary transformation U provides another suitable set, i.e. the equations (3.8) take the same form in terms of the barred quantities such that

$$\hat{\bar{a}}^{\bar{A}}_{\mathbf{k}} = U^{\bar{A}}_{\bar{B}} \hat{a}^B_{\mathbf{k}} \quad \text{and} \quad (3.9)$$

$$\bar{Q}^{\bar{I}}_A = Q^I_B (U^\dagger)^B_{\bar{A}}, \quad \bar{\tilde{P}}_{\bar{I}\bar{A}} = \tilde{P}_{IB} (U^\dagger)^B_{\bar{A}}, \quad (3.10)$$

without changing neither the operators $\hat{Q}^I$ and $\hat{P}_I$ nor the vacuum state $|0\rangle$. This arbitrariness is of course equivalently visible at the level of the quantisation conditions. Indeed, the

commutation relations

$$[\hat{Q}^I(N, \mathbf{x}), \hat{P}_J(N, \mathbf{x}')] = \frac{i\delta_J^I}{a^3(N)} \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \quad (3.11)$$

$$[\hat{Q}^I(N, \mathbf{x}), \hat{Q}^J(N, \mathbf{x}')] = [\hat{P}_I(N, \mathbf{x}), \hat{P}_J(N, \mathbf{x}')] = 0, \quad (3.12)$$

impose the following relations on the mode functions:

$$Q_A^I(N, k) \tilde{P}_{JA}^*(N, k) - \text{c.c.} = \frac{i\delta_J^I}{a^3(N)}, \quad (3.13)$$

$$Q_A^I(N, k) Q_A^{*J}(N, k) - \text{c.c.} = \tilde{P}_{IA}(N, k) \tilde{P}_{JA}^*(N, k) - \text{c.c.} = 0, \quad (3.14)$$

where, as before, the sum over A is implicit.⁶ It is then apparent that two sets of mode functions related by a time-independent unitary matrix like in eq. (3.10) are equally valid and describe the same physics.

Once this quantisation is in place, the two-point vacuum expectation value of the quantum UV operators $\hat{Q}^{\tilde{X}I} = (\hat{Q}^I, \hat{P}^I)$ at a given time N are given by

$$\langle 0 | \hat{Q}^{\tilde{X}I}(N, \mathbf{k}) \hat{Q}^{\tilde{Y}J}(N, \mathbf{k}') | 0 \rangle = (2\pi)^3 \delta^{(3)}(\mathbf{k} + \mathbf{k}') \delta^{AB} Q_A^{\tilde{X}I}(N, k) (Q_B^{\tilde{Y}J}(N, k))^*, \quad (3.15)$$

thus providing the power spectra entering into the properties of the noises (2.23). However, to describe their statistics at time N , only the mode $k_\sigma(N)$ matters. Crucially, this mode is far outside the Hubble radius for $\sigma \ll 1$, which we indeed considered from the start to ensure that the gradient-expansion is valid and that the infrared fields can be considered as classical (see section 2.2). Relatedly, in this regime, the complex mode functions $Q_A^I(N, k)$ and $\tilde{P}_{IA}(N, k)$ become real to a very good accuracy (up to an irrelevant constant unitary matrix), corresponding to fluctuations being in a highly squeezed state [190–193]. This property is well known for a single light scalar field, and we will see in section 5 that it also holds for multiple scalar fields in the massless approximation. More interestingly, we also show there that it is actually valid in the slow-varying approximation for light scalars of masses $m_i < 3/2H$ (see section 5.3), the situation of interest for the stochastic formalism.⁷ Using this, it is thus possible to forget about the complex conjugates $*$ and to consider:

$$\hat{Q}^I(N, \mathbf{k}) \underset{k \ll aH}{\simeq} Q_A^I(N, k) (\hat{a}_{\mathbf{k}}^A + \hat{a}_{-\mathbf{k}}^{A\dagger}), \quad \hat{P}_I(N, \mathbf{k}) \underset{k \ll aH}{\simeq} \tilde{P}_{IA}(N, k) (\hat{a}_{\mathbf{k}}^A + \hat{a}_{-\mathbf{k}}^{A\dagger}). \quad (3.16)$$

It is then natural to define the variables $b_{\mathbf{k}}^A = \hat{a}_{\mathbf{k}}^A + \hat{a}_{-\mathbf{k}}^{A\dagger}$ where we forgot the hat on purpose. Indeed, these are the only “quantum” operators that we are left with on super-Hubble scales and they all commute with one another, i.e. $[b_{\mathbf{k}}^A, b_{\mathbf{k}'}^B] = 0$, hence the fluctuations can be understood as classical.⁸ It can easily be checked that this definition of the $b_{\mathbf{k}}^A$ ’s endows

⁶As usual, these relations, once verified at some initial time, hold at all time by virtue of the equations of motion verified by the mode functions.

⁷In this framework, the presence of heavy degrees of freedom with masses $m_i > 3/2H$, for which eq. (3.16) is not applicable (because the mode functions of heavy fields have genuinely time-dependent phases on super-Hubble scales), is not problematic, as their mode functions are anyway σ -suppressed at coarse-graining scale crossing.

⁸Of course, the canonical commutation relations for fields and momenta still hold, and whether cosmological perturbations completely lost their quantum nature or not is a field of research that has its own dedicated literature, see e.g. refs. [194–197] for recent references. In this paper, we shall be conservative and consider that super-Hubble fluctuations can well be treated classically.

them with Gaussian statistics with $\langle b_{\mathbf{k}}^A \rangle = 0$ and $\langle b_{\mathbf{k}}^A b_{\mathbf{k}'}^B \rangle = (2\pi)^3 \delta^{AB} \delta^{(3)}(\mathbf{k} + \mathbf{k}')$, where the brackets of quantum vacuum expectation values can now be understood as statistical ensemble averages for the stochastic fields $b_{\mathbf{k}}^A$. The noises (2.21) can now be expressed as

$$\xi^{QI}(x) = f_\sigma Q_A^I(N, k_\sigma(N)) \xi^A(x), \quad \xi_P^I(x) = f_\sigma \tilde{P}_{IA}(N, k_\sigma(N)) \xi^A(x), \quad \text{with } f_\sigma = \sqrt{\frac{k_\sigma^3}{2\pi^2} \frac{k_{\sigma'}}{k_\sigma}}, \quad (3.17)$$

where, again, the ratio $k_{\sigma'}/k_\sigma$ may be approximated by unity. We also defined

$$\xi^A(x) = f_\sigma^{-1} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{x}} \frac{d\theta(k - k_\sigma(N))}{dN} b_{\mathbf{k}}^A, \quad (3.18)$$

that are independent Gaussian white noises normalised to almost unity in a given σ -Hubble patch:

$$\langle \xi^A(x) \xi^B(x') \rangle = \frac{\sin k_\sigma r}{k_\sigma r} \delta^{AB} \delta(N - N'), \quad \text{with } r = |\mathbf{x} - \mathbf{x}'|. \quad (3.19)$$

Recalling that the spatial correlation $\sin k_\sigma r / k_\sigma r$ should be approximated by the theta function $\theta(1 - k_\sigma r)$ taking values 1 inside a σ -Hubble patch and 0 outside, one eventually finds

$$\langle \xi^A(x) \xi^B(x') \rangle = \begin{cases} \delta^{AB} \delta(N - N'), & \text{if } r = |\mathbf{x} - \mathbf{x}'| \leq (\sigma a H)^{-1}, \\ 0, & \text{otherwise.} \end{cases} \quad (3.20)$$

Strikingly, these are the same noises ξ^A that appear both in ξ^{QI} and ξ_P^I . This means that we were able to “decorrelate” the $2N_{\text{fields}}$ correlated noises by expressing them in terms of N_{fields} uncorrelated ones. In a mathematical language, one would say that the noise amplitude $A^{\tilde{X}\tilde{Y}IJ}$, with $(\tilde{X}, \tilde{Y}) \in (Q, \tilde{P})$, can be understood as a bilinear form whose matrix is of dimension $2N_{\text{fields}} \times 2N_{\text{fields}}$, but of rank N_{fields} only, and can thus be reduced. The Langevin equations (2.22) are thus rewritten as

$$\varphi^{I'} = \frac{1}{H} G^{IJ} \varpi_J + f_\sigma Q_A^I \circ \xi^A, \quad \mathcal{D}_N \varpi_I = -3\varpi_I - \frac{V_I}{H} + f_\sigma \tilde{P}_{IA} \circ \xi^A, \quad (3.21)$$

where now the Stratonovich interpretation, indicated by the simple symbol $\circ \equiv \circ_{1/2}$, is non-ambiguous as independent noises ξ^A have been identified, and where covariance is respected as the standard chain rule applies. To be precise, there is strictly speaking a family of possible independent noises ξ^A , but, taking into account that we used real $(Q_A^I, \tilde{P}_{IA})$ variables in eq. (3.21), these noises are simply related by a constant rotation U (when restricting eq. (3.9) to real orthogonal matrices). Like in eq. (3.10), this induces a constant rotation U^T of the noises’ amplitudes $(Q_A^I, \tilde{P}_{IA})$, which, as we have seen in section 3.1.2, does not lead to any ambiguity. Modulo this irrelevant rotation, we can hence talk about *the* frame of independent noises used in the Langevin-type equations (3.21). Eventually, one has to be careful there with the covariant time derivative $\mathcal{D}_N$, as it contains stochastic noises through the time derivative $\varphi^{I'}$. It should hence also be discretised in the Stratonovich scheme:

$$\mathcal{D}_N \mathcal{U}^I = \mathcal{U}^{I'} + \Gamma_{JK}^I \mathcal{U}^J \circ \varphi^{K'}, \quad \mathcal{D}_N \mathcal{V}_I = \mathcal{V}_I' - \Gamma_{IJ}^K \mathcal{V}_K \circ \varphi^{J'}, \quad (3.22)$$

where the symbol $\circ$ indicates that when discretised, the term on its left should be evaluated at the midpoint, i.e. one has for instance:

$$\Gamma_{IJ}^K \mathcal{V}_K \circ \varphi^{J'} \equiv \frac{G^{JL}}{H} \Gamma_{IJ}^K \mathcal{V}_K \varpi_L + \left(f_\sigma \Gamma_{IJ}^K \mathcal{V}_K Q_A^I \right) \circ \xi^A. \quad (3.23)$$

Now that we understood that the frame of independent creation-annihilation operators provides the right frame in which to formulate the Langevin equations with a Stratonovich discretisation, all issues of covariance and frame-dependences are solved, but this resolution is still somewhat formal. In order to make this resolution more readily apparent, we will go one step further and derive equivalent Langevin-type equations in the Itô scheme, which are easier to deal with numerically.

3.3 Itô-covariant Langevin equations

In order to go from the Stratonovich Langevin equations (3.21) to Itô ones with the same physical content, one will introduce vielbeins defining a local orthonormal frame along the IR trajectory. This additional structure will eventually disappear from the final Itô Langevin equations, while generating Itô-covariant derivatives, but for this, one has to be careful about their definitions. Let us first consider a given point in field space, say the initial condition for φ^I in a given realisation of the stochastic processes. At this point, it is possible to reduce the metric 2-form G_{IJ} to identity $\delta_{\alpha\beta}$ by using projectors e_α^I from one basis to the other. Then they verify the following relations *at this point*:

$$G_{IJ}e_\alpha^I e_\beta^J = \delta_{\alpha\beta}, \quad \text{and} \quad \delta^{\alpha\beta} e_\alpha^I e_\beta^J = G^{IJ}. \quad (3.24)$$

For these variables to constitute a set of vielbeins, these relations should hold along the whole IR trajectory. We thus ask this property to be conserved along the trajectory, $\mathcal{D}_N(G_{IJ}e_\alpha^I e_\beta^J) = 0$. Because $\mathcal{D}_N G_{IJ} = 0$ by definition, if we write $\mathcal{D}_N e_\alpha^I = \Omega_\alpha^\beta e_\beta^I$, we find that the matrix Ω must be anti-symmetric, parameterizing the local rotation of the orthonormal frame. Then, which anti-symmetric matrix to choose is a matter of convenience. For example, a popular choice is the decomposition in the so-called adiabatic/entropic basis [187, 198], defined by a Gram-Schmidt orthogonalisation process applied to the successive covariant derivatives of $\varphi^{I'}$, in which case the entries of the anti-symmetric matrix correspond to covariant turn rates of the background trajectory in field space. An even simpler choice in some sense is to use *parallel-transported* vielbeins which verify $\mathcal{D}_N e_\alpha^I = 0$, i.e. to chose $\Omega = 0$. These or other choices of vielbeins may have their own advantages for the analytical understanding of the behaviour of UV fluctuations (see sections 5.2 and 5.3). In the following, we make the choice $\Omega = 0$ but we stress that this is merely for convenience, and that the resulting Itô-covariant Langevin equations do not depend on this choice, as any set of vielbeins disappear altogether from the final result.

More important is to note that again, the covariant time derivative $\mathcal{D}_N$ is a stochastic derivative, with an underlying discretisation corresponding to the Stratonovich scheme, as defined in eq. (3.22). Therefore the parallel transport of vielbeins must be realised in the following stochastic way:

$$e_\alpha^{I'} = -\Gamma_{JK}^I e_\alpha^J \circ \varphi^{K'}. \quad (3.25)$$

We call these vielbeins *stochastically-parallel-transported* vielbeins, as this equation defining them is nothing but a Langevin equation. The vielbeins thus really become new stochastic variables, i.e., the collection of stochastic processes reads $\mathcal{S}^n = (\varphi^I, \varpi_I, e_\alpha^I)$: coordinates on the field space, covectors and vectors. Notice that with these definitions the indices α and β can be raised and lowered with the metric $\delta_{\alpha\beta}$, i.e. the up or down position makes no difference. We define the projections of the UV modes along those vielbeins, Q_A^α and $\tilde{P}_A^\alpha$ as

$$Q_A^\alpha = G_{IJ} e^{I\alpha} Q_A^J, \quad \tilde{P}_A^\alpha = e^{I\alpha} \tilde{P}_{IA}. \quad (3.26)$$

These variables are scalars in field space and one deduces from eq. (2.32) and by virtue of our choice $\Omega = 0$ that they verify the simple second-order differential equation:

$$Q_A^{\alpha''} + (3 - \epsilon) Q_A^{\alpha'} + \left(\frac{k^2}{a^2 H^2} \delta_\beta^\alpha + \frac{M^{2\alpha}_\beta}{H^2} \right) Q_A^\beta = 0, \quad \text{with } M^{2\alpha}_\beta = e_I^\alpha e_\beta^J M^{2I}_J. \quad (3.27)$$

An advantage of the parallel-transported vielbeins is thus that the perturbations Q_A^α in such a basis are not kinetically coupled but only mix via the projection of the mass matrix, $M^{2\alpha}_\beta$, which we will use for analytical estimates in section 5. This is of course equivalent to our statement in section 3.2 that these projected fields are independent deep inside the Hubble radius, making easier the quantisation process.

Independently of this, let us now reformulate our system of Langevin equations (3.21) with the new set of stochastic variables augmented by the vielbeins:

$$\begin{cases} \varphi^{I'} = \frac{1}{H} G^{IJ} \varpi_J + f_\sigma e_\alpha^I Q_A^\alpha \circ \xi^A, \\ \varpi_{I'} = -3\varpi_I - \frac{V_I}{H} + \Gamma_{IJ}^K \varpi_K \circ \varphi^{J'} + f_\sigma G_{IJ} e_\alpha^J \tilde{P}_A^\alpha \circ \xi^A, \\ e_\alpha^{I'} = -\Gamma_{JK}^I e_\alpha^J \circ \varphi^{K'}. \end{cases} \quad (3.28)$$

Although it is not manifest, we know these equations respect general covariance, and as is proved in appendix A, it is always possible to move from a given discretisation scheme to another one in the continuous description, by adding a noise-induced deterministic drift of the form (going from Stratonovich to Itô), $\frac{1}{2} (\partial g_A^n / \partial S^m) g_A^m$ to the equation of motion for the process S^n . Let us then find the equivalent Itô description of equations (3.28), keeping in mind that the $Q_A^\alpha, \tilde{P}_{\alpha A}$ are not given functions of the IR stochastic variables, but rather solutions of differential equations that involve them. Using eq. (A.6) with $\alpha = 1/2$, we thus find:

$$\begin{aligned} \varphi^{I'} &= \frac{1}{H} G^{IJ} \varpi_J + f_\sigma e_\alpha^I Q_A^\alpha \xi^A \\ &\quad + \frac{f_\sigma^2}{2} \left(\frac{\partial e_\alpha^I}{\partial e_\beta^J} Q_A^\alpha \right) \times \left(-\Gamma_{KL}^J e_\beta^K e_\gamma^L Q_A^\gamma \right), \end{aligned} \quad [\text{noise of } e_\beta^J] \quad (3.29)$$

$$\begin{aligned} \varpi_{I'} &= -3\varpi_I - \frac{V_I}{H} + \frac{G^{JL}}{H} \Gamma_{IJ}^K \varpi_K \varpi_L + f_\sigma \left(G_{IJ} e_\alpha^J \tilde{P}_A^\alpha + \Gamma_{IJ}^K \varpi_K e_\alpha^J Q_A^\alpha \right) \xi^A \\ &\quad + \frac{f_\sigma^2}{2} \left(\frac{\partial \Gamma_{IJ}^K}{\partial \varphi^L} \varpi_K e_\alpha^J Q_A^\alpha + \frac{\partial G_{IJ}}{\partial \varphi^L} e_\alpha^J \tilde{P}_A^\alpha \right) \times \left(e_\beta^L Q_A^\beta \right) \quad [\text{noise of } \varphi^L] \\ &\quad + \frac{f_\sigma^2}{2} \left(\Gamma_{IJ}^K \frac{\partial \varpi_K}{\partial \varpi_L} e_\alpha^J Q_A^\alpha \right) \times \left(G_{LS} e_\beta^S \tilde{P}_A^\beta + \Gamma_{LS}^R \varpi_R e_\beta^S Q_A^\beta \right) \quad [\text{noise of } \varpi_L] \\ &\quad + \frac{f_\sigma^2}{2} \frac{\partial e_\alpha^J}{\partial e_\beta^K} \left(G_{IJ} \tilde{P}_A^\alpha + \Gamma_{IJ}^K \varpi_K Q_A^\alpha \right) \times \left(-\Gamma_{LM}^K e_\beta^L e_\gamma^M Q_A^\gamma \right), \end{aligned} \quad [\text{noise of } e_\beta^K] \quad (3.30)$$

$$\begin{aligned} e_\alpha^{I'} &= -\frac{G^{KL}}{H} \Gamma_{JK}^I e_\alpha^J \varpi_L - f_\sigma \Gamma_{JK}^I e_\alpha^J e_\beta^K Q_A^\beta \xi^A \\ &\quad + \frac{f_\sigma^2}{2} \left(-\frac{\partial \Gamma_{JK}^I}{\partial \varphi^L} e_\alpha^J e_\beta^K Q_A^\beta \right) \times \left(e_\gamma^L Q_A^\gamma \right) \quad [\text{noise of } \varphi^L] \\ &\quad + \frac{f_\sigma^2}{2} \left(-\Gamma_{JK}^I \frac{\partial (e_\alpha^J e_\beta^K)}{\partial e_\gamma^L} Q_A^\beta \right) \times \left(-\Gamma_{RS}^L e_\gamma^R e_\delta^S Q_A^\delta \right), \end{aligned} \quad [\text{noise of } e_\gamma^L] \quad (3.31)$$

where the absence of a symbol $\circ_\alpha$ means that the underlying discretisation is the Itô scheme. We recognise the appearance of the corrective terms $\propto A^{QQIJ}$ and $A^{Q\bar{P}I}{}_J$ that are needed to make Itô-Langevin equations covariant. For instance, the last term in eq. (3.29), coming from the Stratonovich to Itô conversion, reads $-\frac{1}{2}f_\sigma^2\Gamma_{KL}^I e_\alpha^K Q_A^\alpha e_\gamma^L Q_A^\gamma = -\frac{1}{2}\Gamma_{KL}^I A^{QQKL}$ where

$$A^{QQKL} = f_\sigma^2 Q_A^K(N, k_\sigma(N)) Q_A^L(N, k_\sigma(N)) = \frac{k'_\sigma}{k_\sigma} \mathcal{P}^{QQKL}(N, k_\sigma(N)), \quad (3.32)$$

is intrinsically defined independently of the vielbeins (see eqs. (2.23) and (2.24)).⁹ With similar manipulations, one can rewrite the equations in Itô with use of the covariant derivatives previously defined in eqs. (3.4)–(3.6), as

$$\begin{cases} \mathfrak{D}_N \varphi^I = \frac{\varpi^I}{H} + f_\sigma e_\alpha^I Q_A^\alpha \xi^A, \\ \mathfrak{D}_N \varpi_I = -3\varpi_I - \frac{V_I}{H} + f_\sigma e_I^\alpha \tilde{P}_{\alpha,A} \xi^A, \\ \mathfrak{D}_N e_\alpha^I = 0. \end{cases} \quad (3.33)$$

This self-consistency of the Langevin equations is quite remarkable given the degree of complexity of these stochastic differential equations. In particular, as announced, the vielbeins disappear completely from any physical quantity computed from the first two equations in eq. (3.33), as they do not appear in the Itô-covariant derivatives, and as it is only the auto-correlation of the effective noises ($\xi^{QI} = f_\sigma e_\alpha^I Q_A^\alpha \xi^A = f_\sigma Q_A^I \xi^A$, $\xi_I^{\bar{P}} = f_\sigma e_I^\alpha \tilde{P}_{\alpha,A} \xi^A = f_\sigma \tilde{P}_{I,A} \xi^A$) that matter in Itô. Moreover, the covariance of eqs. (3.33) is manifest.

Now that the question of “stochastic anomalies” is solved, let us present a more rigorous derivation of the Langevin equations in phase space, with use of the coarse-grained effective hamiltonian action in a path-integral approach. As already mentioned, this will enable one to correctly treat the IR-UV interactions at the time of crossing the coarse-graining scale, so that all noises are manifestly real and that UV modes dictating their properties obey the same EoM as in SPT.

4 Coarse-grained effective Hamiltonian action

In this section, we derive the covariant Langevin-type equations of multifield stochastic inflation in a midpoint discretisation scheme, based on functional methods borrowed from non-equilibrium quantum field theory. We will begin by reviewing some of these notions and explaining the roadmap and principles of the computation, before turning to the computation itself. In particular, we will have to deal with several difficulties. First, as usual in cosmology we want to describe the fields dynamics, or their equal-time “in-in” correlation functions. This is different from QFT in Minkowski spacetime where we are interested in scattering “in-out” amplitudes. Thus, the time integration contour should follow a closed-time-path (CTP). Second, we want to compute an effective action for the long wavelength IR modes coupled to the bath of short wavelength UV modes, with interactions that should be specified upon physical arguments. In particular, we will solely consider the IR/UV couplings coming from the flow of UV modes joining the IR sector, i.e. the couplings specific to the

⁹Since we have taken into account the classicalisation of the perturbations on super-Hubble scales and considered the mode functions to be real, notice that here the cross-correlation $A^{Q\bar{P}I}{}_J = f_\sigma^2 Q_A^I P_{JA}$ is automatically real. Anyway, the reality of the auto-correlation of the noises will be rigorously proven from the path-integral approach in section 4.

time-dependent split between the two sectors. Last but not least, we want to pay particular attention to the covariance of the theory. On the UV side, it is known that the perturbations $\delta\phi^I$ do not transform beyond linear order as genuine vectors under field redefinitions. In SPT, this subtlety is only relevant when computing the action at cubic order or higher in perturbations. However, in a stochastic context, we have to take this into account even when considering the action at quadratic order in fluctuations, as the part of the action that is linear in $\delta\phi^I$ does not vanish, but rather plays a crucial role in determining the UV-IR transition. This also applies to momentum perturbations $\delta\pi_I$ that do not even transform as covectors at linear order, and for which quadratic corrections are also needed. On the IR side, based on the arguments developed in the previous section, we will also interpret our path integral as the continuous limit of discrete integrations with an explicit scheme corresponding to the midpoint (Stratonovich-like) discretisation, to ensure that the standard chain rule for changes of variables is applicable.

4.1 Roadmap and principles of the computation

In particle physics, one wishes to compute transition amplitudes between asymptotic “in” states (in the far past) and “out” states (in the far future), which are defined long before interactions are switched on, and long after they are switched off. The situation is crucially different in cosmology, where one is rather interested in vacuum expectation values of quantum operators. Actually, the notion of a future, asymptotic, “out” state is more intricate in a cosmological context as particles keep interacting at least gravitationally in curved spacetimes; boundary conditions can only be imposed in the far past, when the wavelengths of relevant fields are much smaller than the Hubble radius. Expectation values in such time-dependent contexts can be deduced from the “in-in” partition function (rather than the “in-out” one for particle physics) in the presence of external currents, $Z[J_{XI}]$, which is the generating functional of all correlation functions defined as expectation values in the initial (vacuum) state. This “in-in” generating functional, which can be thought of as summing over all possible “out” states, can be computed using a closed-time-path contour of integration [138, 139, 141, 199–202] shown in figure 1, and according to:

$$Z[J_{XI}] = \int_C \mathcal{D}\phi^{XI} \exp\left(iS[\phi^{XI}] + i \int d^4x J_{XI} \phi^{XI}\right), \quad (4.1)$$

where the subscript C precises the contour of integration. Here, in accordance with first principles in the path-integral approach, S denotes the classical action in the Hamiltonian form (2.8), and notations are similar as before: the index X denotes position or momentum in phase space, i.e. the Hamiltonian action depends on the scalar fields $\phi^{XI} = \phi^I$ and on their (contravariant) momenta $\phi^{PI} = G^{IJ}(\phi^K)\pi_J$. Formally, it will prove useful for computations to lower and raise the index X with the appropriate metric $\frac{1}{i}\sigma_{2XY} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and its inverse. Note that contrary to “in-out” partition functions in which $Z[0]$ must be computed as the sum over all vacuum bubbles to enforce a correct normalisation, for “in-in” partition functions, it is trivial to see that $Z[0] = 1$ as the norm of the initial vacuum state should be. Eventually, we note that the condensed notation $\mathcal{D}\phi^{XI}$ that we will use throughout should really be understood as the canonical phase-space measure $\prod_{I,J} \mathcal{D}\phi^I \mathcal{D}\pi_J$.

To avoid the formal path integral along the closed contour C , one can divide it in two path integrals over the forward (+) and backwards (−) parts of the time contour $C = C^+ \cup C^-$. This boils down to doubling the number of degrees of freedom in the path integral, with $\phi^{XI\pm}$ living respectively on C^+ and C^- . The $\pm$ fields and momenta should be considered

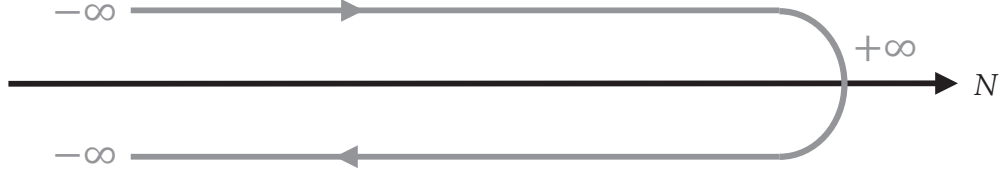


Figure 1. Closed-time-path C of integration used in the “in-in” formalism.

independent, except at future infinity where the time path closes (truly, at any time later than the ones of interest), and where we use the usual boundary conditions that $\pm$ fields coincide, i.e. $\phi^{I+}(+\infty) = \phi^{I-}(+\infty)$, but that momenta $\pi_I^\pm$ are left unconstrained. The time flow being reversed on the C^- branch, the path integral to perform can be rewritten along a forward contour only as

$$Z[J_{XI}^\pm] = \int_{C^+} \mathcal{D}\phi^{XI\pm} \exp\left(iS[\phi^{XI+}] - iS[\phi^{XI-}] + i \int d^4x J_{XI}^+ \phi^{XI+} - i \int d^4x J_{XI}^- \phi^{XI-}\right). \quad (4.2)$$

In practice, we will make use of the so-called Keldysh basis (letting aside the various indices here):

$$\begin{pmatrix} \phi^{\text{cl}} \\ \phi^{\text{q}} \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \phi^+ \\ \phi^- \end{pmatrix} \quad \Leftrightarrow \quad \begin{pmatrix} \phi^+ \\ \phi^- \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 1/2 \\ 1 & -1/2 \end{pmatrix}}_K \begin{pmatrix} \phi^{\text{cl}} \\ \phi^{\text{q}} \end{pmatrix}, \quad (4.3)$$

where ϕ^{cl} and ϕ^{q} are respectively referred to as the classical and quantum components of the fields, and K is the matrix of change of basis. The rationale for this denomination is that among the solutions of the saddle point equations for the Keldysh action $S[\phi^{XI+}] - S[\phi^{XI-}]$, there is always one with vanishing quantum component and classical component obeying the classical equation of motion $\delta S / \delta \phi^{XI} = 0$. Although we are using natural units with $\hbar = 1$, one can intuitively think of the quantum component as $\hbar$ -suppressed, and indeed the stochastic equations we will derive, with classical equations of motion corrected by noises of quantum-mechanical origin, can be seen as semi-classical equations of motion.

Introducing covariant notations, latin indices $a, b, \dots$ for the $\pm$ fields, and Fraktur indices $\mathfrak{a}, \mathfrak{b}, \dots$ for the Keldysh label cl/q, the corresponding change of basis can be summarised as $\phi^a = K^a_{\mathfrak{a}} \phi^{\mathfrak{a}}$. To keep compact expressions, we use the convention of summation over repeated indices, and we will use well-chosen metrics to raise and lower them: the metric $\sigma_{3ab} = \text{diag}(1, -1)_{ab}$ in the $\pm$ basis; and the corresponding one $\sigma_{1\mathfrak{a}\mathfrak{b}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{\mathfrak{a}\mathfrak{b}}$ in the Keldysh basis. Note that in the latter, the matching condition of the CTP branches at future infinity reads $\phi^{\text{Iq}}(+\infty) = 0$, again with no constraint on momenta. The generating functional in this basis reads (note that the Jacobian $|K|$ is unity)

$$Z[J_{XI}^{\mathfrak{a}}] = \int \mathcal{D}\phi^{XI\mathfrak{a}} \exp\left(iS[\phi^{XI\mathfrak{a}}] + i \int d^4x J_{XI}^{\mathfrak{q}} \phi^{XI\text{cl}} + i \int d^4x J_{XI}^{\text{cl}} \phi^{XI\mathfrak{q}}\right), \quad (4.4)$$

where $S[\phi^{XI\mathfrak{a}}] = S[\phi^{XI\text{cl}} + \phi^{XI\mathfrak{q}}/2] - S[\phi^{XI\text{cl}} - \phi^{XI\mathfrak{q}}/2]$.

Formally, the “in-in” vacuum expectation value of any operator at time $t_\star$ can be computed by introducing this operator at this particular time on the closed-time-path of integration and with vanishing currents. Equivalently, n -point functions can be derived by

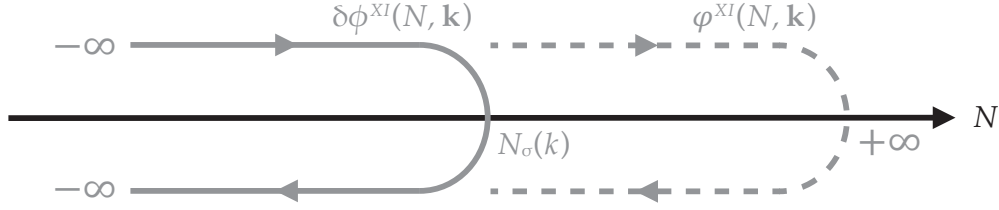


Figure 2. In the stochastic approach, the original path integral along the closed contour C shown in figure 1 is divided for each wavenumber $\mathbf{k}$ into a path integral over UV fields $\delta\phi^{XI}(N, \mathbf{k})$, and into one over IR fields $\varphi^{XI}(N, \mathbf{k})$. Hence, the corresponding UV path is closed at the transition time $N_\sigma(k)$ with the boundary condition $\delta\phi^{Iq}(N_\sigma(k), \mathbf{k}) = 0$ (4.6), while the IR path starts there with the other boundary condition $\varphi^{Icl}(N_\sigma(k), \mathbf{k}) = 0$, and is closed at future infinity with the boundary condition $\varphi^{Iq}(+\infty) = 0$.

calculating the n^{th} functional derivatives of the above generating functional $Z[J_{XI}^a]$ with respect to the external currents J_{XI}^a and evaluating them at $J_{XI}^a = 0$. As for the equations of motion verified by the expectation values of ϕ^{XI} , they can be determined by extremising the quantum effective action, defined as the Legendre transformation of $W[J_{XI}^a] = -i \ln Z[J_{XI}^a]$. However in the following we choose to follow another route: based on the physical distinction between quantum short-wavelength modes and classical long-wavelength ones, we want to derive a classical (albeit stochastic) effective theory for the latter only, and then compute expectation values within this new theory. This amounts in our setup to derive what can be called the “coarse-grained effective Hamiltonian action” that governs the dynamics of the coarse-grained scalar fields in a Hamiltonian language (see e.g. refs. [123, 141, 203] for related concepts). Indeed, based on the scale separation provided by the physical Hubble radius H^{-1} , the original fields can be written in real space as IR+UV: $\phi^{XIa}(x) = \varphi^{XIa}(x) + \delta\phi^{XIa}(x)$, where we have in mind the Fourier cutoff $k_\sigma(N)$ discussed in section 2.¹⁰ The Fourier components of the fields and momenta thus verify:

$$\phi^{XIa}(N, \mathbf{k}) = \begin{cases} \delta\phi^{XIa}(N, \mathbf{k}), & \text{if } N < N_\sigma(k), \\ \varphi^{XIa}(N, \mathbf{k}), & \text{if } N > N_\sigma(k), \end{cases} \quad (4.5)$$

where $N_\sigma(k)$ represents the time at which the modes of modulus k cross the UV/IR cutoff, and hence at which boundary conditions need to be specified for the fields. Because the UV modes $\delta\phi^a(N, \mathbf{k})$ stop being defined at the time $N_\sigma(k)$, their time path actually closes at this particular time, which enforces the boundary condition $\delta\phi^{Iq}(N_\sigma(k), \mathbf{k}) = 0$, like for the full fields whose time path closes at future infinity. Inversely, the time path of IR modes $\varphi^a(N, \mathbf{k})$ begins at that time, with vanishing initial conditions for the classical component of the fields, $\varphi^{Icl}(N_\sigma(k), \mathbf{k}) = 0$ (see figure 2).¹¹ Note that again, neither IR nor UV momenta are constrained at the time $N_\sigma(k)$.

¹⁰Note that the cutoff $k_\sigma(N) = \sigma a(N)H$ is not deterministic because the Hubble parameter depends on the stochastic realisations of the fields. Hence, the cutoff scale has the same status in the path-integral and in the heuristic approaches, i.e. it is understood to be defined self-consistently as mentioned at the end of section 2.2. The following discussion is independent of this subtlety.

¹¹As we will see, the stochastic equations derived heuristically in section 2 actually concern the classical component of the fields, so that the boundary condition $\varphi^{Icl}(N_\sigma(k), \mathbf{k}) = 0$ agrees with the fact that in the stochastic approach, IR fields with wavevectors $\mathbf{k}$ do not exist before the time $N_\sigma(k)$.

Because these conditions will be crucial to specify interactions between IR and UV modes, we rewrite them together:

$$\phi^{I\mathbf{a}}(N_\sigma(k), \mathbf{k}) = \begin{cases} \delta\phi^{I\text{cl}}(N_\sigma(k), \mathbf{k}), & \text{if } \mathbf{a} = \text{cl}, \\ \varphi^{I\mathbf{q}}(N_\sigma(k), \mathbf{k}), & \text{if } \mathbf{a} = \mathbf{q}, \end{cases} \quad (4.6)$$

assigning the Fourier component at the transition time, either fully to the UV part for the classical component, or fully to the IR part for the quantum component. It will become clear when discussing IR-UV interactions in the discretised version of the path integral that, indeed, no boundary condition is required for the momenta, because in the path integral they can be evaluated at intermediate time steps and we can avoid to specify their values at the exact time $N_\sigma(k)$. It was actually shown in the context of a single test scalar field in de Sitter that these boundary conditions at $N_\sigma(k)$ enables the to-be-found stochastic description to correctly reproduce the propagators of the corresponding free QFT [130, 132]. Now that this decomposition into IR and UV fields is fully specified, one may rewrite the generating functional (at vanishing currents for simplicity) as

$$Z = \int \mathcal{D}\varphi^{XI\mathbf{a}} \exp\left(iS_{\text{eff}}\left[\varphi^{XI\mathbf{a}}\right]\right), \quad \text{with} \quad (4.7)$$

$$\exp\left(iS_{\text{eff}}\left[\varphi^{XI\mathbf{a}}\right]\right) = \int \mathcal{D}\delta\phi^{XI\mathbf{a}} \exp\left(iS\left[\varphi^{XI\mathbf{a}} + \delta\phi^{XI\mathbf{a}}\right]\right), \quad (4.8)$$

where the path integral over the UV modes has to be performed explicitly. Then, we will see that upon the introduction of auxiliary stochastic variables describing possible deviations from the classical EoM, one needs not perform the path integral over the IR fields, but simply observe which IR trajectories have non-zero weights in the remaining path integral, and hence obtain the desired Langevin equations. However before that, let us note that eq. (4.8) provides only a “naive” expression, and that one has to be careful about the fact that field perturbations themselves do not transform covariantly under field redefinitions beyond linear order [204, 205]. To ensure that the resulting effective theory respects general covariance, the path integral should be expressed in terms of covariant objects, and we now turn to the identifications of suitable ones in our Hamiltonian formulation.

4.2 Covariant perturbations in the Hamiltonian language

It is well known that field perturbations are not covariant objects beyond linear order. This subtlety is usually irrelevant if one is only interested in the Gaussian properties of the inflationary fluctuations, because SPT is defined around homogeneous fields $\phi_0^{XI}(N)$ that solve the classical equations of motion, $\frac{\delta S}{\delta\phi^{XI}}|_{\phi_0^{XI}} = 0$, and any non-covariant contribution coming from the linear action in terms of $\delta\phi^{XI}$ thus vanishes. However, the aim of stochastic inflation is precisely to take into account the difference between the effective equations of motion verified by the coarse-grained scalar fields and the classical equations of motion verified by $\phi_0^{XI}(N)$ in SPT. In this context, the part of the action that is linear in $\delta\phi^{XI}$ not only does not vanish but actually plays a crucial role. Thus, in stochastic inflation, perturbations should be covariant objects at least up to quadratic order, even to describe only Gaussian statistics and contrary to SPT.

In anticipation of our later setup, we define the perturbations at some spacetime point x by the displacements of the full inflaton fields $\phi^I(x)$ and their conjugate momenta $\pi_I(x)$

from their coarse-grained values $\varphi^I(x)$ and $\varpi_I(x)$ (the homogeneous background ϕ_0 and π_0 would instead be used as reference fields in SPT):

$$\delta\phi^I(x) = \phi^I(x) - \varphi^I(x), \quad \delta\pi_I(x) = \pi_I(x) - \varpi_I(x). \quad (4.9)$$

These finite displacements (4.9) do not transform covariantly under field redefinitions beyond the linear approximation, and therefore one needs to relate them to contravariant/covariant infinitesimal perturbations. The $\delta\phi$'s expansion has been already discussed in ref. [205]. The two neighbouring points in field space $\phi(x)$ and $\varphi(x)$ can be connected by a unique field-space geodesic, which we parameterise by the affine parameter λ such that $\phi(\lambda = 0) = \varphi(x)$ and $\phi(\lambda = 1) = \phi(x)$ (see figure 3). We then define the Vilkovisky-DeWitt-type variable Q^I by the “initial velocity”

$$\left. \frac{d\phi^I}{d\lambda} \right|_{\lambda=0} = Q^I. \quad (4.10)$$

This geometrical definition ensures that Q^I lies in the tangent space of the point $\varphi(x)$, i.e. that it behaves as desired as a vector under field redefinitions. Using the fact that, by definition, $\phi^I(\lambda)$ verifies the geodesic equation

$$\mathcal{D}_\lambda^2 \phi^I(\lambda) = \frac{d^2 \phi^I}{d\lambda^2} + \Gamma_{JK}^I \frac{d\phi^J}{d\lambda} \frac{d\phi^K}{d\lambda} = 0, \quad (4.11)$$

where $\mathcal{D}_\lambda$ represents the covariant derivative with respect to the affine parameter λ , one can express $\phi^I(\lambda)$ in terms of Q^I by using the following expansion around $\lambda = 0$:

$$\begin{aligned} \phi^I(\lambda) &= \phi^I(\lambda = 0) + \left. \frac{d\phi^I}{d\lambda} \right|_{\lambda=0} \lambda + \frac{1}{2} \left. \frac{d^2 \phi^I}{d\lambda^2} \right|_{\lambda=0} \lambda^2 + \dots \\ &= \varphi^I + Q^I \lambda - \frac{1}{2} \Gamma_{JK}^I Q^J Q^K \lambda^2 + \dots, \end{aligned} \quad (4.12)$$

thus obtaining the field perturbations

$$\delta\phi^I = \phi^I(\lambda = 1) - \phi^I(\lambda = 0) = Q^I - \frac{1}{2} \Gamma_{JK}^I Q^J Q^K + \dots. \quad (4.13)$$

The non-tensorial feature of the Christoffel symbols explicitly shows the non-covariance of the finite perturbations $\delta\phi^I$ beyond the linear approximation.

The displacement $\delta\pi_I$ can also be expressed in terms of a truly covariant tensor in a similar way. For that, let us consider a family $\pi_I(\lambda)$ of covectors at each point along the geodesic $\phi^I(\lambda)$, and such that $\pi_I(\lambda = 0) = \varpi_I(x)$ and $\pi_I(\lambda = 1) = \pi_I(x)$. It is then natural to define a second Vilkovisky-DeWitt-type variable $\tilde{P}_I$ by the “initial momentum velocity” along the geodesic as

$$\tilde{P}_I = \mathcal{D}_\lambda \pi_I|_{\lambda=0} = \left(\frac{d\pi_I}{d\lambda} - \Gamma_{IJ}^K \pi_K \frac{d\phi^J}{d\lambda} \right) |_{\lambda=0} = P_I - \Gamma_{IJ}^K \varpi_K Q^J, \quad (4.14)$$

where on the right-hand side, the naive P_I such that $\delta\pi_I = \pi_I(\lambda = 1) - \pi_I(\lambda = 0) = P_I \lambda + \mathcal{O}(\lambda^2)$ does not even transform covariantly at linear order, contrary to $\tilde{P}_I$, whose intrinsic geometrical definition ensures that it transforms as a covector at all order in perturbation theory. If one now imposes that the covectors $\mathcal{D}_\lambda \pi_I$ are parallel-transported along the geodesic:

$$0 = \mathcal{D}_\lambda^2 \pi_I = \frac{d^2 \pi_I}{d\lambda^2} - 2\Gamma_{IJ}^K \frac{d\phi^J}{d\lambda} \frac{d\pi_K}{d\lambda} - (\Gamma_{IJ,K}^S - \Gamma_{IR}^S \Gamma_{JK}^R - \Gamma_{IJ}^R \Gamma_{RK}^S) \pi_S \frac{d\phi^J}{d\lambda} \frac{d\phi^K}{d\lambda}, \quad (4.15)$$

it is possible to express $\delta\pi_I$ in terms of $\tilde{P}_I$. However, we note that imposing $\mathcal{D}_\lambda^2\pi_I = 0$ is *one* simple possible choice, but that others are possible, corresponding to a freedom in the identification of a suitable covariant momentum perturbation. We refer the interested reader to appendix B for more details on this point, to which we will come back, and here just quote the relation between $\delta\pi_I$ and $\tilde{P}_I$ for this particular choice:

$$\delta\pi_I = \tilde{P}_I + \Gamma_{IJ}^K \varpi_K Q^J + \Gamma_{IJ}^K Q^J \tilde{P}_K + \frac{1}{2}(\Gamma_{IJ,K}^S - \Gamma_{IR}^S \Gamma_{JK}^R + \Gamma_{IJ}^R \Gamma_{RK}^S) \varpi_S Q^J Q^K + \dots \quad (4.16)$$

Equipped with these geometrically defined objects, we are now ready to compute the covariant effective action up to second order in the UV fields and momenta as

$$\exp\left(iS_{\text{eff}}[\varphi^{XIa}]\right) = \int \mathcal{D}Q^{\tilde{X}Ia} \exp\left(iS^{(0)}[\varphi^{XIa}] + S^{(1)}[\varphi^{XIa}, Q^{\tilde{X}Ia}] + S^{(2)}[\varphi^{XIa}, Q^{\tilde{X}Ia}]\right), \quad (4.17)$$

with $Q^{\tilde{X}Ia} = (Q^{Ia}, \tilde{P}^{Ia})$ used as a short-hand notation, and like for eq. (4.1), $\mathcal{D}Q^{\tilde{X}Ia}$ truly refers to the canonical phase-space measure $\prod_{I,a,J,b} \mathcal{D}Q^{Ia} \mathcal{D}\tilde{P}_J^b$.

4.3 Covariant CTP action and IR-UV interactions

To investigate the effect of linear UV perturbations on the IR dynamics, we must first covariantly expand the action up to second order in the perturbations. Starting from the Hamiltonian action (2.8), and expanding it up to second order in the fields' covariant UV perturbations $Q^{\tilde{X}I}$ as well as metric UV perturbations $\mathcal{N}_{\text{UV}}$ and ψ ,¹² one finds

$$S^{(0)} = \int d^4x a^3 \left[\varpi_I \varphi^{I'} - \frac{1}{H} \left(\frac{1}{2} G^{IJ} \varpi_I \varpi_J + V + 3M_{\text{Pl}}^2 H^2 \right) \right], \quad (4.18)$$

$$S^{(1)} = \int d^4x a^3 \left[\tilde{P}_I \left(\varphi^{I'} - \frac{\varpi^I}{H} \right) - Q^I \left(\mathcal{D}_N \varpi_I + 3\varpi_I + \frac{V_I}{H} \right) - \mathcal{N}_{\text{UV}} \left(\frac{1}{2} \varpi_I \varpi^I + V - 3M_{\text{Pl}}^2 H^2 \right) \right], \quad (4.19)$$

$$\begin{aligned} S^{(2)} = \int d^4x a^3 & \left[-3M_{\text{Pl}}^2 H^3 \mathcal{N}_{\text{UV}}^2 - \mathcal{N}_{\text{UV}} \left(\varpi_I \tilde{P}^I + V_I Q^I + 2M_{\text{Pl}}^2 H^2 \frac{\partial_i^2}{a^2} \psi \right) + \varpi_I Q^I \frac{\partial_i^2}{a^2} \psi \right. \\ & - \frac{1}{H} \left(\frac{1}{2} \tilde{P}_I \tilde{P}^I - \frac{1}{2} Q_I \frac{\partial_i^2}{a^2} Q^I + \frac{1}{2} V_{;IJ} Q^I Q^J - \frac{1}{2} R_I{}^{JK}{}_L \varpi_J \varpi_K Q^I Q^L \right) + \tilde{P}_I \mathcal{D}_N Q^I \\ & \left. + \left(\varphi^{I'} - \frac{\varpi^I}{H} \right) \frac{1}{2} R_{IJK}{}^L \varpi_L Q^J Q^K \right]. \end{aligned} \quad (4.20)$$

In usual perturbation theory, where the coarse-grained fields and momenta are replaced by their homogeneous values that are solutions of the classical equations of motion dictated by $S^{(0)}$, the linear action $S^{(1)}$ vanishes. It is thus sufficient to use covariant variables at linear order only, and one needs not bother about quadratic terms in $(Q^I, \tilde{P}_I)$ in eqs. (4.13) and (4.16). Here on the contrary, $S^{(1)}$ does not vanish because the time derivatives of the coarse-grained fields and momenta differ slightly from their classical values (by a quantity one can interpret as a classical random noise as we shall find soon). Relatedly, one can check

¹²Let us stress again that the stochastic approach is perturbative in the UV parts of the fields, and we only treat them up to quadratic order in this work (i.e. at the level of linearised perturbation theory). However no expansion is used at this stage for the IR parts of the fields, for which all nonlinearities are kept, at leading order in the gradient expansion.

that the manifest covariance of the result (4.18)–(4.20) would not have hold if one had not expanded $\delta\phi^{XI}$ to quadratic order in covariant perturbations. Let us now examine its three contributions.

Pure IR sector $S^{(0)}$ governs the propagation and self-interactions of the IR fields, without consideration of the UV modes at all. More generally, it should be interpreted as dictating the deterministic drift for the IR fields. Notice that in general, for generic potential V and field-space metric G_{IJ} , this classical drift action can be non-linear in the IR modes. Thus, we will not bother writing explicitly a rather complex expression for $S^{(0)}[\varphi^{XIa}] = S^{(0)}[\varphi^{XIcl} + \varphi^{XIq}/2] - S^{(0)}[\varphi^{XIcl} - \varphi^{XIq}/2]$, given that we will only be interested in its variation evaluated at classical IR solutions, which simply reads

$$\left. \frac{\delta S^{(0)}[\varphi^{XIa}]}{\delta \varphi^{YJq}} \right|_{\varphi^{YJq}=0} = \left. \frac{\delta S^{(0)}[\varphi^{XI}]}{\delta \varphi^{YJ}} \right|_{\varphi^{XI}=\varphi^{XIcl}}. \quad (4.21)$$

In a related manner, one can see that because of its structure, $S^{(0)}[\varphi^{XIa}]$ only contains odd powers of φ^{XIq} , the quantum component of the fields. Thus, its expansion in quantum fields is trivial up to quadratic order, and one can actually write:

$$S^{(0)}[\varphi^{XIa}] = \int d^4x \left. \frac{\delta S^{(0)}[\varphi^{XI}]}{\delta \varphi^{YJ}(x)} \right|_{\varphi^{XI}=\varphi^{XIcl}} \varphi^{YJq}(x) + \mathcal{O}(\varphi^q)^3. \quad (4.22)$$

IR-UV interactions As already stated, we focus in this derivation on the IR-UV interactions stemming from the continuous flow of quantum UV modes to the open system of classical IR ones, which results from the time-dependent Fourier cutoff $k_\sigma(N)$. Interestingly, these interactions are encoded in $S^{(1)}$ in the time derivatives of the IR fields, as seen in the heuristic approach (section 2). We thus focus on those terms and neglect other ones in $S^{(1)}$, which amounts to considering the time derivatives acting as $\delta(N - N_\sigma(k))$ in Fourier space as we shall see now.

However first, because we will write the discretised version of the linear action $S^{(1)}$, it will prove useful to take a step back. The form of $S^{(1)}$ that we displayed in eq. (4.19) is physically appealing because it makes explicitly appear the background EoM for the IR fields, times the UV perturbations, in an explicitly covariant form. However to find it we had first to integrate by parts the term $\int d^4x a^3 Q^{I'} \varpi_I = - \int d^4x a^3 Q^I (\varpi'_I + 3\varpi_I)$ and then combine it with the change from P_I to $\tilde{P}_I = P_I - \Gamma_{IJ}^K \varpi_K Q^J$ to form the covariant time derivative $\mathcal{D}_N \varpi_I$. Thus, going back to this previous version, the relevant terms in $S^{(1)}$ can be more simply expressed (i.e. with less time derivatives) as $S^{(1)} \supset \int d^4x a^3 (\tilde{P}_I \varphi^{I'} - Q^I (\mathcal{D}_N \varpi_I + 3\varpi_I)) = \int d^4x a^3 (P_I \varphi^{I'} + Q^{I'} \varpi_I)$, which we will now take as our starting point to compute IR-UV interactions in the Keldysh basis. Note that each of these two terms is not covariant when taken separately, but that their sum is indeed covariant. Understanding why these terms with time derivatives are peculiar is easier in Fourier space, and requires the investigation of the action in terms of Keldysh fields:

$$\begin{aligned} & S^{(1)}[\varphi^{XIa}, Q^{XIa}] \\ & \supset \int dN \frac{d^3\mathbf{k}}{(2\pi)^3} a^3(N) \left[P_I^{cl}(N, \mathbf{k}) \varphi^{Iq'}(N, \mathbf{k}) + Q^{Icl}(N, \mathbf{k}) \varpi_I^q(N, \mathbf{k}) \right] + (cl \leftrightarrow q). \end{aligned} \quad (4.23)$$

Now, remember that the same Fourier component of UV and IR modes can never be defined at the same time, except at the transition time $N_\sigma(k)$. Of course it means that the support of these terms is of measure zero, and this is actually why terms without derivatives were neglected in $S^{(1)}$.¹³ However the terms with derivatives that we kept play a special role. Let us look for example at the first term, going back to the discrete description of the phase-space path integral for the mode $\mathbf{k}$ around the time $N_\sigma(k)$:

$$\begin{aligned}
 & \int_{N_\sigma(k)-\Delta N}^{N_\sigma(k)+\Delta N} dN a^3(N) P_I^{\text{cl}}(N, \mathbf{k}) \varphi^{Iq'}(N, \mathbf{k}) \\
 &= \Delta N \left[a^3(N_\sigma(k) + \widetilde{\Delta N}) P_I^{\text{cl}}(N_\sigma(k) + \widetilde{\Delta N}, \mathbf{k}) \frac{\varphi^{Iq}(N_\sigma(k) + \Delta N, \mathbf{k}) - \varphi^{Iq}(N_\sigma(k), \mathbf{k})}{\Delta N} \right. \\
 & \quad \left. + a^3(N_\sigma(k) - \Delta N + \widetilde{\Delta N}) P_I^{\text{cl}}(N_\sigma(k) - \Delta N + \widetilde{\Delta N}, \mathbf{k}) \frac{\varphi^{Iq}(N_\sigma(k), \mathbf{k}) - \varphi^{Iq}(N_\sigma(k) - \Delta N, \mathbf{k})}{\Delta N} \right] \\
 &= a^3(N_\sigma(k) - \Delta N + \widetilde{\Delta N}) P_I^{\text{cl}}(N_\sigma(k) - \Delta N + \widetilde{\Delta N}, \mathbf{k}) \varphi^{Iq}(N_\sigma(k), \mathbf{k}),
 \end{aligned} \tag{4.24}$$

with $0 < \widetilde{\Delta N} < \Delta N$ and where we used the conditions (4.5) to get the second equality. Note that while the fields' values φ^I and Q^I are evaluated on the discrete time grid at $N_j = j\Delta N$, the momenta ϖ_I and P_I can be evaluated at intermediate time steps $\widetilde{N}_j = j\Delta N + \widetilde{\Delta N}$, which enables us to compute IR-UV interactions without specifying boundary conditions at the exact time $N_\sigma(k)$ for them. In the same way, we find that the second term contributes $-a^3(N_\sigma(k) + \widetilde{\Delta N}) Q^{I\text{cl}}(N_\sigma(k), \mathbf{k}) \varpi_I^q(N_\sigma(k) + \widetilde{\Delta N}, \mathbf{k})$. As for the third and the fourth term from the (cl-q) permutation in eq. (4.23), they vanish by virtue of the boundary conditions (4.6). Thus, the interaction action that we consider can be rewritten in the continuous limit as

$$\begin{aligned}
 S^{(\text{int})}[\varphi^{XIa}, Q^{XIa}] &= \int d^4x \int \frac{d^3\mathbf{k}}{(2\pi)^3} \delta(N - N_\sigma(k)) e^{i\mathbf{k}\cdot\mathbf{x}} a^3 \left[P_I(x)^{\text{cl}} \varphi^{Iq}(N, \mathbf{k}) - Q^{I\text{cl}}(x) \varpi_I^q(N, \mathbf{k}) \right] \\
 &= \int d^4x a^3 Q^{XIa}(x) \varphi'_{XIa}(x),
 \end{aligned} \tag{4.25}$$

where we introduced the pseudo “time derivatives” $\varphi'_{XIa}(x)$ with lower indices that are defined as

$$\begin{cases} \varphi'_{QIa}(x) := -\delta_a^{\text{cl}} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \delta(N - N_\sigma(k)) e^{i\mathbf{k}\cdot\mathbf{x}} \varpi_I^q(N, \mathbf{k}), \\ \varphi'_{PIa}(x) := \delta_a^{\text{cl}} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \delta(N - N_\sigma(k)) e^{i\mathbf{k}\cdot\mathbf{x}} \varphi_I^q(N, \mathbf{k}), \end{cases} \tag{4.26}$$

thus restricting the couplings to be of the form $\text{UV}^{\text{cl}} \times \text{IR}^q$. Those interaction terms will be the ones responsible for the modification of the classical equations of motion for the IR fields, once the UV perturbations are integrated out. Let us now investigate the dynamics of the latter.

UV dynamics As a first comment, note that the last line of $S^{(2)}$ seemingly goes beyond the approximation of treating UV modes up to quadratic order in the action, as it consists

¹³Strictly speaking this discussion applies only to terms in $S^{(1)}$ that are bilinear in IR and UV fields. Terms that are higher-order in IR quantities contain nonlinear IR-UV mode mixings, but the stochastic formalism does not aim at taking into account these couplings that are also present in Minkowski spacetime.

of a quadratic term in the UV perturbations, multiplied by the “background-like” equation of motion for the IR fields, i.e. by a quantity of order of the to-be-found noise. The careful reader will also have noticed that such a term is exactly of the kind that can ambiguously appear depending on the exact definition of a covariant momentum UV perturbation $\tilde{P}_I$, as we explain in appendix B. Because this arbitrariness can not affect the physics, we are free to make the choice ($\kappa = 1/2$) such that this term proportional to the Riemann tensor of the field space vanishes. This procedure also fixes the form of $S^{(3)}$ as is shown in appendix B, thus we conclude that this term does not affect the Gaussian properties of the theory and we will discard it in what follows, leaving for future work the investigation of this subtlety and of potentially interesting non-Gaussian features related to the geometry of the field space.

Extremising the action (4.18)–(4.20) with respect to the non-dynamical fields $\mathcal{N}_{UV}$ and ψ that appear without any time-derivative, one recovers the local Friedmann equation (2.26) as well as the expressions (2.25) and (2.27) for $\mathcal{N}_{UV}$ and ψ in terms of Q^I and $\tilde{P}_I$. Plugging them back into the second-order action, one can write the latter in the condensed form

$$S^{(2)} = \frac{1}{2} \int d^4x d^4x' Q^{XI}(x) \Lambda_{XYIJ}(x, x') Q^{YJ}(x'), \quad (4.27)$$

where we used the non-covariant variables Q^{XI} that naturally appear in $S^{(\text{int})}$ instead of the covariant perturbations $Q^{\tilde{X}I}$. As a result, some of the following intermediate steps will not be manifestly covariant. However, one is perfectly allowed to use such non-covariant objects to make calculations, and then to switch back to covariant ones using the relation (4.14) $\tilde{P}_I = P_I - \Gamma_{IJ}^K \varpi_K Q^J$. Instead of quoting the kernel Λ_{XYIJ} corresponding to the non-covariant UV modes that only appear in intermediate steps, we rather show its covariant counterpart $\Lambda_{\tilde{X}\tilde{Y}IJ}$, which is given by

$$\begin{pmatrix} \Lambda_{QQIJ}, \Lambda_{Q\tilde{P}IJ} \\ \Lambda_{\tilde{P}QIJ}, \Lambda_{\tilde{P}\tilde{P}IJ} \end{pmatrix} = \delta^{(4)}(x - x') a^3 \begin{pmatrix} \frac{1}{H} \left(G_{IJ} \frac{\partial^2}{a^2} - M_{QQIJ}^2 \right), -G_{IJ}(\mathcal{D}_N + 3) - M_{Q\tilde{P}IJ}^2 \\ G_{IJ} \mathcal{D}_N - M_{\tilde{P}QIJ}^2, -G_{IJ}/H \end{pmatrix}, \quad (4.28)$$

where the differential operators act on the x' coordinates, and with M_{QQIJ}^2 and $M_{Q\tilde{P}IJ}^2 = M_{\tilde{P}QIJ}^2$ already given in eqs. (2.30)–(2.31).

Extremising $S^{(2)}$ with respect to the covariant UV perturbations yields the following classical EoM for the UV fields:

$$\int d^4x' \Lambda_{\tilde{X}\tilde{Y}IJ}(x, x') Q^{\tilde{Y}J}(x') = 0, \Leftrightarrow \begin{cases} \mathcal{D}_N Q^I = \frac{\tilde{P}^I}{H} + M_{\tilde{P}Q}^2{}^I{}_J Q^J, \\ \mathcal{D}_N \tilde{P}_I = -3\tilde{P}_I + \frac{1}{H} \left(G_{IJ} \frac{\partial^2}{a^2} - M_{QQIJ}^2 \right) Q^J - M_{Q\tilde{P}I}^2{}^J \tilde{P}_J, \end{cases} \quad (4.29)$$

which are nothing else than equations (2.28) and (2.29) $E^{QI} = 0 = E_I^{\tilde{P}}$ found in the heuristic approach (section 2). Strikingly, as we shall see in the next subsection, it is sufficient to know the (inverse of the) kernel operator Λ to compute the corrections to the IR dynamics, due to their interactions with UV fluctuations as dictated by $S^{(\text{int})}$. Thus, the UV modes dictating these corrections can be understood as evolving according to $S^{(2)}$ only, hence they verify the EoM (4.29), similar to the one of SPT but with background fields replaced by their infrared counterparts. This is an interesting improvement from the path-integral approach compared to the heuristic one, where we had to *assume* that the dynamics of UV modes was decoupled from the one of IR ones, see the paragraph before eq. (2.21) and the one after eq. (2.31).

Eventually, in the path integral (4.17) with doubled degrees of freedom, the quadratic action written in terms of the fields in the Keldysh basis reads:

$$S^{(2)}[\varphi^{XIa}, Q^{XIa}] = \frac{1}{2} \int d^4x d^4x' Q^{XIa}(x) \Lambda_{XYIJab}(x, x') Q^{YJb}(x'), \quad (4.30)$$

where Λ_{XYIJab} is given by the basis transformation $\Lambda_{XYIJab} = (K^T)_a^a \Lambda_{XYIJab} K_b^b$, with K given in eq. (4.3), and with the $\pm$ basis operator

$$\Lambda_{XYIJab} = \text{diag} \left(\Lambda_{XYIJ}(\varphi^+), -\Lambda_{XYIJ}(\varphi^-) \right). \quad (4.31)$$

Note that, as the differential operator Λ_{XYIJ} depends on the IR fields φ^{XI} , one has in principle to distinguish between its evaluations on $+$ IR fields and on $-$ IR fields: $\Lambda_{XYIJ}(\varphi^+)$ and $\Lambda_{XYIJ}(\varphi^-)$. However, as we already noticed, one can think of the expansion in the quantum components as an expansion in $\hbar$. In this respect, in order to derive the leading-order quantum effects, it is sufficient to use the expression of Λ at zeroth-order:

$$\Lambda_{XYIJab} = \Lambda_{XYIJ}(\varphi^{\text{cl}}) \sigma_{3ab} + \mathcal{O}(\varphi^{\text{q}}) \delta_{ab}. \quad (4.32)$$

Although it may seem a crude approximation, we will check the consistency of this expansion in the next subsection, and explain why higher-order corrections are indeed not needed for our computation.

4.4 Covariant coarse-grained effective Hamiltonian action and Langevin equations

Now we have to gather the three contributions to the covariant coarse-grained Hamiltonian effective action and perform the following path integral:

$$\begin{aligned} \exp(iS_{\text{eff}}[\varphi^{XIa}]) &= \exp(iS^{(0)}[\varphi^{XIa}]) \\ &\times \int \mathcal{D}Q^{XIa} \exp \left[i \int d^4x a^3 \varphi'_{XIa} Q^{XIa} + \frac{i}{2} \int d^4x d^4x' Q^{XIa} \Lambda_{XYIJab} Q^{YJb} \right]. \end{aligned} \quad (4.33)$$

Note that we safely replaced the measure $\mathcal{D}Q^{\tilde{X}Ia}$ by $\mathcal{D}Q^{XIa}$ in the path integral (4.17) as the Jacobian for the transformation $Q^{\tilde{X}Ia} \rightarrow Q^{XIa}$ is exactly one. The Gaussian integral over the UV modes can be performed exactly to give:

$$S_{\text{eff}}[\varphi^{XIa}] = \underbrace{S^{(0)}[\varphi^{XIa}] + \frac{i}{2} \ln [\text{Det}(\Lambda)]}_{S_{\text{ren}}[\varphi^{XIcl}]} - \underbrace{\frac{1}{2} \int d^4x d^4x' \left(a^3 \varphi'_{XIa} \right)_x (\Lambda^{-1})^{XYIJab}_{xx'} \left(a^3 \varphi'_{YJb} \right)_{x'}}_{S_{\text{IA}}[\varphi^{XIa}]}. \quad (4.34)$$

The first term dictates the classical, background dynamics of the IR fields, and contains no new information compared to SPT. The second term is nothing but the usual QFT one-loop correction which can be computed in principle, and then reabsorbed by renormalisations of the bare parameters in the classical action S . We will thus omit this contribution in the following, although the renormalisation procedure is of course highly non-trivial to perform explicitly. More important for us is the third contribution S_{IA} called the *influence action*, describing the influence on the coarse-grained fields of the small-scale UV fluctuations that were integrated out (or more generally, the influence of an environment on the system of

interest [121]). In the rest of this subsection, we compute this influence action, discuss its physical interpretation and derive the resulting stochastic equations for the coarse-grained fields.

As Λ^{-1} is nothing but the closed-time-path-ordered two point correlation function of UV modes, it is easier to express it first in the $\pm$ basis with latin indices $a, b, \dots$, and then translate it into the Keldysh basis with use of the matrix of change of basis K^a_a . So we first focus on

$$\begin{aligned}
 i(\Lambda^{-1})^{XYIJab}(x, x') &= \int \mathcal{D}Q^{XIa} \exp \left[\frac{i}{2} \int d^4x d^4x' Q^{XIa} \Lambda_{XYIJab} Q^{YJb} \right] Q^{XIa}(x) Q^{YJb}(x') \\
 &= \begin{cases} \theta(N - N') \langle \hat{Q}^{XI}(x) \hat{Q}^{YJ}(x') \rangle + \theta(N' - N) \langle \hat{Q}^{YJ}(x') \hat{Q}^{XI}(x) \rangle, & (a = +, b = +), \\ \langle \hat{Q}^{YJ}(x') \hat{Q}^{XI}(x) \rangle, & (a = +, b = -), \\ \langle \hat{Q}^{XI}(x) \hat{Q}^{YJ}(x') \rangle, & (a = -, b = +), \\ \theta(N' - N) \langle \hat{Q}^{XI}(x) \hat{Q}^{YJ}(x') \rangle + \theta(N - N') \langle \hat{Q}^{YJ}(x') \hat{Q}^{XI}(x) \rangle, & (a = -, b = -), \end{cases} \quad (4.35)
 \end{aligned}$$

where the ordering of the quantum operators is determined by the chronological order along the closed-time path C , and the brackets $\langle \dots \rangle$ denote usual vacuum expectation values of UV operators under the φ^{XI} -dependent measure $\mathcal{D}Q^{XI} \exp \left(iS^{(2)} \left[\varphi^{XI}, Q^{XI} \right] \right)$. Note that these expectation values are unambiguously defined in the same way on both branches of the CTP, as we recall that for our computation, it is sufficient to evaluate the kernel Λ with vanishing quantum components of the IR fields, i.e. $\Lambda(\varphi^{\text{cl}})$, see eq. (4.32). Thus, for each component of the Λ^{-1} matrix we are able to forget the $\pm$ indices and we can compute them as in usual perturbation theory, but with background fields replaced by their IR counterparts.

With use of the dimensionless unequal time two-point functions

$$(2\pi)^3 \delta^{(3)}(\mathbf{k} + \mathbf{k}') \frac{2\pi^2}{k^3} \mathcal{P}^{XYIJ}(N, N'; k) = \langle \hat{Q}^{XI}(N, \mathbf{k}) \hat{Q}^{YJ}(N', \mathbf{k}') \rangle, \quad (4.36)$$

Λ^{-1} can be expressed more explicitly as

$$\begin{aligned}
 (\Lambda^{-1})^{XYIJab}(x, x') &= -i \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \frac{2\pi^2}{k^3} \begin{pmatrix} \theta(N - N') \mathcal{P}^{XYIJ}(N, N'; k) & \mathcal{P}^{XYIJ*}(N, N'; k) \\ +\theta(N' - N) \mathcal{P}^{XYIJ*}(N, N'; k) & \theta(N' - N) \mathcal{P}^{XYIJ}(N, N'; k) \\ \mathcal{P}^{XYIJ}(N, N'; k) & +\theta(N - N') \mathcal{P}^{XYIJ*}(N, N'; k) \end{pmatrix}^{ab}, \quad (4.37)
 \end{aligned}$$

where we used that $\mathcal{P}^{YXJI}(N', N; k) = \mathcal{P}^{XYIJ*}(N, N'; k)$ as a consequence of $\hat{Q}^{XI}(x)$ being hermitian operators, and hence $\hat{Q}^{XI\dagger}(N, \mathbf{k}) = \hat{Q}^{XI}(N, -\mathbf{k})$. We now express Λ^{-1} in the Keldysh basis as

$$\begin{aligned}
 (\Lambda^{-1})^{XYIJ}_{ab}(x, x') &= (K^T)_a^a \sigma_{3ab} (\Lambda^{-1})^{XYIJbc}(x, x') \sigma_{3cd} K^d_b \\
 &= -i \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \frac{2\pi^2}{k^3} \begin{pmatrix} 0 & -2i\theta(N' - N) \text{Im} \mathcal{P}^{XYIJ}(N, N'; k) \\ 2i\theta(N - N') \text{Im} \mathcal{P}^{XYIJ}(N, N'; k) & \text{Re} \mathcal{P}^{XYIJ}(N, N'; k) \end{pmatrix}_{ab}, \quad (4.38)
 \end{aligned}$$

where we used $\theta(N' - N) + \theta(N - N') = 1$. The influence action S_{IA} in eq. (4.34) can then be explicitly obtained after contracting twice with $\varphi'_{XI}{}^a(x) \propto \delta_q^a \delta(N - N_\sigma(k))$ (note that the

position of the $\mathbf{a}$ index has been flipped compared to eq. (4.26) with use of the $\sigma_1^{\mathbf{ab}}$ metric), retaining only the q-q component of eq. (4.38) evaluated at equal times $N = N' = N_\sigma(k)$:

$$S_{\text{IA}} = \frac{i}{2} \int d^4x d^4x' \left(a^3 \varphi_{XI}{}^{\mathbf{q}} \right)_x (\text{Re} \Pi^{XYIJ})_{xx'} \left(a^3 \varphi_{YJ}{}^{\mathbf{q}} \right)_{x'}, \quad (4.39)$$

where

$$\begin{aligned} \Pi^{XYIJ}(x, x') &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \frac{2\pi^2}{k^3} \delta(N - N_\sigma) \delta(N' - N_\sigma) \mathcal{P}^{XYIJ}(N, N'; k) \\ &= \frac{k_\sigma'}{k_\sigma} \frac{\sin(k_\sigma |\mathbf{x} - \mathbf{x}'|)}{k_\sigma |\mathbf{x} - \mathbf{x}'|} \mathcal{P}^{XYIJ}(N, k_\sigma) \delta(N - N'), \end{aligned} \quad (4.40)$$

with $\mathcal{P}$ on the second line being simply the usual equal-time dimensionless two-point correlation function. Note that any higher-order correction in the quantum components of the IR fields, coming from evaluating Λ beyond the leading order result (4.32), would generate terms of order $\mathcal{O}(\varphi^{\mathbf{q}})^3$ in the influence action. Put it otherwise, our computation is exact up to quadratic order in the quantum components.

Although we have just seen that the contractions with the “time derivatives” $\varphi'_{XI}{}^{\mathbf{a}}$ only kept the information about the q-q component of $\Lambda^{-1}_{\mathbf{ab}}$, it is still interesting to notice the “causality structure” [141, 201] of this operator.

Classical-Classical component. First, the “cl-cl” component in eq. (4.39) is zero. It is also easy to check that there is no term independent of $\varphi^{\mathbf{q}}$ in the fully nonlinear, purely IR Keldysh action $S^{(0)}[\varphi^{XI\text{cl}}, \varphi^{XI\text{q}}]$, as can be seen for example from its expansion (4.22) in the quantum components of the IR fields. This means that for vanishing quantum components $\varphi^{XI\text{q}} = 0$, the effective action $S_{\text{eff}} = S^{(0)} + S_{\text{IA}}$ is zero: $S_{\text{eff}}[\varphi^{XI\text{cl}}, 0] = 0$. This was expected because for $\varphi^{\mathbf{q}} = 0$, the fields coincide on the forward and backward parts of the closed-time contour and thus the two contributions cancel each other. A last interpretation is that the quantum components do not propagate alone and must mix to classical ones. In this respect, note that although our derivation was done at lowest non-trivial order in the quantum components of the fields and momenta, with $\Lambda \rightarrow \Lambda(\varphi^{\text{cl}})$ in the path integral over UV modes, this property actually holds non-perturbatively. Indeed, any correction to the current computation would be proportional to powers of $\varphi^{\mathbf{q}}$, and thus would still be vanishing when evaluated on configurations with purely classical components.

Classical-Quantum component. This component is interesting because, although non-zero in eq. (4.38), it results in a vanishing contribution to the influence action after contracting with the “time-derivatives” $\varphi'_{XI}{}^{\mathbf{a}} \propto \delta_{\mathbf{q}}^{\mathbf{a}}$, a property inherited from the boundary conditions (4.6). If $\varphi^{I\text{cl}}$ and $Q^{I\text{q}}$ were not vanishing at $N_\sigma(k)$, S_{IA} would be augmented by a cross-term of the form $[\varphi^{\text{cl}} (\Lambda^{-1})_{\text{cl,q}} \varphi^{\mathbf{q}} + (\text{cl} \leftrightarrow \text{q})]$ and proportional to the imaginary part of the power spectrum. The mixed “q-cl”/“cl-q” components in the influence action are more generally known for describing the dissipation of the system (the IR modes) by backreacting on the environment (the UV modes), and being responsible for the famous fluctuation-dissipation theorem. Indeed, if no boundary condition was imposed at the time $N_\sigma(k)$, the classical field configurations $\varphi_{XI}{}^{\text{cl}}(x)$ would get an extra friction term in their equations of motion of the form $-2 \int d^4x' \text{Im} \Pi^{XYIJ}(x, x') a^3(N') \varphi_{YJ}{}^{\text{cl}}(x')$. However in our

setup of stochastic inflation, the continuous flow from UV to IR modes via the time-dependent cutoff $k_\sigma(N)$ is unidirectional and we expect no such backreaction, and thus no dissipation.¹⁴

Quantum-Quantum component. The “q-q” component is the only one that survives in the influence action after contracting with the pseudo “time-derivatives”, and because it is quadratic in the quantum parts of the fields and momenta, it constitutes a non-trivial quantum correction to the classical dynamics, again describing the effects of the integrated out short-scale fluctuations on the IR sector. Let us now discuss its physical implications.

Strikingly, the influence action (4.39) is purely imaginary. This implies that in the path integral (4.7) over the IR components, the weights of configurations with non-zero quantum components are exponentially suppressed. This important fact warrants that our expansion in the quantum components of the fields (and momenta) is well justified. In a related manner, even though we do not use the formalism of density matrices in our paper, it can be shown quite generally that such imaginary “q-q” component in the influence action acts to suppress the off-diagonal terms of the reduced density matrix $\rho_r(\varphi^+, \varphi^-)$ obtained after tracing out the environment (the UV modes here), a process that can be understood as decoherence (see, e.g. refs. [121, 141]). The exponential suppression of the quantum components of the fields in the weight $e^{iS_{\text{IA}}}$ of the path integral is of course reminiscent of statistical field theory. Following the seminal paper of Feynman and Vernon [121], this insight is put to good use by performing what is sometimes called a Hubbard-Stratonovich transformation [206, 207]: introducing auxiliary fields ξ^{XI} , the exponential of the influence action can be rewritten as

$$e^{iS_{\text{IA}}} = \int \mathcal{D}\xi^{XI} P[\xi^{XI}; \varphi^{XI\text{cl}}] e^{i \int d^4x a^3 \xi^{XI} \varphi_{XI}{}^{\text{q}}}, \quad (4.41)$$

where $P[\xi^{XI}; \varphi^{XI\text{cl}}]$ denotes the Gaussian weight

$$P[\xi^{XI}; \varphi^{XI\text{cl}}] = \sqrt{\text{Det}(2\pi \text{Re}\Pi)^{-1}} \exp\left[-\frac{1}{2} \int d^4x d^4x' \xi^{XI} \left(\text{Re}\Pi_{XYIJ}^{-1}\right)_{\varphi^{XI\text{cl}}} \xi^{YJ}\right], \quad (4.42)$$

and where the subscript $\varphi^{XI\text{cl}}$ recalls that Π , as essentially the Green’s function of $\Lambda(\varphi^{XI\text{cl}})$, can thus be seen as a (complicated) functional of the IR classical components $\varphi^{XI\text{cl}}$. The manipulation (4.41)–(4.42) is a simple mathematical identity, in essence the inverse of a Gaussian integration. Yet, it offers a very useful physical insight. Indeed, the partition function (4.7) can now be rewritten as

$$\begin{aligned} Z &= \int \mathcal{D}\varphi^{XI\text{a}} \exp\left(iS_{\text{eff}}[\varphi^{XI\text{a}}]\right) \\ &= \int \mathcal{D}\varphi^{XI\text{cl}} \int \mathcal{D}\xi^{XI} P[\xi^{XI}; \varphi^{XI\text{cl}}] \int \mathcal{D}\varphi^{XI\text{q}} \exp\left(\underbrace{iS^{(0)}[\varphi^{XI\text{a}}] + i \int d^4x a^3 \xi^{XI} \varphi_{XI}{}^{\text{q}}}_{i\tilde{S}_{\text{eff}}[\varphi^{XI\text{a}}, \xi^{XI}]}\right), \end{aligned} \quad (4.43)$$

¹⁴The corresponding mass and friction terms entailed by this classical-quantum component were neglected by hand in refs. [122, 124, 126]. Moss and Rigopoulos cast doubt on the naive way to perform the IR-UV decomposition by a time-dependent window function [129, 161], and indeed, in refs. [130, 132], Tokuda and Tanaka carefully showed that the stochastic theory enables one to recover the free propagators only when choosing the appropriate boundary conditions in the Keldysh basis, with the consequence of prohibiting the classical-quantum component.

with $\int \mathcal{D}\xi^{XI} P[\xi^{XI}; \varphi^{XI\text{cl}}] = 1$ for any realisation of $\varphi^{XI\text{cl}}$. Upon the introduction of the Hubbard-Stratonovich fields ξ^{XI} , the imaginary quadratic interactions of the quantum components in $S_{\text{eff}}[\varphi^{XI\text{a}}]$ have been turned into a real linear coupling between the quantum components and the auxiliary fields in the new real effective action $\tilde{S}_{\text{eff}}[\varphi^{XI\text{a}}, \xi^{XI}]$. Of course, the physical interpretation behind eq. (4.43) is that $P[\xi^{XI}; \varphi^{XI\text{cl}}]$ endows the ξ 's with Gaussian statistics with

$$\begin{cases} \langle \xi^{XI}(x) \rangle \equiv \int \mathcal{D}\xi^{XI} \xi^{XI}(x) P[\xi^{XI}; \varphi^{XI\text{cl}}] = 0, \\ \langle \xi^{XI}(x) \xi^{YJ}(x') \rangle \equiv \int \mathcal{D}\xi^{XI} \xi^{XI}(x) \xi^{YJ}(x') P[\xi^{XI}; \varphi^{XI\text{cl}}] = \text{Re} \Pi^{XYIJ}(x, x') \Big|_{\varphi^{XI\text{cl}}}. \end{cases} \quad (4.44)$$

The delta function $\delta(N - N')$ in $\text{Re}\Pi$, see eq. (4.40), indicates that ξ 's can be interpreted as Gaussian white noises, like in the heuristic approach, with amplitudes determined by the power spectra of the UV modes on the “background” of the IR classical components. Additionally, it is interesting to notice that the reality of the noise is guaranteed in this first-principle derivation, contrary to the heuristic approach where this feature has to be added by hand (see section 2.5). The partition function (4.43) together with equations (4.40) and (4.44) represent one of the main results of this paper.

It is now relatively straightforward to take into account the effect of the quantum components on the classical ones. Indeed, recall that our computation of $S_{\text{eff}}[\varphi^{XI\text{a}}]$ was made up to quadratic order in the quantum components. Consistently neglecting cubic terms in the expression (4.22) for $S^{(0)}$, the quantum components therefore enter only linearly in $\tilde{S}_{\text{eff}}[\varphi^{XI\text{a}}, \xi^{XI}]$, and the path integral over them can hence be performed explicitly, yielding the delta functional $\delta\left(\frac{\delta S^{(0)}[\varphi^{XI}]}{\delta \varphi^{YJ}} \Big|_{\varphi^{XI}=\varphi^{XI\text{cl}}} + a^3 \xi^{YJ}\right)$ in the remaining path integral over the classical components of the IR fields, φ^{cl} , and the auxiliary variables ξ . Thus, the only trajectories with non-zero weights in the path integral are the ones that verify the following equations of motion:

$$\varphi^{I\text{cl}'} = \frac{\varpi^{I\text{cl}}}{H} + \xi^{QI}, \quad \varpi_I^{\text{cl}'} = -3\varpi_I^{\text{cl}} - \frac{V_I(\varphi^{I\text{cl}})}{H} + \frac{1}{H} \Gamma_{IJ}^K(\varphi^{I\text{cl}}) \varpi_K^{\text{cl}} \varpi^{J\text{cl}} + \xi_I^P, \quad (4.45)$$

where we will omit to write explicitly “cl” for simplicity in what follows. While the first equation is already in a manifestly covariant form, the second one is not. However this is not surprising as neither ϖ_I^{cl} nor P_I (that was integrated out), are covariant quantities themselves. However this equation does respect general covariance, as is seen by using $\xi_I^P = \xi_I^{\tilde{P}} + \Gamma_{IJ}^K \varpi_K \xi^{QJ}$, as well as $\varpi_I' = \mathcal{D}_N \varpi_I + \Gamma_{IJ}^K \varpi_K \varphi^{J'}$ and replacing $\varphi^{J'}$ by its value according to the first Langevin equation. Eventually, the stochastic EoM (4.45) can be summarised in an explicitly covariant way as (again, removing the “cl” exponent for conciseness)

$$\varphi^{I'} = \frac{\varpi^I}{H} + \xi^{QI}, \quad \mathcal{D}_N \varpi_I = -3\varpi_I - \frac{V_I}{H} + \xi_I^{\tilde{P}}. \quad (4.46)$$

As we discussed at length in section 3, these Langevin equations should be understood as the continuous limit of a discrete process with a Stratonovich scheme. Moreover, the identification of independent quantum fields in the Bunch-Davies regime provides one, upon classicalisation, with an essentially unique set of independent white noises with which to

formulate these Stratonovich Langevin-type equations. As we also explained there, Itô's discretisation also has a number of advantages, and one can convert the latter equations into the corresponding Itô's ones as:

$$\boxed{\mathfrak{D}_N \varphi^I = \frac{\varpi^I}{H} + \xi^{QI}, \quad \mathfrak{D}_N \varpi_I = -3\varpi_I - \frac{V_I}{H} + \xi_I^{\tilde{P}},} \quad (4.47)$$

with use of the Itô-covariant derivatives (3.4)–(3.6). Let us also remind the reader that the local Hubble parameter H is explicitly given in terms of the IR fields and momenta through the Friedmann constraint (2.26)

$$3M_{\text{Pl}}^2 H^2 = \frac{1}{2} G^{IJ}(\varphi) \varpi_I \varpi_J + V(\varphi), \quad (4.48)$$

without modification compared to the heuristic approach.

Eventually, let us comment on the status of these equations. As the derivation above shows, these are the semi-classical equations governing the trajectories that have a non-zero weight in the closed-time path integral, but they do not yet correspond to physical quantities: the expectation values of the quantum theory are only recovered once taking the ensemble averages over the noises. More precisely, this statistical average exactly reproduces the quantum average only when the initial effective action $S_{\text{eff}}[\varphi^{XIa}]$ is at most quadratic in the quantum components, resulting in the above delta functional (letting aside here the fact that we only integrated out the UV fluctuations at quadratic order in the action). It is in that sense that the stochastic equations (4.47), derived at lowest non-trivial order in the quantum components, can be qualified as “semi-classical”.

As described in section 3, physical quantities derived from Itô's SDE (4.47) only depend on the auto-correlation of the noises, which is physically specified by the UV two-point correlations. The presence of Itô-covariant derivatives also manifestly guarantees general covariance. These equations are thus free from any stochastic anomaly. Furthermore, as we stressed above, the reality of noises is also ensured, as their auto-correlations (4.44) derived from the CTP formalism are automatically given by the real part of the UV two-point functions.

5 Markovian analytical approximations and phase-space Fokker-Planck equation

As we explained in section 2.6, stochastic inflation is strictly speaking not described by a Markov process. Indeed, the noise amplitude is the solution of the differential equation verified by the UV modes which develop on the stochastic IR background, rather than an explicit function of the IR fields themselves. In particular, the noise amplitude *a priori* depends on the whole past history of the stochastic process. However, in some situations, the noise amplitude can be approximately expressed in terms of the instantaneous IR fields, in which case the dynamics can be thought of as Markovian and a powerful tool becomes accessible: the Fokker-Planck equation. In this section, we deal with these Markovian cases. We begin by showing the covariant Fokker-Planck equation that dictates the evolution of the one-point probability density function (PDF) for the IR fields and momenta, that can be inferred from the Langevin equations (4.47) when assuming a Markovian dynamics. Then we show how to approximate the noise amplitude, first in the simpler situation in which the scalar fields are strictly massless, and then in a generic case under the assumption of slow-varying masses.

5.1 Covariant Fokker-Planck equation in phase space

Let us first reemphasise that throughout this work, we treat the fields as locally homogeneous, i.e. at leading order in a gradient expansion. Although this might seem very crude, following the separate universe approach, this nonetheless enables one to capture the full nonlinear dynamics on super-Hubble scales. Hence, as described in section 2.3, the Langevin equations (4.47) govern the stochastic dynamics of a representative σ -Hubble patch. In the Markovian limit, with the assumption that the noise amplitudes are well approximated as functions of the current IR field values (and momenta), these Langevin equations give rise to the corresponding Fokker-Planck (FP) equation, with use of the rule presented in appendix A.3, as

$$\begin{aligned} \partial_N P = & -D_{\varphi^I} \left[\frac{G^{IJ}}{H} \varpi_J P \right] + \partial_{\varpi_I} \left[\left(3\varpi_I + \frac{V_I}{H} \right) P \right] \\ & + \frac{1}{2} D_{\varphi^I} D_{\varphi^J} (A^{QQIJ} P) + D_{\varphi^I} \partial_{\varpi_J} (A^{Q\tilde{P}I}{}_J P) + \frac{1}{2} \partial_{\varpi_I} \partial_{\varpi_J} (A^{\tilde{P}\tilde{P}}{}_{IJ} P). \end{aligned} \quad (5.1)$$

Here we defined a last covariant derivative D_{φ^I} with respect to the IR fields, the phase-space one, whose action on a rank-1 tensor is $D_{\varphi^I} \mathcal{U}^J = \nabla_I \mathcal{U}^J + \Gamma_{IL}^K \varpi_K \partial_{\varpi_L} \mathcal{U}^J$ and generalisation to rank- n tensors is straightforward. As for the $A^{\tilde{X}\tilde{Y}IJ}$'s, these are the noises' auto-correlations at coincident points:

$$A^{\tilde{X}\tilde{Y}IJ}(N) \delta(N - N') = \langle \xi^{\tilde{X}I}(N) \xi^{\tilde{Y}J}(N') \rangle = \frac{k'_\sigma}{k_\sigma} \text{Re}[\mathcal{P}^{\tilde{X}\tilde{Y}IJ}(N, k_\sigma(N))] \delta(N - N'), \quad (5.2)$$

which are here assumed to be functions of $\varphi^I(N)$ and $\varpi_I(N)$, and up to the factor k'_σ/k_σ that may be approximated by unity, are nothing else than the real parts of the UV power spectra.

One should remember that in the FP equation in field space (3.2), which we previously wrote for pedagogical reasons, the scalar PDF P_s is rescaled compared to the PDF P that directly results from the Langevin equations. Here, on the contrary, it is easy to check that the phase-space PDF $P(\varphi^I, \varpi_I, N)$ (truly the transition probability given some initial state), is already a scalar quantity, without the need of any rescaling. In this respect, although we skipped the intermediate steps of the computation, we stress that eq. (5.1) is not postulated, but simply derived from the Langevin equations and eq. (A.19), with covariant phase-space derivatives naturally emerging from the computation. Given the important complexity of the phase-space Itô-Langevin equations (4.47), the manifestly covariant form of the FP equation (5.1) is rather remarkable and provides a non-trivial consistency check of the former. This equation generalises the FP equation that we proposed in our previous paper in a simpler setup [95]: in field space and for test scalar fields in de Sitter space-time only. Also, the “stochastic anomalies” were not solved there, and the form of the FP equation was simply assumed based on the requirement of general covariance. Not only do we present here the derivation of this phase-space FP equation, but we are also confident that it can now be used to compute correlation functions of multifield inflation with curved field space in realistic setups where the fields backreact on the geometry of spacetime. However, it would be restrictive to consider that the virtue of this equation only concerns these situations: the Itô-Stratonovich ambiguity was also plaguing single-field inflation, and our first-principle derivation, with emphasis on manifest covariance, enabled us to solve it in this simpler context as well.

The remaining nontrivial difficulty is now to prescribe values for the auto-correlation of the noises $A^{\tilde{X}\tilde{Y}IJ}$, and in the next two sections, we turn to interesting particular cases where we can give analytical estimates. Note that this will be possible because we assume from now on a slow-varying regime, which was not the case until here. Also, because the dynamics of the UV modes in SPT is conveniently solved in terms of the conformal time τ such that $dN = aHd\tau$, we will also make use of this time variable in what follows. In our context in which H is a stochastic quantity, conformal time is strictly speaking not a deterministic variable like the number of e -folds, but we will nonetheless make this approximation, justified as follows. The noise auto-correlation at time N only depends on the UV fluctuations with wavenumber $k_\sigma(N)$, which exited the Hubble radius $\simeq -\ln(\sigma)$ e -folds before N . As the UV fluctuations follow the Bunch-Davies behaviour until only a few e -folds before Hubble crossing (all the more so for light fields of particular relevance in the stochastic formalism), in practice it is necessary to follow the evolution of a given mode $k_\sigma(N)$ during only for a few e -folds (typically 5), a duration that is not large enough for stochastic effects to accumulate and significantly affect the local Hubble scale.

5.2 Massless limit

For analytically understanding the UV fluctuations, it is particularly useful to use the projections of the mode functions on a set of parallel-transported vielbeins, the Q_A^α introduced in eq. (3.26). They provide independent degrees of freedom deep inside the Hubble radius, only mixing via the projected mass matrix $M^{2\alpha}_\beta$, as can be seen from their EoM (3.27). In this section, we consider that this projected mass matrix is completely negligible. By consistency of the slow-varying approximation, we also use the zeroth-order, locally de-Sitter expression of the scale factor $a(\tau) \simeq -1/(H_\star\tau)$, where $H_\star$ denotes the Hubble scale, considered constant around Hubble crossing, i.e. in the period interpolating between the Bunch-Davies regime and the crossing of the coarse-graining scale, such that $k_\sigma(\tau)\tau \simeq -\sigma(1 + \mathcal{O}(\epsilon))$.

Under these conditions, the mode functions Q_A^α simply provide N_{fields} independent copies ($Q_A^\alpha \propto \delta_A^\alpha$) of the standard single-field massless mode function in quasi de Sitter spacetime, which read, with Bunch-Davies initial condition:

$$Q_A^\alpha(\tau, k) = -i\delta_A^\alpha \frac{e^{-ik\tau}}{a\sqrt{2k}} \left(1 - \frac{i}{k\tau}\right). \quad (5.3)$$

Note that we used the freedom of redefining mode functions with an arbitrary unitary matrix as explained in section 3.2, in order to choose a phase that leads to explicitly real values of Q_A^α (and $\tilde{P}_A^\alpha$) on super-Hubble scales. From these mode functions, and using eq. (3.15), one deduces the multifield power spectrum of the UV modes at coarse-graining scale crossing:

$$\begin{aligned} \mathcal{P}^{QQIJ}(\tau, k_\sigma(\tau)) &= \frac{k_\sigma(\tau)^3}{2\pi^2} e_\alpha^I e_\beta^J Q_A^\alpha(\tau, k_\sigma(\tau)) Q_A^{\beta*}(\tau, k_\sigma(\tau)) \\ &= \left(\frac{H_\star}{2\pi}\right)^2 G^{IJ} (1 + \sigma^2), \end{aligned} \quad (5.4)$$

where we recall that $\sigma \ll 1$, so that the last term should be neglected. Notice that although mass effects are not taken into account in this section, the introduction of the parallel-transported vielbeins enables one to capture the geometrical effects of the curved field space at the level of UV fields ($\mathcal{P}^{QQIJ} \propto G^{IJ}$). Then, neglecting slow-roll suppressed metric per-

turbations $\propto M^2_{\tilde{P}Q}$ in $\tilde{P}$ for consistency, the momentum UV modes read

$$\tilde{P}_A^\alpha(\tau, k) \simeq \frac{d}{d\tau} Q_A^\alpha(\tau, k) = -\delta_A^\alpha \frac{H^2 e^{-ik\tau}}{\sqrt{2k^3}} k^2 \tau^2, \quad (5.5)$$

so that using again eq. (3.15), one obtains, for the power spectra involving momenta:

$$\mathcal{P}^{Q\tilde{P}I}_J(\tau, k_\sigma(\tau)) = -\sigma^2 H_\star \left(\frac{H_\star}{2\pi} \right)^2 \delta_J^I (1 - i\sigma), \quad (5.6)$$

$$\mathcal{P}^{\tilde{P}\tilde{P}}_{IJ}(\tau, k_\sigma(\tau)) = \sigma^4 H_\star^2 \left(\frac{H_\star}{2\pi} \right)^2 G_{IJ}. \quad (5.7)$$

Note that the cross power-spectrum has a non-zero imaginary part $\text{Im}\mathcal{P}^{Q\tilde{P}I}_J = \sigma^3 H_\star \left(\frac{H_\star}{2\pi} \right)^2 \delta_J^I$, remnant from the quantum nature of the scalar fields, and completely fixed by the non-vanishing commutation relation between Q and $\tilde{P}$ in eq. (3.11). Naturally, the fact that it is suppressed by the small parameter σ is related to the highly squeezed state of the fluctuations and to the fact that they “classicalise” on super-Hubble scales. However, notice anyway that the Schwinger-Keldysh derivation shows that only the real parts of the power spectra appear in the statistics of the stochastic noises.

In the strict massless and “slow-roll” regime of this section, the mode functions of the momenta (5.5) at coarse-graining scale crossing are suppressed by σ^2 compared to the ones of the fields (5.3), hence the power spectra involving the former should be self-consistently set to zero in practical computations. However, this property only holds within this framework, and in general, the power spectra involving momenta, while “slow-roll” suppressed, are not σ suppressed and should be considered, as we will show in the next section.

5.3 Slow-varying masses

Let us now go one step further and consider the effects of a non-zero mass matrix $M^{2\alpha}_\beta$. First we notice that at early times the mass term is negligible compared to the gradient term, i.e., $\forall \alpha, \beta, \quad M^{2\alpha}_\beta \ll k^2/a^2$. Thus initial conditions and the first stage of evolution of the perturbations are equivalent to the massless case. However, the behaviour is different around Hubble crossing. To identify these non-trivial mass effects, we make the assumption that the projected mass matrix is approximately constant in the period interpolating between the Bunch-Davies regime and the crossing of the coarse-graining scale, a feature observed in many concrete models of inflation. It is then possible to diagonalise the mass matrix locally, *around the time of Hubble crossing*, making use of the set of mass eigenvalues m_i^2 and corresponding eigenvectors D^α_i such that $M^{2\alpha}_\beta D^\beta_i = m_i^2 D^\alpha_i$ (no sum on i). According to our assumption, these quantities can be considered constant in the interpolating period, so that the vielbein-basis EoM (3.27) result then in the simple set of diagonal equations in the mass eigenbasis:

$$\partial_N^2 Q_A^i + (3 - \epsilon) \partial_N Q_A^i + \left(\frac{k^2}{a^2 H^2} + \frac{m_i^2}{H^2} \right) Q_A^i = 0, \quad (\text{no sum on } i), \quad (5.8)$$

where $Q_A^i = (D^{-1})^\alpha_i Q_A^\alpha$ denotes the projected mode functions on the mass eigenbasis. We here note that the mass matrix $M^{2\alpha}_\beta$ is real and symmetric, hence the mass eigenvalue m_i^2 are real, and one can take the diagonalising matrix D^α_i to be a real orthonormal matrix (with $(D^{-1})^\alpha_i = (D^T)^\alpha_i = D^\alpha_i$). It is important to notice that the mass eigenvalues m_i^2

are scalars in field space, and that they also correspond to eigenvalues of the original mass matrix $M^{2I}{}_J$, with eigenvectors given by $e_i^I = e_\alpha^I D^\alpha{}_i$, i.e.

$$M^{2I}{}_J e_i^J = m_i^2 e_i^I, \quad (\text{no sum on } i). \quad (5.9)$$

Moreover, taking into account the orthonormality of $D^\alpha{}_i$, the set of vectors e_i^I , rotated from the vielbeins e_α^I , constitute another set of vielbeins, hence satisfying $G_{IJ} e_i^I e_j^J = \delta_{ij}$ and $\delta^{ij} e_i^I e_j^J = G^{IJ}$.

The initial conditions for the Q_A^i are simply given by $Q_A^i(\tau, k) \xrightarrow{-k\tau \gg 1} \frac{-i}{a\sqrt{2k}} (D^{-1})^i{}_A e^{-ik\tau}$ with $(D^{-1})^i{}_A = (D^{-1})^\alpha{}_A \delta^\alpha{}_i$, so that the corresponding solution of eq. (5.8) reads, at leading-order in the slow-varying approximation:

$$Q_A^i(\tau, k) = (D^{-1})^i{}_A Q^i(\tau, k), \quad (\text{no sum on } i), \quad (5.10)$$

with Q^i the familiar single-field mode function

$$Q^i(\tau, k) = \frac{e^{i(\nu_i - 1/2)\pi/2}}{2a} \sqrt{-\pi\tau} H_{\nu_i}^{(1)}(-k\tau), \quad \text{with } \nu_i = \begin{cases} \sqrt{\frac{9}{4} - \frac{m_i^2}{H^2}}, & \text{if } \frac{m_i^2}{H^2} < \frac{9}{4}, \\ i\sqrt{\frac{m_i^2}{H^2} - \frac{9}{4}}, & \text{if } \frac{m_i^2}{H^2} \geq \frac{9}{4}. \end{cases} \quad (5.11)$$

expressed in terms of $H_{\nu_i}^{(1)}$, the Hankel function of the first kind and of order ν_i . Hence, one obtains the dimensionless power spectrum of UV modes at the time when $k = \sigma a H$ as

$$\mathcal{P}^{QQIJ}(\tau, k_\sigma(\tau)) = \frac{k_\sigma^3(\tau)}{2\pi^2} \sum_i e_i^I e_i^J |Q^i(\tau, k_\sigma(\tau))|^2, \quad (5.12)$$

where we used the orthonormality of the matrix $D^\alpha{}_i$. The result (5.12) is interesting because intermediate steps like the parallel-transported vielbeins or the diagonalising matrix $D^\alpha{}_i$ disappear altogether: to compute the right-hand side, the only requirement is to know the mass eigenvalues m_i^2 and the corresponding eigenvectors e_i^I forming a set of vielbeins, eq. (5.9), which is easy to obtain numerically from $M^{2I}{}_J$ once a position in phase space (φ^I, ϖ_I) is specified. Moreover, the sum in eq. (5.12) is nicely understood as a mass-weighted metric in field space, and indeed, the massless limit $\propto G^{IJ}$ is easily recovered by setting $\nu_i = 3/2$, $\forall i$. Notice also that $\mathcal{P}^{QQIJ}$ is automatically real and symmetric, as should be from first principles (see section 3.2).

Moving to momenta, and according to the UV EoM (4.29), one obtains

$$\tilde{P}_A^i = H \partial_N Q_A^i - \frac{\varpi^i \varpi_j}{2M_{\text{Pl}}^2 H} Q_A^j, \quad (5.13)$$

where $\varpi_i = e_i^I \varpi_I$. Using the properties of Hankel functions, we note that the time derivative of Q^i can be simply expressed, at leading-order in the slow-varying approximation, as ¹⁵

$$\partial_N Q^i|_{k_\sigma} = q_{\nu_i}(\sigma) Q^i|_{k_\sigma}, \quad \text{with } q_{\nu_i}(\sigma) = \nu_i - \frac{3}{2} - \sigma \frac{H_{\nu_i-1}^{(1)}(\sigma)}{H_{\nu_i}^{(1)}(\sigma)}, \quad (5.14)$$

¹⁵For completeness, at next order one has instead $q_{\nu_i}(\sigma) = (\nu_i - \frac{3}{2}) + \epsilon(\frac{1}{2} - \nu_i) - \sigma \frac{H_{\nu_i-1}^{(1)}(\sigma)}{H_{\nu_i}^{(1)}(\sigma)}$, $\nu_i = \sqrt{9/4 + 3\epsilon - (1+2\epsilon)m_i^2/H^2}$, and assuming both ϵ and m_i^2/H^2 small, one further obtains $q_{\nu_i}(\sigma) = -m_i^2/(3H^2) + O(\epsilon^2) + O(\epsilon \times m_i^2/H^2) + O(\sigma^2)$. However, evaluating q_{ν_i} beyond leading-order is too precise compared to the rest of our computation, as we have anyway considered the projected mass matrix to be constant.

where we evaluated it at the time of crossing of the coarse-graining scale. One therefore obtains

$$\tilde{P}_A^i|_{k_\sigma} = \sum_j \left(H q_{\nu_i}(\sigma) \delta_j^i - \frac{\varpi^i \varpi_j}{2M_{\text{Pl}}^2 H} \right) (D^{-1})^j{}_A Q^j|_{k_\sigma} \equiv \sum_j \mathcal{Q}_j^i (D^{-1})^j{}_A Q^j|_{k_\sigma}, \quad (5.15)$$

so that all power spectra at coarse-graining scale crossing can be summarised as

$$\mathcal{P}^{QQIJ} = \frac{k_\sigma^3}{2\pi^2} \sum_i e_i^I e_i^J |Q^i|_{k_\sigma}^2, \quad (5.16)$$

$$\mathcal{P}^{Q\tilde{P}I}{}_J = \frac{k_\sigma^3}{2\pi^2} \sum_{i,j} e_i^I e_{Jj} \mathcal{Q}^{*j}{}_i |Q^i|_{k_\sigma}^2, \quad (5.17)$$

$$\mathcal{P}^{\tilde{P}\tilde{P}}{}_{IJ} = \frac{k_\sigma^3}{2\pi^2} \sum_{i,j,k} e_{Ii} e_{Jj} \mathcal{Q}_k^i \mathcal{Q}^{*j}{}_k |Q^k|_{k_\sigma}^2. \quad (5.18)$$

One knows from first principles that $\mathcal{P}^{\tilde{P}\tilde{P}}{}_{IJ}$ should be real and symmetric, similarly to $\mathcal{P}^{QQIJ}$, while $\text{Im}\mathcal{P}^{Q\tilde{P}I}{}_J = \sigma^3 H_\star \left(\frac{H_\star}{2\pi}\right)^2 \delta_J^I$. Because our analytical expressions are based on several approximations, these properties are not necessarily precisely verified by eqs. (5.17)–(5.18), a discrepancy that can be used as a quantitative diagnostic of the quality of the approximations in practical numerical computations. However, we note once again that only the real parts of the power spectra anyway enter into the properties of the stochastic noises (see eq. (5.2)).

Although obtained for analytically estimating the noises amplitudes in stochastic multifield inflation, eqs. (5.16)–(5.18) are of more general interest in the context of multifield inflation with slow-varying quantities, replacing σ by k/aH when necessary, and they constitute new results to the best of our knowledge.¹⁶ Given the number of approximations performed, it is difficult to control the degree of accuracy of the above formulae, but they constitute a proof of principle that it is possible to obtain Markovian analytical approximations, and they constitute a basis for future improvements.

The discussion has been kept quite general until now, but as is well known, the behaviour of super-Hubble fluctuations strongly depends on the mass parameter. Hence, from these generically applicable formulas, in the stochastic context, two physically different regimes should be distinguished depending on the various values of m_i^2 , leading either to real positive ν_i for “light” fields (the first line in eq. (5.11)), or imaginary $\nu_i \equiv i\mu_i$ for heavy fields (the second line there). For heavy fields, one can write

$$\frac{k_\sigma^3(\tau)}{2\pi^2} |Q^i(\tau, k_\sigma(\tau))|^2 \underset{\frac{m_i^2}{H^2} \geq \frac{9}{4}}{=} 4\pi e^{-\mu_i \pi} \left(\frac{H}{2\pi}\right)^2 \left(\frac{\sigma}{2}\right)^3 |H_{i\mu_i}^{(1)}(\sigma)|^2, \quad (5.19)$$

with the small argument expansion

$$H_{i\mu}^{(1)}(\sigma) \underset{\sigma \ll 1}{\simeq} -i \frac{\Gamma(i\mu)}{\pi} \left(\frac{\sigma}{2}\right)^{-i\mu} + \frac{1 + \coth(\mu\pi)}{\Gamma(1 + i\mu)} \left(\frac{\sigma}{2}\right)^{i\mu}. \quad (5.20)$$

The factor $|H_{i\mu_i}^{(1)}(\sigma)|^2$ in eq. (5.19) hence describes the characteristic super-Hubble oscillations of heavy fields, but more importantly here, the power spectrum (5.19) is suppressed

¹⁶A related formula for the trace $G_{IJ} \mathcal{P}^{QQIJ}$ has already been used without proof in ref. [208], with excellent agreement with exact numerical computations.

by σ^3 . This explicit dependence on the a priori arbitrary coarse-graining parameter σ is not really worrisome: it simply comes from the fact that fluctuations of heavy fields are strongly suppressed on super-Hubble scales, and should simply be discarded from the stochastic description (and in the sums (5.17)–(5.18)), whose aim is to describe the long-term dynamics generated by light scalars. Turning to them, and using $H_\nu^{(1)}(\sigma) \underset{\sigma \ll 1}{\simeq} -(i/\pi)\Gamma(\nu)(\sigma/2)^{-\nu}$, the last term of $q_{\nu_i}(\sigma)$ in eq. (5.14) should be neglected as of order σ^2 , and one obtains

$$\frac{k_\sigma^3(\tau)}{2\pi^2} |Q^i(\tau, k_\sigma(\tau))|^2 \underset{\substack{m_i^2 < \frac{9}{4} \\ H^2}}{=} \left(\frac{H}{2\pi}\right)^2 \left(\frac{\Gamma(\nu_i)}{\Gamma(3/2)}\right)^2 \left(\frac{\sigma}{2}\right)^{3-2\nu_i}, \quad (5.21)$$

here with only a power-law dependence on σ . This dependence can be neglected, and $(\frac{\sigma}{2})^{3-2\nu_i}$ can be approximated by unity, under the condition that the latter is taken to verify

$$\frac{\sigma}{2} \gg e^{-(3-2\nu_i)^{-1}}, \quad (5.22)$$

which is easily compatible with $\sigma \ll 1$ for a light enough mass (see refs. [57, 162] for discussions in a single-field context). For intermediate masses $0.1 \lesssim m_i^2/H^2 \lesssim 1$, stochastic effects are less important but may not be completely negligible (see, e.g., ref. [166]), and the resulting σ -dependence indicates that the coarse-graining procedure, made at leading-order in the gradient expansion, should be refined in order to properly treat these situations. More precisely, let us add that in theories that are not completely scale invariant, it is expected that the Langevin equations, which describe the distribution of field values in σ -Hubble patches, do depend on σ . Yet another question is to see how σ disappears when computing physical observables on scales much larger than the cutoff scale. It is likely that the stochastic- δN approach needs to be modified to deal with these situations of intermediate masses, but this is largely outside the scope of this paper.

Eventually, as discussed in section 3.2, one can check explicitly that for light scalars with $m_i^2 < 9/4H^2$, the complex mode functions $Q_A^I(N, k)$ and $\tilde{P}_{IA}(N, k)$ (or equivalently, Q_A^i and $\tilde{P}_A^i$) become approximately real up to an irrelevant constant unitary matrix. This stems from the fact that, the Q^α being independent fields inside the Hubble radius, the variables $(D^{-1})^i_\alpha Q^\alpha$, obtained by rotation of the former, equally provide a set of independent variables (and indeed, we have seen that the orthonormal matrix D^α_i drops out of all correlators). Hence, one could also have rotated the annihilation (and creation) operators $\hat{a}^A$ and absorbed in their definitions the individual phase factors $e^{i\nu_i\pi/2}$ of the mode functions (5.11). The corresponding transformation can be described by the relations (3.9)–(3.10) with the unitary matrix

$$U^{\bar{A}}_B = D^{\bar{A}}_i \text{diag} \left(e^{i(\nu_i-3/2)\pi/2} \right)_i (D^{-1})^j_B, \quad (5.23)$$

with which one obtains the expressions

$$\bar{Q}_A^i = (D^{-1})^i_{\bar{A}} e^{-i(\nu_i-3/2)\pi/2} Q^i \quad (\text{no sum on } i), \quad \bar{\tilde{P}}_A^i = \mathcal{Q}^i_j \bar{Q}_A^j \quad (5.24)$$

that become manifestly real on super-Hubble scales.

6 Conclusions

In this paper, we derive an effective stochastic theory for the super-Hubble, coarse-grained, scalar fields during inflation. We do so in a phase-space approach and for the general class

of nonlinear sigma models (1.1), characterised by their potentials and curved field spaces. We first give in section 2 a “heuristic” derivation of the corresponding Langevin equations in phase space, in order to introduce concepts and notations used all the way. We point out the limitations of the heuristic approach that uses the classical equations of motion, as well as the non-Markovian nature of the dynamics. Section 3 is devoted to the resolution of the “inflationary stochastic anomalies” that we pointed out in our previous paper [95]: because of the very quantum nature of the scalar fields, the theory contains a preferred frame that corresponds to the basis of independent creation and annihilation operators. This frame must be used to define independent noises in the Langevin equations, removing the possibility of any ambiguity in the choice of such a frame, and the corresponding Langevin equations should be interpreted according to a Stratonovich, midpoint, discretisation scheme. Along this discussion, we show how the classicalisation of quantum fluctuations on super-Hubble scales enables one to interpret the noises as classical random variables rather than quantum operators. We also show explicitly the transformation of the Stratonovich-Langevin equations to their Itô version by the addition of noise-induced drifts, and explain how these terms can be combined with the usual time-derivatives to define new, covariant in Itô calculus, time-derivatives. With the final form (1.2), the Langevin equations can be readily used in numerical and analytical computations.

Section 4 is devoted to the rigorous derivation of the Langevin equations using a path-integral approach, which solves the remaining conceptual issues of the heuristic one. We begin by recalling that for the intrinsically time-dependent problems of interest in cosmology, like in other nonequilibrium situations, the relevant partition function is the one that dictates “in-in” correlation functions and causal equations of motions, and that it is defined by a closed-time path of integration. Equivalently, in this also called Schwinger-Keldysh formalism, the degrees of freedom are doubled along the conventional path, and we pay particular attention to the boundary conditions that connect them. In accordance with first principles, we also use the Hamiltonian action rather than the Lagrangian one, which is conceptually clearer for our phase-space study and in a stochastic context in which fields and momenta are not time-differentiable in the ordinary sense. Eventually, to deal with the UV parts of the fields and momenta, we identify phase-space covariant Vilkovisky-DeWitt variables, a crucial step to maintain the general covariance of the stochastic theory under redefinitions of the scalar fields. Because we are only interested in the super-Hubble dynamics, we integrate out explicitly the UV fields from the path integral, and find the influence action that describes the deviation of the IR dynamics from the background one of Standard Perturbation Theory. The final result is the Hamiltonian, coarse-grained effective action for the IR fields at first order in quantum corrections, which after a final manipulation consisting of introducing auxiliary classical variables ξ , can be shown to give rise to the noises in the Stratonovich-Langevin equations. The statistics of the noise at a given time is found as the real parts of the UV power spectra at the coarse-graining scale of that time. The fact that the noises are explicitly real is one of the improvements from the path-integral approach compared to the heuristic one. In section 5 we consider cases where the Markovian approximation is valid, and derive the covariant, phase-space Fokker-Planck (FP) equation corresponding to our Langevin equations. Thanks to the resolution of the anomalies, this equation is free from the ambiguities previously present in the literature, even in the single-field case. We also provide explicit analytical formulae for the noises correlations in multifield contexts, for massless scalar fields, as well as in generic situations under a slow-varying approximation.

We are confident that the formalism presented in this paper can be used in many interesting applications, both theoretical and phenomenological. First, the Itô-Langevin equations coupled to the UV EoM could be fully solved numerically without resorting to the Markovian hypothesis. That would however require following the evolutions of as many modes as time steps in the computation, in order to predict the correct noise amplitude at any time, and depending on the previous realisations of the noises and IR dynamics. These simulations should be done a large number of times, in order to compute statistical averages. Although being the most rigorous approach, it may be simpler to first consider the Markovian approximation, replacing the commonly approximated noise amplitude $(H/2\pi)^2$ by the formulae that we give in eqs. (5.16)–(5.18), and only then determine the IR dynamics, either numerically or analytically. Observationally relevant quantities, such as the power spectrum and the full PDF of the curvature perturbation, as well as the mass distribution of PBHs in relevant models, can then be computed by use of the stochastic- δN formalism, either applied to the result of many stochastic simulations in separate universes, or readily working at the level of the FP equation (5.1). We stress that due to the generality of our formalism, such computations can be made, not only in single-field contexts, but in the very large class of multifield models with curved field space, where qualitatively new phenomena can be expected. It would also be interesting to compare the computations of correlation functions made with the stochastic formalism to pure QFT calculations, notably in de Sitter, or to determine equilibrium PDFs in phase space, as well as to study the eigenvalues and eigenvectors of the FP operator in simple multifield contexts.

Eventually, this paper not only provides one with a useful formalism that can be used from now on, but it also paves the way for going further. First, thanks to the rigorous path-integral derivation, corrections to the present stochastic formalism can be in principle computed. Technically, that would require going at next order in the expansion of the Hamiltonian coarse-grained effective action in the quantum components of the fields and momenta. Another interesting avenue is to unveil the effect of non-Gaussianities on the stochastic formalism, by expanding the Hamiltonian action up to cubic order as we do in eqs. (B.15)–(B.18), and considering the effect of non-linear mode couplings. We leave these interesting possibilities for future works.

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A Stochastic calculus

In this appendix, we describe the exotic features of stochastic calculus that are intimately due to the non-differentiability of stochastic random variables. We begin by explaining explicitly

how discretisation schemes are defined, and how moving from one to another changes the continuous description, contrary to what happens for ordinary calculus. Then, we review some properties of Itô calculus, which is very different from the ordinary one as the standard chain rule for the derivative of composite functions does not hold. In particular, we explain how to define covariant derivatives compatible with this stochastic calculus. We eventually give the form of the Fokker-Planck equation corresponding to Langevin equations in any discretisation scheme.

A.1 Going from any scheme α to Itô

Let us consider multiple stochastic processes $\mathcal{S}^n(N)$ that are characterised by a multidimensional Langevin equation of the form

$$\frac{d\mathcal{S}^n}{dN} = h^n(N, \mathcal{S}) + g_A^n(N, \mathcal{S})\xi^A, \quad \langle \xi^A(N)\xi^B(N') \rangle = \delta^{AB}\delta(N - N'), \quad (\text{A.1})$$

where ξ^A are independent normalised Gaussian white noises. Here for notational simplicity we do as if the processes were Markovian and the noise amplitudes g_A^n were functions of the stochastic processes $\mathcal{S}^n$ at the same time N . However, there could be more general cases for which the stochastic processes affect their own noise amplitudes in a more complicated way. As explained in section 2.6, this is actually the case in stochastic inflation for which the amplitude of the noise is dictated by differential equations that simply include the stochastic processes themselves, a situation with implicit dependence that we sometimes refer to by using the expression “Langevin-type” equations. The noise amplitude can also depend explicitly on some subset of the stochastic processes $\mathcal{S}^n$ and implicitly on others, which is the case in eq. (3.28) for example. Keeping this in mind, we will still use the notation $g_A^n(N, \mathcal{S})$ for simplicity in these situations.

The time integration of such stochastic process is first described with use of a discrete time step ΔN , and then evaluated in the continuous limit $\Delta N \rightarrow 0$, like for the ordinary Riemann integral. In this discrete description, the noise term at the step i is first replaced by ΔW_i^A , which are defined as independent random Gaussian variables with variance ΔN :

$$\Delta W_i^A \Delta W_j^B = \delta^{AB} \delta_{ij} \Delta N. \quad (\text{A.2})$$

The fact that $\Delta W_i^A / \Delta N \sim (\Delta N)^{-1/2}$ has the important consequence that the noise, and thus the whole stochastic process, is not differentiable in the mathematical sense. All complexities of stochastic calculus arise from this simple fact. Still, it is possible to write the evolution of $\mathcal{S}^n$ from the step i to $i + 1$ as

$$\Delta \mathcal{S}_i^n = \mathcal{S}_{i+1}^n - \mathcal{S}_i^n = h^n(N_{i+\alpha}, \mathcal{S}_{i+\alpha})\Delta N + g_A^n(N_{i+\alpha}, \mathcal{S}_{i+\alpha})\Delta W_i^A. \quad (\text{A.3})$$

In general, the coefficients h^n and g_A^n can be functions of time N and of the stochastic process $\mathcal{S}^n$ itself. In this case of so-called multiplicative noise, the particular time at which they are evaluated between i and $i + 1$, parametrized by $0 \leq \alpha \leq 1$ as

$$N_{i+\alpha} = N_i + \alpha \Delta N, \quad \mathcal{S}_{i+\alpha}^n = (1 - \alpha)\mathcal{S}_i^n + \alpha \mathcal{S}_{i+1}^n, \quad (\text{A.4})$$

can matter, contrary to the ordinary Riemann integral for differentiable function. Indeed, let us find the transformation law between an arbitrary α discretisation and the so-called

Itô [147], or prepoint, discretisation defined by $\alpha = 0$:

$$\begin{aligned}
 \Delta \mathcal{S}_i^n &= h^n(N_{i+\alpha}, \mathcal{S}_{i+\alpha}) \Delta N + g_A^n(N_{i+\alpha}, \mathcal{S}_{i+\alpha}) \Delta W_i^A \\
 &= \left[h^n + \frac{\partial h^n}{\partial N} \alpha \Delta N + \frac{\partial h^n}{\partial \mathcal{S}^m} \alpha \Delta \mathcal{S}_i^m \right]_{N_i, \mathcal{S}_i} \Delta N + \left[g_A^n + \frac{\partial g_A^n}{\partial N} \alpha \Delta N + \frac{\partial g_A^n}{\partial \mathcal{S}^m} \alpha \Delta \mathcal{S}_i^m \right]_{N_i, \mathcal{S}_i} \Delta W_i^A + \dots \\
 &= \left[h^n + \alpha g_A^m \frac{\partial g_A^n}{\partial \mathcal{S}^m} \right]_{N_i, \mathcal{S}_i} \Delta N + g_A^n(N_i, \mathcal{S}_i) \Delta W_i^A + \mathcal{O}\left((\Delta N)^{3/2}\right). \tag{A.5}
 \end{aligned}$$

Crucially, because of the $(\Delta N)^{1/2}$ -dependence of the discrete noise ΔW_i^A , the term $\alpha(\partial_m g_A^n) \times \Delta \mathcal{S}_i^m \Delta W_i^A$ in the second line, contains a piece linear in ΔN that should be kept for consistency and results in a noise-induced drift $\alpha g_A^m \partial_m g_A^n$. In terms of the continuous description, the Langevin equation is thus properly defined only once a given discretisation scheme α is chosen. However it is always possible to relate it to a different Langevin equation corrected by the noise-induced drift and interpreted in the Itô, $\alpha = 0$, discretisation as

$$\boxed{\alpha\text{-scheme:} \quad \frac{d\mathcal{S}^n}{dN} = h^n + g_A^n \circ_\alpha \xi^A = \left(h^n + \alpha g_A^m \frac{\partial g_A^n}{\partial \mathcal{S}^m} \right) + g_A^n \xi^A,} \tag{A.6}$$

where the implicit sum on m only runs on indices that denote stochastic processes entering *explicitly* in the noise amplitudes g_A^n . We have introduced here the $\circ_\alpha$ symbol to make the α discretisation explicit, while no circle should be understood as the Itô discretisation. Another particular choice is the so-called Stratonovich, or midpoint, $\alpha = 1/2$, scheme [148], which we will represent by the circle $\circ$ without the subscript α . Different discretisation schemes can thus be connected by the induced drift term $\alpha g_A^m \partial_m g_A^n$ in the continuous description. The relation between a Langevin equation interpreted in the Stratonovich scheme, and the equivalent one in the Itô scheme is used in section 3.

A.2 Itô calculus and covariance

In this part we derive useful relations in the continuous description of stochastic processes when the underlying time discretisation is understood in the Itô scheme, taking into account the fact that so-called Itô calculus differs from ordinary calculus. First, the differential form of a function $f(N, \mathcal{S}^n)$ of time and of the stochastic processes $\mathcal{S}^n$, should be consistently expanded at “quadratic” order as

$$df(N, \mathcal{S}^n) = \frac{\partial f}{\partial N} dN + \frac{\partial f}{\partial \mathcal{S}^n} d\mathcal{S}^n + \frac{1}{2} \frac{\partial^2 f}{\partial \mathcal{S}^n \partial \mathcal{S}^m} d\mathcal{S}^n d\mathcal{S}^m. \tag{A.7}$$

Suppose the stochastic processes $\mathcal{S}^n$ verify the following Itô’s Langevin equation:

$$d\mathcal{S}^n = h^n dN + g_A^n dW^A. \tag{A.8}$$

Then, the differential form df can be written with the so-called Itô’s lemma [147],

$$\boxed{\text{Itô's lemma:} \quad df(N, \mathcal{S}^n) = \left(\frac{\partial f}{\partial N} + \frac{1}{2} \frac{\partial^2 f}{\partial \mathcal{S}^n \partial \mathcal{S}^m} A^{nm} \right) dN + \frac{\partial f}{\partial \mathcal{S}^n} d\mathcal{S}^n,} \tag{A.9}$$

where $A^{nm} = g_A^n g_A^m$ is the auto-correlation of the noises. It shows that a function of stochastic variables does not follow the ordinary chain rule of differentiation in Itô calculus. It should

be noted that the scheme conversion (A.6) reveals on the contrary that the Stratonovich discretisation does follow the standard chain rule, as the noise-induced drift compensates for the quadratic correction in Itô's lemma:

$$\begin{aligned} df(N, \mathcal{S}^n) &= \left(\frac{\partial f}{\partial N} + \frac{1}{2} \frac{\partial^2 f}{\partial \mathcal{S}^n \partial \mathcal{S}^m} A^{nm} \right) dN + \left(\frac{\partial f}{\partial \mathcal{S}^n} \circ d\mathcal{S}^n - \frac{1}{2} \frac{\partial^2 f}{\partial \mathcal{S}^n \partial \mathcal{S}^m} d\mathcal{S}^n d\mathcal{S}^m \right) \\ &= \frac{\partial f}{\partial N} dN + \frac{\partial f}{\partial \mathcal{S}^n} \circ d\mathcal{S}^n. \end{aligned} \quad (\text{A.10})$$

That is why the Stratonovich discretisation is useful in physical contexts where changes of variables are ubiquitous.

Motivated by our will to develop a manifestly covariant theory of stochastic multifield inflation, let us now consider a manifold with metric $G_{IJ}(\mathcal{X}^K)$, with coordinates $\mathcal{X}^I$ subject to SDE of the type (A.8). Itô's discretisation does not follow the standard chain rule and therefore it also breaks covariance under coordinate transformation in the ordinary sense. It is however possible to define stochastic covariant derivatives by adding suitable counter terms to ordinary derivatives. For the coordinates $\mathcal{X}^I$, we define

Itô-covariant derivative for coordinates: $\mathfrak{D}\mathcal{X}^I = d\mathcal{X}^I + \frac{1}{2} \Gamma_{JK}^I A^{\mathcal{X}JK} dN,$

(A.11)

where Γ_{JK}^I denote the Christoffel symbols of the metric, and $A^{\mathcal{X}IJ} = g_A^{\mathcal{X}I} g_A^{\mathcal{X}J}$ represents the auto-correlation of the noise $g_A^{\mathcal{X}I}$, assumed to be a vector at $\mathcal{X}^I$. Under the coordinate transformation $\mathcal{X}^I \rightarrow \bar{\mathcal{X}}^{\bar{I}}(\mathcal{X})$, $\mathfrak{D}\mathcal{X}^I$ indeed transforms itself as a vector:

$$\mathfrak{D}\bar{\mathcal{X}}^{\bar{I}} = \frac{\partial \bar{\mathcal{X}}^{\bar{I}}}{\partial \mathcal{X}^I} \mathfrak{D}\mathcal{X}^I, \quad (\text{A.12})$$

as can be shown with use of the Itô's lemma (A.9) for $d\bar{\mathcal{X}}^{\bar{I}}(\mathcal{X})$ and of the transformation law for the Christoffel symbol:

$$\frac{\partial \bar{\mathcal{X}}^{\bar{I}}}{\partial \mathcal{X}^I} \Gamma_{JK}^I = \frac{\partial \bar{\mathcal{X}}^{\bar{J}}}{\partial \mathcal{X}^J} \frac{\partial \bar{\mathcal{X}}^{\bar{K}}}{\partial \mathcal{X}^K} \bar{\Gamma}_{\bar{J}\bar{K}}^{\bar{I}} + \frac{\partial^2 \bar{\mathcal{X}}^{\bar{I}}}{\partial \mathcal{X}^J \partial \mathcal{X}^K}. \quad (\text{A.13})$$

We then also define covariant Itô derivatives for tangent vectors $\mathcal{U}^I$ and covectors $\mathcal{V}_I$. In the new coordinate system $\bar{\mathcal{X}}^{\bar{I}}(\mathcal{X})$, their components read by definition:

$$\bar{\mathcal{U}}^{\bar{I}}(\mathcal{X}, \mathcal{U}) = \frac{\partial \bar{\mathcal{X}}^{\bar{I}}(\mathcal{X})}{\partial \mathcal{X}^I} \mathcal{U}^I, \quad \bar{\mathcal{V}}_{\bar{I}}(\mathcal{X}, \mathcal{V}) = \frac{\partial \mathcal{X}^I(\bar{\mathcal{X}})}{\partial \bar{\mathcal{X}}^{\bar{I}}} \mathcal{V}_I. \quad (\text{A.14})$$

After some algebra, involving derivatives of these transformations as well as the one of the Christoffel symbols (A.13), and using Itô's lemma for $d\bar{\mathcal{U}}^{\bar{I}}(\mathcal{X}, \mathcal{U})$ and $d\bar{\mathcal{V}}_{\bar{I}}(\mathcal{X}, \mathcal{V})$, one finds the following suitable covariant Itô derivatives:

Itô-covariant derivative for vectors:

$$\mathfrak{D}\mathcal{U}^I = \mathcal{D}\mathcal{U}^I + \frac{1}{2} \left(\Gamma_{JS,K}^I - \Gamma_{JS}^M \Gamma_{MK}^I \right) \mathcal{U}^S A^{\mathcal{X}JK} dN + \Gamma_{JK}^I A^{\mathcal{X}IJ} dN,$$

(A.15)

Itô-covariant derivative for covectors:

$$\mathfrak{D}\mathcal{V}_I = \mathcal{D}\mathcal{V}_I - \frac{1}{2} \left(\Gamma_{IJ,K}^S + \Gamma_{IJ}^M \Gamma_{KM}^S \right) \mathcal{V}_S A^{\mathcal{X}JK} dN - \Gamma_{IJ}^K A^{\mathcal{X}J}{}_K dN.$$

(A.16)

Here $A^{\mathcal{X}\tilde{\mathcal{U}}IJ} = g_A^{\mathcal{X}I} g_A^{\tilde{\mathcal{U}}J}$ and $A^{\mathcal{X}\tilde{\mathcal{V}}I}{}_J = g_A^{\mathcal{X}I} g_{JA}^{\tilde{\mathcal{V}}}$ are the cross-correlations between the coordinate noise $g_A^{\mathcal{X}I}$ and the covariant combinations of (co)vector noise:

$$g_A^{\tilde{\mathcal{U}}I} = g_A^{\mathcal{U}I} + \Gamma_{JK}^I \mathcal{U}^J g_A^{\mathcal{X}K}, \quad g_{IA}^{\tilde{\mathcal{V}}} = g_{IA}^{\mathcal{V}} - \Gamma_{IJ}^K \mathcal{V}_K g_A^{\mathcal{X}J}. \quad (\text{A.17})$$

It can be checked that they indeed transform as tensors under Itô calculus, i.e. with:

$$\mathfrak{D}\bar{\mathcal{U}}^{\bar{I}} = \frac{\partial \bar{\mathcal{X}}^{\bar{I}}}{\partial \mathcal{X}^I} \mathfrak{D}\mathcal{U}^I, \quad \mathfrak{D}\bar{\mathcal{V}}_{\bar{I}} = \frac{\partial \mathcal{X}^I}{\partial \bar{\mathcal{X}}^{\bar{I}}} \mathfrak{D}\mathcal{V}_I. \quad (\text{A.18})$$

A.3 From Langevin to Fokker-Planck

When the noise amplitude g_A^n depends only explicitly on the stochastic processes $\mathcal{S}^n$, the whole process is said to be Markovian. Indeed, the distribution from which the noise is drawn at a time N is then fixed by the values of the processes $\mathcal{S}^n$ *at this time N only*, and the past history (the path in the space of the processes that led to this particular point) is irrelevant. Thus, a new useful tool becomes accessible: the Fokker-Planck (FP) equation.

The FP equation is a partial differential equation (PDE) for the transition probability of the stochastic processes $\mathcal{S}^n$. This transition probability $P(\mathcal{S}^n, N | \mathcal{S}_{\text{ini}}^n, N_{\text{ini}})$ is defined as the probability that the stochastic processes take the values $\mathcal{S}^n$ at the time N knowing that they initially had the value $\mathcal{S}_{\text{ini}}^n$ at time N_{ini} . If the processes $\mathcal{S}^n$ verify the Langevin equation (A.6) with a given choice of discretisation α , it can be shown that the transition probability (that can be thought of as a one-point Probability Density Function (PDF) for the processes $\mathcal{S}^n$) verifies the Fokker-Planck equation:

$$\frac{\partial P}{\partial N} = - \frac{\partial}{\partial \mathcal{S}^n} \left[\left(h^n + \alpha g_A^m \frac{\partial g_A^n}{\partial \mathcal{S}^m} \right) P \right] + \frac{1}{2} \frac{\partial^2}{\partial \mathcal{S}^n \partial \mathcal{S}^m} [g_A^n g_A^m P]. \quad (\text{A.19})$$

This is nothing but a convection-diffusion equation for the PDF $P(\mathcal{S}^n, N)$, where the diffusion is due to the stochastic noise while the drift is due to the deterministic force in the Langevin equation (plus a noise-induced drift for discretisations different from Itô, $\alpha = 0$).

B Covariant expansion of the Hamiltonian

In this appendix, we revisit in more detail the choice of covariant UV perturbations. In the main body of the paper, we connect the finite displacements $\delta\phi^I$ and $\delta\pi_I$ and the covariant “initial velocity” $Q^I = d\phi^I/d\lambda|_{\lambda=0}$ and $\tilde{P}_I = \mathcal{D}_\lambda \pi_I|_{\lambda=0}$ through the geodesic-type interpolation $\mathcal{D}_\lambda^2 \phi^I = 0$ and $\mathcal{D}_\lambda^2 \pi_I = 0$. However, the requirement of covariance does not by itself prohibit any curvature invariant term in the corresponding momentum equation. For example, let us consider the transportation of the on-shell solution. Considering the Minkowski limit for simplicity in this discussion, the on-shell momenta are given by $\pi_I = G_{IJ} \dot{\phi}^J$ where a dot represents a generic time derivative (see eq. (2.13)). Therefore, along the field-space geodesic defined by $\mathcal{D}_\lambda^2 \phi^I = 0$, the on-shell π follows

$$\begin{aligned} \mathcal{D}_\lambda^2 \pi_I &= G_{IJ} \mathcal{D}_\lambda^2 \dot{\phi}^J = G_{IJ} \mathcal{D}_\lambda^2 \mathcal{D}_t \phi^J = G_{IJ} \mathcal{D}_\lambda \mathcal{D}_t \mathcal{D}_\lambda \phi^J = G_{IJ} [\mathcal{D}_\lambda, \mathcal{D}_t] \mathcal{D}_\lambda \phi^J \\ &= R_{I\lambda\lambda t} = R_{IJK}^S \pi_S \frac{d\phi^J}{d\lambda} \frac{d\phi^K}{d\lambda} \neq 0 \text{ a priori,} \end{aligned} \quad (\text{B.1})$$

where R_{IJK}^S is the Riemann tensor of the field space:

$$R_{IJK}^S = \Gamma_{IK,J}^S - \Gamma_{IJ,K}^S + \Gamma_{IK}^R \Gamma_{JR}^S - \Gamma_{IJ}^R \Gamma_{KR}^S. \quad (\text{B.2})$$

To derive eq. (B.1), we made use of the general fact $[\mathcal{D}_\lambda, \mathcal{D}_t]\phi^I = 0$ as well as the geodesic equation $\mathcal{D}_\lambda^2 \phi^I = 0$. This new interpolation law obviously yields an additional quadratic term proportional to the Riemann tensor, in the expression of $\delta\pi_I$ in terms of $(Q^I, \tilde{P}_I)$. However the momenta π_I are *a priori* off-shell in the path integral that we perform in section 4. Thus, they have no particular reason to follow the interpolation law (B.1), which is nothing but one of the possible covariant deviations from the geodesic interpolation, and any such covariant deviation is allowed. The point is that the quadratic correction due to the non-trivial “acceleration” $\mathcal{D}_\lambda^2 \pi_I$ can always be absorbed into the definition of the covariant momentum UV perturbation. When the interpolation law is given by eq. (B.1), we will denote the former as $\tilde{P}_{I,1/2}$ for a reason that will soon become clear, and one finds the modification compared to the case where it is $\mathcal{D}_\lambda^2 \pi_I = 0$ that defines $\tilde{P}_I$:

$$\tilde{P}_{I,1/2} = \tilde{P}_I + \frac{1}{2} R_{IJK}{}^L \varpi_L Q^J Q^K. \quad (\text{B.3})$$

Note that this other choice would leave unchanged, both the commutation relation $[Q^I(N, \mathbf{x}), \tilde{P}_{J,1/2}(N, \mathbf{x}')] = i\delta_J^I \delta^{(3)}(\mathbf{x} - \mathbf{x}')$ and the linear UV equations of motion. Interestingly, $\tilde{P}_{I,1/2}$ is the only choice that makes completely disappear the term in “background EoM” $\times$ Riemann $\times$ QQ in $S^{(2)}$, eq. (4.20), and that we discarded in the main text. As already explained, any covariant deviation from the geodesic interpolation law is allowed by the requirement to define a covariant momentum perturbation, so this leaves the possibility of defining for instance a family of covectors

$$\tilde{P}_{I,\kappa} = \tilde{P}_I + \kappa R_{IJK}{}^L \varpi_L Q^J Q^K, \quad (\text{B.4})$$

that all verify the necessary conditions: covariance, standard commutation relation and linear UV equations of motion. We acknowledge that this ambiguity remains in our treatment of stochastic inflation, but the difference between two choices of covariant perturbations goes beyond the usual approximations of stochastic inflation, and in particular the Gaussianity of the noise. However, there might be potentially interesting geometrical effects induced by the curved field space beyond this approximation.

To see the apparent effect of the κ ambiguity, let us explicitly show the cubic Hamiltonian action in terms of the variables $\tilde{P}_{I,\kappa}$. To this end, a geometric approach is more useful than directly expanding the differences $\delta\phi^I = \phi^I - \varphi^I$ and $\delta\pi_I = \pi_I - \varpi_I$. We first note that the action for perturbations $S^{(\text{ptb})}$ is given by the difference between the full action and the IR action as

$$S^{(\text{ptb})} = S[\phi, \pi, \mathcal{N}, \beta] - S[\varphi, \varpi, \mathcal{N}_{\text{IR}}, 0]. \quad (\text{B.5})$$

The non-trivial aspect comes from the fact that the full variables and their IR parts live at the different field-space points $\phi^I(\lambda = 1)$ and $\varphi^I = \phi^I(\lambda = 0)$. That is why their direct differences are not covariant objects. However the action itself is a scalar in field space and thus it is invariant under the parallel transport from $\lambda = 1$ to $\lambda = 0$:

$$S^{(\text{ptb})} = S_{\parallel}[\phi, \pi, \mathcal{N}, \beta]_{\lambda=0} - S[\varphi, \varpi, \mathcal{N}_{\text{IR}}, 0]. \quad (\text{B.6})$$

These transported variables can be directly compared to the IR (co)vectors, and the covariant expansion of the Hamiltonian action is easily derived that way.

Let us describe this approach in detail (see figure 3 for a schematic representation). We first recall that the full field ϕ^I (at $\lambda = 1$) and its IR part φ^I (at $\lambda = 0$) are connected by a

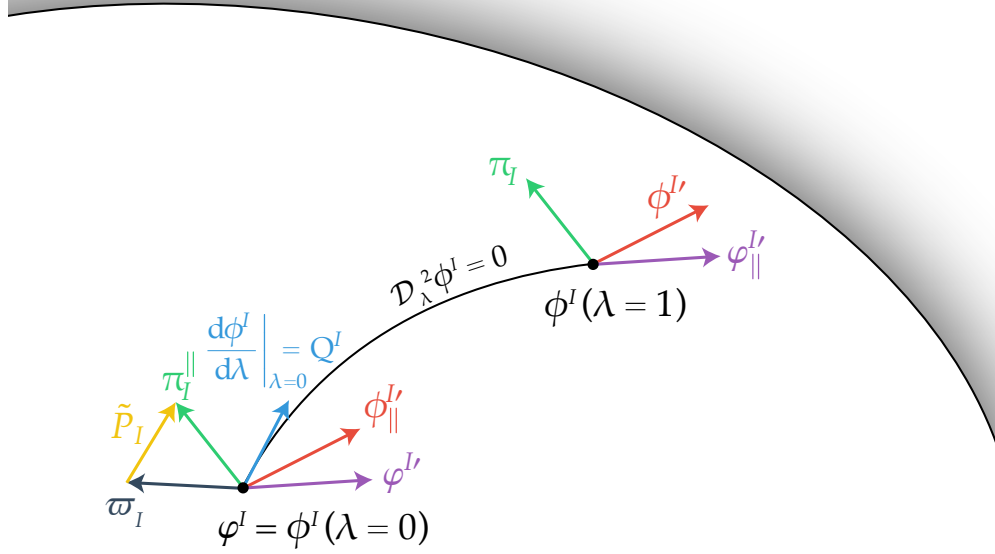


Figure 3. Schematic representation of the Hamiltonian variables on a curved field space. The full (co)vectors $\phi^{I'}$ and π_I are defined at ϕ^I , while their IR parts $\varphi^{I'}$ and ϖ_I live at φ^I . These two points can be connected by the geodesic λ -line $\mathcal{D}_\lambda^2 \phi^I(\lambda) = 0$, characterised by the contravariant UV perturbation $Q^I = d\phi^I/d\lambda|_{\lambda=0}$ which is a vector at φ^I . Along this line, vectors living at each point can be parallel transported to each others (vectors in the same color). This procedure enables one to efficiently expand the action in terms of (co)vectors at the IR point φ^I .

unique geodesic line

$$\mathcal{D}_\lambda^2 \phi^I = 0, \quad \Leftrightarrow \quad \frac{d^2 \phi^I}{d\lambda^2} = -\Gamma_{JK}^I \frac{d\phi^J}{d\lambda} \frac{d\phi^K}{d\lambda}, \quad (\text{B.7})$$

with the affine parameter λ . This geodesic line can be characterised by the contravariant vector at $\lambda = 0$

$$Q^I := \left. \frac{d\phi^I}{d\lambda} \right|_{\lambda=0}. \quad (\text{B.8})$$

Then one can parallel transport, e.g., the full momentum π_I , a covector at $\lambda = 1$, to the IR point $\lambda = 0$ along this λ -line. The transport condition is given by $\mathcal{D}_\lambda \pi_I^{\parallel} = 0$ with the initial condition $\pi_I^{\parallel}|_{\lambda=1} = \pi_I$. The transported momentum $\pi_I^{\parallel}|_{\lambda=0}$ is a covector at $\lambda = 0$, so that it can be directly compared to the other covector there, ϖ_I . Thus one can define the covariant UV momentum by their difference, i.e.:

$$\tilde{P}_I \equiv \pi_I^{\parallel}|_{\lambda=0} - \varpi_I. \quad (\text{B.9})$$

This new definition coincides with the previous one $\tilde{P}_I = \mathcal{D}_\lambda \pi_I|_{\lambda=0}$.

As the scalar product (computed with the field-space metric) between two parallel-transported quantities is constant, the kinetic term in the Hamiltonian, for example, can be

easily expressed as¹⁷

$$\pi_I \pi^I|_{\lambda=1} = \pi_I^\parallel \pi^\parallel|_{\lambda=0} = (\varpi_I + \tilde{P}_I)(\varpi^I + \tilde{P}^I). \quad (\text{B.10})$$

Similarly, all scalar products in the Hamiltonian action such as $\pi_I \pi^I$, $\pi_I \phi'^I$, $\pi_I \partial_i \phi^I$, and $G_{IJ} \partial_i \phi^I \partial_i \phi^J$ can be expanded at $\lambda = 0$ as $\pi_I^\parallel \pi^\parallel|_{\lambda=0}$, $\pi_I^\parallel \phi'^I|_{\lambda=0}$, and so on. Using the geodesic equation (B.7) as well as expansions around $\lambda = 0$ of the Christoffel symbols and their derivatives, it is then straightforward, although tedious, to find the following expressions:

$$\begin{aligned} \phi'^I|_{\lambda=0} &= \varphi'^I + \mathcal{D}_N Q^I + \frac{1}{2} R^I{}_{JKL} \varphi'^L Q^J Q^K \\ &\quad + \frac{1}{6} R^I{}_{JKM;L} \varphi'^M Q^J Q^K Q^L + \frac{1}{6} R^I{}_{JKL} Q^J Q^K \mathcal{D}_N Q^L + \dots, \end{aligned} \quad (\text{B.11})$$

$$(\partial_i \phi^I)|_{\lambda=0} = \partial_i Q^I + \frac{1}{6} R^I{}_{JKL} Q^J Q^K \partial_i Q^L + \dots. \quad (\text{B.12})$$

The scalar potential V can be also expanded in a covariant way as

$$V|_{\lambda=1} = V + V_I Q^I + \frac{1}{2} V_{;IJ} Q^I Q^J + \frac{1}{6} V_{;IJK} Q^I Q^J Q^K + \dots. \quad (\text{B.13})$$

The ADM variables $\mathcal{N}$ and β^i are also scalars in field space but they should be considered independent of ϕ^I and π_I before one takes into account their constraint equations. Thus, one can define their UV parts by the simple differences

$$\mathcal{N}_{\text{UV}} \equiv \mathcal{N} - \mathcal{N}_{\text{IR}}, \quad a^{-2} \partial_i \psi \equiv \beta^i - 0. \quad (\text{B.14})$$

Up to cubic order in the covariant UV perturbations Q^I and $\tilde{P}_I$, the Hamiltonian action then reads¹⁸

$$S^{(0)} = \int d^4 x a^3 \left[\varpi_I \varphi'^I - \frac{1}{H} \left(\frac{1}{2} \varpi_I \varpi^I + V + 3M_{\text{Pl}}^2 H^2 \right) \right], \quad (\text{B.15})$$

$$S^{(1)} = \int d^4 x a^3 \left[\tilde{P}_{I,\kappa} \left(\varphi'^I - \frac{\varpi^I}{H} \right) - Q^I \left(\mathcal{D}_N \varpi_I + 3\varpi_I + \frac{V_I}{H} \right) - \mathcal{N}_{\text{UV}} \left(\frac{1}{2} \varpi_I \varpi^I + V - 3M_{\text{Pl}}^2 H^2 \right) \right], \quad (\text{B.16})$$

$$\begin{aligned} S^{(2)} &= \int d^4 x a^3 \left[\tilde{P}_{I,\kappa} \mathcal{D}_N Q^I - 3M_{\text{Pl}}^2 H^3 \mathcal{N}_{\text{UV}}^2 - \mathcal{N}_{\text{UV}} \left(\varpi_I \tilde{P}_\kappa^I + V_I Q^I + 2M_{\text{Pl}}^2 H^2 \frac{\nabla^2}{a^2} \psi \right) + \varpi_I Q^I \frac{\nabla^2}{a^2} \psi \right. \\ &\quad \left. - \frac{1}{H} \left(\frac{1}{2} \tilde{P}_{I,\kappa} \tilde{P}_\kappa^I - \frac{1}{2} Q_I \frac{\nabla^2}{a^2} Q^I + \frac{1}{2} V_{;IJ} Q^I Q^J - \frac{1}{2} R_I{}^{KL}{}_{J\varpi_K \varpi_L} Q^I Q^J \right) \right. \\ &\quad \left. + \left(\frac{1}{2} - \kappa \right) \left(\varphi'^I - \frac{\varpi^I}{H} \right) R_{IJK}{}^L \varpi_L Q^J Q^K \right], \end{aligned} \quad (\text{B.17})$$

¹⁷The position of the parallel symbol $\parallel$ is arbitrarily raised and lowered without any specific meaning. We put it on the opposite side of the field index I just for clarity.

¹⁸Making use of the linear constraints (2.25) and (2.27), one can check that our cubic Hamiltonian is consistent with results in the literature (see, e.g. refs. [209, 210]), albeit importantly in our stochastic context, no background equation of motion has been used here. Note that, as can be seen in the linear perturbation EoM (4.29), our definition of $\tilde{P}$ differs, even at linear order, from the ordinary notation where the on-shell momentum perturbation is defined as $\tilde{P} \propto \mathcal{D}_N Q$.

$$\begin{aligned}
 S^{(3)} = \int d^4x a^3 \Big[& 3M_{\text{Pl}}^2 H^4 \mathcal{N}_{\text{UV}}^3 + 2M_{\text{Pl}}^2 H^3 \mathcal{N}_{\text{UV}}^2 \frac{\nabla^2}{a^2} \psi + \frac{1}{2} M_{\text{Pl}}^2 H^2 \mathcal{N}_{\text{UV}} \left(\left(\frac{\psi_{ii}}{a^2} \right)^2 - \frac{\psi_{ij}}{a^2} \frac{\psi_{ij}}{a^2} \right) \\
 & - \frac{1}{a^2} \psi_i \tilde{P}_{I,\kappa} \partial_i Q^I - \mathcal{N}_{\text{UV}} \left(\frac{1}{2} \tilde{P}_{I,\kappa} \tilde{P}_\kappa^I + \frac{1}{2a^2} \partial_i Q^I \partial_i Q_I + \frac{1}{2} V_{;IJ} Q^I Q^J - \kappa R_I{}^{KL}{}_{;J} \varpi_K \varpi_L Q^I Q^J \right) \\
 & + \mathcal{N}_{\text{IR}} \left(\left(\frac{1}{2} + \kappa \right) R^L{}_{IJ}{}^K \varpi_L Q^I Q^J \tilde{P}_{K,\kappa} - \frac{1}{6} V_{;IJK} Q^I Q^J Q^K + \frac{1}{6} R^L{}_{IJ}{}^M{}_{;K} \varpi_L \varpi_M Q^I Q^J Q^K \right) \\
 & + \frac{1}{6} \left(\varphi'^I - \frac{\varpi^I}{H} \right) \left(3R_{IJK}{}^L Q^J Q^K \tilde{P}_{L,\kappa} + R_{IJK}{}^M{}_{;L} \varpi_M Q^J Q^K Q^L \right) \\
 & + \left(\frac{1}{6} - \kappa \right) R^L{}_{IJK} \varpi_L Q^I Q^J \mathcal{D}_N Q^K \Big]. \tag{B.18}
 \end{aligned}$$

Here we use the generalised momentum $\tilde{P}_{I,\kappa}$ (B.4), allowing a shift from the original momentum (B.9). As mentioned before, $\kappa = 1/2$ eliminates the term proportional to the “background-like” EoM $\varphi'^I - \varpi^I/H$ in the quadratic action $S^{(2)}$. On the other hand, if one chooses $\kappa = 1/6$, there is no term containing $\mathcal{D}_N Q^I$ in the cubic action, which indicates that $\tilde{P}_{I,1/6}$ might enjoy interesting properties. Although not directly used in this paper, we hope these results can be useful for future works.

C Covariant notations

We gather in this appendix the various covariant notations that we use in the paper.

C.1 Manifolds, indices and related metrics

To use compact and covariant notations, we had to introduce several types of indices denoting coordinates on various manifolds. To help the reader, here we show a comprehensive list of these notations together with the corresponding metrics that must be used to raise and lower indices.

Manifold	Index	Metric	Dimension
Spacetime	μ	$g_{\mu\nu}$	4
3-dimensional spatial hypersurfaces	i	$\gamma_{ij} = a^2 \delta_{ij}$ in flat gauge	3
Field space	I	G_{IJ} evaluated at ϕ^I or φ^I	N_{fields}
Phase space	X or $\tilde{X}$	$-i\sigma_{2XY} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	2
Set of creation-annihilation operators	A	δ_{AB}	N_{fields}
Vielbeins' frame	α	$\delta_{\alpha\beta}$	N_{fields}
Mass squared matrix eigenvalues	i	δ_{ij}	N_{fields}
Set $\{+, -\}$ of CTP branches	a	$\sigma_{3ab} = \text{diag}(1, -1)_{ab}$	2
Keldysh basis $\{\text{cl}, \text{q}\}$	$\mathfrak{a}$	$\sigma_{1\mathfrak{a}\mathfrak{b}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	2

C.2 Covariant derivatives

Motivated by our will to have a manifestly covariant theory of multifield stochastic inflation, we have to use a certain number of covariant derivatives. Here we list all of them and show their actions on an IR stochastic vector in phase space $\mathcal{U}^I(\varphi^I, \varpi_I)$ from which their actions on any IR stochastic tensor can be deduced. Note that $A^{Q\tilde{U}JK} = A^{QUJK} + \Gamma_{LM}^K \mathcal{U}^L A^{QQJM}$.

Name	Notation	Action on a field-space vector
Field space	∇_J	$\nabla_J \mathcal{U}^I = \partial_J \mathcal{U}^I + \Gamma_{JK}^I \mathcal{U}^K$
Phase space	D_{φ^J}	$D_{\varphi^J} \mathcal{U}^I = \nabla_J \mathcal{U}^I + \Gamma_{JL}^K \varpi_K \partial_{\varpi_L} \mathcal{U}^I$
Time (deterministic or Stratonovich scheme)	$\mathcal{D}_N$	$\mathcal{D}_N \mathcal{U}^I = \partial_N \mathcal{U}^I + \Gamma_{JK}^I (\partial_N \varphi^J) \mathcal{U}^K$
Time (Itô scheme)	$\mathfrak{D}_N$	$\mathfrak{D}_N \mathcal{U}^I = \mathcal{D}_N \mathcal{U}^I + \frac{1}{2} (\Gamma_{JS,K}^I - \Gamma_{JS}^M \Gamma_{MK}^I) \mathcal{U}^S A^{QQJK} + \Gamma_{JK}^I A^{Q\tilde{U}JK}$

C.3 Covariant perturbations?

Under redefinitions of the scalar fields, naive perturbations of the full fields ϕ^I and π_I around a classical background (or IR) value, do not transform covariantly beyond linear order. This subtlety was discussed in section 4.2 and in appendix B. Here we summarise our notations for “perturbations” including the naive ones, $\delta\phi^I = \phi^I - \varphi^I$ and $\delta\pi_I = \pi_I - \varpi_I$, as well as the true covariant objects such as Q^I and $\tilde{P}_I$. Their covariance (“Yes”, “No”, or at “Linear order” only) is also explicitly shown.

Notation	Definition	Covariant?
$\delta\phi^I$	$\phi^I - \varphi^I = Q^I - \frac{1}{2} \Gamma_{JK}^I Q^J Q^K + \dots$	Linear order
$\delta\pi_I$	$\pi_I - \varpi_I = \tilde{P}_I + \Gamma_{IJ}^K \varpi_K Q^J + \Gamma_{IJ}^K Q^J \tilde{P}_K$ $+ \frac{1}{2} (\Gamma_{IJ,K}^S - \Gamma_{IR}^S \Gamma_{JK}^R + \Gamma_{IJ}^R \Gamma_{RK}^S) \varpi_S Q^J Q^K + \dots$	No
Q^I	$\left. \frac{d\phi^I}{d\lambda} \right _{\lambda=0}$	Yes
P_I	$\left. \frac{d\pi_I}{d\lambda} \right _{\lambda=0}$	No
$\tilde{P}_I$	$\mathcal{D}_\lambda \pi_I _{\lambda=0} = P_I - \Gamma_{IJ}^K \varpi_K Q^J$	Yes
$\tilde{P}_{I,\kappa}$	$\tilde{P}_I + \kappa R_{IJK}{}^L \varpi_L Q^J Q^K$	Yes

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Part IV

Cosmological reheating: the transition

Chapter 8

Single-field (p)reheating and the growth of small-scale perturbations

This part discusses different physical aspects of the theory of cosmic reheating that must take place at the end of single-field inflation, in order to convert the energy density stored in the potential of the inflaton into Standard Model particles and dark matter and avoid an empty, bitter cold Universe [108–114]. I find surprising that such a crucial cosmological epoch is so poorly known and studied. A justification however might be that single-field inflation constitutes a particular case for which the details of the reheating mechanism only mildly impact cosmological observables. Indeed, since the comoving curvature perturbation is constant on super-Hubble scales in single-field attractor scenarios, the only effect of reheating is to add up more expansion between the time of horizon exit of the modes observed in the CMB and the beginning of the radiation-domination epoch. This purely kinematic effect can however be studied: it shifts the interpretation of the observational constraints that one can put on the single-field models of inflation, as it indeed effectively changes the parameter N_* described in Sec. 3.3, see *e.g.* Refs. [113, 263–265]. But there are a few exceptions for which even cosmological and astrophysical observables may be considerably impacted by the details of reheating. The first one has to do with small scales, even in the single-field case, and is studied in this Chapter. Another one is when multiple degrees of freedom are present and interact at the end of inflation, and this is studied in the next one, Chapter 9.

In this chapter, the main scientific content is a peer-reviewed publication, Ref. [6], in Sec. 8.1, because it contains itself a pedagogical introduction to reheating and in particular to three particular scenarios that are not self-exclusive: perturbative reheating through the continuous decays of a scalar field into another degree of freedom, as well as non-perturbative aspects of the usual preheating mechanism and of the more particular metric preheating case. After these generalities, the core of the mechanism at play for the small scales at the end of inflation is studied: scalar perturbations are exponentially amplified due to a parametric resonance provoked by the oscillations of the background

scalar field when it reaches the bottom of his potential. In order to dynamically stop the instability, the scalar field is also continuously decaying in a cosmological fluid, therefore bridging the gap between the two physical phenomena of (p)reheating.

Sec. 8.2 then builds on the definitions and the physical phenomena explained in this first section, in order to discuss the results and replace them in the context of the current research, such as the (over)production of Primordial Black Holes (PBH) with the metric preheating instability.

8.1 Generalities and growth of small-scale perturbations during (p)reheating (article)

In this section, we explain the general idea behind reheating at the end of single-field inflation in the introduction of Ref. [6],

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that is reproduced below.

Then, we first show in section 2 that, by adding an additional degree of freedom which can either be an other scalar field χ constituting a proxy for Standard Model and dark matter particles, or a cosmological fluid with constant equation of state w_f , as well as perturbative interactions between it and the inflaton ϕ , one can transfer energy from the potential part of the inflaton to actual particles that will later reach thermal equilibrium and therefore “reheat” the Universe. But this mechanism, called “perturbative reheating” is by nature poorly efficient, and much more powerful physical phenomena might also take place at the same time, in particular quantum ones. It is the aim of “preheating” to study this quantum-mechanical production of χ -particles whose number densities are indeed subject to a parametric resonance due to the oscillations of the background inflaton $\bar{\phi}(t)$ when it necessarily reaches the bottom of its potential (note that in this regime the potential may be approximated by a parabola around the minimum at $\phi = \sigma$, $V(\phi) = V(\sigma) + m^2(\phi - \sigma)^2 + \mathcal{O}[(\phi - \sigma)^3]$, and the potential is not quadratic only if it is tuned to have a vanishing curvature at σ), and this amplification, which is even more severe due to Bose enhancement for such bosonic scalar field χ as a decay product, is shortly reviewed too in section 2.2. Although very efficient (almost instantaneous), this decay can only partially transfer the energy density of the inflaton because the instability quickly stops, and one must eventually resort to perturbative reheating again. Eventually, we explain in detail in section 2.3 how a similar amplification mechanism due to parametric resonance, takes place for the inflaton’s fluctuations on sub-Hubble scales that verify the condition $H^2 < k^2/a^2 < 3Hm$, even though a crucial difference is that the narrow band instability is a dynamical attractor in the sense that more and more modes eventually join the instability.

It therefore seems evident that some other physical phenomenon must take place, otherwise the Universe would eventually become so much unstable that it would entirely

collapse in a gigantic PBH. It is the aim of section 3 below to study the continuous decays of the inflaton into a cosmological fluid with constant equation of state w_f (constant, but several interesting cases are investigated: $w_f \in \{0, 1/3, 1\}$) by allowing them to have covariant interactions described by the absence of conservation of their individual stress-energy tensors $T_{(\alpha)}^{\mu\nu}$ with a constant of proportionality Γ corresponding to the decay rate, *together with* the metric preheating instability. An important conclusion of this paper is that the perturbative reheating does not entirely spoil the instability, but rather provides a natural way to dynamically end it around a time N_{reh} corresponding to $H(N_{\text{reh}}) \sim \Gamma$. We propose an analytical formalism¹ together with a full numerical resolution of the system at hand, both at the level of the background dynamics and the ones of linear fluctuations, respectively in subsections 3.1 and 3.2, which results in a continuous description of the (p)reheating mechanism, as can be seen from the plot in Fig. 8.1 that is reproduced from the article and that shows the energy budget in the Universe at the end of inflation and through reheating. Eventually, in the subsection 3.3 we discuss aspects related to PBH formation, which are further explained in the next, Sec. 8.2, but constituted the initial motivation for this work.

The original article as published in JCAP is now displayed. Notations should be transparent.

¹This formalism is only shortly reviewed in the article reproduced here, for a more pedagogical introduction of it, in a much more general setup with any number of scalar fields and cosmological fluids, and potentially more diverse interactions, the interested reader is referred to the next, Sec. 9, where this is better explained.

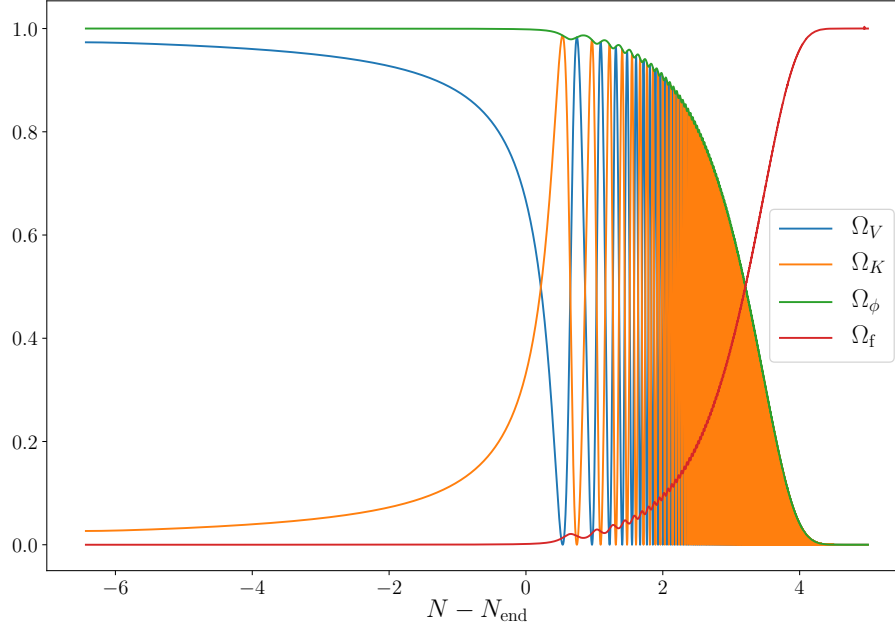


Figure 8.1: Energy budget in the Universe at the end of single-field inflation, with $\Omega_{(\alpha)} = \bar{\rho}_{(\alpha)}/\bar{\rho}_{\text{tot}}$. The universe is made of a scalar field ϕ and a cosmological fluid f , and the scalar field is split into two fictitious cosmological fluids with constant equations of state (eos): a kinetic fluid K with eos $w_K = 1$ and a potential one V with $w_V = -1$. During inflation, the scalar field is in slow roll and thus its potential part largely dominates over the other contributions. The end of inflation at $N = N_{\text{end}}$ coincides with the time at which the kinetic and potential energy densities of the inflaton each make up for half of the total one. The inflaton then begins to oscillate with almost equipartition on average between its kinetic and potential parts, but its overall contribution eventually decreases due to it decaying into the cosmological fluid that gradually becomes dominant and imposes its own equation of state as being the one of the entire Universe: if $w_f = 1/3$, it is the beginning of the radiation-dominated epoch. In this example, one has $N_{\text{reh}} \sim N_{\text{end}} + 3$, which can be used to render more precise the theoretical predictions of the inflationary model in the CMB. The visible oscillations of the background inflaton field is responsible for a parametric amplification of its perturbations in the comoving instability band $H < k/a < \sqrt{3Hm}$ as explained in the text and in the article.

Metric preheating and radiative decay in single-field inflation

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Abstract. At the end of inflation, the inflaton oscillates at the bottom of its potential and these oscillations trigger a parametric instability for scalar fluctuations with wavelength λ comprised in the instability band $(3Hm)^{-1/2} < \lambda < H^{-1}$, where H is the Hubble parameter and m the curvature of the potential at its minimum. This “metric preheating” instability, which proceeds in the narrow resonance regime, leads to various interesting phenomena such as early structure formation, production of gravitational waves and formation of primordial black holes. In this work we study its fate in the presence of interactions with additional degrees of freedom, in the form of perturbative decay of the inflaton into a perfect fluid. Indeed, in order to ensure a complete transition from inflation to the radiation-dominated era, metric preheating must be considered together with perturbative reheating. We find that the decay of the inflaton does not alter the instability structure until the fluid dominates the universe content. As an application, we discuss the impact of the inflaton decay on the production of primordial black holes from the instability. We stress the difference between scalar field and perfect fluid fluctuations and explain why usual results concerning the formation of primordial black holes from perfect fluid inhomogeneities cannot be used, clarifying some recent statements made in the literature.

Keywords: inflation, physics of the early universe, primordial black holes

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1 Introduction

Cosmic inflation [1–5] is presently the most promising paradigm to describe the physical conditions that prevailed in the very early universe. It consists of two stages. First, there is a phase of accelerated expansion. In the simplest models, it is driven by a scalar field, the inflaton, slowly rolling down its potential, and the background spacetime almost exponentially expands. Second, there is the reheating epoch [6–12] (see refs. [13, 14] for reviews) during which the inflaton field oscillates around the minimum of its potential and decays into other degrees of freedom it couples to. Then, after thermalisation of these decay products, the radiation-dominated era of the hot big-bang phase starts.

One of the main successes of the inflationary scenario is that it provides a convincing mechanism for the origin of the structures in our universe [15, 16]. According to the inflationary paradigm, they stem from quantum fluctuations born on sub-Hubble scales and subsequently amplified by gravitational instability and stretched to super-Hubble distances by cosmic expansion. During this process, which occurs in the slow-roll phase, cosmological perturbations acquire an almost scale-invariant power spectrum, which is known to provide an excellent fit to the astrophysical data at our disposal [17, 18].

In the simplest models where inflation is driven by a single scalar field with canonical kinetic term, on large scales, the curvature perturbation is conserved [15, 16], which implies that the details of the reheating process do not affect the inflationary predictions or, in other words, that “metric preheating” is inefficient on those scales. Since these models are well compatible with the data [19–22], the stage of reheating is usually not considered as playing an important role in the evolution of cosmological perturbations [23]. For the scales observed in the Cosmic Microwave Background (CMB), the only effect of reheating is through the amount of expansion that proceeds during this epoch, which relates physical scales as we observe today to the time during inflation when they emerge. This thus determines the part of the inflationary potential that we probe with the CMB. In practice, there is a single combination [24] of the reheating temperature and of the mean equation-of-state parameter, that sets the location of the observational window along the inflationary potential. Given the restrictions on the shape of the potential now available [20, 25], this can be used to constrain

the kinematics of reheating [26–29]. In multiple-field scenarios, on the contrary, large-scale curvature perturbations can be strongly distorted by the reheating process [30–34], which means that metric preheating can be important and, thus, can have more impact on CMB observations.

The situation is very different for scales smaller than those observed in the CMB, more precisely for scales crossing back in the Hubble radius during reheating (or never crossing out the Hubble radius during inflation). In particular, it was shown in ref. [35] (see also ref. [36]) that the density contrast of the scalar field fluctuations can grow on small scales during preheating, due to a parametric instability sourced by the oscillations of the inflaton at the bottom of its potential. This mechanism demonstrates that metric preheating can be important even in single-field inflation, although not on large scales. It can give rise to different interesting phenomena such as early structure formation [35], gravitational waves production [37] and even Primordial Black Holes (PBHs) [38, 39] formation [40] (PBHs formation from scalar fields was considered in ref. [41], in the case of two-fields models in ref. [42] and in the case of single-field tachyonic preheating in ref. [43]).

These phenomena can lead to radical shifts in the standard picture of how reheating proceeds. Indeed, in ref. [40], it was shown that the production of light PBHs from metric preheating is so efficient that they can quickly come to dominate the universe content, such that reheating no longer occurs because of the inflaton decay, as previously described, but rather through PBHs Hawking evaporation. This conclusion, however, was reached by neglecting the decay products of the inflaton throughout the instability phase, and by simply assuming that they would terminate the instability abruptly at the time when they dominate the energy budget (if PBHs have not come to dominate the universe before then). However, as will be made explicit below, the instability of metric preheating proceeds in the narrow resonance regime. One may therefore be concerned that it requires a delicate balance in the dynamics of the system, and that even a small amount of produced radiation could be enough to distort or jeopardise the instability mechanism. The goal of this paper is therefore to investigate how the presence of inflaton decay products (modelled as a perfect fluid), produced by perturbative reheating, affects the metric preheating instability.

The paper is organised as follows. In section 2, we briefly review metric preheating, which leads to the growth of the inflaton density contrast at small scales. Then, in section 3, we study whether a small amount of radiation, originating from the inflaton decay, can modify this growth. For this purpose, we introduce a covariant coupling model between the inflaton scalar field and a perfect fluid, leading to equations of motion at the background (see section 3.1) and perturbative (see section 3.2) levels that feature no substantial change in the instability structure until the fluid dominates. In section 3.3, we discuss the application of the previous results to the production of PBHs during reheating, which, we stress, cannot be described as originating from perfect fluid inhomogeneities, contrary to what is sometimes argued. Finally, in section 4, we briefly summarise our main results and present our conclusions.

2 Preheating in single-field inflation

In this work, we consider single scalar field models of inflation, with a canonical kinetic term. In these models, a homogeneous inflaton field $\phi(t)$ drives the expansion of a flat Friedmann-Lemaître-Robertson-Walker (FLRW) space-time, described by the metric $ds^2 = -dt^2 + a^2(t)d\mathbf{x}^2$, where $a(t)$ is the FLRW scale factor. The corresponding equations of motion

are the Friedmann and Klein-Gordon equations, namely

$$H^2 = \frac{1}{3M_{\text{Pl}}^2} \left[\frac{\dot{\phi}^2}{2} + V(\phi) \right], \quad \ddot{\phi} + 3H\dot{\phi} + V_\phi(\phi) = 0, \quad (2.1)$$

where $H = \dot{a}/a$ is the Hubble parameter, V_ϕ the derivative of the potential with respect to ϕ , M_{Pl} the reduced Planck mass and a dot denotes a derivative with respect to cosmic time t . The inflaton field potential $V(\phi)$ must be such that the potential energy dominates over the kinetic energy of the inflaton, and inflation ($\ddot{a} > 0$) ends when they become comparable, that is to say when the first slow-roll parameter $\epsilon_1 \equiv -\dot{H}/H^2$ reaches one. This usually happens in the vicinity of a local minimum of the potential. There, most potentials can be approximated by a quadratic function, $V(\phi) \sim m^2\phi^2/2$, where m is the curvature of the potential at its minimum. In fact, this expression can be seen as a leading-order Taylor expansion of the potential around its minimum, and it is not valid only for potentials having an exactly vanishing mass at their minimum, for which the leading term is of higher order. When the inflaton reaches this region of the potential, it oscillates according to $\phi(t) \propto a^{-3/2} \sin(mt)$, the expansion becomes, on average, decelerated, and similar to that of a matter-dominated universe [9], i.e. $\langle \rho \rangle \propto a^{-3}$ (where $\langle \cdot \rangle$ denotes averaging over one oscillation).

2.1 Perturbative reheating

These considerations however ignore the possible coupling of the inflaton with other degrees of freedom. In order to incorporate it, several descriptions are possible. A simple way, which corresponds to “perturbative reheating”, consists in introducing a term “ $\Gamma\dot{\phi}$ ” (where Γ is a decay rate) in the Klein-Gordon equation to account for the decay of the inflaton into a perfect fluid (typically radiation) [6–8, 12]. In this case, the friction term becomes $(3H + \Gamma/2)\dot{\phi}$. Initially, $H \gg \Gamma$ and the effect of the inflaton decay is negligible, until H crosses down Γ , at a time around which most of the decay of the inflaton occurs. In the next section, we explain how to introduce Γ covariantly, thus allowing us to perform a consistent treatment both at the background and perturbative levels. Microscopically, if one considers for instance that ϕ is coupled to another scalar field χ through the interaction Lagrangian $\mathcal{L}_{\text{int}} = -2g^2\sigma\phi\chi^2$, where g is a dimensionless coupling constant and σ a new mass scale, the corresponding decay rate can be calculated within perturbation theory and one finds $\Gamma = g^4\sigma^2/(4\pi m)$ [12]. If this process occurs at sufficiently high energy, the mass of the χ -particles are small compared to the Hubble parameter at decay and, effectively, the inflaton field decays into relativistic matter or radiation.

2.2 Non-perturbative preheating

The above perturbative description is however not sufficient since non-perturbative effects can also play an important role [10–12]. This can be simply illustrated if one considers the case where the interaction Lagrangian reads $\mathcal{L}_{\text{int}} = -g^2\phi^2\chi^2/2$. If one denotes the monotonously decreasing amplitude of the inflaton oscillations as $\phi_0(t)$, such that $\phi \simeq \phi_0(t) \sin(mt)$, then the equation of motion of the Fourier transform $\chi_{\mathbf{k}}$ of the field χ reads

$$\ddot{\chi}_{\mathbf{k}} + 3H\dot{\chi}_{\mathbf{k}} + \left[\frac{k^2}{a^2(t)} + m_\chi^2 + g^2\phi_0^2(t) \sin^2(mt) \right] \chi_{\mathbf{k}} = 0, \quad (2.2)$$

where m_χ is the mass of χ and $\mathbf{k}$ the wavenumber of the mode under consideration. Writing $X_{\mathbf{k}} = a^{3/2}\chi_{\mathbf{k}}$ and using the variable $z \equiv mt$, the above equation can also be written under

the following form

$$\frac{d^2 X_{\mathbf{k}}}{dz^2} + [A_{\mathbf{k}} - 2q \cos(2z)] X_{\mathbf{k}} = 0, \quad (2.3)$$

where the quantities $A_{\mathbf{k}}$ and q are defined by

$$A_{\mathbf{k}} = \frac{k^2}{a^2 m^2} + \frac{m_\chi^2}{m^2} - \frac{3}{2} \frac{H^2}{m^2} \left(\frac{3}{2} - \epsilon_1 \right) + 2q, \quad q = \frac{g^2 \phi_0^2}{4m^2}. \quad (2.4)$$

As a first step, in order to gain intuition about the behaviour of the solutions, it is convenient to analyse the above equation in the Minkowski space-time (for simplicity, we also consider the massless case $m_\chi = 0$). In that situation, the coefficients $A_{\mathbf{k}} = k^2/m^2 + 2q$ and q are constant and eq. (2.3) is a Mathieu equation [44]. This equation possesses unstable, exponentially growing solutions $\chi_{\mathbf{k}} \propto \exp(\mu_{\mathbf{k}} z)$. In figure 1, known as the Mathieu instability chart, we display the value of $\mu_{\mathbf{k}}$, the so-called Floquet index of the unstable mode (namely the maximum of the two Floquet indices), as a function of $A_{\mathbf{k}}$ and q . Unstable regions correspond to where $\mu_{\mathbf{k}} > 0$, and are organised in several “bands”, which can be identified as the non dark-blue regions in figure 1. Since $A_{\mathbf{k}} = k^2/m^2 + 2q$, the parameter space of interest is such that $A_{\mathbf{k}} > 2q$, which corresponds to the region above the white line in figure 1. At a given q , one can see in figure 1 that there are several ranges of values of $A_{\mathbf{k}}$, hence several ranges of wavenumbers k , where an instability develops. One also notices that the band with the smallest value of $A_{\mathbf{k}}$ is the most pronounced one. When $q \gg 1$, the range of excited modes is large, which corresponds to being in the “broad-resonance” regime. When $q \ll 1$, on the contrary, there is only a small range of values of k being excited, which correspond to the “narrow-resonance” regime. In that limit, the boundaries of the first band correspond to $1 - q \lesssim A_{\mathbf{k}} \lesssim 1 + q$.

Then, space-time dynamics must be restored and its impact on the previous considerations discussed. In that case, three time scales play a role in eq. (2.2): the inflaton oscillation period m^{-1} , the Hubble time H^{-1} , and the $\mathbf{k}$ -mode period, a/k . The quantities $A_{\mathbf{k}}$ and q now become functions of time [notice that the oscillating phase starts when $m \sim H$, and since H decreases afterwards, one quickly reaches the regime where $H \ll m$ and, as a consequence, the term $\propto H^2/m^2$ in the definition (2.4) of $A_{\mathbf{k}}$ can be neglected]. This means that eq. (2.3) is no longer a Mathieu equation: a given mode $\mathbf{k}$ now follows a certain path in the map of figure 1. What is then the fate of the two regimes (narrow and broad resonance) identified before? Since more time is being spent in the wide bands than in the narrow ones, the broad resonance regime is the most important one to amplify the χ field. However, this regime is also crucially modified by space-time expansion and gives rise to the so-called “stochastic-resonance regime”, discovered in ref. [12]. Preheating effects have also been studied in other contexts, for instance when the curvature of (some region of) the inflationary potential is negative, as it is the case, for instance, in small-field inflation, leading to tachyonic preheating [45, 46].

2.3 Metric preheating

So far we have discussed preheating at the background level only, without including the inflaton and metric perturbations. They however play an important role, in a mechanism known as “metric preheating” [23, 30–34]. Including scalar fluctuations only, in the longitudinal gauge, the perturbed metric can be written as $ds^2 = a^2(\eta) [-(1 + 2\Phi) d\eta^2 + (1 - 2\Phi) \delta_{ij} dx^i dx^j]$,

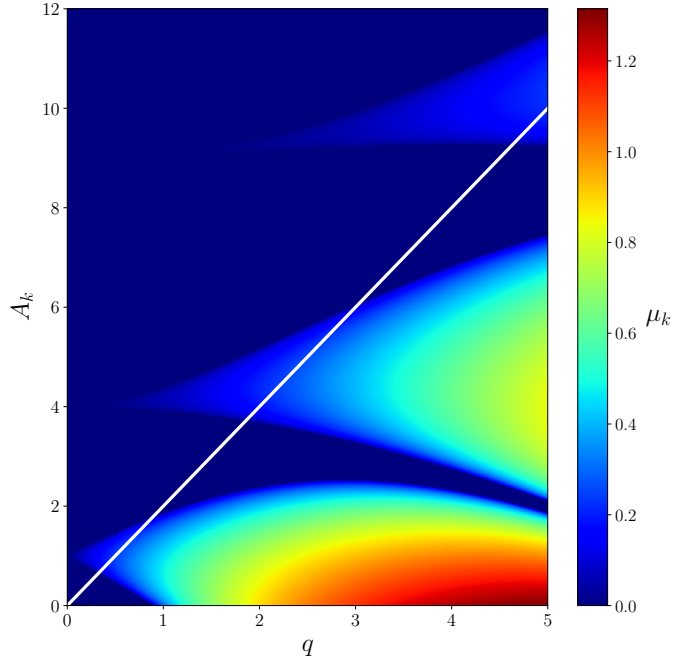


Figure 1. Instability chart of the Mathieu equation. The colour code (see the colour bar on the right hand side of the plot) represents the value of the Floquet exponent μ_k of the unstable mode. In the present case, stable solutions corresponds to $\mu_k = 0$ and are represented by the dark blue regions. The other regions, structured in different bands, correspond to unstable solutions.

where η is the conformal time related to the cosmic time by $dt = a d\eta$. As is apparent in the previous expression, the scalar perturbations are described by a single quantity, namely the Bardeen potential Φ . Matter perturbations, which, in the context of inflation, boil down to scalar field perturbations, are also characterised by a single quantity, the perturbed scalar field $\delta\phi^{(\text{gi})}$, where the “gi” indicates that this is a gauge-invariant quantity ($\delta\phi^{(\text{gi})} = \delta\phi$ in the longitudinal gauge and is mapped by gauge transformations otherwise). Using the perturbed Einstein equations, the whole scalar sector can in fact be described by a single quantity, which is a combination of metric and matter perturbations. This single quantity is the Mukhanov-Sasaki variable [15, 16] $v \equiv a [\delta\phi^{(\text{gi})} + \phi'\Phi/\mathcal{H}]$, where $\mathcal{H} = a'/a$ (a prime denotes a derivative with respect to conformal time) is the conformal Hubble parameter, and is directly related to the comoving curvature perturbation $\mathcal{R}$ by $v = Z\mathcal{R}$, where $Z \equiv \sqrt{2\epsilon_1}aM_{\text{Pl}}$. The Fourier component v_k evolves according to the equation of a parametric oscillator where the time dependence of the frequency is determined by the dynamics of the background [47]

$$v_k'' + \left(k^2 - \frac{Z''}{Z}\right) v_k = 0, \quad (2.5)$$

with

$$\frac{Z''}{Z} = a^2 H^2 \left[\left(1 + \frac{\epsilon_2}{2}\right) \left(2 - \epsilon_1 + \frac{\epsilon_2}{2}\right) + \frac{\epsilon_2 \epsilon_3}{2} \right], \quad (2.6)$$

where $\epsilon_2 \equiv d \ln \epsilon_1 / dN$ and $\epsilon_3 \equiv d \ln \epsilon_2 / dN$ are the second and the third slow-roll parameters respectively.

The question is then whether eq. (2.5) allows for parametric resonance when the inflaton field oscillates at the bottom of its potential. One might indeed expect that the oscillations in $\phi(t)$ induce oscillations in the Hubble parameter H , hence in the slow-roll parameters, hence in Z''/Z . In this case, eq. (2.5) could be of the Mathieu type, or more generally of the Hill type, and could lead to parametric resonance. This was first thought not to be the case, the main argument being that, despite the oscillations in Z''/Z , the curvature perturbation has to remain constant and, as a consequence, there cannot be any growth of scalar perturbations [23]. It has also been stressed that the situation can be drastically different in multiple-field inflation [33], where entropy fluctuations source the evolution of curvature perturbations. If the entropy fluctuations are parametrically amplified, they can also cause a parametric amplification of adiabatic perturbations. This is the reason why metric preheating was first mostly studied in the context of multiple-field (and in practice, mostly two-field) inflation, see for instance ref. [33].

It was then realised in ref. [35] (see also ref. [36]) that eq. (2.5) can be put under the form

$$\frac{d^2}{dz^2} (\sqrt{a} v_{\mathbf{k}}) + [A_{\mathbf{k}} - 2q \cos(2z)] (\sqrt{a} v_{\mathbf{k}}) = 0, \quad (2.7)$$

with

$$A_{\mathbf{k}} = 1 + \frac{k^2}{m^2 a^2}, \quad q = \frac{\sqrt{6}}{2} \frac{\phi_{\text{end}}}{M_{\text{Pl}}} \left(\frac{a_{\text{end}}}{a} \right)^{3/2}, \quad (2.8)$$

where a_{end} is the scale factor at the end of inflation and $z \equiv mt + \pi/4$. Although, strictly speaking, this equation is not of the Mathieu type because of the time dependence of the parameters $A_{\mathbf{k}}$ and q , it was shown in ref. [35] that this time dependence is sufficiently slow so that eq. (2.7) can be analysed using Mathieu equations techniques. At the end of inflation and at the onset of the oscillations, $\phi_0(t_{\text{end}}) = \phi_{\text{end}}$ is of the order of the Planck mass, so eq. (2.8) indicates that q starts out being of order one and quickly decreases afterwards. In contrast to the situation of non-perturbative preheating discussed in section 2.2, the narrow-resonance regime $q \ll 1$ is therefore always the relevant one for metric preheating. In that regime, and contrary to the case of broad resonance, space-time expansion does not blur the resonance but, on the contrary, reinforces its effectiveness, in a sense that we will explain below. As mentioned above, in the $q \ll 1$ limit, the boundaries of the first instability band are given by $1 - q < A_{\mathbf{k}} < 1 + q$, which here translates into

$$k < a\sqrt{3Hm}. \quad (2.9)$$

One notices the appearance of a new scale in the problem, namely $\sqrt{3Hm}$. Since the universe behaves as matter dominated during the oscillations of the inflaton, $a\sqrt{H} \propto a^{1/4}$, and the upper bound (2.9) increases with time. This means that the range of modes subject to the instability widens up as time proceeds, hence the above statement that space-time expansion strengthens the resonance effect.

Inside the first instability band, the Floquet index of the unstable mode is given by $\mu_{\mathbf{k}} \simeq q/2$, so $v_{\mathbf{k}} \propto a^{-1/2} \exp(\int \mu_{\mathbf{k}} dz) \propto a$ [23, 35]. The comoving curvature perturbation, $\mathcal{R}_{\mathbf{k}} = v_{\mathbf{k}}/(M_{\text{Pl}} a \sqrt{2\epsilon_1})$, is thus conserved for modes satisfying eq. (2.9). Notice that, since $H \ll m$ during the oscillatory phase, this comprises super-Hubble modes, $k < aH$, for which the conservation of $\mathcal{R}$ is a well-known result [15, 16]. However, the conservation of $\mathcal{R}$ also applies for those sub-Hubble modes having $k < a\sqrt{3Hm}$, and for which this leads

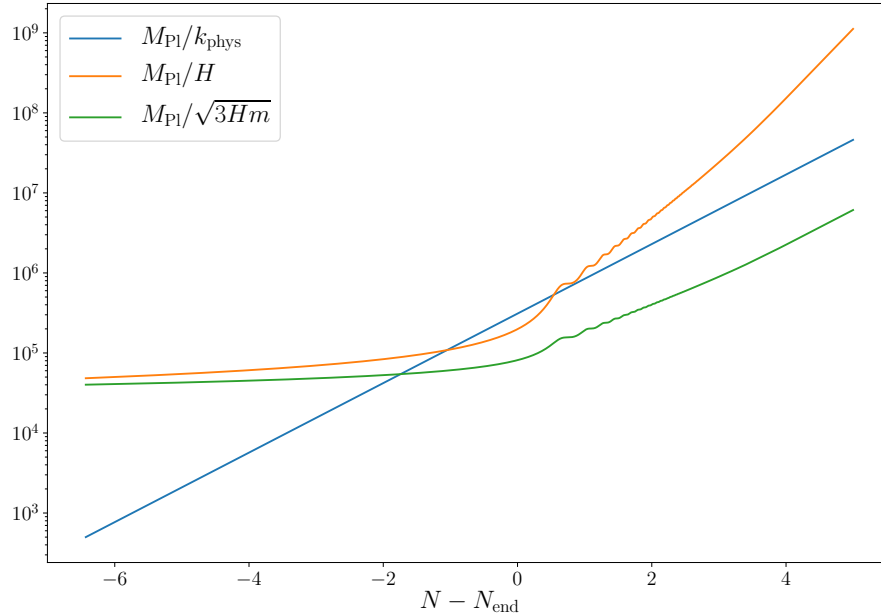


Figure 2. Evolution of the physical scales appearing in eq. (2.12), with time parameterised by the number of e -folds (counted from the end of inflation). The orange solid line represents the Hubble radius $1/H$, the solid green line the new length scale $1/\sqrt{3Hm}$ and the solid blue line the physical wavelength of a mode of interest, which enters the instability band from above. In all figures of this work, we study the comoving scale $k/a_{\text{ini}} = 0.002M_{\text{Pl}}$, where the initial time of integration is set 6 e -folds before the end of inflation, in a quadratic potential model $V(\phi) = m^2\phi^2/2$ with $m = 10^{-5}M_{\text{Pl}}$. The inflaton decay constant (the definition of which is detailed in section 3.1) is given by $\Gamma = 10^{-7}M_{\text{Pl}}$. Here, we consider the case where the inflaton decays into a radiation fluid, with equation-of-state parameter $w_f = 1/3$.

to an increase of the density contrast. Indeed, if $\mathcal{R}$ is constant, and given that the pressure vanishes on average, the fractional energy density perturbation $\delta_{\mathbf{k}} = \delta\rho_{\mathbf{k}}/\rho$ (where ρ is the background energy density of the scalar field) in the Newtonian gauge is related to the curvature perturbation via [35]

$$\delta_{\mathbf{k}} = -\frac{2}{5} \left(\frac{k^2}{a^2 H^2} + 3 \right) \mathcal{R}_{\mathbf{k}}. \quad (2.10)$$

On super-Hubble scales, the first term in the braces can be neglected, hence $\delta_{\mathbf{k}}$ is constant as $\mathcal{R}_{\mathbf{k}}$. On sub-Hubble scales however, the first term becomes the dominant one, and since $a^2 H^2 \propto a^{-1}$, the density contrast grows like

$$\delta_{\mathbf{k}} \propto a. \quad (2.11)$$

This corresponds to a physical instability (notice that, at sub-Hubble scales, there are no gauge ambiguities in the definition of the density contrast), which therefore operates at scales

$$aH < k < a\sqrt{3Hm}. \quad (2.12)$$

The scales appearing in this relation are displayed in figure 2. An instability is triggered if the physical wavelength of a mode (blue line) is smaller than the Hubble radius (orange

line) during the oscillatory phase and larger than the new scale $1/\sqrt{3Hm}$ (green line). This implies that the instability only concerns modes that are inside the Hubble radius at the end of the oscillatory phase, which is not the case for the scales probed in the CMB. It is therefore true that metric preheating does not operate at CMB scales, although it plays a crucial role at smaller scales (typically those crossing out the Hubble radius a few e -folds before the end of inflation) where it triggers an instability in the narrow-resonance regime. The growth of the density contrast along eq. (2.11) may have several important consequences such as early structure formation [35], emission of gravitational waves [37] and, as recently studied in ref. [40], formation of PBHs that may themselves contribute to the reheating process, via Hawking evaporation.

As already mentioned, preheating effects cannot by themselves ensure a complete transition to the hot big-bang phase [12, 13, 48, 49] (except if reheating occurs by Hawking evaporation of the very light primordial black holes produced from the instability if they come to dominate the universe content [40]), which also requires perturbative decay of the inflaton to complete. Metric preheating has however been investigated only in the context of purely single-field setups, and it is not clear whether or not the narrow resonant structure of metric preheating is immune to the decay of the inflaton into other degrees of freedom. This is why in the next sections, we study metric preheating and perturbative reheating altogether, in order to determine if and how the later can spoil the former.

3 Metric preheating and radiative decay

We have seen before that perturbations entering the instability band (2.12) undergo a growth of their density contrast proportional to the FLRW scale factor, see eq. (2.11), and that this can lead to a variety of interesting phenomena. At some stage, however, the inflaton field decays and the growth of the density contrast, sourced by the oscillations of the inflaton condensate, should come to an end. In ref. [40] this was simply modelled by abruptly stopping the oscillating phase at a certain time (e.g., when H becomes smaller than a certain value that can be identified with the decay rate Γ) and by assuming instantaneous production of radiation at that time. However, clearly, the inflaton decay should proceed continuously. Although it is true that the production of radiation becomes sizeable when the Hubble parameter becomes of the order of the decay rate, tiny amounts of radiation are present before and one may wonder whether or not they can destroy the delicate balance which is responsible for the presence of the modes in the instability band. Indeed, the instability proceeds in the narrow resonance regime, which means that the instability band spans a small, fine-tuned volume of parameter space. In this section, we investigate these questions.

3.1 Setup and background

In order to study the influence of fluid production, we must first modify the equations of motion of the system and introduce an explicit coupling between the inflaton field and a perfect fluid, both at the background and perturbative levels. This poses non-trivial problems at the technical level and we now review the formalism that can be used in order to tackle them. Let us consider a collection of fluids in interaction. The presence of interactions break the energy-momentum conservation for each fluid. On very general grounds, their non-conservations can be described non-perturbatively by detailed balance equations of the

form [50–56]

$$\nabla_\nu T_{(\alpha)}^{\mu\nu} = \sum_\beta \left[Q_{(\alpha) \rightarrow (\beta)}^\mu - Q_{(\beta) \rightarrow (\alpha)}^\mu \right], \quad (3.1)$$

where the transfer coefficients $Q_{(\alpha) \rightarrow (\beta)}^\mu$ are responsible for the non-conservation of energy-momentum originating from the interaction between the fluids. The indices between parenthesis [such as “ (α) ”] label the different fluid components. The term $Q_{(\alpha) \rightarrow (\beta)}^\mu$ describes a loss due to the decay of the fluid α into the fluids β while, on the contrary, the term $Q_{(\beta) \rightarrow (\alpha)}^\mu$ corresponds to a gain originating from the decay of the fluids β into α . The evolution of the stress-energy tensor of the fluid α , which is denoted $T_{(\alpha)}^{\mu\nu}$, is then controlled by the detailed balance between those two effects. The transfer coefficient $Q_{(\alpha) \rightarrow (\beta)}^\mu$ can always be decomposed as

$$Q_{(\alpha) \rightarrow (\beta)}^\mu = Q_{(\alpha) \rightarrow (\beta)} u^\mu + f_{(\alpha) \rightarrow (\beta)}^\mu, \quad (3.2)$$

where $Q_{(\alpha) \rightarrow (\beta)}$ is a scalar quantity and $f_{(\alpha) \rightarrow (\beta)}^\mu$ a vector orthogonal to the matter flow, that is to say $f_{(\alpha) \rightarrow (\beta)}^\mu u_\mu = 0$ where u^μ is the total velocity of matter. In an FLRW universe it is given by $u^\mu = (1/a, \mathbf{0})$, $u_\mu = (-a, \mathbf{0})$, which immediately implies that $f_{(\alpha) \rightarrow (\beta)}^0 = 0$ at the background level. Furthermore, in an homogeneous and isotropic background, one must have $f_{(\alpha) \rightarrow (\beta)}^i = 0$ to respect the symmetries of space-time, hence $f_{(\alpha) \rightarrow (\beta)}^\mu = 0$. This allows us to write $Q_{(\alpha) \rightarrow (\beta)}^0 = Q_{(\alpha) \rightarrow (\beta)}/a$ and $Q_{(\alpha) \rightarrow (\beta)}^i = 0$. At the background level, the energy transfer is therefore entirely specified by the scalar $Q_{(\alpha) \rightarrow (\beta)}$.

Let us now apply these considerations to a system made of one scalar field (the inflaton field) and a perfect fluid assumed to be the inflaton decay product. In order to consistently couple the scalar field ϕ with the fluid, one must view the scalar field as a collection of two fictitious fluids, the “kinetic” one, with energy density and pressure given by $\rho_K = p_K = \dot{\phi}^2/(2a^2)$, and the “potential” one, with $\rho_V = -p_V = V(\phi)$, each of them having a constant equation-of-state, one and minus one, respectively. The energy density and pressure of the scalar field are just the sums of the energy densities and pressures of the two fluids, namely $\rho_\phi = \rho_K + \rho_V$ and $p_\phi = p_K + p_V$. In order to recover the standard equations for a scalar field, one must also consider that the fictitious kinetic and potential fluids are coupled, the coupling being described by [50]

$$aQ_{K \rightarrow V} = -\phi' V_\phi, \quad aQ_{V \rightarrow K} = 0. \quad (3.3)$$

Then, we consider the “real” interaction between the scalar field and the perfect fluid (in practice radiation). The crucial idea [50, 57] is that it is obtained by coupling the fluid only to the fictitious kinetic fluid related to ϕ and introduced above (and not to the potential fluid). This implies that $Q_{V \rightarrow f}^\mu = Q_{f \rightarrow V}^\mu = 0$. In practice, we consider the case where the covariant interaction between “ K ” and “ f ” can be described non-perturbatively by the following energy four-momentum transfer:

$$Q_{K \rightarrow f}^\mu = \Gamma T_K^{\mu\nu} u_\nu^K, \quad Q_{f \rightarrow K}^\mu = 0, \quad (3.4)$$

where Γ is the decay rate and is the only new parameter introduced in order to account for the interaction. Note that this description should be understood as a phenomenological parametrisation of the decays of scalar fields in cosmological fluids, and not as a concrete microphysical model. At the background level, one recovers the picture described in section 2.1,

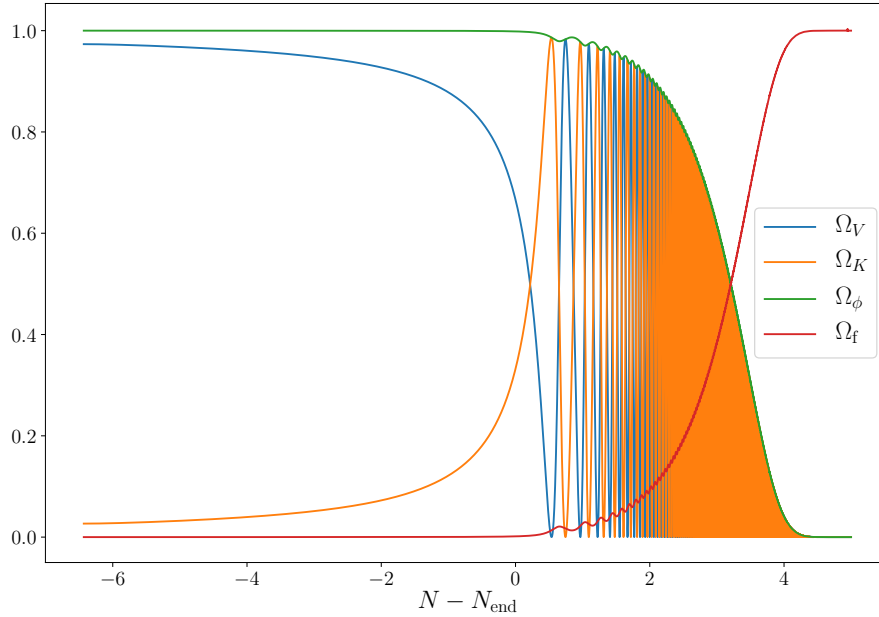


Figure 3. Evolution of the different energy density contributions as a function of the number of e -folds. The solid orange line represents the contribution of the fictitious kinetic fluid, the solid blue line the contribution of the fictitious potential fluid and the solid green line the contribution of the physical scalar field which is the sum of those two. The solid red line corresponds to the contribution of radiation. Before the end of inflation, the scalar field dominates the energy budget and, then, when its decay becomes effective, radiation takes over. The parameter values are the same as in figure 2.

since the equations of motion (3.1) of the system (namely the energy conservation equation, since the momentum conservation equation is trivial) can be written as

$$\phi'' + 2\mathcal{H}\phi' + \frac{a\Gamma}{2}\phi' + a^2V_\phi = 0, \quad (3.5)$$

$$\rho'_f + 3\mathcal{H}(1 + w_f)\rho_f - \frac{\Gamma}{2a}\phi'^2 = 0. \quad (3.6)$$

The first equation is the modified Klein-Gordon equation while the second one is the modified conservation equation for the fluid with equation-of-state parameter w_f (in practical applications, unless stated otherwise, we take $w_f = 1/3$). These equations are usually introduced in a phenomenological way. The fact that we are able to derive them from a covariant formulation, eq. (3.1), will allow us to describe perturbations in the same framework, by assuming that eq. (3.1) also holds at the perturbative (and in principle, even non-perturbative) level, see section 3.2.

We have numerically integrated eqs. (3.5) and (3.6) for $V(\phi) = m^2\phi^2/2$ with $m = 10^{-5}M_{\text{Pl}}$, $w_f = 1/3$ and $\Gamma = 10^{-7}M_{\text{Pl}}$. For a quadratic potential, inflation stops when $\phi_{\text{end}}/M_{\text{Pl}} \simeq \sqrt{2}$ and the (slow-roll) trajectory reads $\phi(N)/M_{\text{Pl}} \simeq \sqrt{2 - 4(N - N_{\text{end}})}$ where N is the number of e -folds. Here, we want to focus on the last e -folds of inflation and, therefore, the initial conditions are chosen such that the evolution is started on the slow-roll attractor at $\phi_{\text{ini}}/M_{\text{Pl}} \simeq 5$, corresponding to $N_{\text{end}} - N_{\text{ini}} \simeq 6$, and $\rho_f^{\text{ini}} = 0$ (as we will show below, the precise choice of the time at which we set $\rho_f = 0$ does not matter since ρ_f quickly reaches an attractor during inflation). The result is represented in figures 3 and 4, where inflation

ends when $N - N_{\text{end}} = 0$. Then starts the oscillation phase. In figure 3, $\Omega_K \equiv \rho_K/(\rho_\phi + \rho_f)$, $\Omega_V \equiv \rho_V/(\rho_\phi + \rho_f)$, $\Omega_\phi \equiv \Omega_K + \Omega_V$ and $\Omega_f \equiv \rho_f/(\rho_\phi + \rho_f)$ are displayed as a function of time. Initially, we have $\Omega_\phi \simeq \Omega_V \simeq 1$ and $\Omega_f \simeq \Omega_K \simeq 0$. Indeed, in the slow-roll phase, the potential energy largely dominates over the kinetic energy, since the first slow-roll parameter can be expressed as $\epsilon_1 = 3[(1+w_f)\Omega_f + 2\Omega_K]/2$, hence both Ω_f and Ω_K need to be very small. In this regime, we also have $H \gg \Gamma$ and the amount of radiation being produced is very small. Then, inflation stops and Ω_K and Ω_V become of comparable magnitude and start oscillating. During that phase, radiation still provides a small, though non-vanishing, contribution. Finally, when $H \simeq \Gamma$, at the time $N \equiv N_\Gamma$, radiation starts to be produced in a sizeable amount and cannot be neglected anymore. After the end of inflation, the universe expands, on average, as in a matter-dominated era, for which $H \propto a^{-3/2}$, that is to say $H \propto H_{\text{end}} \exp[-3(N - N_{\text{end}})/2]$. Writing the condition $H = \Gamma$ thus leads to an estimate of N_Γ , namely

$$N_\Gamma - N_{\text{end}} \simeq \frac{2}{3} \ln \left(\frac{\sqrt{2} m}{2 \Gamma} \right). \quad (3.7)$$

With the values used in figure 3, one obtains $N_\Gamma - N_{\text{end}} \simeq 2.8$, which is in good agreement with what can be observed in this figure. Then, within a few e -folds, radiation takes over and the radiation-dominated era starts. In figure 4, the transparent blue line displays the total equation-of-state parameter for the background, namely $w_{\text{bg}} = (p_\phi + p_f)/(\rho_\phi + \rho_f)$. The same remarks as in figure 3 apply. Initially, $w_{\text{bg}} \simeq -1$ and inflation proceeds in the slow-roll regime, until w_{bg} crosses $-1/3$ and inflation stops. After inflation, w_{bg} oscillates, and finally asymptotes $1/3$ when the transition towards the radiation-dominated era is completed. In order to factor out the effect of oscillations and only study their envelope, we also display the averaged value of w_{bg} , i.e. $\langle w_{\text{bg}} \rangle$, for two different time scales of averaging. The orange curve corresponds to w_{bg} convolved with a Gaussian kernel of standard deviation given by 0.2 e -fold, while the green one follows the same procedure but with standard deviation 0.1 e -fold. Interestingly, right after the onset of the oscillatory phase, $\langle w_{\text{bg}} \rangle$ is close to zero, which confirms that the background expands on average as in a matter-dominated era, until the production of radiation becomes effective.

The behaviour of $\langle w_{\text{bg}} \rangle$ when radiation is still subdominant (i.e. during inflation and during the first stage of the oscillating phase) can be described analytically as follows. A first remark is that eq. (3.6) can be solved exactly,

$$\rho_f(t) = \frac{\Gamma}{2} \int_{t_{\text{in}}}^t \dot{\phi}^2(\tilde{t}) \left[\frac{a(\tilde{t})}{a(t)} \right]^{3(1+w_f)} d\tilde{t}. \quad (3.8)$$

This expression can be cast as a perturbative expansion in Γ . At leading order, the integrand should be evaluated with $\Gamma = 0$, i.e. using the background dynamics in the absence of the radiation fluid, which we know how to describe.

During inflation, using the formula given above for the slow-roll trajectory, one can compute eq. (3.8) explicitly in terms of error functions. The resulting expression is not particularly illuminating so we do not reproduce it here, but we note that if the initial time is chosen sufficiently far in the past, it converges to¹

$$\rho_f \simeq \frac{m M_{\text{Pl}}^2 \Gamma}{3} \sqrt{\frac{\pi}{2(1+w_f)}} e^{\frac{3}{2}(1+w_f)[1-2(N-N_{\text{end}})]} \text{erfc} \left\{ \sqrt{\frac{3}{2}(1+w_f)[1-2(N-N_{\text{end}})]} \right\}. \quad (3.9)$$

¹This convergence proves that, as mentioned above, after a few e -folds in slow-roll inflation, ρ_f reaches an attractor, which implies that our results do not depend on our choice of initial time of integration.

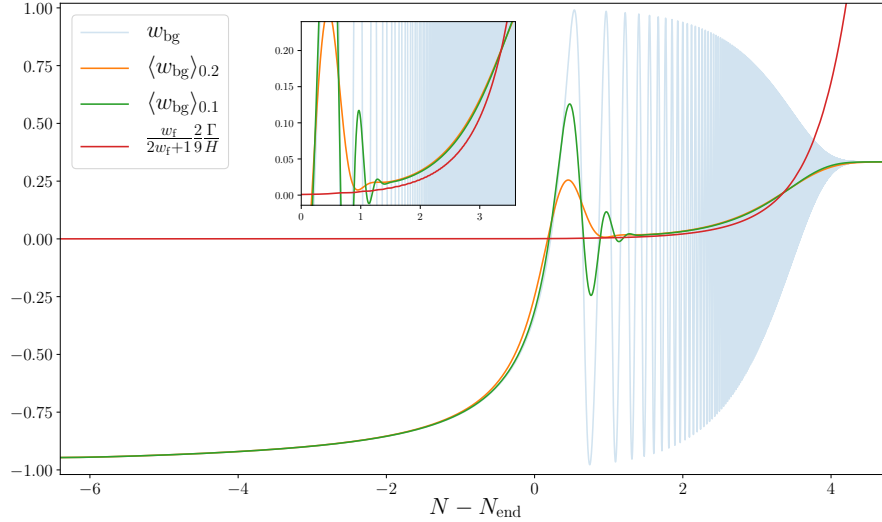


Figure 4. Evolution of the instantaneous (transparent blue line) and time-averaged equation-of-state parameters as a function of the number of e -folds, in the same setup as in figure 3. The averaging procedure consists in convolving the instantaneous signal with a Gaussian kernel of constant standard deviation given by 0.2 e -folds (orange line) and 0.1 e -folds (green line), such that oscillations on shorter time scales are averaged out. The analytical approximation eq. (3.12) is also displayed (red line), and the inset plot zooms in its regime of validity (i.e. at the onset of the oscillating phase).

At the end of inflation, ρ_f is therefore of order $mM_{\text{Pl}}^2\Gamma$, hence Ω_f is of order Γ/H_{end} , so radiation can indeed be neglected when the decay rate is much smaller than the Hubble scale during inflation. For instance, with the parameter values used in figure 3, eq. (3.9) gives $\Omega_f(t_{\text{end}}) \simeq 8.1 \times 10^{-4}$ while the numerical integration performed in figure 3 gives $\Omega_f(t_{\text{end}}) \simeq 9.8 \times 10^{-4}$, which allows us to check the validity of our approach (the small difference between these two values is explained by the fact that the slow-roll approximation breaks down towards the end of inflation).

During the oscillating phase, in the absence of fluid, as explained above $\phi(t) \propto \sin(mt)a^{-3/2}$. Plugging this formula into eq. (3.8), and after averaging over the oscillating term, one obtains

$$\Omega_f \simeq \Omega_f(t_{\text{end}})e^{-3w_f(N-N_{\text{end}})} + \frac{\Gamma}{12H_{\text{end}}} \frac{\phi_{\text{end}}^2}{M_{\text{Pl}}^2} \left\{ \frac{3}{4(w_f - \frac{1}{2})} \left[e^{-\frac{3}{2}(N-N_{\text{end}})} - e^{-3w_f(N-N_{\text{end}})} \right] + \frac{m^2}{3(w_f + \frac{1}{2})H_{\text{end}}^2} \left[e^{\frac{3}{2}(N-N_{\text{end}})} - e^{-3w_f(N-N_{\text{end}})} \right] \right\}. \quad (3.10)$$

After a few e -folds, if $w_f > -1/2$, the first term on the second line is the dominant one, which leads to

$$\Omega_f \simeq \frac{1}{18(2w_f + 1)} \frac{\phi_{\text{end}}^2 m^2}{M_{\text{Pl}}^2 H_{\text{end}}^2} \frac{\Gamma}{H}. \quad (3.11)$$

In a quadratic potential, using the slow-roll formula $\phi_{\text{end}} \simeq \sqrt{2}M_{\text{Pl}}$, one has $H_{\text{end}} \simeq m/\sqrt{2}$ and the equation-of-state parameter $w_{\text{bg}} \simeq w_f\Omega_f$ is given by

$$w_{\text{bg}} \simeq \frac{2w_f}{9(2w_f + 1)} \frac{\Gamma}{H}. \quad (3.12)$$

Because of the slow-roll violation at the end of inflation, this formula is expected to provide an accurate description only up to an overall factor of order one (for instance in m/H_{end}), and in figure 4 one can check that this is indeed the case, see the inset in particular (the agreement in the case of other fluid equation-of-state parameters can be checked in figure 6 below). When Γ becomes of order H , i.e. when $N \sim N_\Gamma$, the approximation breaks down and eq. (3.12) cannot be trusted anymore.

3.2 Perturbations

Having established how the background evolves, we now turn to the behaviour of the perturbations. Since the equations we started from, eqs. (3.1) and (3.4), have a covariant form, they can be perturbed. As stressed above, this is not the case of the background equations of motion, eqs. (3.5) and (3.6), which explains why these two equations cannot be used as a starting point, and why it was necessary to re-derive them from a covariant principle. For more explanations about this formalism, we refer the interested reader to refs. [50, 57]. By perturbing eq. (3.1), one obtains

$$\delta \left[\nabla_\nu T_{(\alpha)}^{\mu\nu} \right] = \sum_\beta \left[\delta Q_{(\alpha) \rightarrow (\beta)}^\mu - \delta Q_{(\beta) \rightarrow (\alpha)}^\mu \right]. \quad (3.13)$$

In this formula, the perturbed energy transfer $\delta Q_{(\alpha) \rightarrow (\beta)}^\mu$, using eq. (3.2), can be written as

$$\delta Q_{(\alpha) \rightarrow (\beta)}^\mu = \delta Q_{(\alpha) \rightarrow (\beta)} u^\mu + Q_{(\alpha) \rightarrow (\beta)} \delta u^\mu + \delta f_{(\alpha) \rightarrow (\beta)}^\mu. \quad (3.14)$$

The constraint that the four-vector $f_{(\alpha) \rightarrow (\beta)}^\mu$ is orthogonal to the Hubble flow must also be satisfied at the perturbed level, and this leads to $\delta[f_{(\alpha) \rightarrow (\beta)}^\mu u_\mu] = 0$. As a consequence, $\delta f_{(\alpha) \rightarrow (\beta)}^0 = 0$ and only $\delta f_i^{(\alpha) \rightarrow (\beta)} \neq 0$. Since we consider scalar perturbations, we write $\delta f_i^{(\alpha) \rightarrow (\beta)} = \partial_i \delta f_{(\alpha) \rightarrow (\beta)}$ and work in terms of the function $\delta f_{(\alpha) \rightarrow (\beta)}$.

Let us now perturb the gradient of the stress energy tensor for a scalar field in interaction with a perfect fluid. At the perturbed level, the kinetic and potential fictitious fluids associated to ϕ have perturbed energy density and pressure given by

$$\delta \rho_K^{(\text{gi})} = \delta p_K^{(\text{gi})} = \frac{\phi'}{a^2} \delta \phi^{(\text{gi})'} - \frac{\phi'^2}{a^2} \Phi, \quad (3.15)$$

$$\delta \rho_V^{(\text{gi})} = -\delta p_V^{(\text{gi})} = V_\phi \delta \phi^{(\text{gi})}, \quad (3.16)$$

and the perturbed gradient of the stress energy tensor also involves the velocity potential $v_{(\alpha)}^{(\text{gi})}$, related to the spatial component of the perturbed velocity by $v_{(\alpha),i}^{(\text{gi})} = \partial_i v_{(\alpha)}^{(\text{gi})}$, and the rescaled velocity $\varsigma_{(\alpha)}^{(\text{gi})}$ defined by $\varsigma_{(\alpha)}^{(\text{gi})} \equiv [\rho_{(\alpha)} + p_{(\alpha)}] v_{(\alpha)}^{(\text{gi})}$,

$$v_K^{(\text{gi})} = -\frac{\delta \phi^{(\text{gi})}}{\phi'}, \quad \varsigma_K^{(\text{gi})} = -\frac{\phi'}{a^2} \delta \phi^{(\text{gi})}. \quad (3.17)$$

Notice that we do not need to specify $v_V^{(\text{gi})}$ since it does not appear in the equations. In these expressions, as already mentioned, the superscript “(gi)” means that the corresponding quantity is gauge-invariant and coincides with its value in the longitudinal gauge. At the

perturbed level, the energy-momentum transfer coefficients between the kinetic and potential fluids are given by

$$a\delta Q_{K \rightarrow V} = -V_\phi \delta\phi^{(\text{gi})'} + V_\phi \phi' \Phi - V_{\phi\phi} \phi' \delta\phi^{(\text{gi})}, \quad a\delta Q_{V \rightarrow K} = 0, \quad (3.18)$$

$$\delta f_{K \rightarrow V} = \delta f_{V \rightarrow K} = 0. \quad (3.19)$$

As will be shown below, these formulas are indeed needed to recover the standard equation of motion for the scalar field fluctuation (i.e. the equation of motion in absence of coupling with a fluid, for which a Lagrangian formulation of the theory exists and the equation of motion is well prescribed). Regarding the interaction between the kinetic and potential fluids on one hand, and the perfect fluid on the other hand, we have from perturbing eq. (3.4)

$$\delta Q_{K \rightarrow f} = -\Gamma \delta\rho_K^{(\text{gi})}, \quad \delta Q_{f \rightarrow K} = \delta Q_{V \rightarrow f} = \delta Q_{f \rightarrow V} = 0, \quad (3.20)$$

and

$$\delta f_{K \rightarrow f} = a\Gamma \left[v_{\text{tot}}^{(\text{gi})} - v_K^{(\text{gi})} \right] \rho_K, \quad \delta f_{f \rightarrow K} = \delta f_{V \rightarrow f} = \delta f_{f \rightarrow V} = 0, \quad (3.21)$$

where the total velocity $v_{\text{tot}}^{(\text{gi})}$ is defined by the following expression

$$v_{\text{tot}}^{(\text{gi})} = \frac{1}{\rho + p} \sum_{\alpha} [\rho_{(\alpha)} + p_{(\alpha)}] v_{(\alpha)}^{(\text{gi})}, \quad (3.22)$$

with ρ and p the total energy density and pressure.

Endowed with these definitions and assumptions one can then derive the perturbed equations of motion. For the scalar field, one obtains the perturbed Klein-Gordon equation

$$\delta\phi^{(\text{gi})''} + 2\mathcal{H}\delta\phi^{(\text{gi})'} + \frac{a\Gamma}{2}\delta\phi^{(\text{gi})'} - \nabla^2\delta\phi^{(\text{gi})} + a^2V_{\phi\phi}\delta\phi^{(\text{gi})} = 4\phi'\Phi' - 2a^2V_\phi\Phi - \frac{a\Gamma}{2}\phi'\Phi. \quad (3.23)$$

For the perfect fluid, one has two equations, namely the time and space components of the conservation equation, yielding an equation for the perturbed energy density and the perturbed velocity respectively, which read

$$\delta\rho^{(\text{gi})'} + 3\mathcal{H}(1+w_f)\delta\rho^{(\text{gi})} - 3(1+w_f)\rho\Phi' + (1+w_f)\rho\nabla^2v^{(\text{gi})} - \frac{\Gamma}{a} \left[\phi'\delta\phi^{(\text{gi})'} - \frac{1}{2}\phi'^2\Phi \right] = 0, \quad (3.24)$$

$$\varsigma^{(\text{gi})'} + 4\mathcal{H}\varsigma^{(\text{gi})} + \rho(1+w_f)\Phi + w_f\delta\rho^{(\text{gi})} + \frac{\Gamma}{2a}\phi'\delta\phi^{(\text{gi})} = 0. \quad (3.25)$$

One also needs an equation to track the evolution of the Bardeen potential and this is provided by the perturbed Einstein equations,

$$\Phi' = -\mathcal{H}\Phi - \frac{a^2}{2M_{\text{Pl}}^2} \left[-\frac{1}{a^2}\phi'\delta\phi^{(\text{gi})} + \varsigma^{(\text{gi})} \right]. \quad (3.26)$$

In figure 5, we have numerically integrated the above equations using the same parameters as in figures 3 and 4 and for the mode $k/a_{\text{ini}} = 0.002M_{\text{Pl}}$, the physical wavelength of which is displayed in figure 2. The solid blue line in figure 5 represents the scalar field density contrast $k^3|\delta\phi_{\mathbf{k}}|^2 = k^3|\delta\rho_{\phi,\mathbf{k}}^{(\text{gi})}/\rho_\phi|^2$, the solid orange line corresponds to the radiation

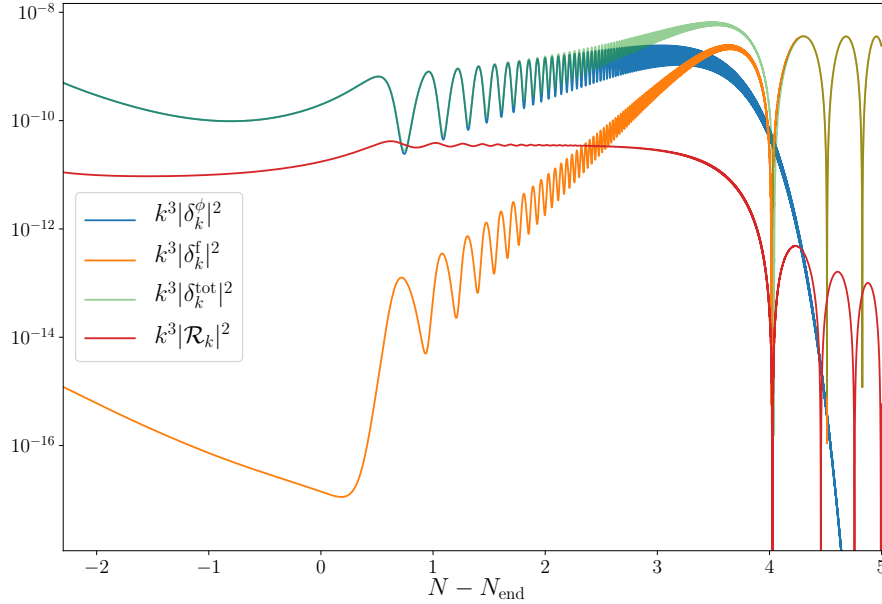


Figure 5. Evolution of the modulus of the gauge invariant perturbative quantities δ_k^ϕ (inflaton density contrast, blue line), δ_k^f (radiation density contrast, orange line), δ_k^{tot} (total, i.e. scalar field plus radiation, density contrast, green line) and $\mathcal{R}_k$ (comoving curvature perturbation, red line) as a function of the number of e -folds, in the same setup as the one displayed in the previous figures. Soon after perturbative reheating becomes effective (which, according to the discussion around figure 3, occurs when $N_\Gamma - N_{\text{end}} \simeq 2.8$), the scalar field density contrast decreases, the curvature perturbation stops being constant and decreases as well, hence the total density contrast stops increasing, which signals the end of the instability.

fluid density contrast $k^3|\delta_k^f|^2 = k^3|\delta\rho_{f,\mathbf{k}}^{(\text{gi})}/\rho_f|^2$, while the green line is the total density contrast $k^3|\delta_k^{\text{tot}}|^2 = k^3|[\delta\rho_{\phi,\mathbf{k}}^{(\text{gi})} + \delta\rho_{f,\mathbf{k}}^{(\text{gi})}]/(\rho_\phi + \rho_f)|^2$. When the mode enters the instability band around $N - N_{\text{end}} \simeq 0.5$ e -fold, we see that the scalar field density contrast grows and one can check that this growth is proportional to the scale factor $a(t)$. This is a first consistency check. Originally, this growth was derived from an analysis based on the Mathieu-like equation for the Mukhanov-Sasaki variable, see ref. [35]. Here, we recover it using the conservation equations. We also notice that, initially, the total density contrast is equal to the scalar field density contrast which is of course expected since the production of radiation has not yet started in a sizeable way. When the amount of radiation starts being substantial, the two density contrasts become different as revealed by the fact that the green and blue curves separate. Then, the scalar field density contrast strongly decreases and becomes quickly negligible. This means that the total density contrast is given by the radiation density contrast and we see that, when the transition is completed, it stays constant. In figure 5, we have also represented the comoving curvature perturbation $\mathcal{R}_k = \Psi_k - aHv_{\text{tot},\mathbf{k}}^{(\text{gi})}$ with the red line. At the onset of the instability phase, it is, as expected from the above analysis, constant, and then it decreases as expected for sub-sonic perturbations in a radiation-dominated universe.

The main conclusion of this analysis is a confirmation that perturbative reheating effects do not destroy the metric preheating instability, since the instability stops only when, at the background level, the radiation fluid dominates the energy budget of the universe. The tiny

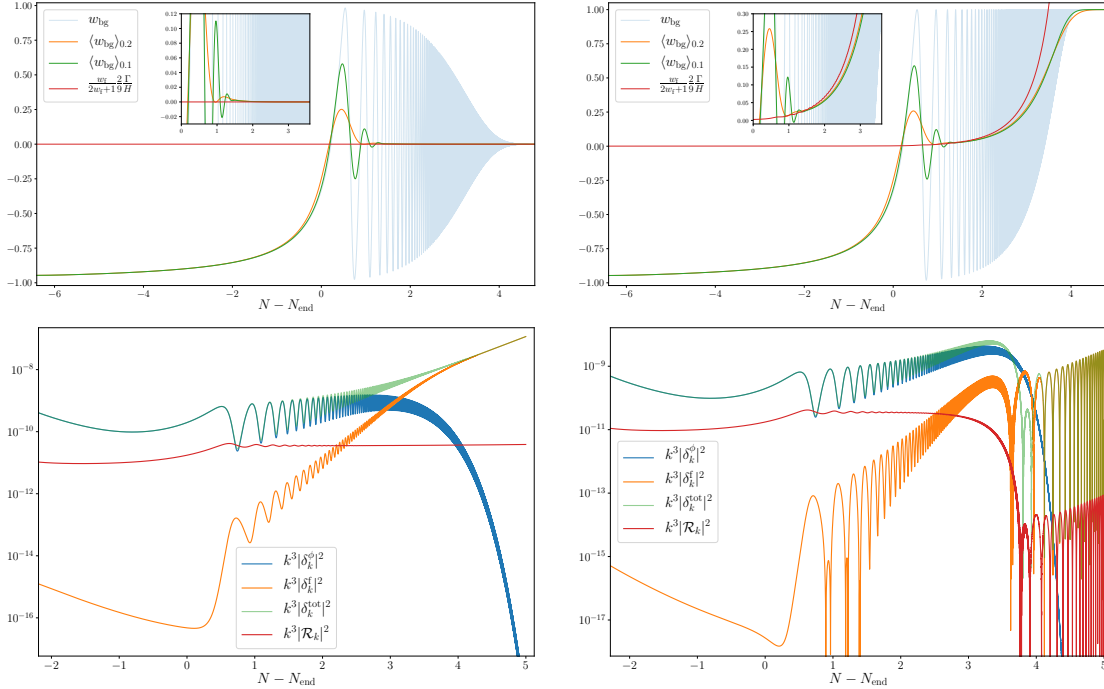


Figure 6. Time evolution of the background equations-of-state parameters (upper panels), with the insets zooming in the regime of validity of the analytical approximation (3.12), as well as scalar perturbations (lower panels), as a function of the number of e -folds, in the cases of decay into pressureless matter $w_f = 0$ (left panels) and into a stiff fluid $w_f = 1$ (right panels). Apart from the value of w_f , the setup and parameter values are the same as in all previous figures.

amount of radiation that is initially present is not sufficient to blur the narrow-resonance regime and to remove the system from the first, and very thin, instability band of the Mathieu equation chart. Notice that this supports the treatment of ref. [40] where the instability was simply stopped at the time when the universe becomes radiation dominated. This also demonstrates the robustness of the results obtained in ref. [35] and the generic, unavoidable presence of an instability in single-field models of inflation at small scales.

Another way to test this robustness is to study whether the above conclusion is still valid when the inflaton decays into a fluid with an equation of state that differs from the one of radiation. We have therefore considered two additional cases corresponding to a decay into a fluid with $w_f = 0$ (pressureless matter) and a decay into a fluid with $w_f = 1$ (stiff matter). The results are displayed in figure 6 and confirm that our description of the instability generalises to arbitrary equation-of-state parameters w_f . On the upper panels, we show the total equations of state w_{bg} and their averaged values, as well as the analytical approximation eq. (3.12), as a function of the number of e -folds. One verifies that the equation-of-state parameter indeed asymptotes $w_{bg} = 0$ (left panel) and $w_{bg} = 1$ (right panel) at late time. On the lower panels, we have displayed the time evolution of the density contrasts and of the curvature perturbation. The growth $\delta_k \propto a$ is still observed until the universe is dominated by the fluid,² regardless of its equation of state.

²In the case where the decay product is a pressureless fluid, the growth $\delta_k \propto a$ still continues afterwards for all scales. In the case where $w_f = 1$, stiff fluid density fluctuations also grow like $\delta_k \propto a$ on sub-Hubble scales, see the relation above eq. (3.33).

3.3 Radiative decay and PBH formation from metric preheating

In the covariant description developed in section 3, two fluids were necessary to fully describe the scalar field fluctuations. This shows that cosmological inhomogeneities of a scalar field and of a perfect fluid are a priori two very different physical systems, featuring different properties. It is therefore rather intriguing that, during the oscillatory phase, the averaged equation of state is the one of pressureless matter, and that inside the instability band, the density contrast behaves as the one of pressureless matter too, since it grows linearly with the scale factor.

The formation of primordial black holes has mostly been studied in the context of perfect fluids, so if this correspondence between an oscillating scalar field and a pressureless perfect fluid does hold (and even in the presence of additional radiation), it would have important practical consequences [58] for studying the production of PBHs from the metric preheating instability. This is why, in this section, we compare more carefully the behaviour of the cosmological perturbations of the system at hand with those of a single perfect fluid sharing the same equation-of-state parameter.

A key concept in this comparison is the one of the equation of state “felt” by the perturbations, if they are interpreted as perturbations of a single perfect fluid. We start by recalling the behaviour of the density contrast for a perfect fluid with a given equation-of-state parameter w . This will allow us to extract the equation-of-state parameter from the time dependence of the density contrast, and to apply this formula to the system studied in section 3 in order to derive the effective “equation of state” felt by the density perturbations. We will then compare it with the equation of state of the background.

In order to implement this program, a remark is in order regarding the definition of the density contrast. So far, we have worked in terms of the density contrast $\delta^{(\text{gi})}$ (noted δ_g in ref. [59]), which consists in measuring the energy density relative to the hypersurface which is as close as possible to a “Newtonian” time slicing. However, for a single perfect fluid, this density contrast usually stays constant at large scales and, as a consequence, cannot be used as a tracer of the equation-of-state parameter. Fortunately, as is well-known, there are other possible definitions, in particular δ_{com} (noted δ_m in ref. [59]), which measures the amplitude of energy density from the point of view of matter, and corresponds to the density contrast in the comoving-orthogonal gauge. The behaviour of δ_{com} does depend on w on large scales and, therefore, it is a useful quantity for our purpose. The relationship between $\delta^{(\text{gi})}$ and δ_{com} is given by

$$\delta^{(\text{gi})} = \delta_{\text{com}} - \frac{\rho'}{\rho} v^{(\text{gi})} = \delta_{\text{com}} \left[1 + 3 \frac{a^2 H^2}{k^2} \left(1 + \frac{\Phi'}{aH\Phi} \right) \right], \quad (3.27)$$

which shows that, although they behave differently on super-Hubble scales, their evolution is identical on small scales. To prove this relation, we have used that the density contrast δ_{com} is related to the Bardeen potential through the Poisson equation [59]

$$\delta_{\text{com}} = - \frac{2k^2 M_{\text{Pl}}^2}{a^2 \rho} \Phi. \quad (3.28)$$

If the space-time expansion is driven by a perfect fluid with constant equation-of-state parameter w , the energy density scales as $\rho = \rho_{\text{end}} (a_{\text{end}}/a)^{3(1+w)}$, which leads to

$$\delta_{\text{com}} = \delta_{\text{com}}^{\text{end}} \left(\frac{a}{a_{\text{end}}} \right)^{1+3w} \frac{\Phi}{\Phi_{\text{end}}}, \quad (3.29)$$

where the Bardeen potential follows the equation of motion [47]

$$\frac{d^2}{d(k\eta)^2} [(k\eta)^\nu \Phi] + \frac{2}{k\eta} \frac{d}{dk\eta} [(k\eta)^\nu \Phi] + \left[w - \frac{\nu(\nu+1)}{(k\eta)^2} \right] (k\eta)^\nu \Phi = 0, \quad (3.30)$$

with $\nu = 2/(1+3w)$. The solution to this equation is given by

$$\Phi_{\mathbf{k}} = (wk\eta)^\alpha [A_{\mathbf{k}} J_\alpha(wk\eta) + B_{\mathbf{k}} J_{-\alpha}(wk\eta)], \quad (3.31)$$

with $\alpha = -(5+3w)/[2(1+3w)]$, J_α being a Bessel function and $A_{\mathbf{k}}$, $B_{\mathbf{k}}$ two integration constants fixed by the initial conditions. The behaviour of this solution depends on whether $|wk\eta| \ll 1$ or $|wk\eta| \gg 1$, i.e. on whether the mode wavelength is larger or smaller than the sound horizon w/H .

On super-sonic scales, $|wk\eta| \ll 1$, the Bessel functions can be expanded according to $J_\alpha(z) \propto z^\alpha$. Since $\alpha < 0$ for $w > -1/3$, eq. (3.31) features a constant mode and a decaying mode. The Bardeen potential thus asymptotes to a constant, and $\delta_{\text{com}} \propto a^{1+3w}$, see eq. (3.29). If $w = 0$, then $\delta_{\text{com}} \propto a$, which is a well-known result.

On sub-sonic scales, $|wk\eta| \gg 1$, the Bessel functions can be expanded according to $J_\alpha(z) \simeq \sqrt{2/(\pi z)} \cos[z - \pi(1+2\alpha)/4]$. This leads to $\delta_{\text{com}} \simeq a^{-1/2+3w/2} \cos[wk\eta - \pi(1+2\alpha)/4]$. The density contrast thus oscillates as a result of the competition between gravity and pressure, and compared to the super-sonic case, the overall amplitude also scales differently with the scale factor. One also notices that this formula cannot be applied if $w = 0$. Indeed, in that case, the argument of the Bessel functions vanishes. Physically, if $w = 0$, there is no sound horizon anymore (since the pressure vanishes), and all scales are “super-sonic” by definition.

These two limiting expressions of the density contrast can be used to define an effective equation-of-state parameter “felt” by the perturbations. Since $\delta_{\text{com}} \propto a^{1+3w}$ on super-sonic scales, we define

$$w_{\text{eff}}^{\text{super}} \equiv \frac{1}{6} \frac{d \ln (k^3 \langle \delta_{\text{com}}^2 \rangle)}{d \ln a} - \frac{1}{3}, \quad (3.32)$$

where $\langle \cdot \rangle$ stands for time averaging over possible background oscillations. On sub-sonic scales, $\delta_{\text{com}} \simeq a^{-1/2+3w/2} \cos[wk\eta - \pi(1+2\alpha)/4]$, so we introduce

$$w_{\text{eff}}^{\text{sub}} \equiv \frac{1}{3} \frac{d \ln (k^3 \langle \delta_{\text{com}}^2 \rangle)}{d \ln a} + \frac{1}{3}. \quad (3.33)$$

Which of these two effective equations of state is relevant depends on whether the mode k is sub-sonic and super-sonic. In figure 7, we display these two quantities, $w_{\text{eff}}^{\text{super}}$ and $w_{\text{eff}}^{\text{sub}}$, from the value of δ_{com} numerically obtained as in the previous figures, and compare them with the (averaged) equation-of-state parameter of the background. In all cases, the time averaging is performed with a Gaussian kernel of constant standard deviation given by 0.2 e -folds. Let us also stress again that, on sub-Hubble scales, the density contrast in the comoving-orthogonal gauge, δ_{com} , coincides with the one in the longitudinal gauge displayed in figures 5 and 6.

During the first oscillations, the equation-of-state parameter vanishes (on average) in the background, and recalling that all modes are super-sonic for a vanishing equation-of-state parameter, one can check that the relevant equation of state, $w_{\text{eff}}^{\text{super}}$, indeed vanishes, and that the red and orange curves in figure 7 are indeed close. This however lasts for a few e -folds only, after which neither of the effective equations of state correctly reproduces the behaviour of the (averaged) equation of state of the background. In addition, for the

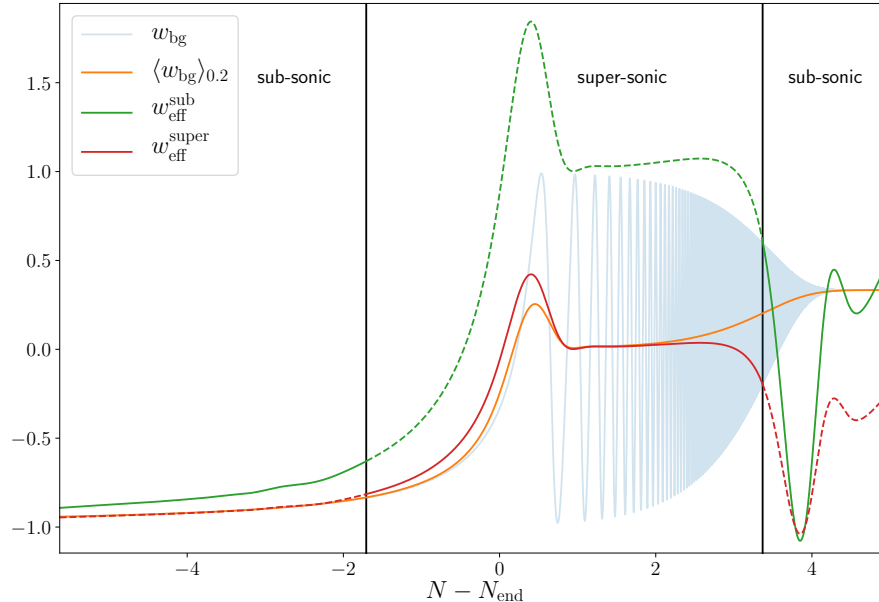


Figure 7. Effective equation-of-state parameters for the perturbations as a function of the number of e -folds. When the mode k is super-sonic, its effective equation-of-state parameter is given by $w_{\text{eff}}^{\text{super}}$ (red line), and respectively by $w_{\text{eff}}^{\text{sub}}$ (green line) when it is sub-sonic. In order to facilitate the reading of the figure, the effective equation-of-state parameters are displayed with dashed lines in the regimes where they are not relevant. The instantaneous background equation of state (transparent blue line) and its averaged value (orange line) are also represented for comparison. When $\langle w_{\text{bg}} \rangle \approx 0$, the sound horizon is very small and the super-sonic effective equation of state (red line) is the relevant one. As expected, it is close to 0. However when $\langle w_{\text{bg}} \rangle$ starts to depart from zero, since the physical mode k/a is within the Hubble radius (see figure 2), the sub-sonic equation of state (green line) becomes the relevant one and, as expected, it quickly converges to $1/3$. Note however that between these two asymptotic regimes, the effective equation of state for the perturbation does not match the one of the background.

sub-sonic scales that lie inside the instability band, $\langle w_{\text{bg}} \rangle$ does not coincide at all with $w_{\text{eff}}^{\text{sub}}$ during the oscillating phase until radiation strongly dominates the universe content and both converge to $1/3$. Therefore, despite the fact that the inflaton background effectively behaves as pressureless matter on average, and that its decay product is a perfect fluid, the perturbations of the system are not those of perfect fluids. This confirms that the system made of a decaying, oscillating scalar field has different behaviour from a pure perfect fluid, and cannot be simply modelled as such.

Let us note that this fundamental difference is even more striking in the case where the inflaton potential is quartic close to its minimum, since in that case the correspondence between the inflaton perturbations and those of a perfect fluid with the same background equation of state breaks down even in the absence of inflaton radiative decay. As shown in ref. [35] indeed, while $\langle w_{\text{bg}} \rangle = 1/3$ in such a case, the instability of metric preheating is still present, and the density contrast grows even faster than that of pressureless matter (namely, exponentially with the scale factor) in the instability band, while the density contrast for a perfect fluid having $w = 1/3$ is constant on sub-sonic scales.

As mentioned above, this implies that, in order to study the production of PBHs that arises from the increase of the density contrast in the instability band, one cannot rely on techniques developed for perfect fluids. In ref. [58] for instance, it was used that an overdensity of a perfect fluid with constant equation-of-state parameter w collapses into a black hole if it exceeds the critical density contrast³ [62, 63]

$$\delta_c = \frac{3(1+w)}{5+3w} \sin^2 \left(\frac{\pi\sqrt{w}}{1+3w} \right), \quad (3.34)$$

in which w was replaced with $w \sim \Gamma/H$ [see eq. (3.12)]. If $w = 0$, eq. (3.34) indicates that any local overdensity ends up forming a black hole, which is indeed the case in the absence of any pressure force. The analysis of ref. [58] thus suggests that what limits the formation of PBHs from the instability of metric preheating is the presence of (even small amounts of) radiation, which provide a non-vanishing value to the equation-of-state parameter, and hence to δ_c . However, the results of the present work cast some doubt on such a treatment since we showed that an oscillating scalar field decaying into a radiation fluid cannot be treated as a collection of perfect fluids at the perturbed level [furthermore, the background equation of state for such a system is strongly time dependent, see eq. (3.12), while eq. (3.34) only applies to constant equation-of-state parameters].

In ref. [40], the formation of PBHs from the overdensities of an oscillating scalar field was studied in the context of metric preheating, and it was found that what limits the formation of PBHs is rather the fact that the instability does not last for ever, since it stops when radiation takes over. Indeed, although it is true that any overdensity inside the instability band develops towards forming a black hole, the amount of time needed for a black hole to form depends on (and decreases with) the initial value of the density contrast. By requiring that it takes less time than what is available before the complete inflaton decay (which, as we have established in section 3.2, signals the end of the instability phase that is otherwise not affected by the presence of radiation being produced), one obtains a lower bound on the density contrast, which however has nothing to do with eq. (3.34).

4 Conclusions

Preheating effects are often believed to be observationally irrelevant in single-field models of inflation. Although this is true at large scales, where the curvature perturbation is merely conserved, the situation is different at small scales, namely those leaving the Hubble radius a few e -folds before the end of inflation. Such scales are subject to a persistent instability proceeding in the narrow-resonance regime [35], which causes the density contrast to grow, leading to various possible effects such as early structure formation or even PBHs formation [40].

In contrast to the case of background preheating, where the narrow-resonance regime is irrelevant since, in a time-dependent background, the system spends very little time in the thin instability band and the resonance effects are wiped out, in the metric preheating case, the presence of the instability is actually caused by cosmic expansion itself (see figure 2). This is the reason why this mechanism is both atypical and very efficient.

This fact was known to be true [35] only if the inflaton is uncoupled to other degrees of freedom. However, in order for reheating to proceed, the inflaton field must decay into

³The criterion for PBH formation is expressed in terms of the density contrast rather than curvature perturbation, the latter being affected by environmental effects [60], see also ref. [61].

radiation, and the goal of this paper was to determine whether this decay could spoil the instability. Using the formalism of cosmological perturbations in the presence of interactions between fluids, we have shown that it is not the case, and that the growth of the density contrast inside the instability band remains unaffected until the radiation fluid dominates the universe content.

We have also stressed that there is a fundamental difference between the cosmological perturbations of an oscillating scalar field and those of a perfect fluid, and that techniques developed to study the formation of PBHs from perfect fluid overdensities cannot be applied to the present context. Instead, a dedicated analysis such as the one of ref. [40] must be performed. Our results have confirmed that the presence of radiation can simply be ignored until it comes to dominate the energy budget, thus stopping the instability.

The results of this work therefore confirm that the instability of metric preheating is unavoidable in single-field models of inflation, since it only requires an oscillating scalar field in a cosmological background, which is the state of the universe at the end of most inflationary models, and given that it is robust against perturbative decay of this field.

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8.2 Metric preheating and formation of Primordial Black Holes

In the previous section, it has been shown that single-field inflation generic leads to a parametric amplification of sub-Hubble inflaton's fluctuations in the range $H < k/a < \sqrt{3Hm}$ where m is the curvature of the scalar potential at its minimum. This instability was first investigated in Ref. [266] (see also Ref. [267]), and later on it was realised that the scalar instability could lead to a cosmological production of primordial gravitational waves via second-order effects [268] as well Primordial Black Holes (PBH) [269, 270] that can themselves produce primordial gravitational waves [271]. In this section, one slightly elaborates, although staying qualitative, on the PBH production mechanism, mainly rephrasing the results of Ref. [269] and replacing them in the wider context of perturbative reheating together with metric preheating that was presented in the previous section.

A given wavenumber k enters the instability band at a time denoted $t_{bc}(k)$ where “bc” stands for band-crossing, and evaluating time-dependent quantities at this time will now simply be denoted $bc(k)$ where the k -dependence may be implicit. If the instability stops at the time t_{stop} , then there is a minimum and a maximum wavenumber that are amplified (they “enter” the instability band, respectively from above and from below in Fig. 2 of Sec. 8.1, at the time when the instability stops), corresponding to $k_{min} = a_{stop}H_{stop}$ and $k_{max} = a_{stop}\sqrt{3H_{stop}m}$. Of course, the range $[k_{min}, k_{max}]$ corresponds to physical scales that are much smaller than the ones probed in the CMB and that exited the horizon approximately 60 e -folds before the end of inflation. Actually note that the unstable modes in the range $[a_{end}H_{end}, k_{max}]$ are so small that they have never exited the horizon, hence their status is unclear: should they still be described quantum-mechanically? Given the exponential amplification of the density contrast, $\delta_k \propto a$, a given mode with wavenumber k reaches the critical value at which it collapses into a PBH after an amount of time $\Delta t_{collapse}(k) = t_{collapse}(k) - t_{bc(k)}$ spent in the instability band, that can be predicted by spherical collapse models: [269, 272]

$$\Delta t_{collapse}(k) = \frac{\pi}{\left(H\delta_k^{3/2}\right)\Big|_{bc(k)}}. \quad (8.1)$$

Note that if the initial overdensity at the onset of the instability is larger, it obviously takes less time for it to collapse. Therefore one is left with a criterion for a given mode to end up collapsing into a PBH before the instability stops:

$$\Delta t_{collapse}(k) < \Delta t_{instab}(k) = t_{stop} - t_{bc(k)}. \quad (8.2)$$

PBHs are interesting because they constitute a probe of the small-scale physics of inflation (and of reheating as one just understood), and therefore of a very different part of the scalar potential of the inflaton, as well as of the other degrees of freedom and interactions in the early Universe. For example, the PBH mass fraction from the metric preheating instability is crucially dependent on the duration of the instability, a duration

that is set by the value of the decay parameter Γ of the scalar field into the cosmological fluid as one understood in Sec. 8.1. For low values of this decay parameter, the instability lasts for a long time and thus overproduces PBHs in such a way that the entire Universe becomes filled with PBHs. It however needs not mean that our current Universe should be filled with PBHs (and it seems not to be), since those PBHs are so light that they are expected to disappear very quickly due to Hawking evaporation. Actually, reheating could even be due to the Hawking evaporation of these PBHs. Indeed, a PBH associated to a collapsed scale k , and of mass $M(k) \propto k^{-3}$, evaporates in an amount of time [273]:

$$\Delta t_{\text{evap}}(k) = \frac{10240}{g} \frac{M^3(k)}{M_{\text{Pl}}^4}, \quad (8.3)$$

where g is the number of degrees of freedom, and which therefore results in a different criterion, this time for PBHs to survive until the instability stops:

$$\Delta t_{\text{collapse}}(k) + \Delta t_{\text{evap}}(k) > \Delta t_{\text{instab}}(k). \quad (8.4)$$

This time, one can see that the higher the initial density contrast at the onset of the instability, the less PBH at the end of instability. Together with the formation criterion, they provide both a lower bound and an upper bound on $\delta_k^{\text{bc}(k)}$ for observing PBH related to the scale k at the end of the instability.

Then of course, the amount of PBHs and their masses keep evolving in the remaining of the cosmological history, due to gravitational interactions such as clustering, but also Hawking evaporation that is still taking place, all this being modeled by the time-evolving mass fraction. By considering the absence so far of unquestionable observation of PBHs, one can then place theoretical constraints on the model at hand, such as restricting the range of allowed values for Γ . But the above reasoning assumes that the instability takes place independently of the details of the mechanism that stops the instability at the particular time t_{stop} , which may well simply be the usual perturbative reheating when the inflaton decays into another scalar field or into a cosmological fluid. It is in order to explore this scenario and validate the results of Ref. [269] that we investigated the dynamics of radiative decay *during* metric preheating in Ref. [6] reproduced above in Sec. 8.1: the important conclusion is that the instability is unspoiled by these decays that simply provide a natural and dynamical way to stop the instability around the time $t_{\text{stop}} = t_{\Gamma} \sim \Gamma^{-1}$.

A sketch of the relevant dynamical energy scales and peculiar times of interest for this section, is represented in Fig. 8.2.

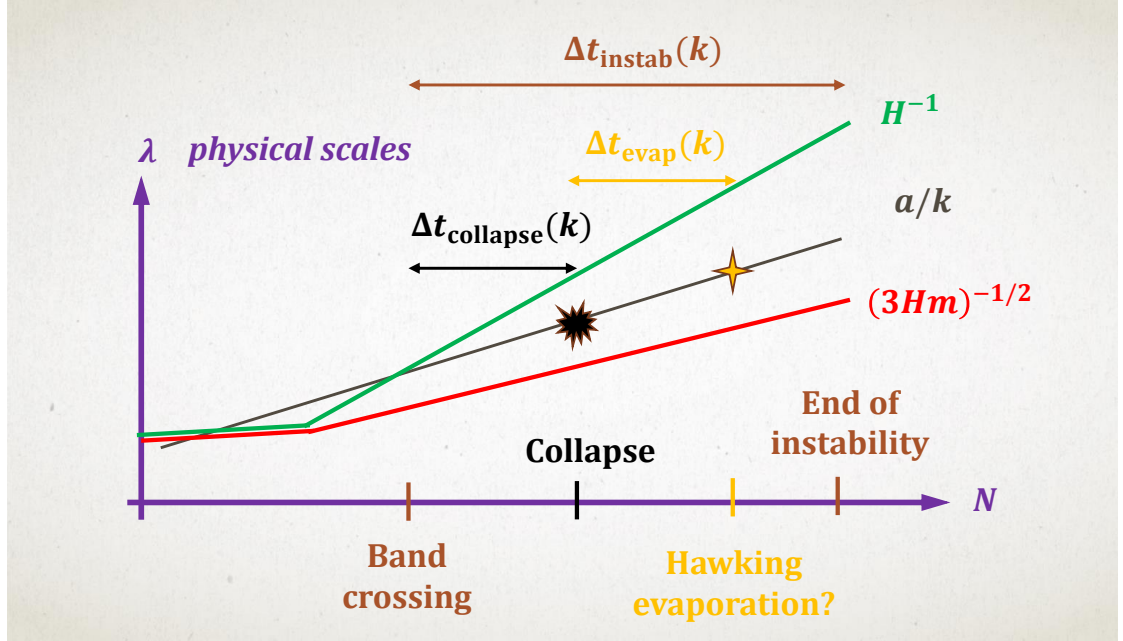


Figure 8.2: Physical scales at the end of inflation and during preheating where the background oscillates but behaves on average as a pressure-less Universe. The two scales representing the boundaries of the instability band are depicted in green (Hubble radius H^{-1}) and in red $[(3Hm)^{-1/2}]$, while a physical scale of size $\lambda(t) = a(t)/k$, stretched from under the horizon to super-Hubble scales and then re-entering the horizon and thus the instability band “by above” at a time $t_{bc(k)}$, is in black. Assuming that the density contrast at the onset of the instability, $\delta_k^{bc(k)}$, is large enough to collapse before the end of the instability, the time of collapse is represented. If the Hawking evaporation is efficient enough, the corresponding PBH will have evaporated after a time $\Delta t_{evap}(k)$ that may be before the end of the instability, which is supposed here on this sketch.

8.3 Temperature of reheating

In sec. 8.1, one has understood that the metric preheating instability is stopped when the reheating process is complete and all the energy of the inflaton field has been transferred to a decay product, modeled there to be a perfect cosmological fluid. Indeed, because the Hubble parameter H is quickly decreasing when universe dominated by the oscillating scalar field, it reaches the threshold value Γ of the decay rate after a few e -folds. How many e -folds exactly depends on the ratio between the Hubble parameter at the end of inflation, H_{end} , and the value of Γ which fixes the temperature of the Universe when reheating as terminated (note that knowing this duration of reheating is important to find the correct value of $N_*(k_{pivot})$, the time at which the pivot scale exited the horizon during inflation). Indeed, assuming that the decay products of the inflaton

instantaneously thermalise, they are described by a fluid at thermal equilibrium with temperature T_{reh} such that:

$$\begin{aligned}\rho_{\text{reh}} &= \rho(N_{\text{reh}}) = 3\Gamma^2 M_{\text{Pl}}^2 \\ &= \frac{\pi^2}{30} g_* T_{\text{reh}}^4,\end{aligned}\tag{8.5}$$

where g_* is the number of primordial relativistic degrees of freedom just after the decay, and therefore one finds the

(Temperature of reheating): $T_{\text{reh}} = \left(\frac{90}{g_*}\right)^{1/4} \sqrt{\frac{\Gamma M_{\text{Pl}}}{\pi}}.$

(8.6)

Obviously, this very simplistic treatment neglects many interesting aspects of reheating, such as the issue of thermalisation of the decay products [274–279] and turbulence [280, 281], the possibility to produce cosmological defects [282] or feature a tachyonic preheating phase [283], as well as plenty of other ones. For a recent and pedagogical review on these topics, I recommend Ref. [284].

Chapter 9

Multifield – multi-fluids reheating and the evolution of isocurvature perturbations

This chapter deals with the multi-species reheating scenario. It mainly consists in a scientific publication where we study the perturbative reheating of the Universe by the decays of the multiple scalar fields responsible for inflation, into several cosmological fluids. It proposes not only a generic formalism to describe those interactions, but also a systematic method to study the behaviour of the background and of the linear fluctuations both in the sub-Hubble and super-Hubble regime, the latter being relevant in multi-species reheating. Moreover, it is explained that for most cases, a numerical resolution of the many coupled differential equations, is necessary in order to derive precise enough predictions for the initial conditions of CMB physics.

9.1 General formalism and application to double inflation (article)

This section proposes to follow both analytically and numerically the evolution of isocurvature fluctuations through multifield–multi-fluids reheating, see Ref. [7],

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arXiv:submit/3733831,

that is reproduced below.

We begin by explaining the formalism that enables us to couple scalar fields with cosmological fluids and that has been inspired from Ref. [150]. It consists in treating a collection of N_{field} scalar fields with canonical kinetic terms as a collection of $N_{\text{field}} + 1$ perfect fluids with constant equations of state, by separating them into N_{field} kinetic fluids with $w_K = 1$ and one potential fluid with $w_V = -1$. This is only possible if

each of the resulting stress-energy tensors, $T_{(\alpha)}^{\mu\nu}$ with $(\alpha) \in \{K_1, \dots, K_{N_{\text{field}}}, V\}$, is not individually conserved: $\nabla_\mu T_{(\alpha)}^{\mu\nu} = Q_{(\alpha)}^\nu$ where $Q_{(\alpha)}^\nu$ is a covariant energy-momentum flow describing the transfers between kinetic and potential fluids, and that is uniquely fixed by the scalar potential and the background quantities. Until now, this simply consists in a fluid formalism to describe scalar fields. But then, one can add to these “fictitious” kinetic and potential fluids, a collection of N_{fluid} “real” cosmological fluids, typically radiation, dark matter, baryons, neutrinos, dark energy, etc. For simplicity, we restrict ourselves to cosmological fluids that do not possess an anisotropic stress, although our equations could be easily extended to this case. The idea is that the two sectors made of fictitious and real cosmological fluids are not decoupled: first of course gravity mixes them, but one can also add direct couplings by allowing new kinds of non-conservation laws $Q_{(\alpha)}^\nu$, that can be chosen such that the scalar fields indeed decay into cosmological fluids at the end of inflation, as it is supposed to happen during reheating. Note that in principle the formalism can be used for other cosmological scenarios than reheating, such as warm inflation [285, 286], or inverse decays where the cosmological fluids produce scalar fields, etc.

Crucially, because those non-conservation laws are written in a covariant way, they can be used to describe interactions at the level of perturbations too, just like the Einstein equations that describe the evolution of the spacetime geometry in a Universe filled by such system of $N_{\text{field}} + N_{\text{fluid}} + 1$ fluids. Doing so, we show the full set of closed differential equations that must be solved at the level of the background but also of linear fluctuations, and explain that contrary to what could be thought, one must follow the evolution of velocity perturbations and describe not only the energy exchanges but also the momentum ones, in order to correctly encompass all physical effects. We define both adiabatic and isocurvature fluctuations, for energy densities’ perturbations but also for the velocities (that are inherently perturbative) of the various fluids. Because the fluid description of the scalar fields allows for an unified description, we check that these definitions are compatible with the usual ones used in multifield inflation, and recover various formulas relating those fluctuations and the non-adiabatic pressure perturbation. We then apply the formalism explicitly to the case of reheating at the end of multifield inflation, showing the equations in terms of concrete quantities like the scalar potential of the scalar fields, the equations of state of the real cosmological fluids and the decay rates of the fields–fluids interactions. We also recall how to quantise a system of several scalar fields and extend it heuristically to the multi-fluids case.

The remainder of this piece of work specialises to a particular multifield model that is double quadratic inflation, in which $N_{\text{field}} = 2$ scalar fields only have a mass term in their potential, and that each couples to a cosmological fluid: the heavy field first decays into a dark matter fluid with $w_m = 0$, actually *during* inflation, and the light field decays at the end of inflation into a radiation fluid $w_\gamma = 1/3$. This model is simply chosen in order to display a simple representative example of the formalism, and to show that even in the simplest case, although a sophisticated analytical treatment is proposed both for the background and the linear fluctuations (but it seems unlikely that one could extend it to more complicated multifield models), it is barely precise enough to accurately match

the full numerical resolution. In particular, we revisit the generation and the evolution of non-adiabatic, isocurvature fluctuations before, during and after reheating in this two-field scenario and argue that the numerical treatment that we propose seems unavoidable in most cases. Although it has not yet been done, we plan to publicly release our code that enables one to solve for the coupled multifield–multi-fluids system.

In order to grasp the background physics and the many cosmological eras that are encapsulated in our single numerical treatment, I chose to reproduce in Fig. 9.1, one of the many figures of the article, because it shows the evolution of the energy budget between the five effective fluids during the whole time evolution.

The original article as put online in arXiv is now displayed, note that contrary to the other articles reproduced in this thesis manuscript, it has not been peer-reviewed yet. Notations should be transparent.

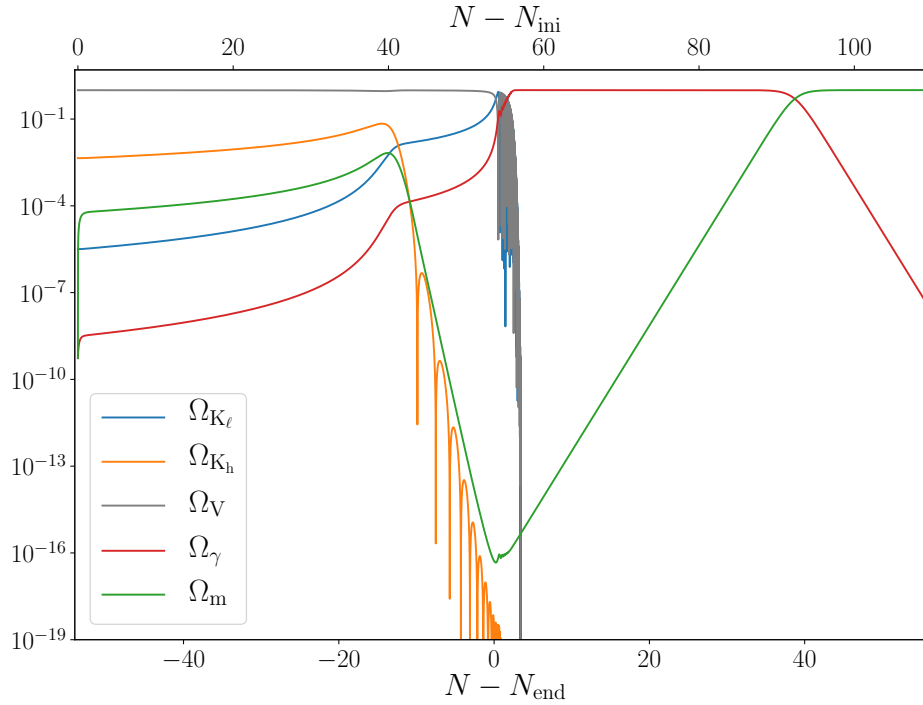


Figure 9.1: Energy budget $\Omega_{(\alpha)} = \rho_{(\alpha)}/\rho$ between the “fictitious” and “real” fluids in the universe during inflation, reheating, radiation domination and matter domination. During inflation, the potential fluid is always dominating, and the second most important contribution comes from the kinetic fluid corresponding to the scalar field that is driving inflation at that time. As already mentioned, the contributions from the cosmological fluids are then negligible but not extremely small. Clearly, when the heavy field reaches the minimum of its potential, it begins to oscillate and redshift, and completes its transfer of energy to the matter fluid (however the latter quickly begins to decay a bit less rapidly than a^{-3} because it is then only sustained by the exponentially decreasing kinetic energy of the heavy field). At the end of inflation, both the kinetic energy of the light scalar field and the potential energy oscillate with opposite phases but equal amplitudes, and the universe therefore behaves on average and on large scales as in a matter-dominated epoch. This large kinetic energy of the light scalar field is efficiently transferred to the radiation fluid, whose contribution rapidly grows during reheating. Around 3 e -folds after the end of inflation, reheating is complete and it is the onset of the radiation-dominated era, which lasts until radiation has so much redshifted (as a^{-4}) that the small remaining quantity of matter at the end of reheating (that redshifts slower as a^{-3}) eventually dominates, thus setting the stage for the radiation-dominated era.

Opening the reheating box in multifield inflation

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Abstract. The robustness of multifield inflation to the physics of reheating is investigated. In order to carry out this study, reheating is described in detail by means of a formalism which tracks the evolution of scalar fields and perfect fluids in interaction (the inflatons and their decay products). This framework is then used to establish the general equations of motion of the background and perturbative quantities controlling the evolution of the system during reheating. Next, these equations are solved exactly by means of a new numerical code and new analytical techniques, allowing us to interpret and approximate these solutions, are developed. As an illustration of a physical prediction that could be affected by the micro-physics of reheating, the amplitude of non-adiabatic perturbations in double inflation is considered. It is found that ignoring the fine-structure of reheating, as usually done in the standard approach, can lead to differences as big as $\sim 50\%$, while our semi-analytic estimates can reduce this error to $\sim 10\%$. We conclude that, in multifield inflation, tracking the perturbations through the details of the reheating process is important and, to achieve good precision, requires the use of numerical calculations.

Keywords: physics of the early universe, inflation

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1 Introduction

One of the most important result recently obtained in the field of Cosmology is that the physical conditions that prevailed in the very early Universe can be convincingly described by the theory of cosmic inflation [1–10]. Moreover, and this is even more impressive, detailed pieces of information about the mechanism responsible for this inflationary phase have started to be gathered. So far, all astrophysical data are compatible with single-field models [11] and the corresponding potential is known to be of the plateau shape (or close to it) [12–14], the prototypical scenario satisfying these physical requirements being the Starobinsky model [1].

Does that mean that the final word has been said about the mechanism that drives inflation? There are reasons to believe this is not the case. In particular, since inflation proceeds at very high energies, much higher than the energies probed in accelerators, its description must be based on extensions of the standard model of particle physics. Generically, these frameworks predict the presence of several (scalar) fields. So a natural arena for designing well-motivated models seems to be multifield inflation (see, *e.g.*, Refs. [15–25] for works that are particularly relevant for the present article). In this sense, a fundamental and so far open problem consists in explaining how, from this multifield description, an effective single-field scenario emerges, as revealed by the data.

It is also interesting to realize that the above described situation could, maybe, change in the near future. Indeed, the next generation of experiments will probe even further the micro-physics of inflation, for instance by measuring in refined details the properties of the large scale structures and/or of the Cosmic Microwave Background (CMB) anisotropies [26–28]. These experiments will soon come on line. They could reveal that the physical nature of inflation, so far compatible (and, to some extent, hidden) in an effective single-field framework, is in fact multifield at a deeper level. Given the present efficiency of the single-field description, however, the corresponding observational signatures, if ever detected, are likely to manifest themselves as small deviations.

The previous considerations indicate that it is important to know what physical predictions are expected from multifield inflation and to calculate those predictions with enough accuracy.

The typical signatures of multifield inflation, namely those that would allow us to distinguish multifield inflation from single-field inflation, have already been studied in great details in the literature. Among the emblematic predictions of multifield inflation that are not compatible with a single-field description are a violation of consistency relation $r = -8n_T$ (r is the tensor to scalar ratio and n_T is the tensor spectral index) [21], the presence, at a level to be determined, of Non-Gaussianity (NG) [29] and of non-adiabatic perturbations [30, 31]. In fact, to be more precise, NG is also compatible with single-field models provided the fields have non-canonical terms but non-canonical and multifield NG may be of different type and therefore can be, at least in principle, distinguished (see, *e.g.*, Refs. [32–46] for specific signatures of multifield inflation in the NG signal). On the other hand, the presence of non-adiabatic modes in the data would establish, beyond any doubt, that the dynamics during inflation involves several degrees of freedom.

At this stage, it ought to be mentioned that there is a fundamental difference between single-field and multifield inflation: in multifield inflation, the details of what happens during the reheating epoch [47–55] affect the behaviour of the perturbations even of super-Hubble scales [56] (note, however, that even in single-field inflation, the small scales can be affected by the details of metric preheating [57–60]; for interesting references on preheating in multifield inflation, see Refs. [61–63]). Technically, this is because, in presence of non-adiabatic perturbations, curvature perturbations can evolve, even on large scales. This implies that calculating the behaviour of the system during inflation is *a priori* not sufficient to establish the predictions of a multifield scenario: we need to model the reheating and to follow the perturbations during this phase. What we have just described has important implications for the above discussion. Since the reheating phase is *a priori* complicated, so is an accurate calculation of the corresponding properties of multifield scenarios. However, as we have already mentioned, we need such accurate estimates in order to optimize the use of cosmological data and to constrain inflationary scenarios beyond the single-field framework.

In the literature, considerable efforts have been made to understanding what happens during the (multifield) inflationary phase but much less efforts have been devoted to investigating the influence of reheating. This will be the main focus of the present paper. Very often, the dynamics of reheating is simply ignored and the predictions follow from simple assumptions about the continuity of the relevant quantities used to describe the inflationary scenario under scrutiny. In this article, on the contrary, we will model reheating in detail by carefully following the decay of the inflaton fields during this epoch. This will require the use of a formalism which explicitly includes interactions between scalar field and perfect fluids (since perfect fluids will be assumed to be a good description of the inflaton fields decay products) both at the background and perturbative levels [56, 64, 65]. Then, we will follow the fate of the perturbations through this detailed description of reheating and study how it depends on the parameters of

the models, for instance the decay rates. This will also allow us to compare approaches where the details of reheating are ignored to the framework of this article where the dynamics of reheating is taken into account. As a consequence, we will be able to assess how much precision on the final predictions of a model is lost by using a simplified treatment of reheating. As already mentioned, since curvature perturbation is not necessarily conserved during reheating, the corresponding effect is expected to be relevant.

As notice above, multifield inflationary scenarios can be quite complicated and lead to several predictions that differ from those of single-field models. As a simple illustration of how the predictions in multifield inflation depend on reheating, we will therefore not try to be exhaustive nor to consider only fully realistic scenarios (that is to say, necessarily fully compatible with the most recent astrophysical data) but, rather, we will concentrate on one observable, namely the amplitude of non-adiabatic perturbations. Moreover, when it comes to concrete numbers, we will focus a specific scenario, namely double inflation [15–17, 20]. We will calculate exactly the evolution of the system by mean of two numerical codes (in order to check our conclusions). Then, we will compare these exact results with several analytical approaches, some of them being already present in the literature [15, 17] some others being introduced here. The previous program will allow us to address the main question of the paper, namely assessing the robustness of the predictions in multifield inflation to changes in the physics of reheating.

This article is organized as follows. After this foreword, Sec. 1, we discuss in Sec. 2 how exchanges between fluids can be introduced and modeled. We first present general considerations in Sec. 2.1. Then, in Sec. 2.2, we show that a collection of scalar fields can be viewed as a collection of “fictitious” perfect fluids, provided these fluids are in interaction. In Sec. 2.3, we explain how the exchanges between scalar fields and, this time, “real” perfect fluids can be modeled. In Sec. 2.4, we apply the previous considerations to a homogeneous and isotropic Universe. We discuss scalar fields in Sec. 2.4.1 and the exchanges between scalar fields and “real” fluids in Sec. 2.4.2. In Sec. 3, we consider the theory of cosmological perturbations. In Sec. 3.1, we present generalities and explain how an exchange 4-vector can be defined at the perturbed level. In Sec. 3.2, we give the perturbed conservation equations in presence of exchanges between fluids. We apply these considerations to scalar fields in Sec. 3.3 where we derive the form of the exchange perturbed 4-vectors in order for a collection of perturbed scalar fields to be equivalent to a collection of perturbed “fictitious” perfect fluids in interaction. Then, in Sec. 3.4, we consider the same question but, this time, for the interaction between perturbed scalar fields and “real” perfect fluids. In Sec. 3.5 and in Sec. 3.5.1, we introduce and discuss conserved quantities for individual scalar fields and fluids. We also introduce the corresponding total conserved quantities. In Sec. 3.5.2, we use these definitions to define non-adiabatic perturbations. In Sec. 4, we apply the previous formalism to the case of reheating after, in order to be concrete, two-field inflation, although this formalism is valid for an arbitrary number of fields. In Sec. 4.1, we introduce the model and the parameters that characterize the phase of inflation and the decay of the inflaton fields. Then, in Sec. 4.1.1, we derive the background equations of motion and in Sec. 4.1.2, the perturbed equations of motion. In Sec. 4.2, we discuss the theory

of cosmological perturbations of quantum-mechanical origin and in Sec. 4.3, we explain how these considerations can allow us to fix the initial conditions. We exemplify how this can be done in the case where there is a single fluid in Sec. 4.3.1 and, in Sec. 4.3.2, we consider the many fluids case. In Sec. 4.4, we briefly describe the numerical codes that are used in this paper in order to integrate the equations of motion. In Sec. 5, we apply the formalism developed before to a specific model, namely double inflation. In Sec. 5.1, we introduce the model and define its parameters. In Sec. 5.2, we discuss the dynamics of the background and, in Sec. 5.2.1, we present the corresponding equations of motion. In Sec. 5.2.2, we solve numerically these equations, compute the inflaton field trajectories and compare these results with an analytical approach based on the slow-roll approximation. In Sec. 5.2.3, we describe the evolution of the inflaton decay products (concretely, radiation and pressure-less fluids) during inflation. Then, in Sec. 5.2.4, we study the behaviour of the system during the decay of the inflaton fields. In particular, we show that a simple approach to this question is not very accurate which motivates the need to do better, a problem which is considered later in the paper. In Sec. 5.2.5, we present other ways to describe the evolution of the system, first in field space and, then, in Sec. 5.2.6, using the energy density of individual fluids to total energy density ratios. In Sec. 5.3, we discuss the evolution of the perturbations in the double inflation model. In Sec. 5.3.1, we split the perturbations into adiabatic and non-adiabatic perturbations during double inflation. In Ref. 5.3.2, we explain how the initial conditions can be fixed in the particular case of double inflation. In Sec. 5.3.3, we discuss the large scale solutions and, finally, in Sec. 5.3.4, we match the inflationary perturbations to the perturbations in the post-inflationary epochs. This will allow us to derive an analytical formula for the amplitude of non-adiabatic perturbations after inflation. In Sec. 6, we compare our results to the results existing in the literature. In Sec. 7, we briefly present our conclusions and try to establish general lessons from our study. We conclude the paper in an appendix A where we develop analytical techniques to describe the behaviour of the background at the time of the heavy field decay. In Sec. A.1, we present the equations of motion and, in Sec. A.2, we explain how the WKB formalism can be used to solve these equations. These considerations are applied to the evolution of matter in Sec. A.3. In Sec. A.4, we use these results to derive precisely the time at which the heavy field decays. This quantity is important since it determines the amplitude of the non-adiabatic perturbations.

2 Scalar fields and fluids in presence of energy-momentum exchanges

2.1 General equations

In this paper, we consider a situation where there are several fluids living in a space-time described by the four-dimensional metric tensor $g_{\mu\nu}(x^\kappa)$; each fluid is characterized by its own energy-momentum tensor, $T_{\mu\nu}^{(\alpha)}$. The index “ (α) ” is written between parenthesis to indicate that it is not a space-time index but a label identifying the fluid. However, in the following, when no confusion is possible, we will not write the parenthesis in order to avoid cluttered notations. Also, the fluid label will indifferently appear either up or

down. Concretely, the different fluids will be either scalar fields or perfect fluids with constant equations of state (although one could easily accommodate time-dependent equations of state). A crucial aspect of the physical situation considered in the present article is that energy-momentum transfers between the fluids will be possible. This will be described by the following conservation equations, based on a detailed balance analysis [56, 64, 65]

$$\nabla_\nu T_{(\alpha)}^{\mu\nu} = \sum_{(\beta)} \left[Q_{(\alpha) \rightarrow (\beta)}^\mu - Q_{(\beta) \rightarrow (\alpha)}^\mu \right], \quad (2.1)$$

where ∇_ν denotes the covariant derivative associated with the metric $g_{\mu\nu}$. The vector $Q_{(\alpha) \rightarrow (\beta)}^\mu$ describes the transfer from the fluid “ (α) ” to the fluid “ (β) ” while, evidently, the vector $Q_{(\beta) \rightarrow (\alpha)}^\mu$ describes the transfer from the fluid “ (β) ” to the fluid “ (α) ”. The vector $Q_{(\alpha) \rightarrow (\beta)}^\mu$ can always be written in a covariant, non-perturbative way, as [56, 64, 65]

$$Q_{(\alpha) \rightarrow (\beta)}^\mu = Q_{(\alpha) \rightarrow (\beta)} u^\mu + f_{(\alpha) \rightarrow (\beta)}^\mu, \quad (2.2)$$

with $f_{(\alpha) \rightarrow (\beta)}^\mu u_\mu = 0$ where u^μ is the total velocity of matter. We see that $Q_{(\alpha) \rightarrow (\beta)}^\mu$ has been decomposed in terms of a scalar, $Q_{(\alpha) \rightarrow (\beta)}$, and a vector, $f_{(\alpha) \rightarrow (\beta)}^\mu$.

We have just mentioned that individual energy momentum tensors are not conserved due to the presence of possible transfers between the fluids. But, clearly, the total energy momentum tensor must be conserved because it sources Einstein equations

$$G_{\mu\nu} = \frac{1}{M_{\text{Pl}}^2} \sum_{(\alpha)} T_{\mu\nu}^{(\alpha)}, \quad (2.3)$$

where, of course, $G_{\mu\nu} \equiv R_{\mu\nu} - Rg_{\mu\nu}/2$ is the Einstein tensor ($R_{\mu\nu}$ is the Ricci tensor and R the scalar curvature) while M_{Pl} is the reduced Planck mass. In order to satisfy the Bianchi identities, one must have $\nabla_\nu [\sum_{(\alpha)} T_{(\alpha)}^{\mu\nu}] = 0$. Physically, as already mentioned, this expresses the fact that, if energy momentum transfers can occur among fluids, the total energy momentum must be conserved and the net sum of all transfers must equal zero.

2.2 Scalar fields

In this section, we consider the case where the fluids under consideration are all scalar fields. Therefore, we assume that we have N_{field} scalars with canonical kinetic terms, that we denote ϕ_a with $a = 1, \dots, N_{\text{field}}$ (as it was the case in the last subsection for indices between parenthesis, a is not a spacetime index and, in the following, for notational convenience, will be displayed either up or down). As is well-known, the corresponding stress energy tensor can be written as

$$T_{\mu\nu} = \sum_{a=1}^{N_{\text{field}}} \left(\partial_\mu \phi_a \partial_\nu \phi_a - \frac{1}{2} g_{\mu\nu} g^{\alpha\beta} \partial_\alpha \phi_a \partial_\beta \phi_a \right) - g_{\mu\nu} V(\phi_1, \dots, \phi_{N_{\text{field}}}), \quad (2.4)$$

where $V(\phi_a)$ is the potential function that we do not need to specify at this stage. A crucial remark is that, because the potential term $V(\phi_a)$ is *a priori* non-separable, the above stress-energy tensor cannot be written as the sum of individual stress-energy tensors, namely cannot be written as $\sum_{a=1}^{N_{\text{field}}} T_{\mu\nu}^a$ where $T_{\mu\nu}^a$ would be the stress-energy tensor associated with the field ϕ_a . However, a collection of N_{field} scalar fields can also be viewed as a collection of $N_{\text{field}}+1$ perfect fluids with constant equation of state [56, 64, 65]. In this approach, we have N_{field} “kinetic fluids” with stress-energy tensor¹

$$T_{\mu\nu}^{K_a} = \partial_\mu \phi_a \partial_\nu \phi_a - \frac{1}{2} g_{\mu\nu} g^{\alpha\beta} \partial_\alpha \phi_a \partial_\beta \phi_a, \quad (2.5)$$

and one “potential fluid” with stress-energy tensor

$$T_{\mu\nu}^V = -g_{\mu\nu} V(\phi_1, \dots, \phi_{N_{\text{field}}}), \quad (2.6)$$

and the total stress-energy tensor can be expressed as the sum of the stress-energy tensors of the kinetic and potential fluids, $T_{\mu\nu} = \sum_{a=1}^{N_{\text{field}}} T_{\mu\nu}^{K_a} + T_{\mu\nu}^V$. More precisely, the kinetic fluids have energy density and pressure

$$\rho_{K_a} = p_{K_a} = -\frac{1}{2} g^{\alpha\beta} \partial_\alpha \phi_a \partial_\beta \phi_a, \quad (2.7)$$

which shows that each of them has a constant, “stiff”, equation of state, $w_{K_a} \equiv p_{K_a}/\rho_{K_a} = 1$. The kinetic fluids have velocity $u_\mu^{K_a}$ defined by $u_\mu^{K_a} u_\nu^{K_a} = -\partial_\mu \phi_a \partial_\nu \phi_a / (g^{\alpha\beta} \partial_\alpha \phi_a \partial_\beta \phi_a)$ and, clearly, one verifies that $u_\mu^{K_a} u_\mu^{K_a} = -1$ as expected. On the other hand, the energy density and pressure of the potential fluid are given by

$$\rho_V = -p_V = V(\phi_1, \dots, \phi_{N_{\text{field}}}), \quad (2.8)$$

which means that this fluid has a vacuum equation of state, namely $w_V = -1$. The velocity of the potential fluid is not defined, which is not problematic since it will be shown that, in fact, this quantity never appears in the equations of motion and is, therefore, not relevant.

For the previous description to hold, there is however a price to pay: we must assume that the kinetic and potential fluids interact. This is indeed necessary in order to recover the correct equations of motion (namely, the Klein-Gordon equation) of the scalar fields. This can be shown as follows. Using Eqs. (2.1) and (2.6), the conservation equation for the potential fluid can be expressed as

$$\nabla_\nu T_V^{\mu\nu} = -g^{\mu\nu} \partial_\nu V = - \sum_{a=1}^{N_{\text{field}}} \partial^\mu \phi_a \frac{\partial V}{\partial \phi_a} = \sum_{a=1}^{N_{\text{field}}} (Q_{V \rightarrow K_a}^\mu - Q_{K_a \rightarrow V}^\mu), \quad (2.9)$$

which is satisfied by

$$Q_{V \rightarrow K_a}^\mu = 0, \quad Q_{K_a \rightarrow V}^\mu = \partial^\mu \phi_a \frac{\partial V}{\partial \phi_a}, \quad (2.10)$$

¹In accordance with the remark made in Sec. 2.1, we have written the stress-energy tensors without a parenthesis around the labels “ K_a ” and “ V ” since, in this case, there is no possible confusion with a space-time index.

where no sum is meant despite the repeated index “ a ” (recall that “ a ” is not a space-time index). Then, if one writes the conservation equation for the kinetic fluids, using Eq. (2.5), one arrives at

$$\nabla_\nu T_{K_a}^{\mu\nu} = \partial^\mu \phi_a \nabla_\nu \nabla^\nu \phi_a = \sum_{b \neq a} \left(Q_{K_a \rightarrow K_b}^\mu - Q_{K_b \rightarrow K_a}^\mu \right) + Q_{K_a \rightarrow V}^\mu - Q_{V \rightarrow K_a}^\mu, \quad (2.11)$$

and, recalling Eqs. (2.10), this reduces to the known Klein-Gordon equation only if $Q_{K_a \rightarrow K_b}^\mu = 0$ for any index a and b .

We conclude that a situation with N_{field} scalar fields is in fact equivalent to a situation with $N_{\text{field}} + 1$ perfect fluids (with constant equations of state) in interaction [56, 64, 65]. This effective interaction is such that the interaction among kinetic fluids vanishes and the energy-momentum transfer only proceeds from the kinetic fluids to the potential one (and not the opposite).

2.3 Scalar fields and perfect fluids in interaction

In this article, since our goal is to study the reheating in multifield inflationary models, where, at the end of inflation, the inflaton fields decay in various channels the physical properties of which can be described by means of hydrodynamical considerations, we are interested in a situation where there are scalar fields and perfect fluids in the Universe. We have just seen that scalar fields can in fact be viewed as a collection of perfect fluids, provided those fluids interact in a specific way. Therefore, a situation with scalar fields and perfect fluids is in fact equivalent to a situation where there are only perfect fluids, some of them being “fictitious” and some others being “real”. In the previous section 2.2, we have written the interactions between the “fictitious” kinetic and potential fluids obtained from the requirement that the usual equations of motion describing the behavior of scalar fields are recovered. In this section, we consider the “real” interaction between a scalar field and a “real” fluid.

Firstly, we notice that, on general grounds, the interaction between two fluids can be characterized in a covariant, non-perturbative way, by the following exchange vector [56, 64, 65]

$$Q_{(\alpha) \rightarrow (\beta)}^\mu = \Gamma_{(\alpha) \rightarrow (\beta)} T_{(\alpha)}^{\mu\nu} u_\nu^{(\alpha)}, \quad (2.12)$$

where $\Gamma_{(\alpha) \rightarrow (\beta)} > 0$ is a coefficient that controls the strength of the interaction and which can also be interpreted as a decay rate. If the fluid has a perfect fluid form (in this article, we do not consider fluids which have anisotropic stress), namely $T_{\mu\nu}^{(\alpha)} = [\rho_{(\alpha)} + p_{(\alpha)}] u_\mu^{(\alpha)} u_\nu^{(\alpha)} + p_{(\alpha)} g_{\mu\nu}$ then, it is easy to show that

$$Q_{(\alpha) \rightarrow (\beta)}^\mu = -\Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} u_{(\alpha)}^\mu. \quad (2.13)$$

Secondly, we can apply the previous considerations to the questions studied in this article. The crucial ingredient is to realize that the interaction between a scalar field and a “real” fluid can in fact be viewed as an interaction between the corresponding

“fictitious” kinetic fluid and the “real” fluid. In other words, this interaction will be characterized by $Q_{K_a \rightarrow (\beta)}^\mu$ given by Eq. (2.12) and $Q_{(\beta) \rightarrow K_a}^\mu = 0$. The “fictitious” potential fluid will remain decoupled from all the “real” fluids present in space-time, namely $Q_{V \rightarrow (\beta)}^\mu = Q_{(\beta) \rightarrow V}^\mu = 0$.

2.4 The Homogeneous and Isotropic FLRW Universe

The results discussed in the previous subsections are valid for any metric tensor, namely for any space-time. We now assume that the Universe is homogeneous and isotropic on large scales and, therefore, is described by a Friedmann-Lemaître-Robertson-Walker (FLRW) metric $ds^2 = -dt^2 + a^2(t)\delta_{ij}dx^i dx^j$, where t is the cosmic time and $a(t)$ is the scale factor. The metric can also be written $ds^2 = a^2(\eta)(-d\eta^2 + \delta_{ij}dx^i dx^j)$, where η is the conformal time related to cosmic time t by $dt = a(\eta)d\eta$. For a FLRW Universe (using conformal time), the total velocity of matter is given by $u^\mu = (1/a, \mathbf{0})$, $u_\mu = (-a, \mathbf{0})$. On very general grounds, for any type of fluid, the relation $f_{(\alpha) \rightarrow (\beta)}^\mu u_\mu = 0$ implies that, in Eq. (2.2), one has $f_{(\alpha) \rightarrow (\beta)}^0 = 0$ and, since $f_{(\alpha) \rightarrow (\beta)}^i$ must vanish in an homogeneous and isotropic background², we reach the conclusion that $f_{(\alpha) \rightarrow (\beta)}^\mu = 0$. Therefore, this quantity simply does not appear at the background level. As a consequence, for any kind of fluid living in a FLRW Universe, one has (using conformal time) $Q_{(\alpha) \rightarrow (\beta)}^0 = Q_{(\alpha) \rightarrow (\beta)}/a$ and $Q_{(\alpha) \rightarrow (\beta)}^i = 0$, with, using Eq. (2.2),

$$Q_{(\alpha) \rightarrow (\beta)} = -\Gamma_{(\alpha) \rightarrow (\beta)} \rho(\alpha), \quad (2.14)$$

since at the background level $u_{(\alpha)}^\mu = u^\mu$ for any (α) and as we have just seen $f_{(\alpha) \rightarrow (\beta)}^\mu = 0$.

2.4.1 Scalar fields in the FLRW Universe

Now, let us see how the formalism described in Secs. 2.1, 2.2 and 2.3 can be applied in an homogeneous and isotropic Universe filled with N_{field} scalar fields. The total energy density and pressure can be written as

$$\rho = \sum_{a=1}^{N_{\text{field}}} \frac{\phi_a'^2}{2a^2} + V(\phi_1, \dots, \phi_{N_{\text{field}}}), \quad p = \sum_{a=1}^{N_{\text{field}}} \frac{\phi_a'^2}{2a^2} - V(\phi_1, \dots, \phi_{N_{\text{field}}}), \quad (2.15)$$

where a prime denotes a derivative with respect to conformal time. As already discussed, it is not possible to decompose ρ and p as a sum over N_{field} individual energy densities and pressures ρ_a and p_a , one for each scalar field, unless the potential is separable, namely unless we deal with the particular case where $V(\phi_1, \dots, \phi_{N_{\text{field}}}) = \sum_{a=1}^{N_{\text{field}}} V_a(\phi_a)$. Then, the conservation equation leads to the equations of motion for the fields ϕ_a , namely

$$\sum_{a=1}^{N_{\text{field}}} \frac{\phi_a'}{a} (\phi_a'' + 2\mathcal{H}\phi_a' + a^2 V_{\phi_a}) = 0, \quad (2.16)$$

²Indeed, this quantity can be decomposed into a scalar and a transverse 3-vector, $f_{(\alpha) \rightarrow (\beta)}^i = \partial_i f_{(\alpha) \rightarrow (\beta)} + \tilde{f}_{(\alpha) \rightarrow (\beta)}^i$ with $\partial_i \tilde{f}_{(\alpha) \rightarrow (\beta)}^i = 0$. At the background level, the scalar part must vanish because the universe is homogeneous and the transverse 3-vector must also vanish because the universe is isotropic.

where the quantity $\mathcal{H} = a'/a$ is the conformal Hubble parameter, related to the Hubble parameter $H = \dot{a}/a$ (a dot standing for a derivative with respect to cosmic time) by $\mathcal{H} = aH$ and where $V_{\phi_a} \equiv \partial V / \partial \phi_a$. Eq. (2.16) is satisfied if, for each field ϕ_a , one has

$$\phi_a'' + 2\mathcal{H}\phi_a' + a^2 V_{\phi_a} = 0, \quad (2.17)$$

which is the standard form of the Klein-Gordon equations in a FLRW Universe.

As discussed in the previous sections 2.2 and 2.3, another way to proceed is to introduce N_{field} kinetic fluids and one potential fluid, which are perfect fluids with energy density and pressure given by

$$\rho_{K_a} = \frac{\phi_a'^2}{2a^2} = p_{K_a}, \quad \rho_V = V = -p_V. \quad (2.18)$$

Then, one can write the total energy density and pressure as $\rho = \sum_{a=1}^{N_{\text{field}}} \rho_{K_a} + \rho_V$ and $p = \sum_{a=1}^{N_{\text{field}}} p_{K_a} + p_V$. In order to recover the Klein-Gordon equations, we must introduce interactions between these $N_{\text{field}} + 1$ fluids which, in an homogeneous and isotropic Universe, take the following form [we recall that all $Q_{(\alpha) \rightarrow (\beta)}^i = 0$ at the background level]

$$aQ_{K_a \rightarrow V} = -\phi_a' V_{\phi_a}, \quad aQ_{V \rightarrow K_a} = 0, \quad aQ_{K_a \rightarrow K_b} = 0. \quad (2.19)$$

Indeed, with the above transfert vectors, the most general conservation equation for the kinetic fluid, namely

$$\rho'_{K_a} + 3\mathcal{H}(\rho_{K_a} + p_{K_a}) = a(Q_{K_a \rightarrow V} - Q_{V \rightarrow K_a}) + a \sum_{b \neq a} (Q_{K_a \rightarrow K_b} - Q_{K_b \rightarrow K_a}), \quad (2.20)$$

simply reproduces the Klein-Gordon equation (2.17) for ϕ_a . On the other hand, the conservation equation for the potential fluid

$$\rho'_V = a \sum_{a=1}^{N_{\text{field}}} (Q_{V \rightarrow K_a} - Q_{K_a \rightarrow V}) = \sum_{a=1}^{N_{\text{field}}} \phi_a' V_{\phi_a}, \quad (2.21)$$

is identically satisfied.

2.4.2 Scalar fields and perfect fluids in interactions in the FLRW Universe

We now take into account the interactions between N_{field} scalar fields and N_{fluid} “real” fluids. Since we have these “fictitious” and “real” fluids in the Universe, the total energy density and pressure can now be expressed as

$$\rho = \sum_{a=1}^{N_{\text{field}}} \rho_{K_a} + \rho_V + \sum_{(\alpha)=1}^{N_{\text{fluid}}} \rho_{(\alpha)}, \quad p = \sum_{a=1}^{N_{\text{field}}} p_{K_a} + p_V + \sum_{(\alpha)=1}^{N_{\text{fluid}}} P_{(\alpha)}. \quad (2.22)$$

Then, one must rewrite the conservation equation (2.20) for the kinetic fluid and add the terms describing the exchanges between fields (or “fictitious” fluids) and “real” fluids. This leads to

$$\begin{aligned} \rho'_{K_a} + 3\mathcal{H}(\rho_{K_a} + p_{K_a}) = & a(Q_{K_a \rightarrow V} - Q_{V \rightarrow K_a}) + a \sum_{b \neq a} (Q_{K_a \rightarrow K_b} - Q_{K_b \rightarrow K_a}) \\ & + a \sum_{(\alpha)=1}^{N_{\text{fluid}}} [Q_{K_a \rightarrow (\alpha)} - Q_{(\alpha) \rightarrow K_a}], \end{aligned} \quad (2.23)$$

where $Q_{K_a \rightarrow (\alpha)}$ is given by Eq. (2.14), $Q_{(\alpha) \rightarrow K_a} = 0$ and other interactions verify Eq. (2.19). As a consequence, one obtains the following modified Klein-Gordon equation

$$\phi''_a + \left[2\mathcal{H} + \frac{a}{2} \sum_{(\alpha)=1}^{N_{\text{fluid}}} \Gamma_{K_a \rightarrow (\alpha)} \right] \phi'_a + a^2 V_{\phi_a} = 0, \quad (2.24)$$

where it is clear that these new interactions result in extra friction terms for the scalar fields, parameterized by the decay rates $\Gamma_{K_a \rightarrow (\alpha)}$. On the other hand, the conservation equation for ρ_V is not modified by any new terms since the potential fluid does not interact with the “real” fluids. As a consequence, it is still identically satisfied.

If we now consider the “real” fluids, the conservation equation (2.1) leads to only one non-trivial equation, its time-component. In a homogeneous and isotropic Universe, it reads

$$\rho'_{(\alpha)} + 3\mathcal{H}[\rho_{(\alpha)} + p_{(\alpha)}] = a \sum_{a=1}^{N_{\text{field}}} [Q_{(\alpha) \rightarrow K_a} - Q_{K_a \rightarrow (\alpha)}] + a \sum_{(\beta)=1}^{N_{\text{fluid}}} [Q_{(\alpha) \rightarrow (\beta)} - Q_{(\beta) \rightarrow (\alpha)}], \quad (2.25)$$

where we recall that $\rho_{(\alpha)}$ and $p_{(\alpha)}$ are the energy density and pressure of the “real” fluid (α) . Using again Eq. (2.14), one obtains

$$\rho'_{(\alpha)} + 3\mathcal{H}[\rho_{(\alpha)} + p_{(\alpha)}] - \sum_{a=1}^{N_{\text{field}}} \frac{\Gamma_{K_a \rightarrow (\alpha)}}{2a} \phi'^2_a + a \sum_{(\beta)=1}^{N_{\text{fluid}}} [\Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} - \Gamma_{(\beta) \rightarrow (\alpha)} \rho_{(\beta)}] = 0, \quad (2.26)$$

where the decays of the scalar fields result in an enhancement of the “real” fluids energy densities, as should be the case during reheating, while the self-interactions of the “real” fluids can add extra complexity in the system with positive and negative contributions. As already mentioned, the space component of the conservation equation is identically satisfied.

The formalism described above is particularly well suited to describe the transfers of energy that occur, at the background level, from scalar fields to cosmological fluids at the end of inflation, namely during the reheating. This formalism will therefore be very

useful to study this epoch of the inflationary scenario which, we recall, is the main target of this paper. Notice also that the interactions introduced before need not be turned on by hand at the end of inflation: they are negligible but present during inflation and dynamically become relevant only when the decay rates become of the order of the Hubble parameter. This will be exemplified in the following when we study the case of double inflation. Finally, as an additional remark, let us stress that this formalism can also be used for the warm inflation scenario [66, 67].

We now turn to the description of linear fluctuations around a FLRW background in the presence of interactions between scalar fields and “real” fluids. This is indeed crucial in order to establish reliable cosmological predictions in multifield models since, in that case, and contrary to single-field scenarios, curvature perturbation can evolve during reheating, even on super-Hubble scales. It is therefore important to track the behaviour of the perturbations when the interactions between the inflaton fields and their decay products play an important role in the dynamics of the Universe. This is the goal of the next section.

3 Theory of cosmological perturbations in presence of energy-momentum exchanges

3.1 General equations

In this section, we consider a Universe which is no longer homogeneous and isotropic and which is filled with various fluids that can interact with each other. We assume that the deviations from homogeneity and isotropy are small and, therefore, can be treated perturbatively [68]. This leads to the theory of cosmological perturbations in presence of energy-momentum exchanges [56, 64, 65]. As expected, this only differs from the standard approach to cosmological perturbations in the fact that the perturbed conservation equations of the various fluids (“fictitious” ones describing scalar fields, “real” fluids, etc.) acquire new terms to describe these exchanges, in very much the same way as described before for the background. As a consequence, the corresponding perturbed line element is written in the standard way, namely $ds^2 = a^2(\eta)\{- (1 - 2\phi)d\eta^2 + 2(\partial_i B)dx^i d\eta + [(1 - 2\psi)\delta_{ij} + 2\partial_i\partial_j E]dx^i dx^j\}$ and is characterized by four functions, ϕ , B , ψ and E that are time and space dependent. Here, we have taken into account only scalar perturbations and, in principle, the perturbed line element should also contain a vector and a tensor parts. In this article, we focus on the scalar sector only, that is decoupled from vectors and tensors at this order of perturbation theory. In order to be consistent, the matter sector is also perturbed and we introduce perturbed scalar fields $\delta\phi_a(\eta, \mathbf{x})$ and/or perturbed energy density $\delta\rho_{(\alpha)}(\eta, \mathbf{x})$ and pressure, $\delta p_{(\alpha)}(\eta, \mathbf{x})$, for the fluids. For the velocity, one has $\delta u_{(\alpha)}^\mu = (-\phi/a, v_{(\alpha)}^i/a)$ [and $\delta u_{\mu}^{(\alpha)} = (-a\phi, av_i^{(\alpha)} + a\partial_i B)$], where the index of v_i is raised by δ_{ij} at this order of perturbation theory. One can check that it preserves the normalization of the four-velocity at the perturbative level. As usual, not all perturbed quantities are physically meaningful because of the gauge problem. In the following, we will deal with this issue by making use of the so-called gauge-invariant formalism for cosmological perturbations [68, 69].

The gravity sector will be described by the Bardeen potentials, $\Phi = \phi + [a(B - E')]' / a$ and $\Psi = \psi - \mathcal{H}(B - E')$. In the matter sector, as is well-known [69], there are different ways to define gauge-invariant perturbed energy densities. Here, we work in terms of $\delta\rho_{(\alpha)}^{(\text{gi})} = \delta\rho_{(\alpha)} + \rho'_{(\alpha)}(B - E')$. For the pressure, we have $\delta p_{(\alpha)}^{(\text{gi})} = \delta p_{(\alpha)} + p'_{(\alpha)}(B - E')$ and for the velocity, $v_{(\alpha)}^{(\text{gi})} = v_{(\alpha)} + E'$ with $v_i^{(\alpha)} = \partial_i v^{(\alpha)}$ (and a similar definition for the gauge-invariant part) since we consider scalar perturbations only. Finally, if matter is described by scalar fields, the inhomogeneous field fluctuations can be described in terms of the quantity $\delta\phi_a^{(\text{gi})} = \delta\phi_a + \phi'_a(B - E')$. It can be checked that all these quantities, Φ, Ψ and all the perturbations with a “(gi)” symbol are gauge-invariant at linear order in cosmological perturbation theory [69].

Let us now examine the equations of motion controlling the behaviour of the perturbations. We obviously have the perturbed Einstein equations

$$\delta G_{\mu\nu} = \frac{1}{M_{\text{Pl}}^2} \sum_{(\alpha)} \delta T_{\mu\nu}^{(\alpha)}, \quad (3.1)$$

and, perturbing the conservation equation (2.1), we also obtain another set of equations, namely

$$\delta \left[\nabla_\nu T_{(\alpha)}^{\mu\nu} \right] = \sum_{(\beta)} \left[\delta Q_{(\alpha) \rightarrow (\beta)}^\mu - \delta Q_{(\beta) \rightarrow (\alpha)}^\mu \right]. \quad (3.2)$$

In this formula, the perturbed stress-energy tensor can be calculated in the standard way and expressed in terms of the gauge-invariant quantities introduced before. For the exchange vector, using the covariant, non-perturbative Eq. (2.2), one has

$$\delta Q_{(\alpha) \rightarrow (\beta)}^\mu = \delta Q_{(\alpha) \rightarrow (\beta)} u^\mu + Q_{(\alpha) \rightarrow (\beta)} \delta u^\mu + \delta f_{(\alpha) \rightarrow (\beta)}^\mu. \quad (3.3)$$

As it was the case for the background, we must satisfy the constraint that the vector $f_{(\alpha) \rightarrow (\beta)}^\mu$ is perpendicular to the total velocity of matter. At the perturbative level, this means that $\delta \left[f_{(\alpha) \rightarrow (\beta)}^\mu u_\mu \right] = 0$. This implies that

$$\delta f_{(\alpha) \rightarrow (\beta)}^\mu u_\mu + f_{(\alpha) \rightarrow (\beta)}^\mu \delta u_\mu = 0. \quad (3.4)$$

The second term is vanishing because we have seen that, at the background level, $f_{(\alpha) \rightarrow (\beta)}^\mu = 0$. Moreover, $u_0 \neq 0$, $u_i = 0$ and, therefore, one has $\delta f_{(\alpha) \rightarrow (\beta)}^0 = 0$. From the above considerations, we deduce that the time and space components of $\delta Q_{(\alpha) \rightarrow (\beta)}^\mu$ are given by

$$\delta Q_{(\alpha) \rightarrow (\beta)}^0 = \frac{1}{a} \delta Q_{(\alpha) \rightarrow (\beta)} - \frac{\phi}{a} Q_{(\alpha) \rightarrow (\beta)}, \quad (3.5)$$

$$\delta Q_{(\alpha) \rightarrow (\beta)}^i = Q_{(\alpha) \rightarrow (\beta)} \delta u^i + \delta f_{(\alpha) \rightarrow (\beta)}^i. \quad (3.6)$$

In the following, since we consider scalar perturbations, we will work in terms of v and $\delta f_{(\alpha) \rightarrow (\beta)}$ defined by $v_i = \partial_i v$ and $\delta f_i^{(\alpha) \rightarrow (\beta)} = \partial_i \delta f_{(\alpha) \rightarrow (\beta)}$. Let us emphasize again that,

in the above expressions, δu^i is the space component of the total velocity and not the space component of the velocity of some individual fluid. In order to clarify further this point, let us explain how these quantities are related. The time-space component of the perturbed Einstein equations can be written as

$$\Psi' + \mathcal{H}\Phi = -\frac{a^2}{2M_{\text{Pl}}^2} \sum_{(\alpha)} [\rho_{(\alpha)} + p_{(\alpha)}] v_{(\alpha)}^{(\text{gi})} = -\frac{a^2}{2M_{\text{Pl}}^2} (\rho + p) v^{(\text{gi})}, \quad (3.7)$$

where $\rho = \sum_{(\alpha)} \rho_{(\alpha)}$ and $p = \sum_{(\alpha)} p_{(\alpha)}$ are the total energy density and pressure, respectively. This immediately implies that

$$v^{(\text{gi})} = \frac{1}{\rho + p} \sum_{(\alpha)} [\rho_{(\alpha)} + p_{(\alpha)}] v_{(\alpha)}^{(\text{gi})}, \quad (3.8)$$

can be understood as describing the total velocity.

Finally, we must define gauge-invariant exchange vectors or, rather, define them in terms of gauge-invariant quantities. For the scalar $\delta Q_{(\alpha) \rightarrow (\beta)}$, we introduce the gauge-invariant expressions $\delta Q_{(\alpha) \rightarrow (\beta)}^{(\text{gi})} = \delta Q_{(\alpha) \rightarrow (\beta)} + Q'_{(\alpha) \rightarrow (\beta)}(B - E')$. This expression is similar to the definition of the gauge-invariant scalar field fluctuations, perturbed energy densities, etc. and this is of course due to the fact that, in all these cases, we deal with scalar quantities. Regarding $\delta f_{(\alpha) \rightarrow (\beta)}$, the situation is even simpler: this quantity is already gauge-invariant since it has no background counterpart.

3.2 Perturbed conservation equations for fluids

We now consider Eq. (3.2) and write it explicitly for a perfect fluid. Let us first start with the time component. It can be expressed as

$$\begin{aligned} \delta \rho_{(\alpha)}^{(\text{gi})'} + 3\mathcal{H} \left[\delta \rho_{(\alpha)}^{(\text{gi})} + \delta p_{(\alpha)}^{(\text{gi})} \right] - 3 [\rho_{(\alpha)} + p_{(\alpha)}] \Psi' + [\rho_{(\alpha)} + p_{(\alpha)}] \nabla^2 \left[v_{(\alpha)}^{(\text{gi})} \right] \\ = \sum_{(\beta)} \left[a \delta Q_{(\alpha) \rightarrow (\beta)}^{(\text{gi})} + a Q_{(\alpha) \rightarrow (\beta)} \Phi - a \delta Q_{(\beta) \rightarrow (\alpha)}^{(\text{gi})} - a Q_{(\beta) \rightarrow (\alpha)} \Phi \right]. \end{aligned} \quad (3.9)$$

It is interesting to notice that, even if the velocity appears in the left hand side of this equation, the scalar $\delta f_{(\alpha) \rightarrow (\beta)}$ is absent. Contrary to the background case, the space component of the conservation equation leads, at the perturbative level, to an interesting equation which controls the evolution of the perturbed velocity. It reads

$$\begin{aligned} [\rho_{(\alpha)} + p_{(\alpha)}] v_{(\alpha)}^{(\text{gi})'} + [\rho'_{(\alpha)} + p'_{(\alpha)}] v_{(\alpha)}^{(\text{gi})} + 4\mathcal{H} [\rho_{(\alpha)} + p_{(\alpha)}] v_{(\alpha)}^{(\text{gi})} + [\rho_{(\alpha)} + p_{(\alpha)}] \Phi + \delta p_{(\alpha)}^{(\text{gi})} \\ = \sum_{(\beta)} \left[a Q_{(\alpha) \rightarrow (\beta)} v^{(\text{gi})} + \delta f_{(\alpha) \rightarrow (\beta)} - a Q_{(\beta) \rightarrow (\alpha)} v^{(\text{gi})} - \delta f_{(\beta) \rightarrow (\alpha)} \right]. \end{aligned} \quad (3.10)$$

Eqs. (3.9) and (3.10) are two equations which, when considered together with the perturbed Einstein equations, form a complete set allowing us to follow the evolution of cosmological perturbations.

It will also turn useful to introduce another quantity related to the perturbed velocity, namely the rescaled velocity for the fluid “ (α) ”, which is defined by

$$\varsigma_{(\alpha)} \equiv [\rho_{(\alpha)} + p_{(\alpha)}] v_{(\alpha)}^{(\text{gi})} \quad (3.11)$$

If, quite naturally, the total rescaled velocity is defined by $\varsigma \equiv (\rho + p)v^{(\text{gi})}$ where ρ , p and v are respectively the total energy density, pressure and velocity, then one has $\varsigma = \sum_{(\alpha)} \varsigma_{(\alpha)}$ and $\Psi' + \mathcal{H}\Phi = -a^2/(2M_{\text{Pl}}^2)\varsigma$. The equations of motion written in terms of this rescaled velocity read

$$\begin{aligned} \delta\rho_{(\alpha)}^{(\text{gi})'} + 3\mathcal{H} \left[\delta\rho_{(\alpha)}^{(\text{gi})} + \delta p_{(\alpha)}^{(\text{gi})} \right] - 3 [\rho_{(\alpha)} + p_{(\alpha)}] \Psi' + \nabla^2 [\varsigma_{(\alpha)}] \\ = \sum_{(\beta)} \left[a\delta Q_{(\alpha)\rightarrow(\beta)}^{(\text{gi})} + aQ_{(\alpha)\rightarrow(\beta)}\Phi - a\delta Q_{(\beta)\rightarrow(\alpha)}^{(\text{gi})} - aQ_{(\beta)\rightarrow(\alpha)}\Phi \right], \end{aligned} \quad (3.12)$$

$$\begin{aligned} \varsigma'_{(\alpha)} + 4\mathcal{H}\varsigma_{(\alpha)} + [\rho_{(\alpha)} + p_{(\alpha)}] \Phi + \delta p_{(\alpha)}^{(\text{gi})} \\ = \sum_{(\beta)} \left[aQ_{(\alpha)\rightarrow(\beta)} \frac{\varsigma}{\rho + p} + \delta f_{(\alpha)\rightarrow(\beta)} - aQ_{(\beta)\rightarrow(\alpha)} \frac{\varsigma}{\rho + p} - \delta f_{(\beta)\rightarrow(\alpha)} \right]. \end{aligned} \quad (3.13)$$

In the following, we will use the rescaled velocities $\varsigma_{(\alpha)}$ for numerical integration.

3.3 Perturbed conservation equations for scalar fields

We now consider a collection of N_{field} scalar fields. As explained in Sec. 2.2, N_{field} scalar fields can always be seen as $N_{\text{field}} + 1$ perfect fluids provided those ones interact in a specific way. Of course, this “technical trick” remains true at the perturbative level and one of the goals of this section is to determine the form of the corresponding perturbed exchange vectors. As it was the case for the background, this is achieved by requiring the equations of motion to reduce to the equations of motion for perturbed scalar fields, namely the perturbed Klein-Gordon equation. The great advantage of working with $N_{\text{field}} + 1$ fluids (as opposed to N_{field} scalar fields) is that, as it was the case for the background before, this allows us to consistently implement the interaction between fields and “real” fluids at the perturbative level.

The perturbed kinetic fluids energy density, pressure and velocity are given by the following expressions

$$\delta\rho_{K_a}^{(\text{gi})} = \delta p_{K_a}^{(\text{gi})} = \frac{\phi_a'}{a^2} \delta\phi_a^{(\text{gi})'} - \frac{\phi_a'^2}{a^2} \Phi, \quad v_{K_a}^{(\text{gi})} = -\frac{\delta\phi_a^{(\text{gi})}}{\phi_a'}, \quad \varsigma_{K_a} = -\frac{\phi_a'}{a^2} \delta\phi_a^{(\text{gi})}, \quad (3.14)$$

while the same quantities for the potential fluid can be expressed as

$$\delta\rho_V^{(\text{gi})} = -\delta p_V^{(\text{gi})} = \sum_{a=1}^{N_{\text{field}}} V_{\phi_a} \delta\phi_a^{(\text{gi})}. \quad (3.15)$$

Notice that, given the form of its individual energy-momentum tensor, it is impossible to define a velocity $v_V^{(\text{gi})}$ for the potential fluid. However, since this quantity never appears

in the equations of motion, this is actually not an issue. We also notice that the sound speed, defined by $c_s^2 \equiv p'/\rho'$, of the kinetic and potential fluids is equal to the equation of state parameter, $c_s^2 = w$, and (anticipating a little bit over the following considerations) that those fluids have no intrinsic entropy perturbations.

Our next move is to consider Eq. (3.12). We take the expression of the energy density, pressure and velocity for the kinetic fluids given by Eqs. (3.14) and insert them in Eq. (3.12). This leads to the standard perturbed Klein-Gordon equation

$$\delta\phi_a^{(\text{gi})''} + 2\mathcal{H}\delta\phi_a^{(\text{gi})'} - \nabla^2 \left[\delta\phi_a^{(\text{gi})} \right] + a^2 \sum_{b=1}^{N_{\text{field}}} V_{\phi_a\phi_b} \delta\phi_b^{(\text{gi})} = 4\phi_a' \Psi' - 2a^2 V_{\phi_a} \Psi, \quad (3.16)$$

provided the perturbed exchanges take the following form

$$a\delta Q_{K_a \rightarrow V} = -V_{\phi_a} \delta\phi_a^{(\text{gi})'} + V_{\phi_a} \phi_a' \Psi - \sum_{b=1}^{N_{\text{field}}} V_{\phi_a\phi_b} \phi_a' \delta\phi_b^{(\text{gi})}, \quad (3.17)$$

$$a\delta Q_{V \rightarrow K_a} = 0, \quad a\delta Q_{K_a \rightarrow K_b} = 0. \quad (3.18)$$

If one does the same for the potential fluid, namely insert the perturbed energy density and perturbed pressure given by Eq. (3.15) in Eq. (3.12) with the exchanges just established in Eqs. (3.17), (3.18), then one verifies that the corresponding equation is identically satisfied. The choices (3.17) and (3.18) are therefore consistent. The next step is to proceed in a similar fashion for the coefficients $\delta f_{(\alpha) \rightarrow (\beta)}$. Clearly, this has to be done by considering the momentum conservation equation. Therefore, we insert the expressions (3.14) in Eq. (3.13) and find that it is automatically satisfied provided one takes

$$\delta f_{K_a \rightarrow V} = V_{\phi_a} \delta\phi_a^{(\text{gi})} - \phi_a' V_{\phi_a} \frac{1}{\sum_{b=1}^{N_{\text{field}}} \phi_b'^2} \sum_{c=1}^{N_{\text{field}}} \phi_c' \delta\phi_c^{(\text{gi})}, \quad \delta f_{V \rightarrow K_a} = \delta f_{K_a \rightarrow K_b} = 0. \quad (3.19)$$

The expression for the only non-vanishing coefficient, $\delta f_{K_a \rightarrow V}$, is quite complicated but can be simplified if one notices that, in the case under consideration in this section where one has only scalar fields (and no “real” fluids), the total velocity reads

$$v^{(\text{gi})} = \sum_{(\alpha)} \frac{\rho_{(\alpha)} + p_{(\alpha)}}{\rho + p} v_{(\alpha)}^{(\text{gi})} = \frac{1}{\sum_b \phi_b'^2 / a^2} \sum_{a=1}^{N_{\text{field}}} \frac{\phi_a'^2}{a^2} \left[-\frac{\delta\phi_a^{(\text{gi})}}{\phi_a'} \right]. \quad (3.20)$$

We see that this reproduces exactly the expression appearing in Eq. (3.19). As a consequence, it follows that

$$\begin{aligned} \delta f_{K_a \rightarrow V} &= -\phi_a' V_{\phi_a} v_{K_a}^{(\text{gi})} + \phi_a' V_{\phi_a} v^{(\text{gi})} = -aQ_{K_a \rightarrow V} \left[v^{(\text{gi})} - v_{K_a}^{(\text{gi})} \right] \\ &= aQ_{K_a \rightarrow V} \left(\frac{\varsigma_{K_a}}{\phi_a'^2 / a^2} - \frac{\varsigma}{\sum_b^{N_{\text{field}}} \phi_b'^2 / a^2} \right). \end{aligned} \quad (3.21)$$

It is important to keep in mind that, here, $v^{(\text{gi})}$ (or ς) is the total velocity in the case where they are only scalar fields. In a situation where they are scalar fields and fluids, we have the same formula (3.21) but the expression of $v^{(\text{gi})}$ is modified since the velocities of the fluids participate to the total velocity. However, it is fair to acknowledge that another inequivalent possibility would be to define the momentum exchange with Eq. (3.19). Moreover, let us notice that the exchanges between the fictitious kinetic and potential fluids cannot be written in the form used in Eq. (2.12).

3.4 Perturbed conservation equations in presence of scalar fields and fluids in interaction

We now consider the situation which is probably the most relevant for the present article, namely the case where there are scalar fields and “real” fluids in interaction. As already mentioned, this interaction is described covariantly and non-perturbatively by Eq. (2.13), modelling the exchange between the “fictitious” fluids representing the scalar fields and the “real” fluids, as well as the “real” fluids self-interactions. We have already shown that this implies $Q_{(\alpha) \rightarrow (\beta)} = -\Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)}$ for the background, see Eq. (2.14). Then, at the perturbed level, one has

$$\delta Q_{(\alpha) \rightarrow (\beta)}^\mu = -\Gamma_{(\alpha) \rightarrow (\beta)} \delta \rho_{(\alpha)} u^\mu - \Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} \delta u^\mu. \quad (3.22)$$

This implies that the time component of the perturbed exchange vector can be expressed as

$$\delta Q_{(\alpha) \rightarrow (\beta)}^0 = -\frac{1}{a} \Gamma_{(\alpha) \rightarrow (\beta)} \delta \rho_{(\alpha)} + \Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} \frac{\phi}{a}, \quad (3.23)$$

and, comparing to Eq. (3.5), this leads to

$$\delta Q_{(\alpha) \rightarrow (\beta)}^{(\text{gi})} = -\Gamma_{(\alpha) \rightarrow (\beta)} \delta \rho_{(\alpha)}^{(\text{gi})}. \quad (3.24)$$

Then, the scalar $\delta f_{(\alpha) \rightarrow (\beta)}$ which is associated with the spatial component of the exchange vector remains to be determined. This last one can be written as

$$\delta Q_{(\alpha) \rightarrow (\beta)}^i = -\Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} \delta u_{(\alpha)}^i = -\Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} \delta u^i + \Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} \left[\delta u^i - \delta u_{(\alpha)}^i \right].$$

Comparing to Eq. (3.6), this implies that $\delta f_{(\alpha) \rightarrow (\beta)}^i = \Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} \left[\delta u^i - \delta u_{(\alpha)}^i \right]$, that is to say

$$\delta f_{(\alpha) \rightarrow (\beta)} = a \Gamma_{(\alpha) \rightarrow (\beta)} \rho_{(\alpha)} \left[v^{(\text{gi})} - v_{(\alpha)}^{(\text{gi})} \right]. \quad (3.25)$$

This completes our derivation of the exchange vector describing the interaction between scalar field and “real” fluids.

3.5 Conserved quantities for scalar fields and fluids

3.5.1 General case

In this section, we turn to the definition of the so-called “conserved quantities” (a name which might not be totally appropriate in the present case since these quantities will not always be “conserved”, or “constant”, in the presence of several scalar fields and fluids). These quantities play an important role in the theory of cosmological perturbations for two reasons. Firstly, their behaviour is, at least in some regimes, quite simple which is of great help to understand the behaviour of the perturbations and to test and check numerical calculations. Secondly, they appear in the definition of non-adiabatic or entropy perturbations which are a typical signature of a multi-fluids system.

We introduce two gauge-invariant “conserved” quantities for a given fluid “(α)”, $\zeta_{(\alpha)}$ and $\mathcal{R}_{(\alpha)}$, which are related to the individual energy density contrast and velocity perturbation, respectively. Their definition reads [56, 64, 65, 68, 69]

$$\zeta_{(\alpha)} = -\Psi - \mathcal{H} \frac{\delta\rho_{(\alpha)}^{(\text{gi})}}{\rho'_{(\alpha)}}, \quad \mathcal{R}_{(\alpha)} = \Psi - \mathcal{H} v_{(\alpha)}^{(\text{gi})}. \quad (3.26)$$

One can also introduce the corresponding “total” quantities (as opposed to individual) by means of the following expressions, $\zeta = -\Psi - \mathcal{H} \delta\rho^{(\text{gi})}/\rho'$ and $\mathcal{R} = \Psi - \mathcal{H} v^{(\text{gi})}$, where we recall that $\delta\rho^{(\text{gi})} = \sum_{(\alpha)} \delta\rho_{(\alpha)}^{(\text{gi})}$, $\rho' = \sum_{(\alpha)} \rho'_{(\alpha)}$ and $v^{(\text{gi})}$ is the total velocity defined in Eq. (3.8). It is then easy to show that

$$\zeta = \sum_{(\alpha)} \frac{\rho'_{(\alpha)}}{\rho'} \zeta_{(\alpha)}, \quad \mathcal{R} = \sum_{(\alpha)} \frac{\rho_{(\alpha)} + p_{(\alpha)}}{\rho + p} \mathcal{R}_{(\alpha)}, \quad (3.27)$$

where ρ and p are the total energy density and pressure, respectively. The quantities ζ and $\mathcal{R}$ are nothing but the weighted sum of the individual $\zeta_{(\alpha)}$ and $\mathcal{R}_{(\alpha)}$. We notice, however, that the weight is not the same for ζ and $\mathcal{R}$ unless the individual fluids are separately conserved in which case $\rho'_{(\alpha)}/\rho' = [\rho_{(\alpha)} + p_{(\alpha)}]/(\rho + p)$. The quantities ζ and $\mathcal{R}$ correspond to the well-known curvature perturbation on constant energy density slices ($\zeta = -\psi|_{\delta\rho=0}$) and on comoving slices ($\mathcal{R} = \psi|_{v+B=0}$), respectively.

Our next move is to derive the equation of motion for the individual conserved quantities. Using the equations of motion established before, straightforward but lengthy calculations lead to

$$\begin{aligned} \zeta'_{(\alpha)} = & -\frac{1}{3\mathcal{H}} \nabla^2 [\Psi - \mathcal{R}_{(\alpha)}] + \frac{3\mathcal{H}^2}{\rho'_{(\alpha)}} \delta p_{\text{nad}}^{(\alpha)} - \frac{a}{3\mathcal{H}\rho'_{(\alpha)}} \sum_{(\beta)} [Q_{(\alpha)\rightarrow(\beta)} - Q_{(\beta)\rightarrow(\alpha)}] \nabla^2 \mathcal{R}_{(\alpha)} \\ & - \frac{a}{\rho'_{(\alpha)}} \left(\mathcal{H} - \frac{\mathcal{H}'}{\mathcal{H}} \right) \sum_{(\beta)} [Q_{(\alpha)\rightarrow(\beta)} - Q_{(\beta)\rightarrow(\alpha)}] [\zeta_{(\alpha)} - \zeta] \\ & - \frac{a\mathcal{H}}{\rho'_{(\alpha)}} \sum_{(\beta)} \left\{ \delta Q_{(\alpha)\rightarrow(\beta)}^{(\text{gi})} - \delta Q_{(\beta)\rightarrow(\alpha)}^{(\text{gi})} - \frac{\delta\rho_{(\alpha)}}{\rho'_{(\alpha)}} [Q'_{(\alpha)\rightarrow(\beta)} - Q'_{(\beta)\rightarrow(\alpha)}] \right\}. \end{aligned} \quad (3.28)$$

Several comments are in order at this stage. Firstly, the quantity $\delta p_{\text{nad}}^{(\alpha)}$ is defined by $\delta p_{\text{nad}}^{(\alpha)} = \delta p_{(\alpha)} - c_{(\alpha)}^2 \delta \rho_{(\alpha)}$, where $c_{(\alpha)}$ is the sound speed for the fluid “(α)” [the sound speed has already been defined in the text, after Eq. (3.15)]. Physically, it represents intrinsic entropy (or non adiabatic -nad-) perturbations. For a perfect fluid with constant equation of state, such that the “real” and “fictitious” fluids considered before, this quantity is vanishing. However, this is not the case for a scalar field as can be checked by direct inspection. Secondly, the term between curled brackets in the last line of the above equation can be seen as a kind of “intrinsic exchange perturbations”. For interactions characterized by Eqs. (2.12), (2.13) and (2.14), it vanishes. For more complicated interactions, such as the ones we have introduced between the “fictitious” fluids, it is not necessarily zero and can contribute to the evolution of $\zeta_{(\alpha)}$. Thirdly, in absence of exchanges between the fluids and in absence of intrinsic entropy perturbations, we see that $\zeta_{(\alpha)}$ is a conserved quantity on large scales. However, if interactions between the fluids are present, $\zeta_{(\alpha)}$ can evolve even on large scales, thanks to the term in the second line. Fourthly, it is also possible to establish the equation satisfied by the “total” ζ . Indeed, ζ corresponds to a fluid which is conserved (since its energy momentum tensor has to satisfy the Einstein equations, see above). As a consequence, all terms related to exchange vectors have to disappear. Moreover, for the same reason, ρ' can be replaced with $-3\mathcal{H}(\rho + p)$. It follows that ζ obeys the equation

$$\zeta' = -\frac{1}{3\mathcal{H}}\nabla^2(\Psi - \mathcal{R}) - \frac{\mathcal{H}}{\rho + p}\delta p_{\text{nad}}, \quad (3.29)$$

with $\delta p_{\text{nad}} = \delta p - c_s^2 \delta \rho$ and $c_s^2 = p'/\rho'$, these definitions involving the total physical quantities (namely total, background and perturbed, energy density and pressure). We see that ζ can evolve on large scales in presence of non-adiabatic pressure.

Let us now present the equation of motion of the individual quantity $\mathcal{R}_{(\alpha)}$. Straightforward but quite lengthy manipulations lead to

$$\begin{aligned} \mathcal{R}'_{(\alpha)} = & \left(\mathcal{H} - \frac{\mathcal{H}'}{\mathcal{H}} \right) [\mathcal{R} - \mathcal{R}_{(\alpha)}] - c_{(\alpha)}^2 \frac{\rho'_{(\alpha)}}{\rho_{(\alpha)} + p_{(\alpha)}} [\mathcal{R}_{(\alpha)} + \zeta_{\alpha}] \\ & + \frac{a}{\rho_{(\alpha)} + p_{(\alpha)}} \sum_{(\beta)} [Q_{(\alpha) \rightarrow (\beta)} - Q_{(\beta) \rightarrow (\alpha)}] [\mathcal{R} - \mathcal{R}_{(\alpha)}] + \frac{\mathcal{H}}{\rho_{(\alpha)} + p_{(\alpha)}} \delta p_{\text{nad}}^{(\alpha)} \\ & - \frac{\mathcal{H}}{\rho_{(\alpha)} + p_{(\alpha)}} \sum_{(\beta)} [\delta f_{(\alpha) \rightarrow (\beta)} - \delta f_{(\beta) \rightarrow (\alpha)}]. \end{aligned} \quad (3.30)$$

We remark that, contrary to the case of $\zeta_{(\alpha)}$, the scalar $\delta f_{(\alpha) \rightarrow (\beta)}$ now participates to the equation of motion of $\mathcal{R}_{(\alpha)}$. The same reasoning as the one used for ζ allows us to derive the equation of motion of $\mathcal{R}$: all terms depending on the exchange vectors should not be present in that equation since this is an equation for a fluid (the total fluid) which is conserved and ρ' can be replaced by $-3\mathcal{H}(\rho + p)$. One obtains that

$$\mathcal{R}' = 3\mathcal{H}c_s^2(\mathcal{R} + \zeta) + \frac{\mathcal{H}}{\rho + p}\delta p_{\text{nad}}. \quad (3.31)$$

As it was already the case before, we notice that the presence of non-adiabatic pressure can cause the evolution of $\mathcal{R}$ on large scales. However, in the present case, one may also wonder about the impact of the first term in Eq. (3.31). At first sight, it could also be responsible for an evolution of $\mathcal{R}$ on large scales. However, one can show that this term can in fact be expressed in terms of the gradient of the Bardeen potential, see for instance Eq. (4.40). Therefore, the presence of non-adiabatic pressure is the only cause for a potential evolution of $\mathcal{R}$ on large scales, as it was the case for ζ .

3.5.2 Definitions of non-adiabatic perturbations

We conclude this section 3.5 by introducing the definitions of non-adiabatic perturbations. These definitions are directly related to the individual conserved quantities discussed before. The energy density entropy perturbations $S_{(\alpha)(\beta)}$ and the velocity perturbations $V_{(\alpha)(\beta)}$ are respectively defined by

$$S_{(\alpha)(\beta)} = 3 [\zeta_{(\alpha)} - \zeta_{(\beta)}], \quad V_{(\alpha)(\beta)} = \mathcal{R}_{(\alpha)} - \mathcal{R}_{(\beta)}. \quad (3.32)$$

Using Eq. (3.26), one can also write $S_{(\alpha)(\beta)} = -3\mathcal{H}[\delta\rho_{(\alpha)}^{(\text{gi})}/\rho'_{(\alpha)} - \delta\rho_{(\beta)}^{(\text{gi})}/\rho'_{(\beta)}]$ which, if each fluid is separately conserved, reduces to

$$S_{(\alpha)(\beta)} = \frac{\delta\rho_{(\alpha)}^{(\text{gi})}}{\rho_{(\alpha)} + p_{(\alpha)}} - \frac{\delta\rho_{(\beta)}^{(\text{gi})}}{\rho_{(\beta)} + p_{(\beta)}}. \quad (3.33)$$

This matches the standard expression for energy density entropy perturbations. In the same way, velocity entropy perturbations can be re-expressed as

$$V_{(\alpha)(\beta)} = -\mathcal{H} \left[v_{(\alpha)}^{(\text{gi})} - v_{(\beta)}^{(\text{gi})} \right], \quad (3.34)$$

and, as expected (and as the name indicates), is related to the difference in velocities of the two fluids.

4 Reheating after multifield inflation

Having introduced the formalism describing a physical situation where scalar fields and fluids are present and interacting, we are now in a position where we can make use of this formalism to study reheating after multifield inflation. The equations derived in the previous sections are completely general and can, in principle, be applied to a situation with an arbitrary number of fields and fluids in interaction. In this section, however, we restrict ourselves to two-field inflationary scenarios where each field can decay into two fluids with constant but otherwise arbitrary equation of state. This does not restrict the generalities of the results established in this article since, as already mentioned, from the previous equations, it would be straightforward to apply the following considerations to a scenario with more fields and/or fluids. The main advantage of this assumption is that this will allow to write and work with concrete equations of motion and to discuss several physical questions in an especially convenient manner. Moreover, this simple framework covers in fact a very large landscape of models.

4.1 Equations of motion

In the following, the two fields will be denoted ϕ_ℓ and ϕ_h and the two perfect fluids will be named “fluid 1” and “fluid 2”. ϕ_ℓ and ϕ_h is the notation used for the double inflation model where one field is said to be “light” and the other “heavy”. We will consider this model in great details in what follows, see Sec. 5, but, at this stage, the potential of the model $V(\phi_\ell, \phi_h)$ remains arbitrary and the indices “ ℓ ” and “ h ” must only be viewed as a convenient way to distinguish the two fields without carrying the meaning it will acquire when, later, we come explicitly to double inflation. The model we have just introduced is described by the following Lagrangian

$$\mathcal{L}_{\text{twofields-inf}} = -\frac{1}{2}\partial^\mu\phi_\ell\partial_\mu\phi_\ell - \frac{1}{2}\partial^\mu\phi_h\partial_\mu\phi_h - V(\phi_\ell, \phi_h) + \mathcal{L}_{\text{matter}} + \mathcal{L}_{\text{int}}. \quad (4.1)$$

As explained before, the two fields responsible for inflation also interact with other components of matter that, phenomenologically, we represent by perfect fluids. These fluids are described by $\mathcal{L}_{\text{matter}}$ and the interaction between matter and the inflaton fields is supposed to be given by the term $\mathcal{L}_{\text{int}}$. Although evidently ever-present, it becomes relevant only at the end of inflation and will account for the desintegration of the two inflaton fields explaining the “graceful exit”, *i.e.* how the Universe smoothly evolves from inflation to the standard Big Bang model. Following the formalism used in this article, we will not describe the interaction between the scalar fields and the fluid by specifying $\mathcal{L}_{\text{int}}$ but we will proceed as reviewed earlier, at the level of the non-conservation of the individual energy-momentum tensors. Indeed, according to the previous considerations, the two scalar fields are in fact equivalent to three fluids, two kinetic ones and one potential one, with energy densities and pressures given by

$$\rho_{K_\ell} = \frac{\phi_\ell'^2}{2a^2} = p_{K_\ell}, \quad \rho_{K_h} = \frac{\phi_h'^2}{2a^2} = p_{K_h}, \quad \rho_V = V(\phi_\ell, \phi_h) = -p_V. \quad (4.2)$$

We know from Eqs. (3.17) and (3.18) that the exchanges between those three fluids are given by

$$aQ_{K_\ell \rightarrow V} = -\phi_\ell' V_{\phi_\ell}, \quad aQ_{V \rightarrow K_\ell} = 0, \quad aQ_{K_h \rightarrow V} = -\phi_h' V_{\phi_h}, \quad aQ_{V \rightarrow K_h} = 0, \quad (4.3)$$

in order to recover the usual equations of motion for the fields. Then, as already discussed at length before, the crucial ingredient is that the interactions between scalar fields and fluids is obtained by coupling “real” cosmological fluids to the “fictitious” kinetic ones only (and not to the potential fluid). In practice, using Eq. (2.14), one takes

$$\begin{aligned} Q_{K_\ell \rightarrow (1)} &= -\Gamma_{\ell 1} \rho_{K_\ell}, & Q_{(1) \rightarrow K_\ell} &= 0, & Q_{K_\ell \rightarrow (2)} &= -\Gamma_{\ell 2} \rho_{K_\ell}, & Q_{(2) \rightarrow K_\ell} &= 0, \\ Q_{K_h \rightarrow (1)} &= -\Gamma_{h 1} \rho_{K_h}, & Q_{(1) \rightarrow K_h} &= 0, & Q_{K_h \rightarrow (2)} &= -\Gamma_{h 2} \rho_{K_h}, & Q_{(2) \rightarrow K_h} &= 0, \end{aligned} \quad (4.4)$$

Finally, we make also the hypothesis that the decay products (the “real” fluids) can interact amongst themselves. This will be described by

$$Q_{(1) \rightarrow (2)} = -\Gamma_{12} \rho_1, \quad Q_{(2) \rightarrow (1)} = -\Gamma_{21} \rho_2. \quad (4.5)$$

To summarize, the parameters of the model will be the parameters appearing in the potential $V(\phi_\ell, \phi_h)$ that, as already mentioned, we do not specify, the equation of state of the two perfect “real” fluids, w_1 and w_2 , the parameters describing the decay of the scalar fields into fluids one and two, $\Gamma_{\ell 1}$, $\Gamma_{\ell 2}$, Γ_{h1} , Γ_{h2} and the possible interaction between the decay products, Γ_{12} , Γ_{21} .

4.1.1 Background equations of motion for two-field inflation

We now describe the equations that controls the evolution of this system at the background and perturbative levels. At the background level, we have the Friedman equation

$$H^2 = \frac{1}{3M_{\text{Pl}}^2} (\rho_{K_\ell} + \rho_{K_h} + \rho_V + \rho_1 + \rho_2) = \frac{1}{3M_{\text{Pl}}^2} \left[\frac{1}{2} \dot{\phi}_\ell^2 + \frac{1}{2} \dot{\phi}_h^2 + V(\phi_h, \phi_\ell) + \rho_1 + \rho_2 \right], \quad (4.6)$$

where ρ_1 and ρ_2 are the energy densities associated with the fluids one and two, respectively. We also have the two Klein-Gordon equations for the ϕ_ℓ and ϕ_h fields, namely

$$\ddot{\phi}_\ell + \left[3H + \frac{1}{2} (\Gamma_{\ell 1} + \Gamma_{\ell 2}) \right] \dot{\phi}_\ell + \frac{\partial V}{\partial \phi_\ell} = 0, \quad \ddot{\phi}_h + \left[3H + \frac{1}{2} (\Gamma_{h1} + \Gamma_{h2}) \right] \dot{\phi}_h + \frac{\partial V}{\partial \phi_h} = 0. \quad (4.7)$$

Finally, we have the two conservation equations for fluid one and fluid two which can be written as

$$\dot{\rho}_1 + 3H(1 + w_1)\rho_1 = \frac{1}{2}\Gamma_{\ell 1}\dot{\phi}_\ell^2 + \frac{1}{2}\Gamma_{h1}\dot{\phi}_h^2 - \Gamma_{12}\rho_1 + \Gamma_{21}\rho_2, \quad (4.8)$$

$$\dot{\rho}_2 + 3H(1 + w_2)\rho_2 = \frac{1}{2}\Gamma_{\ell 2}\dot{\phi}_\ell^2 + \frac{1}{2}\Gamma_{h2}\dot{\phi}_h^2 + \Gamma_{12}\rho_1 - \Gamma_{21}\rho_2. \quad (4.9)$$

The previous formulas form a closed set of equations which, when solved, provides a complete solution for the background behaviour.

4.1.2 Perturbed equations of motion for two-field inflation

We now turn to the equations of motion for the perturbations. We have seen that, at the perturbative level, the exchanges between the inhomogeneous fluids are described by the two scalars $\delta Q_{(\alpha) \rightarrow (\beta)}^{(\text{gi})}$ and $\delta f_{(\alpha) \rightarrow (\beta)}$. In the case considered here, upon using Eqs. (3.24), these coefficients can be expressed as

$$\begin{aligned} \delta Q_{K_\ell \rightarrow (1)}^{(\text{gi})} &= -\Gamma_{\ell 1} \delta \rho_{K_\ell}^{(\text{gi})}, & \delta Q_{K_\ell \rightarrow (2)}^{(\text{gi})} &= -\Gamma_{\ell 2} \delta \rho_{K_\ell}^{(\text{gi})}, \\ \delta Q_{K_h \rightarrow (1)}^{(\text{gi})} &= -\Gamma_{h1} \delta \rho_{K_h}^{(\text{gi})}, & \delta Q_{K_h \rightarrow (2)}^{(\text{gi})} &= -\Gamma_{h2} \delta \rho_{K_h}^{(\text{gi})}, \\ \delta Q_{(1) \rightarrow (2)}^{(\text{gi})} &= -\Gamma_{12} \delta \rho_1^{(\text{gi})}, & \delta Q_{(2) \rightarrow (1)}^{(\text{gi})} &= -\Gamma_{21} \delta \rho_2^{(\text{gi})}, \end{aligned} \quad (4.10)$$

all the other quantities $\delta Q_{(\alpha) \rightarrow (\beta)}^{(\text{gi})}$ being zero. Regarding the coefficients related to momentum transfers, they are given by Eq. (3.25) and read

$$\delta f_{K_\ell \rightarrow (1)} = a\Gamma_{\ell 1} \frac{\phi'_\ell{}^2}{2a^2} \left[v^{(\text{gi})} - v_{K_\ell}^{(\text{gi})} \right], \quad \delta f_{K_\ell \rightarrow (2)} = a\Gamma_{\ell 2} \frac{\phi'_\ell{}^2}{2a^2} \left[v^{(\text{gi})} - v_{K_\ell}^{(\text{gi})} \right], \quad (4.11)$$

$$\delta f_{K_h \rightarrow (1)} = a\Gamma_{h1} \frac{\phi'_h{}^2}{2a^2} \left[v^{(\text{gi})} - v_{K_h}^{(\text{gi})} \right], \quad \delta f_{K_h \rightarrow (2)} = a\Gamma_{h2} \frac{\phi'_h{}^2}{2a^2} \left[v^{(\text{gi})} - v_{K_h}^{(\text{gi})} \right], \quad (4.12)$$

$$\delta f_{(1) \rightarrow (2)} = a\Gamma_{12}\rho_1 \left[v^{(\text{gi})} - v_1^{(\text{gi})} \right], \quad \delta f_{(2) \rightarrow (1)} = a\Gamma_{21}\rho_2 \left[v^{(\text{gi})} - v_2^{(\text{gi})} \right], \quad (4.13)$$

the other coefficients $\delta f_{(\alpha) \rightarrow (\beta)}$ vanishing. In the above expressions, $v^{(\text{gi})}$ is the total velocity defined by Eq. (3.8) which, in the present context, reads

$$v^{(\text{gi})} = \frac{1}{\phi'_h{}^2/a^2 + \phi'_\ell{}^2/a^2 + (1+w_1)\rho_1 + (1+w_2)\rho_2} \left[-\frac{\phi'_h{}^2}{a^2} \frac{\delta\phi_h^{(\text{gi})}}{\phi'_h} - \frac{\phi'_\ell{}^2}{a^2} \frac{\delta\phi_\ell^{(\text{gi})}}{\phi'_\ell} + (1+w_1)\rho_1 v_1^{(\text{gi})} + (1+w_2)\rho_2 v_2^{(\text{gi})} \right]. \quad (4.14)$$

We see that quantities related to fluids and scalar fields all participate to the expression of the total velocity.

We are now in a position where the equations of motion can be derived. From the perturbed Einstein equations (the time-space component), we get

$$\frac{\dot{\Phi}}{H} = -\Phi - \frac{1}{2M_{\text{Pl}}^2 H} \left[-\dot{\phi}_\ell \delta\phi_\ell^{(\text{gi})} - \dot{\phi}_h \delta\phi_h^{(\text{gi})} + a\rho_1(1+w_1)v_1^{(\text{gi})} + a\rho_2(1+w_2)v_2^{(\text{gi})} \right]. \quad (4.15)$$

Notice that, in the present context, the two Bardeen potentials are equal: $\Phi = \Psi$. From the time component of the conservation equations (3.9), (3.12) for the perturbed “fictitious” kinetic fluids, we obtain the perturbed Klein-Gordon equations for the two fields in presence of energy-momentum exchanges. They read

$$\begin{aligned} \ddot{\delta\phi}_\ell^{(\text{gi})} + \left[3H + \frac{1}{2}(\Gamma_{\ell 1} + \Gamma_{\ell 2}) \right] \dot{\delta\phi}_\ell^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_\ell^2} \delta\phi_\ell^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_\ell \partial \phi_h} \delta\phi_h^{(\text{gi})} + \frac{k^2}{a^2} \delta\phi_\ell^{(\text{gi})} + 2\frac{\partial V}{\partial \phi_\ell} \Phi \\ + \frac{1}{2}(\Gamma_{\ell 1} + \Gamma_{\ell 2}) \dot{\phi}_\ell \Phi - 4\dot{\phi}_\ell \dot{\Phi} = 0, \end{aligned} \quad (4.16)$$

$$\begin{aligned} \ddot{\delta\phi}_h^{(\text{gi})} + \left[3H + \frac{1}{2}(\Gamma_{h1} + \Gamma_{h2}) \right] \dot{\delta\phi}_h^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_h^2} \delta\phi_h^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_h \partial \phi_\ell} \delta\phi_\ell^{(\text{gi})} + \frac{k^2}{a^2} \delta\phi_h^{(\text{gi})} + 2\frac{\partial V}{\partial \phi_h} \Phi \\ + \frac{1}{2}(\Gamma_{h1} + \Gamma_{h2}) \dot{\phi}_h \Phi - 4\dot{\phi}_h \dot{\Phi} = 0. \end{aligned} \quad (4.17)$$

In a similar way, Eqs. (3.9), (3.12) written for the fluid one and two lead to the equations

controlling the evolution of the perturbed energy density for those fluids

$$\begin{aligned} \dot{\delta\rho}_1^{(\text{gi})} + 3H(1+w_1)\delta\rho_1^{(\text{gi})} - 3(1+w_1)\rho_1\dot{\Phi} - a(1+w_1)\rho_1\frac{k^2}{a^2}v_1^{(\text{gi})} - \Gamma_{\ell 1} [\delta\rho_{K_\ell}^{(\text{gi})} + \rho_{K_\ell}\Phi] \\ - \Gamma_{h1} [\delta\rho_{K_h}^{(\text{gi})} + \rho_{K_h}\Phi] + \Gamma_{12} [\delta\rho_1^{(\text{gi})} + \rho_1\Phi] - \Gamma_{21} [\delta\rho_2^{(\text{gi})} + \rho_2\Phi] = 0, \end{aligned} \quad (4.18)$$

$$\begin{aligned} \dot{\delta\rho}_2^{(\text{gi})} + 3H(1+w_2)\delta\rho_2^{(\text{gi})} - 3(1+w_2)\rho_2\dot{\Phi} - a(1+w_2)\rho_2\frac{k^2}{a^2}v_2^{(\text{gi})} - \Gamma_{\ell 2} [\delta\rho_{K_\ell}^{(\text{gi})} + \rho_{K_\ell}\Phi] \\ - \Gamma_{h2} [\delta\rho_{K_h}^{(\text{gi})} + \rho_{K_h}\Phi] + \Gamma_{21} [\delta\rho_2^{(\text{gi})} + \rho_2\Phi] - \Gamma_{12} [\delta\rho_1^{(\text{gi})} + \rho_1\Phi] = 0. \end{aligned} \quad (4.19)$$

Notice that the quantity $\delta\rho_{K_a}^{(\text{gi})} + \rho_{K_a}\Phi$ that often appears in the above formulas can also be re-written as $\delta\rho_{K_a}^{(\text{gi})} + \rho_{K_a}\Phi = \dot{\phi}_a\delta\dot{\phi}_a^{(\text{gi})} - \dot{\phi}_a^2\Phi/2$. We also remark that the time component of the conservation equation does not explicitly depend on the coefficients $\delta f_{(\alpha)\rightarrow(\beta)}$. As a consequence, if one only tracks perturbed energy densities (and/or energy density non-adiabatic perturbations), one could be under the impression that they can be ignored and that the above equations are sufficient. However, this is not the case because the velocities affect the evolution of the energy densities and the velocities equation of motion, see for instance Eq. (3.10), do depend on the coefficients $\delta f_{(\alpha)\rightarrow(\beta)}$. Therefore, even if at the end one is only interested in the density perturbations, the momentum exchanges must be specified.

Finally, we now turn to the space components of the conservation equations, see Eqs. (3.10) and (3.13). Let us first write the space component of the conservation equation for the “fictitious” kinetic fluid associated to, say, ϕ_ℓ (the conclusion is the same for ϕ_h). Using Eqs. (3.14), this gives

$$\begin{aligned} -\frac{\phi_\ell''}{a^2}\delta\phi_\ell^{(\text{gi})} - \frac{2}{a^2}\mathcal{H}\phi_\ell'\delta\phi_\ell = a [Q_{K_\ell\rightarrow V} + Q_{K_\ell\rightarrow(1)} + Q_{K_\ell\rightarrow(2)}] v^{(\text{gi})} + \delta f_{K_\ell\rightarrow V} \\ + \delta f_{K_\ell\rightarrow(1)} + \delta f_{K_\ell\rightarrow(2)}. \end{aligned} \quad (4.20)$$

However, the time component of the background equation of motion gives $\phi_{K_\ell}' (\phi_{K_\ell}'' + 2\mathcal{H}\phi_{K_\ell}')/a^2 = a [Q_{K_\ell\rightarrow V} + Q_{K_\ell\rightarrow(1)} + Q_{K_\ell\rightarrow(2)}]$. Plugging this expression in the space component of the conservation equation leads to

$$\delta f_{K_\ell\rightarrow V} + \delta f_{K_\ell\rightarrow(1)} + \delta f_{K_\ell\rightarrow(2)} = a [Q_{K_\ell\rightarrow V} + Q_{K_\ell\rightarrow(1)} + Q_{K_\ell\rightarrow(2)}] [v_{K_\ell}^{(\text{gi})} - v^{(\text{gi})}], \quad (4.21)$$

which is automatically satisfied, thanks to Eq. (4.11). This result makes sense because, for scalar fields, there is no other equation of motion than the Klein-Gordon equation, which is of second order in time and which we have already derived before.

Let us now study the space component of the conservation equation for the “real”

fluids. Making use of Eqs. (3.10) and (3.13), one arrives at

$$\begin{aligned}
\dot{v}_1^{(\text{gi})} + (1 - 3w_1) H v_1^{(\text{gi})} + \frac{\Phi}{a} + \frac{w_1}{1 + w_1} \frac{1}{a} \frac{\delta \rho_1^{(\text{gi})}}{\rho_1} = & - \frac{w_1}{(1 + w_1) \rho_1} Q_{(1) \rightarrow (2)} v_1^{(\text{gi})} \\
& + \frac{1}{\rho_1} Q_{K_\ell \rightarrow (1)} \left[v_1^{(\text{gi})} - \frac{v_{K_\ell}^{(\text{gi})}}{1 + w_1} \right] + \frac{1}{\rho_1} Q_{K_h \rightarrow (1)} \left[v_1^{(\text{gi})} - \frac{v_{K_h}^{(\text{gi})}}{1 + w_1} \right] \\
& + \frac{1}{\rho_1} Q_{(2) \rightarrow (1)} \left[v_1^{(\text{gi})} - \frac{v_2^{(\text{gi})}}{1 + w_1} \right], \tag{4.22}
\end{aligned}$$

$$\begin{aligned}
\dot{v}_2^{(\text{gi})} + (1 - 3w_2) H v_2^{(\text{gi})} + \frac{\Phi}{a} + \frac{w_2}{1 + w_2} \frac{1}{a} \frac{\delta \rho_2^{(\text{gi})}}{\rho_2} = & - \frac{w_2}{(1 + w_2) \rho_2} Q_{(2) \rightarrow (1)} v_2^{(\text{gi})} \\
& + \frac{1}{\rho_2} Q_{K_\ell \rightarrow (2)} \left[v_2^{(\text{gi})} - \frac{v_{K_\ell}^{(\text{gi})}}{1 + w_2} \right] + \frac{1}{\rho_2} Q_{K_h \rightarrow (2)} \left[v_2^{(\text{gi})} - \frac{v_{K_h}^{(\text{gi})}}{1 + w_2} \right] \\
& + \frac{1}{\rho_2} Q_{(1) \rightarrow (2)} \left[v_2^{(\text{gi})} - \frac{v_1^{(\text{gi})}}{1 + w_2} \right]. \tag{4.23}
\end{aligned}$$

Eqs. (4.15), (4.16), (4.17), (4.18), (4.19), (4.22) and (4.23) represent a complete set allowing us to track the perturbations during inflation and afterwards. We stress that these equations are valid for any model of two-field inflation and, in this sense, are quite general. To our knowledge, although implicitly present in Ref. [70], this is the first time that they are written explicitly. Similar equations have been studied in Ref. [71] but for one scalar field and one fluid only. Maybe the closest related work is Ref. [23] which investigates the generation of entropy fluctuations after multifield inflation (this paper studies models where there is a large number of fields during inflation). But the derivation of the conservation equations does not follow from a systematic formalism as we have done and, moreover, the space component of the conservation equations is not presented because Ref. [23] does not study how velocity non-adiabatic perturbations are produced (although, as we have discussed before, it is not possible to ignore them since they influence the evolution of the perturbed density contrasts). We notice that, when the comparison is possible, the equations presented here are consistent with those of Ref. [23].

4.2 Quantization of cosmological perturbations in multifield inflation

According to the theory of inflation, all the inhomogeneities (CMB anisotropies, large scale structures, ...) that we observe today originate from quantum fluctuations that were amplified by gravitational instability and stretched to astrophysical distances by the cosmic expansion during inflation [7–9] (see also Refs. [72–74]).

In the context of single-field inflation, this means that the perturbed metric, $\delta \hat{g}_{\mu\nu}(\eta, \mathbf{x})$ [in practice, the Bardeen potential $\hat{\Phi}(\eta, \mathbf{x})$] and the quantity representing matter, the scalar field fluctuations $\delta \hat{\phi}(\eta, \mathbf{x})$, must be quantum operators. In that case,

everything can be reduced to the study of a single variable, the so-called Mukhanov-variable [7, 68, 75]³, $\hat{Q}(\eta, \mathbf{x}) = z(\eta)\hat{\mathcal{R}}(\eta, \mathbf{x})$, where $z(\eta) = a(\eta)\sqrt{2\epsilon_1}M_{\text{Pl}}$. Then, this quantity is expanded in terms of creation and annihilation operators,

$$\hat{Q}(\eta, \mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} \left[Q_k(\eta)\hat{c}_{\mathbf{k}} + Q_k^*(\eta)\hat{c}_{-\mathbf{k}}^\dagger \right] e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (4.24)$$

with $[\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}^\dagger] = \delta^{(3)}(\mathbf{k} - \mathbf{k}')$. We have also introduced the mode function $Q_k(\eta)$ that controls the evolution of the operator $\hat{Q}(\eta, \mathbf{x})$. Notice that, here, we denote the mode function with the same symbol as the corresponding quantum operator. No confusion can arise with the Fourier transform of the quantum operator (which also carries an index $\mathbf{k}$) since the mode function does not carry the hat symbol. In this framework, the perturbed Einstein equations discussed in the previous sections must be viewed as operator equations. However, upon inserting the expansion (4.24) in these operator equations, one obtains ordinary differential equations for the mode functions $Q_k(\eta)$. Of course, the differential equations for the mode functions have in fact the same form as the operator differential equations. The two-point correlation function of the Mukhanov-Sasaki variable leads to the definition of the power spectrum $\mathcal{P}_Q$, namely

$$\langle \hat{Q}^2(\eta, \mathbf{x}) \rangle = \int_0^{+\infty} \frac{dk}{k} \mathcal{P}_Q(k), \quad (4.25)$$

with

$$\mathcal{P}_Q = \frac{k^3}{2\pi^2} |Q_k(\eta)|^2. \quad (4.26)$$

This procedure can be extended to more degrees of freedom, for instance in a multifield inflationary setup, which is the case of interest in this paper. With N_{field} scalar fields labelled by a , there exists a set of N_{field} independent annihilation and creation operators that, however, need not be aligned with scalar fields themselves, i.e. there exists a frame labelled by numbers A in which $[\hat{c}_{\mathbf{k}}^A, \hat{c}_{\mathbf{k}'}^{\dagger B}] = \delta^{AB}\delta^{(3)}(\mathbf{k} - \mathbf{k}')$. Then, the multifield Sasaki-Mukhanov variables $Q^a(\eta, \mathbf{x})$ are promoted to quantum operators and we have the expansion [19, 24, 76]:

$$\hat{Q}^a(\eta, \mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} \sum_{A=1}^{N_{\text{field}}} \left[Q_{A,k}^a(\eta)\hat{c}_{A,\mathbf{k}} + Q_{A,k}^{a*}(\eta)\hat{c}_{A,-\mathbf{k}}^\dagger \right] e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (4.27)$$

where we now have N_{field}^2 mode functions $Q_{A,\mathbf{k}}^a(\eta)$. The calculation of the two-point correlation function,

$$\langle \hat{Q}^a(\eta, \mathbf{x}) \hat{Q}^b(\eta, \mathbf{x}) \rangle = \int_0^{+\infty} \frac{dk}{k} \mathcal{P}_Q^{ab}(k), \quad (4.28)$$

³Here, we denote this variable by $Q(\eta, \mathbf{x})$ and not by the more traditional symbol $v(\eta, \mathbf{x})$ in order to avoid a possible confusion with the velocities of the fluids.

leads to a definition of the “generalized” power spectrum $\mathcal{P}_Q^{ab}$ which reads

$$\mathcal{P}_Q^{ab} = \frac{k^3}{2\pi^2} \sum_{A=1}^{N_{\text{field}}} Q_{A,k}^a(\eta) \left[Q_{A,k}^b(\eta) \right]^*. \quad (4.29)$$

Interestingly enough, we see that the two-point correlation function receives contributions from all independent modes labelled by “ A ”.

In this article, we deal with a situation which is slightly different from what was described before. The reason is of course that we have, at the same time, the presence of scalar fields and fluids and their associated fluctuations. Cosmological fluids can be quantized in a way that is very similar to what was described above, once their Mukhanov-Sasaki variables with canonical kinetic terms have been identified, see Refs. [68, 75] for details. As for a scalar field, in the case of a single fluid, the Mukhanov-Sasaki variable is defined from the conserved quantity, $\mathcal{R}$, by $Q(\eta, \mathbf{x}) = z(\eta)\mathcal{R}(\eta, \mathbf{x})$, with $z(\eta) = a(\eta)\sqrt{2\epsilon_1}M_{\text{Pl}}/c_S$, see Ref. [68, 75]. Notice that the quantity $z(\eta)$ differs from the case of a scalar field since there is an additional factor c_S participating to its expression. In the present context, the situation is more complicated since we deal with several fluids. One should, therefore, introduce several Mukhanov-Sasaki variables, one for each fluid. To our knowledge, this question has not been (yet) studied in a comprehensive manner in the literature but it is clear that each degree of freedom is related to the individual $\mathcal{R}_{(\alpha)}$. We will come back to this problem in the section where we discuss the initial conditions for the perturbations, see Sec. 4.3. In any case, the individual $\mathcal{R}_{(\alpha)}$ becomes a quantum operator $\hat{\mathcal{R}}_{(\alpha)}(\eta, \mathbf{x})$ that can be expanded in terms of creation and annihilation operators and that possesses its own mode functions.

As explained before, once the system has been quantized, the individual $\hat{\mathcal{R}}_{(\alpha)}$ becomes quantum operators with their associated mode functions. Clearly, for consistency, this is also the case for any other quantity participating to the description of matter since they are all related to the $\mathcal{R}_{(\alpha)}$. For instance, in the case of scalar fields, the field fluctuations $\delta\hat{\phi}^a(\eta, \mathbf{x})$ can be expanded as

$$\delta\hat{\phi}^a(\eta, \mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} \sum_{A=1}^{N_{\text{field}}+N_{\text{fluid}}} \left[\delta\phi_{A,k}^a(\eta)\hat{c}_{A,\mathbf{k}} + \delta\phi_{A,k}^{a*}(\eta)\hat{c}_{A,-\mathbf{k}}^\dagger \right] e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (4.30)$$

where $\delta\phi_{A,k}^a(\eta)$ are the associated mode functions. In a similar way, for a hydrodynamical fluid, the perturbed energy density $\delta\hat{\rho}_{(\alpha)}$ and/or the perturbed velocity $\hat{v}_{(\alpha)}$..., must also be viewed as quantum operators. For instance the perturbed energy density can be expressed as

$$\delta\rho_{(\alpha)}(\eta, \mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d\mathbf{k} \sum_{A=1}^{N_{\text{field}}+N_{\text{fluid}}} \left[\delta\rho_{A,k}^{(\alpha)}(\eta)\hat{c}_{A,\mathbf{k}} + \delta\rho_{A,k}^{(\alpha)*}(\eta)\hat{c}_{A,-\mathbf{k}}^\dagger \right] e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (4.31)$$

where we have introduced the mode functions $\delta\rho_{A,k}^{(\alpha)}(\eta)$ that are obviously different from, say, the mode functions of the perturbed scalar field. However, it is crucial to remark

that the creation and annihilation operators in Eqs. (4.30) and (4.31) are really the same quantities. In general, with N_{field} scalar fields and N_{fluid} cosmological fluids, the index A runs from 1 to $N_{\text{field}} + N_{\text{fluid}}$. In our case of interest with 2 scalar fields and 2 cosmological fluids, the index A runs on the 4 independent oscillators.

The derivation of the differential equations obeyed by the mode functions of the system is straightforward. As already mentioned, Eqs. (4.15), (4.16), (4.17), (4.18), (4.19), (4.22) and (4.23) must now be viewed as differential equations for quantum operators. Then, we can insert the canonical expansions of each operators and the same equations for the mode functions is obtained, however duplicated for each oscillator “ A ”. Concretely, this gives for the perturbed Einstein equations

$$\frac{\dot{\Phi}_A}{H} = -\Phi_A - \frac{1}{2M_{\text{Pl}}^2 H} \left[-\dot{\phi}_\ell \delta\phi_{\ell,A}^{(\text{gi})} - \dot{\phi}_h \delta\phi_{h,A}^{(\text{gi})} + a\rho_1(1+w_1)v_{1,A}^{(\text{gi})} + a\rho_2(1+w_2)v_{2,A}^{(\text{gi})} \right]. \quad (4.32)$$

Since, as already mentioned, A runs on four independent oscillators, the above equation really means four independent equations. For the mode functions of the field fluctuations operators, one obtains

$$\begin{aligned} \ddot{\delta\phi}_{\ell,A}^{(\text{gi})} + \left[3H + \frac{1}{2}(\Gamma_{\ell 1} + \Gamma_{\ell 2}) \right] \dot{\delta\phi}_{\ell,A}^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_\ell^2} \delta\phi_{\ell,A}^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_\ell \partial \phi_h} \delta\phi_{h,A}^{(\text{gi})} + \frac{k^2}{a^2} \delta\phi_{\ell,A}^{(\text{gi})} + 2 \frac{\partial V}{\partial \phi_\ell} \Phi_A \\ + \frac{1}{2}(\Gamma_{\ell 1} + \Gamma_{\ell 2}) \dot{\phi}_\ell \Phi_A - 4\dot{\phi}_\ell \dot{\Phi}_A = 0, \end{aligned} \quad (4.33)$$

$$\begin{aligned} \ddot{\delta\phi}_{h,A}^{(\text{gi})} + \left[3H + \frac{1}{2}(\Gamma_{h 1} + \Gamma_{h 2}) \right] \dot{\delta\phi}_{h,A}^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_h^2} \delta\phi_{h,A}^{(\text{gi})} + \frac{\partial^2 V}{\partial \phi_h \partial \phi_\ell} \delta\phi_{\ell,A}^{(\text{gi})} + \frac{k^2}{a^2} \delta\phi_{h,A}^{(\text{gi})} + 2 \frac{\partial V}{\partial \phi_h} \Phi_A \\ + \frac{1}{2}(\Gamma_{h 1} + \Gamma_{h 2}) \dot{\phi}_h \Phi_A - 4\dot{\phi}_h \dot{\Phi}_A = 0. \end{aligned} \quad (4.34)$$

Finally, it remains the equations of motion controlling the behaviour of the mode functions associated to the “real” fluids present in the system. They read

$$\begin{aligned} \dot{\delta\rho}_{1,A}^{(\text{gi})} + 3H(1+w_1)\delta\rho_{1,A}^{(\text{gi})} - 3(1+w_1)\rho_1\dot{\Phi}_A - a(1+w_1)\rho_1\frac{k^2}{a^2}v_{1,A}^{(\text{gi})} \\ - \Gamma_{\ell 1} \left[\delta\rho_{K_\ell,A}^{(\text{gi})} + \rho_{K_\ell}\Phi_A \right] - \Gamma_{h 1} \left[\delta\rho_{K_h,A}^{(\text{gi})} + \rho_{K_h}\Phi_A \right] + \Gamma_{12} \left[\delta\rho_{1,A}^{(\text{gi})} + \rho_1\Phi_A \right] \\ - \Gamma_{21} \left[\delta\rho_{2,A}^{(\text{gi})} + \rho_2\Phi_A \right] = 0, \end{aligned} \quad (4.35)$$

$$\begin{aligned} \dot{\delta\rho}_{2,A}^{(\text{gi})} + 3H(1+w_2)\delta\rho_{2,A}^{(\text{gi})} - 3(1+w_2)\rho_2\dot{\Phi}_A - a(1+w_2)\rho_2\frac{k^2}{a^2}v_{2,A}^{(\text{gi})} \\ - \Gamma_{\ell 2} \left[\delta\rho_{K_\ell,A}^{(\text{gi})} + \rho_{K_\ell}\Phi_A \right] - \Gamma_{h 2} \left[\delta\rho_{K_h,A}^{(\text{gi})} + \rho_{K_h}\Phi_A \right] + \Gamma_{21} \left[\delta\rho_{2,A}^{(\text{gi})} + \rho_2\Phi_A \right] \\ - \Gamma_{12} \left[\delta\rho_{1,A}^{(\text{gi})} + \rho_1\Phi_A \right] = 0, \end{aligned} \quad (4.36)$$

$$\begin{aligned}
\dot{v}_{1,A}^{(\text{gi})} + (1 - 3w_1) H v_{1,A}^{(\text{gi})} + \frac{\Phi_A}{a} + \frac{w_1}{1 + w_1} \frac{1}{a} \frac{\delta \rho_{1,A}^{(\text{gi})}}{\rho_1} = & - \frac{w_1}{(1 + w_1) \rho_1} Q_{(1) \rightarrow (2)} v_{1,A}^{(\text{gi})} \\
& + \frac{1}{\rho_1} Q_{K_\ell \rightarrow (1)} \left[v_{1,A}^{(\text{gi})} - \frac{v_{K_\ell,A}^{(\text{gi})}}{1 + w_1} \right] + \frac{1}{\rho_1} Q_{K_h \rightarrow (1)} \left[v_{1,A}^{(\text{gi})} - \frac{v_{K_h,A}^{(\text{gi})}}{1 + w_1} \right] \\
& + \frac{1}{\rho_1} Q_{(2) \rightarrow (1)} \left[v_{1,A}^{(\text{gi})} - \frac{v_{2,A}^{(\text{gi})}}{1 + w_1} \right], \tag{4.37}
\end{aligned}$$

$$\begin{aligned}
\dot{v}_{2,A}^{(\text{gi})} + (1 - 3w_2) H v_{2,A}^{(\text{gi})} + \frac{\Phi_A}{a} + \frac{w_2}{1 + w_2} \frac{1}{a} \frac{\delta \rho_{2,A}^{(\text{gi})}}{\rho_2} = & - \frac{w_2}{(1 + w_2) \rho_2} Q_{(2) \rightarrow (1)} v_{2,A}^{(\text{gi})} \\
& + \frac{1}{\rho_2} Q_{K_\ell \rightarrow (2)} \left[v_{2,A}^{(\text{gi})} - \frac{v_{K_\ell,A}^{(\text{gi})}}{1 + w_2} \right] + \frac{1}{\rho_2} Q_{K_h \rightarrow (2)} \left[v_{2,A}^{(\text{gi})} - \frac{v_{K_h,A}^{(\text{gi})}}{1 + w_2} \right] \\
& + \frac{1}{\rho_2} Q_{(1) \rightarrow (2)} \left[v_{2,A}^{(\text{gi})} - \frac{v_{1,A}^{(\text{gi})}}{1 + w_2} \right]. \tag{4.38}
\end{aligned}$$

The above differential equations are the equations to be integrated in order to follow the evolution of the system. In particular, once the mode functions are known, the two-point correlation functions of any combination of operators can be evaluated. However, in order to be able to carry out this task, we need to know the initial conditions for each quantity. We now turn to this question.

4.3 Initial conditions for the perturbations

4.3.1 Warm-up: the case of a single fluid

One of the great advantage of the inflationary theory is its ability to suggest natural and well-defined initial conditions. These initial conditions can be introduced in several different ways. Here, as a warm-up, we discuss one method and show how it is related to the formalism introduced before in the simple (and standard) case where there is only one scalar field or one perfect fluid.

Let us start with the case of one scalar field. The equations for the conserved quantities ζ and $\mathcal{R}$ (here, obviously, the total ζ and $\mathcal{R}$ are the same as the individual conserved quantities since, in our example, there is only one fluid) are given by Eq. (3.29) and Eq. (3.31). In the present context, the non-adiabatic pressure that appears in those equations is the intrinsic non-adiabatic pressure of a scalar field. It is given by

$$\delta p_{\text{nad}} = -2M_{\text{Pl}}^2 (1 - c_s^2) \frac{k^2}{a^2} \Phi_{\mathbf{k}}. \tag{4.39}$$

We see that it is non-vanishing unless $c_s = 1$, namely a scalar field is a fluid with non-vanishing intrinsic non-adiabatic pressure, but it is proportional to k^2/a^2 and, therefore, becomes irrelevant on large scales. Then, using the above expression of δp_{nad} in Eq. (3.31)

and the fact that the Bardeen potential can be written as

$$\Phi_{\mathbf{k}} = -\frac{3}{2} \frac{a^2(\rho + p)}{k^2 M_{\text{Pl}}^2} (\zeta_{\mathbf{k}} + \mathcal{R}_{\mathbf{k}}), \quad (4.40)$$

it is easy to establish that the quantity $\mathcal{R}'_{\mathbf{k}}$ can be re-expressed as $\mathcal{R}'_{\mathbf{k}} = 3\mathcal{H}(\mathcal{R}_{\mathbf{k}} + \zeta_{\mathbf{k}})$. Then, deriving this expression once, and using the δp_{nad} -independent expression of $\zeta'_{\mathbf{k}} + \mathcal{R}'_{\mathbf{k}}$ obtained by summing up Eq. (3.29) and Eq. (3.31), one arrives at

$$\mathcal{R}''_{\mathbf{k}} + 2\frac{z'}{z}\mathcal{R}'_{\mathbf{k}} + k^2\mathcal{R}_{\mathbf{k}} = 0, \quad (4.41)$$

where we recall that $z \equiv aM_{\text{Pl}}\sqrt{2\epsilon_1}$. Finally, introducing the Mukhanov-Sasaki variable, see above, $Q = z\mathcal{R}$, we obtain the following equation of a parametric oscillator

$$Q''_{\mathbf{k}} + \left(k^2 - \frac{z''}{z}\right) Q_{\mathbf{k}} = 0. \quad (4.42)$$

At the beginning of inflation, the physical wavelengths of Fourier modes of astrophysical interest today were much smaller than the Hubble radius, meaning that $k^2 \gg z''/z$. As a consequence, in this regime, the solution of Eq. (4.42) reads

$$Q_{\mathbf{k}}(\eta) = A_{\mathbf{k}} e^{ik(\eta - \eta_{\text{ini}})} + B_{\mathbf{k}} e^{-ik(\eta - \eta_{\text{ini}})}, \quad (4.43)$$

where $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are integration constants. Then, quantizing the fluctuations and assuming that the initial state is the vacuum, adiabatic or Wentzel Kramer Brillouin (WKB), Bunch-Davies state, it follows that $A_{\mathbf{k}} = (2k)^{-1/2}$ and $B_{\mathbf{k}} = 0$.

The above reasoning can easily be repeated if one now assumes that there is only one perfect fluid in the Universe. The main difference with the scalar field calculation presented above is that we now have $\delta p_{\text{nad}} = 0$. Let us restart from Eq. (3.31) and take the derivative of this equation and, then, replace $\zeta'_{\mathbf{k}}$ using Eq. (3.29). One arrives at

$$\mathcal{R}''_{\mathbf{k}} = \frac{\mathcal{H}'}{\mathcal{H}} \mathcal{R}'_{\mathbf{k}} + \frac{(c_s^2)'}{c_s^2} \mathcal{R}'_{\mathbf{k}} + 3\mathcal{H}c_s^2 \mathcal{R}'_{\mathbf{k}} - c_s^2 k^2 \mathcal{R}_{\mathbf{k}} + c_s^2 k^2 \Psi_{\mathbf{k}}. \quad (4.44)$$

The last term in the above equation can be expressed in terms of $\zeta_{\mathbf{k}} + \mathcal{R}_{\mathbf{k}}$ using Eq. (4.40) (here, we recall that we do not distinguish between $\Psi_{\mathbf{k}}$ and $\Phi_{\mathbf{k}}$) and, thanks to Eq. (3.31), $\zeta_{\mathbf{k}} + \mathcal{R}_{\mathbf{k}}$ is proportional to $\mathcal{R}'_{\mathbf{k}}$. As a consequence, one obtains a closed equation for $\mathcal{R}_{\mathbf{k}}$ which reads

$$\mathcal{R}''_{\mathbf{k}} = \left[\frac{\mathcal{H}'}{\mathcal{H}} + \frac{(c_s^2)'}{c_s^2} + 3\mathcal{H}c_s^2 - \mathcal{H}\epsilon_1 \right] \mathcal{R}'_{\mathbf{k}} - c_s^2 k^2 \mathcal{R}_{\mathbf{k}} = -2\frac{z'}{z} \mathcal{R}'_{\mathbf{k}} - c_s^2 k^2 \mathcal{R}_{\mathbf{k}}, \quad (4.45)$$

where $z = aM_{\text{Pl}}\sqrt{2\epsilon_1}/c_s$. Notice that z is not well-defined for a pressure-less fluid. Then, as we did for the case of a scalar field, we define the Mukhanov-Sasaki variable of the fluid, Q , by $Q = z\mathcal{R}$ and it follows that

$$Q''_{\mathbf{k}} + \left(c_s^2 k^2 - \frac{z''}{z}\right) Q_{\mathbf{k}} = 0. \quad (4.46)$$

This equation is very similar to Eq. (4.43), the only difference being the appearance of the sound velocity in the gradient term and in the definition of $z(\eta)$ (which, if c_s is constant, cancels out in the term z''/z). If the Fourier mode under consideration is such that its wavelength is much smaller than the Hubble horizon initially, then the solution of the above equation reads $Q_{\mathbf{k}}(\eta) = A_{\mathbf{k}}e^{icsk(\eta-\eta_{\text{ini}})} + B_{\mathbf{k}}e^{-icsk(\eta-\eta_{\text{ini}})}$. Quantizing the hydrodynamical fluctuations and assuming that they are initially placed in the vacuum state leads to the following initial conditions: $A_{\mathbf{k}} = (2c_s k)^{-1/2}$ and $B_{\mathbf{k}} = 0$.

Endowed with the initial conditions for the quantity $Q_{\mathbf{k}}(\eta)$ determined above, one can infer the initial conditions of any other variable. However, this is not straightforward and, as a preparation to the multi-fluid case, we explain how it can be done in the single fluid case. Let us first assume that there is only one scalar field. We have two methods to derive the initial conditions of the Bardeen potential. Using Eq. (4.40) and the fact that $\mathcal{R}_{\mathbf{k}} + \zeta_{\mathbf{k}} = \mathcal{R}'_{\mathbf{k}}/(3\mathcal{H})$, one can easily establish that (notice that this equation is exact)

$$\Phi_{\mathbf{k}} = -\frac{\mathcal{H}\epsilon_1}{k^2} \left(\frac{Q_{\mathbf{k}}}{z} \right)', \quad (4.47)$$

or

$$a\Phi_{\mathbf{k}} = -\frac{1}{2k^2} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} \left(Q'_{\mathbf{k}} - \frac{z'}{z} Q_{\mathbf{k}} \right), \quad (4.48)$$

from which one can write

$$\Phi_{\mathbf{k}} = -\frac{i}{(2k)^{3/2}} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} \left(1 - \frac{z'}{ikz} \right) e^{ik(\eta-\eta_{\text{ini}})} \simeq -\frac{i}{(2k)^{3/2}} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} e^{ik(\eta-\eta_{\text{ini}})}, \quad (4.49)$$

the second term between the parenthesis in the above equation being negligible in the small-scale limit. Therefore, we have that $\Phi_{\mathbf{k}} \sim (2k)^{-3/2}$. Then, since $a\delta\phi_{\mathbf{k}} = Q_{\mathbf{k}} - z\Phi_{\mathbf{k}}$, one has $\delta\phi_{\mathbf{k}} \sim (2k)^{-1/2}$, the second term proportional to the Bardeen potential giving a sub-dominant contribution.

A second way to derive those results, which was also the method used in Ref. [71], consists in the following. The single-field version of the Einstein equation, see Eq. (4.32), can be written as

$$\Phi'_{\mathbf{k}} = -\mathcal{H}\Phi_{\mathbf{k}} + \frac{\phi'}{2M_{\text{Pl}}^2} \delta\phi_{\mathbf{k}}. \quad (4.50)$$

We are interested in the sub-Hubble behaviour of $\Phi_{\mathbf{k}}$ and $\delta\phi_{\mathbf{k}}$. In this regime, given the solution found above for $Q_{\mathbf{k}}$, one can write $\Phi_{\mathbf{k}} = \mathcal{A}_{\Phi} e^{ik(\eta-\eta_{\text{ini}})}$ and $\delta\phi_{\mathbf{k}} = \mathcal{A}_{\delta\phi} e^{ik(\eta-\eta_{\text{ini}})}$, where $\mathcal{A}_{\Phi}$ and $\mathcal{A}_{\delta\phi}$ are slowly varying overall amplitudes. Inserting these expressions into Eq. (4.50) and using the definition of $Q_{\mathbf{k}}$, $Q_{\mathbf{k}} = a\delta\phi_{\mathbf{k}} + z\Phi_{\mathbf{k}}$, in order to express $\mathcal{A}_{\delta\phi}$ in terms of $Q_{\mathbf{k}}$ and $\mathcal{A}_{\Phi}$, one obtains

$$a\mathcal{A}'_{\Phi} + ik \left[1 + \frac{\mathcal{H}(1+\epsilon_1)}{ik} \right] a\mathcal{A}_{\Phi} = \frac{1}{2} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} Q_{\mathbf{k}}. \quad (4.51)$$

In this equation, the derivative $\mathcal{A}'_{\Phi}$ can be neglected since $\mathcal{A}_{\Phi}$ is changing very slowly; moreover, given that $k/\mathcal{H} \gg 1$ on sub-Hubble scales, one arrives at exactly Eq. (4.49). Therefore, this also completely determines the initial conditions of $\Phi_{\mathbf{k}}$ in terms of those of $Q_{\mathbf{k}}$ and gives results similar to the first method. As a consequence, as announced before, once the initial conditions for the Mukhanov-Sasaki variable are known, the initial conditions for any other relevant quantities can be automatically inferred.

The same reasoning can also be applied to the situation where there is only one perfect fluid in the Universe. In that case, an exact result is

$$\Phi_{\mathbf{k}} = -\frac{\mathcal{H}\epsilon_1}{c_s^2 k^2} \left(\frac{Q_{\mathbf{k}}}{z} \right)', \quad (4.52)$$

or

$$a\Phi_{\mathbf{k}} = -\frac{c_s}{2c_s^2 k^2} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} \left(Q'_{\mathbf{k}} - \frac{z'}{z} Q_{\mathbf{k}} \right). \quad (4.53)$$

Then, we introduce the same WKB ansatz already discussed before with one important difference though. Instead of oscillatory terms $\propto e^{ik\eta}$, one needs to take into account the fact that, in a fluid, fluctuations propagate with a speed which not the speed of light. As a consequence, the relevant quantities characterizing the fluid will be written as a slow-varying amplitude times $e^{icsk(\eta-\eta_{\text{ini}})}$. Then, repeating the previous considerations leads to the following equation

$$\Phi_{\mathbf{k}} = -\frac{ics}{(2c_s k)^{3/2}} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} \left(1 - \frac{z'}{icskz} \right) e^{icsk(\eta-\eta_{\text{ini}})} \simeq -\frac{ics}{(2c_s k)^{3/2}} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} e^{icsk(\eta-\eta_{\text{ini}})}, \quad (4.54)$$

and, therefore, that $\Phi_{\mathbf{k}} \propto (2c_s k)^{-3/2}$. Notice, as expected, that the above equation is exactly Eq. (4.49) if one takes $c_s = 1$.

The second method can also be used to check the validity of the result. In case of one perfect fluid, Eq. (4.32) reduces to

$$\Phi'_{\mathbf{k}} = -\mathcal{H}\Phi_{\mathbf{k}} - \frac{a^2}{2M_{\text{Pl}}^2} \rho(1+w)v^{(\text{gi})}, \quad (4.55)$$

and using similar considerations as the ones presented before in the case of a single scalar field, we obtain

$$a\mathcal{A}'_{\Phi} + icsk \left[1 + \frac{\mathcal{H}(1+\epsilon_1)}{icsk} \right] a\mathcal{A}_{\Phi} = \frac{c_s}{2} \frac{\mathcal{H}}{M_{\text{Pl}}} \sqrt{2\epsilon_1} Q_{\mathbf{k}}. \quad (4.56)$$

that is to say the same formula as for a scalar field except for the presence of the sound velocity. In the large scale limit, one obtain exactly Eq. (4.54) for the Bardeen potential and we conclude that $\Phi_{\mathbf{k}} \propto (2c_s k)^{-3/2}$. For the velocity, we can use the definition of $Q_{\mathbf{k}}$, namely $\mathcal{H}\mathcal{A}_v = \mathcal{A}_{\Phi} - Q_{\mathbf{k}}/z$ and, therefore, $\mathcal{A}_v \propto (2c_s k)^{-1/2}$. In particular, the contribution coming from the Bardeen potential is sub-dominant as expected.

Finally, the initial conditions for the density contrast remains to be discussed. In the single fluid case, the perturbed energy density conservation equation, see Eq. (4.35), reads (again, neglecting the exchange terms)

$$\delta\rho' + 3\mathcal{H}(1+w)\delta\rho - 3(1+w)\rho\Phi' - (1+w)\rho k^2 v = 0, \quad (4.57)$$

yielding

$$\mathcal{A}'_{\delta\rho} + ikc_s \left[1 + \frac{3\mathcal{H}(1+w)}{ikc_s} \right] \mathcal{A}_{\delta\rho} = 3(1+w)\rho (\mathcal{A}'_\Phi + ikc_s \mathcal{A}_\Phi) + (1+w)\rho k^2 \mathcal{A}_v. \quad (4.58)$$

In the right hand side, the dominant term is the term proportional to $\mathcal{A}_v$ which scales as $\propto k^{3/2}$ since the term proportional to $\mathcal{A}_\Phi$ “only” scales $\propto k^{-1/2}$. As a consequence, one can write

$$\mathcal{A}_{\delta\rho} = \frac{(1+w)\rho}{ic_s^2} c_s k \mathcal{A}_v, \quad (4.59)$$

and deduce that $\mathcal{A}_{\delta\rho} \propto k^{1/2}$. It is interesting to test the consistency of this result with the other conservation equation which, in the single fluid case, reads [see Eq. (4.37)]

$$v' + 3\mathcal{H}(1-3w)v + \Phi + \frac{w}{1+w} \frac{\delta\rho}{\rho} = 0. \quad (4.60)$$

Inserting the WKB ansatz in this equation, one obtains

$$\mathcal{A}'_v + ic_s k \left[1 + \frac{3\mathcal{H}(1-3w)}{ic_s k} \right] \mathcal{A}_v = -\mathcal{A}_\Phi - \frac{w}{(1+w)\rho} \mathcal{A}_{\delta\rho}. \quad (4.61)$$

In the right hand side the term proportional to $\mathcal{A}_\Phi$ is subdominant since it scales $\propto k^{-3/2}$ while the term proportional to $\mathcal{A}_{\delta\rho}$ is proportional to $k^{-1/2}$. As a consequence, one obtains

$$\mathcal{A}_{\delta\rho} = -\frac{(1+w)\rho}{w} ic_s k \mathcal{A}_v, \quad (4.62)$$

which is exactly Eq. (4.59) since $w = c_s^2$ for a perfect fluid with constant equation of state. We conclude that this is entirely consistent with the results obtained from the energy density contrast conservation equation and that the relevant initial conditions have now been completely specified.

4.3.2 The many fluid case

In the previous section, we have shown how to connect the formalism presented in Sec. 3 to the approach utilizing the Mukhanov-Sasaki variable. In principle, the generalization to the many fluid case is straightforward.

The first step consists in defining a Mukhanov-Sasaki variable for each fluid present in the system. For scalar fields, this is known to be $Q_a = a\delta\phi_a + z_a\Phi$ with $z_a = a\phi'_a/\mathcal{H}$,

see Ref. [18]. In the case of a single scalar field, we recall that $Q = a\delta\phi + z\Phi$, where, as already introduced before, $z = a\sqrt{2\epsilon_1}M_{\text{Pl}} = a\phi'/a$. In some sense, z_a is a generalization of the second manner of writing the z variable (namely a generalization of $a\phi'/\mathcal{H}$ and “not” of $aM_{\text{Pl}}\sqrt{2\epsilon_1}$).

For perfect fluids, to our knowledge, the question has not been studied as thoroughly as in the case of scalar fields. We recall that, for a single fluid $Q = z\mathcal{R} = z[\Psi - \mathcal{H}v_{(\text{gi})}]$, with $z = a\sqrt{2\epsilon_1}M_{\text{Pl}}/c_s$. The question is then to define a variable $Q_{(\alpha)}$ and a quantity $z_{(\alpha)}$ for each fluid. One possibility for $z_{(\alpha)}$ would be $z_{(\alpha)} = a\sqrt{2\epsilon_1}M_{\text{Pl}}/c_{(\alpha)}$. However, there is also another possibility which seems closer to what is done in the case of scalar fields. Indeed the one-fluid definition of z can also be written as $z = a^2/\mathcal{H}\sqrt{(\rho+p)/(\rho'/p')}$, where, here, ρ and p are the total energy density and pressure, respectively, which (obviously!) are also the energy density and the pressure of the fluid under consideration since we assumed there is only one fluid. In the multi-fluid situation, this suggests the introduction of the quantity $z_{(\alpha)}$ defined by

$$z_{(\alpha)} = \frac{a^2}{\mathcal{H}} \sqrt{\frac{\rho_{(\alpha)} + p_{(\alpha)}}{p'_{(\alpha)}/\rho'_{(\alpha)}}}. \quad (4.63)$$

It is important to notice that $z_{(\alpha)}$ can no longer be expressed in terms of ϵ_1 because ϵ_1 is now determined by the total energy density and pressure. Then, one can define $Q_{(\alpha)}$ by $Q_{(\alpha)} = z_{(\alpha)}\mathcal{R}_{(\alpha)} = z_{(\alpha)}[\Psi - \mathcal{H}v_{(\alpha)}^{(\text{gi})}]$.

Having defined the generalized Mukhanov-Sasaki variables for each fluid of the system, the next step consists in establishing from the general equations of Sec. 3, the equations satisfied by the Q_a and the $Q_{(\alpha)}$. These equations will obviously be coupled. Finally, one needs to take the large scale limit, $k/\mathcal{H} \rightarrow \infty$, in order to guess the initial conditions for the Q_a and the $Q_{(\alpha)}$.

However, there exists a route which is much easier. First of all, we can remark that, initially, the couplings between the scalar fields and the fluids can be neglected. As a consequence, the N_{field} scalar fields and the N_{fluid} fluids can be treated separately. The initial conditions for a collection of N_{field} perturbed fields have been studied in great details in the literature and it is standard to show that one has [19, 24, 76]

$$Q_{a,k}^A(\eta) \rightarrow \frac{1}{\sqrt{2k}} e^{ik(\eta-\eta_{\text{ini}})} \delta_a^A. \quad (4.64)$$

In this expression, it is worth noticing the presence of δ_a^A which means that, initially, the canonical variables are not “mixed”. Only the time evolution of those variables, in presence of an interaction between them, will be able to mix them.

The treatment of a collection of N_{fluid} fluids is less standard. As already mentioned, in principle, one should establish the equations of motion of the variables $Q_{(\alpha)}$. However, in the large scale limit, we expect the Bardeen potential not to play an important role. As a consequence, one can introduce a simplified version of $Q_{(\alpha)}$, $\mathcal{Q}_{(\alpha)}$, defined by $\mathcal{Q}_{(\alpha)} = -z_{(\alpha)}\mathcal{H}v_{(\alpha)}^{(\text{gi})}$. Assuming that each fluid has a constant equation of state, which is

the case of interest in this paper, we find that $\mathcal{Q}_{(\alpha)}$ obeys the equation

$$\mathcal{Q}_{(\alpha)}'' + \mathcal{Q}_{(\alpha)} \left[w_\alpha k^2 - \frac{z_{(\alpha)}''}{z_{(\alpha)}} + \mathcal{H}^2 \epsilon_1 \epsilon_2 \right] = 0. \quad (4.65)$$

This equation is sufficient to fix the initial conditions in the sub-Hubble regime and we take

$$\mathcal{Q}_{(\alpha),k}^A \rightarrow \frac{1}{\sqrt{2c_{(\alpha)}}k} e^{ic_{(\alpha)}k(\eta-\eta_{\text{ini}})} \delta_{(\alpha)}^A, \quad (4.66)$$

where, as it was the case for the case of scalar fields, we have introduced “non-mixing” initial conditions, see the presence of $\delta_{(\alpha)}^A$. When the Bardeen potential is sub-dominant on sub-Hubble scales, one expects $\mathcal{Q}_{(\alpha),k}^A \simeq Q_{(\alpha),k}^A$.

Here, a comment is in order. We see that Eq. (4.66) is ill-defined when $c_{(\alpha)} = 0$, namely in the case where the fluid under consideration is pressure-less, which is clearly relevant in the present context. In that case, however, there is no oscillatory modes anymore and, moreover, the physical wavelengths of the Fourier amplitudes are never inside the sonic horizon (which simply vanishes), a necessary criterion to be able to single out well-defined initial conditions. Carrying out the quantization of such a system seems therefore difficult. On the other hand, we need to choose some initial conditions in order to perform numerical calculations. Here, we will simply take a small but non-vanishing pressure for the matter fluid: $c_m = 0.01$. Although it may be interesting to discuss this question more deeply, at the practical level, we have noticed that the numerical behaviour of the system does not depend on those initial conditions. Therefore the physical conclusions obtained in this paper will not be sensitive to this issue.

Having chosen the initial conditions for the “canonical variables” Q_a and $Q_{(\alpha)}$, we now discuss how the initial conditions for the other relevant quantities can be determined. This is done with the method presented in Sec. 4.3.1. Notice, however, that the scalar field fluctuations and perfect fluid fluctuations propagate with different speed. The different perfect fluid perturbations also propagate with different speed since, *a priori*, the fluids do not have the equation of state. To deal with this issue, we write $\Phi^A = \mathcal{A}_\Phi^A e^{ic_A k(\eta-\eta_{\text{ini}})}$, with $c_A = (1, 1, c_1, c_2)$. In the same manner, we write the two perturbed scalar fields as $\delta\phi_{\ell,h}^A = \mathcal{A}_{\ell,h}^A e^{ic_A k(\eta-\eta_{\text{ini}})}$, the two perturbed energy densities as $\delta\rho_{1,2}^A = \mathcal{A}_{1,2}^A e^{ic_A k(\eta-\eta_{\text{ini}})}$ and, finally, the two velocities as $v_{1,2,A}^{(\text{gi})} = \mathcal{A}_{v_1,v_2}^A e^{ic_A k(\eta-\eta_{\text{ini}})}$. It is interesting to see that the scalar field fluctuations which, *a priori*, propagate $\propto e^{ik(\eta-\eta_{\text{ini}})}$ can also acquire modes $\propto e^{ic_1 k(\eta-\eta_{\text{ini}})}$ and $\propto e^{ic_2 k(\eta-\eta_{\text{ini}})}$ (the same remark could be done for perfect fluids perturbations). Whether we initially populate the mode, say, $\Phi^1 = \mathcal{A}_\Phi^1 e^{ic_1 k(\eta-\eta_{\text{ini}})}$ is precisely the choice of the initial conditions. In a standard situation, one could also decide to populate this type of mode but, without interactions between scalar fields and perfect fluids, this is not physically very relevant and, in any case, does not correspond to the usual choice of initial conditions. In the present context, however, this discussion is much more relevant since the interactions are able to sustain such a mode.

The next step consists in inserting the above expressions of Φ^A , $\delta\phi_{\ell,h}^A$, $\delta\rho_{1,2}^A$ and $v_{1,2,A}^{(\text{gi})}$ in Eqs. (4.32), (4.33), (4.34), (4.35), (4.36), (4.37) and (4.38), and neglect the interactions terms. As in Sec. 4.3.1, we consider that the amplitudes $\mathcal{A}_\Phi^A$, $\mathcal{A}_{\ell,h}^A$, $\mathcal{A}_{1,2}^A$ and $\mathcal{A}_{v_1,v_2}^A$ are slowly varying functions of time. Moreover, we use the initial conditions obtained from the quantum-mechanical considerations presented earlier in this section. In particular, the requirement (4.64) implies that

$$\mathcal{A}_\ell^A = \frac{K_\ell}{a} \delta_\ell^A - \frac{z_\ell}{a} \mathcal{A}_\Phi^A, \quad \mathcal{A}_h^A = \frac{K_h}{a} \delta_h^A - \frac{z_h}{a} \mathcal{A}_\Phi^A, \quad (4.67)$$

and we also have

$$\mathcal{A}_{v_1}^A = -\frac{K_1}{\mathcal{H}z_1} \delta_1^A + \frac{1}{\mathcal{H}} \mathcal{A}_{\Phi,1}^A, \quad \mathcal{A}_{v_2}^A = -\frac{K_2}{\mathcal{H}z_2} \delta_2^A + \frac{1}{\mathcal{H}} \mathcal{A}_{\Phi,2}^A, \quad (4.68)$$

where the precise definitions of the background functions z_ℓ , z_h , z_1 and z_2 have been introduced before. In fact, at this stage, all we need to know is that these quantities are background quantities and we will see that they do not play a crucial role in determining the initial conditions. The quantities K_ℓ , K_h , K_1 and K_2 , on the contrary, determine the scaling of the initial conditions and are fixed by the quantum-mechanical considerations described above, namely $K_\ell = K_h = (2k)^{-1/2}$ and $K_{1,2} = (2c_{1,2}k)^{-1/2}$.

Let us start with the equation for Φ^A . Substituting the previous WKB ansatz in Eq. (4.32), one arrives at

$$\begin{aligned} & \mathcal{A}_\Phi^A + ic_A k \left\{ 1 + \frac{\mathcal{H}}{ic_A k} + \frac{1}{2M_{\text{Pl}}^2 ic_A k} \left[\frac{\Phi'_\ell z_\ell}{a} + \frac{\Phi'_h z_h}{a} + \frac{a^2 \rho_1 (1+w_1)}{\mathcal{H}} + \frac{a^2 \rho_2 (1+w_2)}{\mathcal{H}} \right] \right\} \mathcal{A}_\Phi^A \\ &= \frac{1}{2M_{\text{Pl}}^2} \left[\frac{\phi'_\ell}{a} K_\ell \delta_\ell^A + \frac{\phi'_h}{a} K_h \delta_h^A + \frac{a^2 \rho_1 (1+w_1)}{\mathcal{H}z_1} K_1 \delta_1^A + \frac{a^2 \rho_2 (1+w_2)}{\mathcal{H}z_2} K_2 \delta_2^A \right], \end{aligned} \quad (4.69)$$

from which one obtains

$$\mathcal{A}_\Phi^A \simeq \frac{1}{2M_{\text{Pl}}^2 ic_A k} \left[\frac{\phi'_\ell}{a} K_\ell \delta_\ell^A + \frac{\phi'_h}{a} K_h \delta_h^A + \frac{a^2 \rho_1 (1+w_1)}{\mathcal{H}z_1} K_1 \delta_1^A + \frac{a^2 \rho_2 (1+w_2)}{\mathcal{H}z_2} K_2 \delta_2^A \right]. \quad (4.70)$$

We see that each component of $\mathcal{A}_\Phi^A$ is determined by the corresponding fluid, that is to say the component $\mathcal{A}_\Phi^\ell$ is determined by K_ℓ , $\mathcal{A}_\Phi^h$ is determined by K_h and so on. As for the single fluid case, one has $\mathcal{A}_\Phi^A \propto k^{-3/2}$. Then, using Eqs. (4.67) and (4.68), one deduces that, at leading order, $\mathcal{A}_\ell^A \propto k^{-1/2} \delta_\ell^A$, $\mathcal{A}_h^A \propto k^{-1/2} \delta_h^A$, $\mathcal{A}_{v_1}^A \propto k^{-1/2} \delta_1^A$ and $\mathcal{A}_{v_2}^A \propto k^{-1/2} \delta_2^A$. At this stage, a comment is in order about the off-diagonal terms of the components $\mathcal{A}_\ell^A$, $\mathcal{A}_h^A$, $\mathcal{A}_{v_1}^A$ and $\mathcal{A}_{v_2}^A$. According to the previous considerations, these quantities are next-to-leading order. For instance, according to Eq. (4.67), if $A \neq \ell$, one has $\mathcal{A}_\ell^A \propto -z_\ell \mathcal{A}_\Phi^A/a$, which means a scaling $\propto k^{-3/2}$ instead of $\propto k^{-1/2}$ for the diagonal component ($A = \ell$). However, one has to remember that these conclusions are based on the quantization of the variable $\mathcal{Q}_{(\alpha)}$ introduced before, which is equivalent to $Q_{(\alpha)}$ only if the Bardeen contribution is neglected. As a consequence, rigorously, the

present considerations do not allow us to derive the sub-leading contributions exactly. In the following, for convenience, we will just assume that the off-diagonal terms initially vanish. Again, at the practical level, this point does not play an important role in the following since the evolution of the system is largely independent of those initial conditions.

Finally, the initial conditions for the energy density contrasts remain to be established. Using Eqs. (4.35) and (4.36), it is easy to show that

$$\mathcal{A}_1^{A'} + ikc_A \left[1 + \frac{3\mathcal{H}(1+w_1)}{ic_A k} \right] \mathcal{A}_1^A = 3(1+w_1)\rho_1 (\mathcal{A}_\Phi^{A'} + ic_A k \mathcal{A}_\Phi^A) + (1+w_1)\rho_1 k^2 \mathcal{A}_{v_1}^A, \quad (4.71)$$

and a similar equation for $\mathcal{A}_2^A$. It follows that

$$\mathcal{A}_1^A \simeq \frac{(1+w_1)\rho_1}{ic_A^2} c_A k \mathcal{A}_{v_1}^A \simeq -\frac{(1+w_1)\rho_1}{ic_A^2 \mathcal{H} z_1} c_A k K_1 \delta_1^A, \quad (4.72)$$

and, again, a similar expression for $\mathcal{A}_2^A$. This gives the following scaling $\mathcal{A}_{1,2} \propto k^{1/2} \delta_{1,2}^A$, at leading order. As in the single fluid case, one can check that the above expression can also be recovered from (or is consistent with) the conservation equations involving the velocity of the fluids. Again, for the off-diagonal terms, which are next-to-leading order, we assume that they initially vanish. The previous comments on this assumption are also valid in the present case.

4.4 Numerical Codes

It is clear that Eqs. (4.15), (4.16), (4.17), (4.18), (4.19), (4.22) and (4.23) are too complicated to permit the obtention of analytical solutions. We have therefore integrated them numerically and, in this section, we briefly present the methods that we have used to find numerical solutions. Actually, we have written two independent codes to follow the evolution of the background and linear fluctuations in these kinds of setups, in order to be able to cross-check the numerical results. One code is using **Python3** and the other is using **Fortran**.

The Python code uses the **LSODA** method from the routine `solve_ivp` of the package `scipy.integrate`, in order to numerically evolve the two-fields-two-fluids system of 8 coupled background functions $(a, H, \phi_\ell, \phi_h, \pi_\ell, \pi_h, \rho_1, \rho_2)$ and $72 = 9 \times 2 \times 4$ coupled linear perturbations $\text{Re/Im}(\Phi^A, \delta\phi_\ell^A, \delta\phi_h^A, \delta\pi_\ell^A, \delta\pi_h^A, \delta\rho_1^A, \delta\rho_2^A, v_1^A, v_2^A)_{A=\ell, h, 1, 2}$. The time variable for the integration is chosen to be the number of e -folds N , which constrains the value of the scale factor a at each time step. Moreover, the Hubble parameter H is evolved with the dynamical Friedmann equation $\dot{H} = -(\rho + P)/(2M_{\text{Pl}}^2)$ with ρ, P the total energy density and pressure, while the other Friedmann equation is used as a diagnosis of the accuracy (energy conservation) of the numerical computation: $\mathcal{E} = |1 - 3H^2 M_{\text{Pl}}^2 / \rho|$ provides a dimensionless quantity measuring the numerical error. During inflation, $\mathcal{E}$ is of order 10^{-11} in our fiducial two-field model of Sec. 5, showing that the numerical implementation is evidently very accurate, even though it

grows quickly up to $\lesssim 1\%$ after the oscillations of the lightest field at the end of inflation. Indeed, to follow the dynamics of the fluids (background and linear fluctuations) after the end of reheating, we abruptly drop the scalar fields in the numerical evolution in order for the code not to try to resolve the tiny oscillations that must remain even though they constitute a negligible amount of the total energy density, and we believe that this violent procedure (the derivative of H is formally infinite at this point) is at the origin of the quite important decrease in the numerical accuracy. Although more clever solutions might be possible in order to keep a good numerical accuracy during radiation and matter domination, this does not play an important role since we can still compute accurately each quantity at the end of reheating, a few e -folds after the end of inflation, which is the main goal of this article, and only numerical predictions well within the radiation era (or even in the matter era) should be taken more cautiously.

Our Fortran code integrates the same equations (and, therefore, calculate the behaviour of the same variables) with a time parameter which is also taken to be the number of e -folds. The method of integration is a fifth-order Runge-Kutta method with adaptative step size control [77]. As in the Phyton code, when it becomes difficult to follow the evolution of the inflaton fields after reheating, their contribution is automatically put to zero when the corresponding energy density becomes smaller than a chosen threshold. This is done at the background and perturbed level.

As mentioned before, we have cross-checked our results and no significative difference between the results of the two codes has been found.

5 Application: double inflation

5.1 Description of the model

In this section, we apply the formalism studied before to a specific model of multifield inflation. In order to remain as simple as possible, we consider that the phase of inflation is well-described by the “double inflation” model [15–17, 20] characterized by the following Lagrangian

$$\mathcal{L}_{\text{dbl-inf}} = -\frac{1}{2}\partial^\mu\phi_\ell\partial_\mu\phi_\ell - \frac{1}{2}\partial^\mu\phi_h\partial_\mu\phi_h - \frac{1}{2}m_\ell^2\phi_\ell^2 - \frac{1}{2}m_h^2\phi_h^2 + \mathcal{L}_{\text{matter}} + \mathcal{L}_{\text{int}}. \quad (5.1)$$

In this model there are two fields, ϕ_ℓ and ϕ_h and the main difference with the general case of two-field inflation considered before is that, now, the potential is separable $V(\phi_\ell, \phi_h) = V_\ell(\phi_\ell) + V_h(\phi_h)$, each individual term being simply the potential for a massive field. The mass of ϕ_ℓ is m_ℓ and that of ϕ_h is m_h with $m_h = Rm_\ell$ and $R > 1$ which explains why one field is called “light”, ϕ_ℓ , and the other “heavy”, ϕ_h . As explained before, the two fields responsible for inflation also interact with other components of matter represented here by $\mathcal{L}_{\text{matter}}$. In the present context, we interpret $\mathcal{L}_{\text{matter}}$ as the Lagrangian describing the decay products of the inflaton fields, the interaction between the inflaton fields and those decay products being given by $\mathcal{L}_{\text{int}}$. *A priori*, a complete model requires the microscopic description of the decay products (especially if a perturbative calculation is carried out), namely an explicit form for $\mathcal{L}_{\text{matter}}$ in terms of other fundamental fields. One possibility

would be that the inflaton fields decay in other scalar fields. For instance, the light field could decay into the field χ with $-\mathcal{L}_{\text{matter}} = (\partial\chi)^2/2 + V(\chi)$ and

$$V(\chi) \propto e^{-\sqrt{3}(1+w)^{1/2}\chi/M_{\text{Pl}}}, \quad (5.2)$$

where w is a free parameter [78]. This potential is used in the model of power-law inflation. An important feature of this model is that the equation of state of χ is constant and given by w (hence the name). In the context of power-law inflation, w is chosen sufficiently close to minus one which makes the potential very flat as required for an inflationary model. However, if $w = 1/3$, and, therefore, if the potential is rather steep, then when the inflaton fields have decayed away and the energy budget of the Universe is dominated by the field χ , a radiation-dominated epoch starts. In other words, a field χ with the potential (5.2) provides an example of a microscopic description of radiation. Then, the interaction between χ and the inflaton field could typically be taken as $-\mathcal{L}_{\text{int}} = \sigma\phi_\ell\chi^2$, where σ is a constant of dimension one. This Lagrangian describes the decay of one “ ϕ_ℓ -particle” into two “ χ -particles”. This represents an interesting example where the Lagrangian (5.1) is entirely explicit.

In this article, however, we follow a different route and use a phenomenological description in which the decay products are modelled by perfect fluids, see Secs. 2, 3. In this section, we will consider two fluids with constant equations of state: the first fluid will be radiation with $w_\gamma = 1/3$ and the second fluid will be pressure-less with vanishing equation of state $w_m = 0$. Moreover, as already discussed before, we assume that the light field can only desintegrate into radiation and the heavy field into pressure-less matter. Finally, we also make the hypothesis that the decay products cannot interact among themselves. As described before, the two scalar fields are in fact equivalent to three fluids, two “kinetic fluids” and one “potential fluid” with energy densities and pressures given by

$$\rho_{K_\ell} = \frac{\phi_\ell'^2}{2a^2} = p_{K_\ell}, \quad \rho_{K_h} = \frac{\phi_h'^2}{2a^2} = p_{K_h}, \quad \rho_V = V = -p_V. \quad (5.3)$$

We know from the previous considerations, see Sec. 2, that the exchanges between those three fluids are given by

$$aQ_{K_\ell \rightarrow V} = -\phi_\ell' V_{\phi_\ell}, \quad aQ_{V \rightarrow K_\ell} = 0, \quad aQ_{K_h \rightarrow V} = -\phi_h' V_{\phi_h}, \quad aQ_{V \rightarrow K_h} = 0, \quad (5.4)$$

in order to recover the usual equations of motion for the fields. The above assumptions concerning the interaction between fields and fluids, using Eq. (2.14), are equivalent to

$$Q_{K_\ell \rightarrow \gamma} = -\Gamma_{\ell\gamma}\rho_{K_\ell}, \quad Q_{\gamma \rightarrow K_\ell} = 0, \quad Q_{K_h \rightarrow m} = -\Gamma_{hm}\rho_{K_h}, \quad Q_{m \rightarrow K_h} = 0, \quad (5.5)$$

all other, *a priori* possible, terms vanishing. To summarize, the model is characterized by four parameters, m_ℓ , m_h (or m_ℓ and R), $\Gamma_{\ell\gamma}$ and Γ_{hm} .

5.2 Background Evolution

5.2.1 Generalities

The equations of motion controlling the evolution of the background fields $\phi_\ell(t)$, $\phi_h(t)$ and of the fluid energy densities, $\rho_\gamma(t)$, $\rho_m(t)$ are the Friedman equation

$$H^2 = \frac{1}{3M_{\text{Pl}}^2} \left[\frac{\dot{\phi}_\ell^2}{2} + \frac{\dot{\phi}_h^2}{2} + V_\ell(\phi_\ell) + V_h(\phi_h) + \rho_\gamma + \rho_m \right], \quad (5.6)$$

the two Klein-Gordon equations for the light and heavy fields, namely

$$\ddot{\phi}_\ell + \left(3H + \frac{1}{2}\Gamma_{\ell\gamma} \right) \dot{\phi}_\ell + m_\ell^2 \phi_\ell = 0, \quad \ddot{\phi}_h + \left(3H + \frac{1}{2}\Gamma_{hm} \right) \dot{\phi}_h + m_h^2 \phi_h = 0, \quad (5.7)$$

and the two conservation equations for the radiation and pressure-less fluids

$$\dot{\rho}_\gamma + 4H\rho_\gamma = \frac{1}{2}\Gamma_{\ell\gamma}\dot{\phi}_\ell^2, \quad \dot{\rho}_m + 3H\rho_m = \frac{1}{2}\Gamma_{hm}\dot{\phi}_h^2. \quad (5.8)$$

We now describe the different epochs of evolution of the scenario. Initially, the terms $\Gamma_{\ell\gamma}$ and Γ_{hm} are chosen to be negligible, $\Gamma_{\ell\gamma} \ll H$ and $\Gamma_{hm} \ll H$. This implies that any pre-existing amount of radiation and/or matter (if any) plays no role during the initial phase of the model. In that case, we are left with two standard Klein-Gordon equations, $\ddot{\phi}_{\ell,h} + 3H\dot{\phi}_{\ell,h} + m_{\ell,h}^2\phi_{\ell,h} = 0$ and a simplified Friedman equation, $H^2 = (\dot{\phi}_\ell^2/2 + \dot{\phi}_h^2/2 + V_\ell + V_h)/(3M_{\text{Pl}}^2)$. Nevertheless, no exact, analytical, solution, to this system of equations is known and we will have to rely on numerical calculations, see below. However, the exact numerical solutions can be well-understood by means of the slow-roll approximation. We therefore introduce the (hierarchy of) Hubble-flow parameters ϵ_n defined by [79]

$$\epsilon_{n+1} = \frac{d \ln |\epsilon_n|}{dN}, \quad (5.9)$$

with $\epsilon_0 = \dot{H}/H$. In particular, the first Hubble-flow parameter, $\epsilon_1 = -\dot{H}/H^2 = 1 - \ddot{a}/(aH^2)$ indicates whether inflation occurs since $\epsilon_1 < 1$ is equivalent to $\ddot{a} > 0$. In the present case, one has

$$\epsilon_1 = \frac{1}{2H^2 M_{\text{Pl}}^2} (\dot{\phi}_\ell^2 + \dot{\phi}_h^2) = 3 \frac{\dot{\phi}_\ell^2/2 + \dot{\phi}_h^2/2}{\dot{\phi}_\ell^2/2 + \dot{\phi}_h^2/2 + V(\phi_\ell, \phi_h)}. \quad (5.10)$$

Therefore, in order to have inflation, one needs $\dot{\phi}_\ell^2/(H^2 M_{\text{Pl}}^2) \ll 1$ and $\dot{\phi}_h^2/(H^2 M_{\text{Pl}}^2) \ll 1$ and, as usual, this corresponds to a situation where the fields have sub-dominant kinetic energy compared to their potential energy. This also implies that the slow-roll Friedman equation can be approximated as $H^2 \sim (m_\ell^2 \phi_\ell^2 + m_h^2 \phi_h^2)/(6M_{\text{Pl}}^2)$.

The validity of the slow-roll approximation also depends on field acceleration, a piece of information which is encoded in the second Hubble-flow parameter given by

$$\epsilon_2 = 2\epsilon_1 + \frac{2}{H} \frac{\ddot{\phi}_\ell \dot{\phi}_\ell + \ddot{\phi}_h \dot{\phi}_h}{\dot{\phi}_\ell^2 + \dot{\phi}_h^2}. \quad (5.11)$$

Interestingly enough, and contrary to the single-field case, $\epsilon_2 \ll 1$ does not necessarily imply that $\ddot{\phi}_h/(H\dot{\phi}_h) \ll 1$ and $\ddot{\phi}_\ell/(H\dot{\phi}_\ell) \ll 1$ separately. In the following, we will nevertheless assume that this is true, in which case the two Klein-Gordon equations can be approximated as $3H\dot{\phi}_{\ell,h} + m_{\ell,h}^2\phi_{\ell,h} \sim 0$.

The previous considerations also allow us to re-write the first Hubble flow parameter as

$$\epsilon_1 \sim 2M_{\text{Pl}}^2 \frac{\phi_\ell^2 + R^4\phi_h^2}{(\phi_\ell^2 + R^2\phi_h^2)^2}. \quad (5.12)$$

As a consistency check, one verifies that, if the heavy field dominates, $m_h\phi_h \gg m_\ell\phi_\ell$, or $R\phi_h \gg \phi_\ell$, then the expression (5.12) reduces to $\epsilon_1 \simeq 2M_{\text{Pl}}^2/\phi_h^2$ which is, as expected, the single-field expression of the first Hubble flow parameter. If, on the contrary, the light field dominates, $\phi_\ell \gg R\phi_h$, then $\epsilon_1 \simeq 2M_{\text{Pl}}^2/\phi_\ell^2$ and, again, one recovers the single-field result (even though strictly speaking this rather requires the more constraining inequality $\phi_\ell \gg R^2\phi_h$).

5.2.2 Slow-roll evolution of the background

As already mentioned, if the slow-roll approximation is satisfied, then the equations of motion can be analytically integrated. Let us briefly (since this solution is standard in the literature) recall how this is derived, mainly in order to clarify the role of the integration constants. Summing up the two slow-roll Klein-Gordon equations (5.7) (where, in accordance with the previous discussion, we do not - yet - take into account the decay terms) and using the Friedmann equation, one arrives at

$$3H^2 \left(\phi_\ell \frac{d\phi_\ell}{dN} + \phi_h \frac{d\phi_h}{dN} \right) = -m_\ell^2\phi_\ell^2 - m_h^2\phi_h^2 = -6M_{\text{Pl}}^2 H^2, \quad (5.13)$$

which results in $d(\phi_\ell^2/M_{\text{Pl}}^2 + \phi_h^2/M_{\text{Pl}}^2)/ds = 4$. Here, the variable s is such that $ds/dN = -1$ which means that $s = -\ln(a/a_p) = -N + N_p$, a_p being the scale factor at a particular time “ t_p ” that we do not need to specify for the moment. Then, if one chooses the parameterisation, $\phi_\ell = r(s)\cos[\theta(s)]$, $\phi_h = r(s)\sin[\theta(s)]$, the above equation becomes a differential equation for $r(s)$ only, which can easily be solved. One finds $r(s) = \sqrt{r_0^2 + 4M_{\text{Pl}}^2(s - s_0)}$ where r_0 and s_0 are constants of integration. Moreover, using the slow-roll equation for the light field, one can show that the angle $\theta(s)$ obeys

$$\frac{2M_{\text{Pl}}^2}{r^2(s)}(R^2 - 1) \frac{ds}{d\theta} = \frac{1 + R^2 \tan^2 \theta}{\tan \theta}, \quad (5.14)$$

which can also be solved exactly, leading to

$$s = s_0 + \frac{r_0^2}{4M_{\text{Pl}}^2} \left[-1 + \frac{\cos^2 \theta_0}{\cos^2 \theta} \left(\frac{\tan \theta}{\tan \theta_0} \right)^{\frac{2}{R^2 - 1}} \right], \quad (5.15)$$

where $\theta_0 = \theta(s_0)$. As a consequence, the solutions for the light and heavy fields can be expressed as

$$\phi_\ell = 2M_{\text{Pl}} C^{1/2} (\tan \theta)^{1/(R^2-1)}, \quad \phi_h = 2M_{\text{Pl}} C^{1/2} (\tan \theta)^{R^2/(R^2-1)}, \quad (5.16)$$

where C is a constant given by

$$C = \frac{r_0^2}{4M_{\text{Pl}}^2} \frac{\cos^2 \theta_0}{(\tan \theta_0)^{2/(R^2-1)}}. \quad (5.17)$$

At this stage, without loss of generality, we can use our freedom to choose the peculiar time N_p in order to simplify the above expressions. A convenient choice is $N_p = N_0 + r_0^2/(4M_{\text{Pl}}^2)$ which implies that $s_0 = r_0^2/(4M_{\text{Pl}}^2)$. Then, it immediately follows that the expression for s simplifies to

$$s = C \frac{(\tan \theta)^{2/(R^2-1)}}{\cos^2 \theta}. \quad (5.18)$$

It is also interesting to express the quantity C in a way which is more convenient, in particular when numerical and analytical estimates are compared. Using the above expression of C , it is easy to establish that

$$C = N_{\text{tot}} \frac{\cos^2 \theta_{\text{ini}}}{(\tan \theta_{\text{ini}})^{2/(R^2-1)}} \left[1 - \frac{\cos^2 \theta_{\text{ini}}}{\cos^2 \theta_{\text{end}}} \left(\frac{\tan \theta_{\text{end}}}{\tan \theta_{\text{ini}}} \right)^{2/(R^2-1)} \right]^{-1}, \quad (5.19)$$

where θ_{ini} and θ_{end} are the value of θ at the beginning and at the end of inflation, respectively. The quantity $N_{\text{tot}} = N_{\text{end}} - N_{\text{ini}}$ is the total number of e-folds during inflation. At this point, one needs to elaborate a little bit on what we exactly mean by the end of inflation. Of course, the end of inflation is defined by $\epsilon_1 = 1$. However, the previous considerations are based on the slow-roll approximation which, *a priori*, ceases to be valid when the heavy field starts oscillating (in this regime, its kinetic energy equals its potential energy and the slow-roll approximation breaks down). However, when it is the case, the energy density of the heavy field becomes negligible and the Universe is dominated by the light field which is still slow-rolling. As a consequence, the slow-roll expression for ϕ_ℓ and for the Hubble parameter H found above can be extended in this regime. As mentioned before, in this case, $\epsilon_1 \simeq 2M_{\text{Pl}}^2/\phi_\ell^2$ and the end of inflation is given by $\tan \theta_{\text{end}} \simeq (2C)^{(1-R^2)/2}$, which implies $s_{\text{end}} = 1/2$ and, therefore, $N_p = N_{\text{end}} + 1/2$. Another reasoning is, however, possible. We can also say that the end of inflation cannot be predicted accurately within the slow-roll approximation but that it certainly happens when $\theta_{\text{end}} \ll 1$. As a consequence, given Eq. (5.18), $s_{\text{end}} = -N_{\text{end}} + N_p \simeq 0$, namely $N_p = N_{\text{end}}$. We conclude that analytical approximations lead to $N_p = N_{\text{end}} + \mathcal{O}(1)$ but that the extra factor of order one cannot be unambiguously determined in this framework. For simplicity, in the following, we will ignore it and take $N_p \simeq N_{\text{end}}$, which, with the help of Eq. (5.19), results in $C = N_{\text{tot}} \cos^2 \theta_{\text{ini}} / (\tan \theta_{\text{ini}})^{2/(R^2-1)}$. Let us also

notice that this last expression can be used to estimate the total number of e-folds in terms of the initial values of the fields. Straightforward manipulations lead to

$$N_{\text{tot}} = \frac{\phi_\ell^2|_{\text{ini}}}{4M_{\text{Pl}}^2} \left[1 + \left(\frac{\phi_h|_{\text{ini}}}{\phi_\ell|_{\text{ini}}} \right)^2 \right]. \quad (5.20)$$

Finally, with the choice $N_p = N_0 + r_0^2/(4M_{\text{Pl}}^2)$, one has $r(s) = 2M_{\text{Pl}}\sqrt{s}$ and the Hubble parameter can be written as

$$H^2(s) = \frac{2}{3}sm_\ell^2 [1 + (R^2 - 1)\sin^2\theta], \quad (5.21)$$

an expression which is a good approximation of the exact Hubble parameter during the whole inflation duration even when the heavy field is no longer slow-rolling (as explained above).

It is also interesting to relate the variable θ to the cosmic time. Using the chain equation

$$dt = \frac{dN}{H} = \frac{dN}{ds} \frac{ds}{d\theta} \frac{1}{H} d\theta = -\frac{ds}{d\theta} \frac{1}{H} d\theta, \quad (5.22)$$

the cosmic time can be expressed by mean of the following integral

$$\frac{m_\ell}{\sqrt{6}}(t - t_p) = -\frac{C^{1/2}}{R^2 - 1} \int_{\theta_p}^{\theta} \frac{\sqrt{1 + R^2 \tan^2 \theta}}{\sin \theta \cos \theta} (\tan \theta)^{\frac{1}{R^2-1}} d\theta, \quad (5.23)$$

which can be explicitly calculated. As a consequence, the relation between θ and t can be expressed as

$$\begin{aligned} \frac{m_\ell}{\sqrt{6}}(t - t_p) = & -C^{1/2} (\tan \theta)^{\frac{1}{R^2-1}} {}_2F_1 \left[-\frac{1}{2}, \frac{1}{2(R^2-1)}, 1 + \frac{1}{2(R^2-1)}; -R^2 \tan^2 \theta \right] \\ & + C^{1/2} (\tan \theta_p)^{\frac{1}{R^2-1}} {}_2F_1 \left[-\frac{1}{2}, \frac{1}{2(R^2-1)}, 1 + \frac{1}{2(R^2-1)}; -R^2 \tan^2 \theta_p \right], \end{aligned} \quad (5.24)$$

where ${}_2F_1(\cdot)$ is an hypergeometric function [80, 81]. In this expression, one is of course free to choose the peculiar time as one wishes.

Let us now study the exact solutions of the Friedmann and Klein-Gordon equations and how the approximations developed above perform. In the following, unless specified otherwise, we will always work with the “fiducial” parameters $m_\ell = 10^{-5}M_{\text{Pl}}$, $R = 5$, $\Gamma_{\ell\gamma} = 10^{-6}M_{\text{Pl}}$ and $\Gamma_{\text{hm}} = 10^{-5}M_{\text{Pl}}$. The initial conditions are chosen so that $\phi_\ell|_{\text{ini}} = 8M_{\text{Pl}}$, $\phi_h|_{\text{ini}} = 12M_{\text{Pl}}$ and a negligible amount of radiation and pressure-less matter (we come back to this question below). The velocities of the scalar fields are fixed according to the slow-roll approximation of their Klein-Gordon equation. This implies the following initial value for the Hubble parameter, $H_{\text{ini}} = 2.5 \times 10^{-4}M_{\text{Pl}}$. The corresponding exact, numerical, solutions for $\phi_\ell(N)$ (solid blue line), $\phi_h(N)$ (solid orange line) and the Hubble

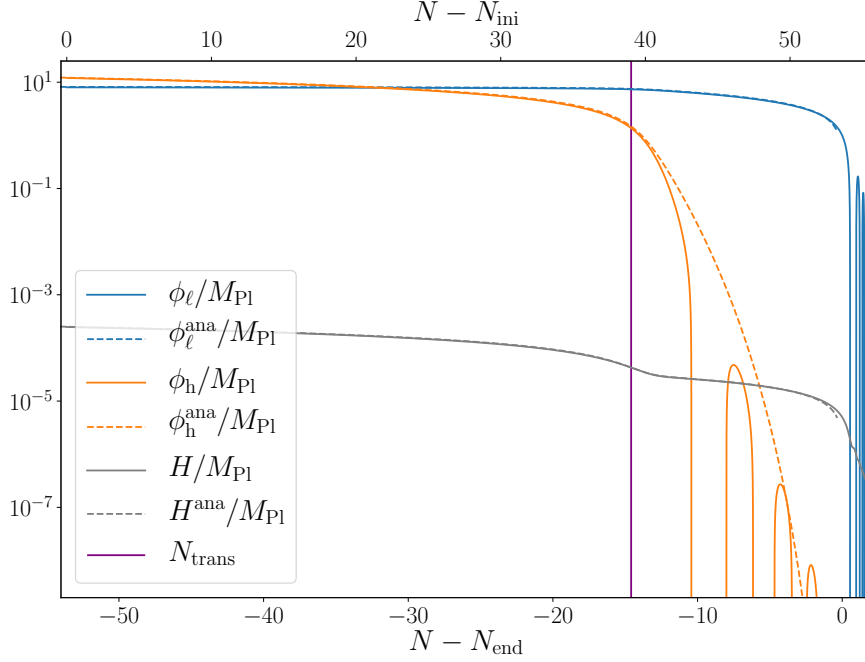


Figure 1: Light and heavy scalar fields and Hubble parameter during inflation, in Planck mass units. Exact numerical solutions (solid lines, respectively blue, orange and grey) and approximate, slow-roll, analytical solutions “ana” (dashed lines, respectively blue, orange and grey) given by Eqs. (5.16)–(5.21) are both displayed. The vertical purple line indicates the transition between the regime dominated by the heavy field and the regime dominated by the light field.

parameter $H(N)$ (solid grey line) during inflation are presented in Fig. 1. We have also plotted the slow-roll approximated evolution of the fields, Eqs. (5.16)–(5.21), see the dashed blue, orange and grey lines. In brief, the approximation evidently appears to be very good in the slow-roll regime. *A priori*, this regime is left when the fields start oscillating and, as a result, we see that the solid and dashed lines separate. Note, however, as already mentioned above, that even when the heavy field has started its oscillations, the slow-roll solutions for the light field and the Hubble parameter are still valid approximations because the universe becomes quickly dominated by the light field which is still slowly rolling.

Let us now describe Fig. 1 in more quantitative terms. One first sees that the heavy field has initially a vacuum expectation value higher than that of the light field and, therefore, starts “higher” in the potential. This regime can be understood by means of Eqs. (5.16) and (5.21). One can indeed assume that, initially, the heavy field completely dominates the energy budget of the universe. This is a good approximation as can be

checked if, for instance, one uses it to calculate the initial value of the Hubble parameter. This gives $H_{\text{ini}}/M_{\text{Pl}} \simeq m_{\text{h}}\phi_{\text{h}}|_{\text{ini}}/(\sqrt{6}M_{\text{Pl}})$ leading, with the fiducial parameters of Fig. 1, to $H_{\text{ini}} \simeq 2.5 \times 10^{-4}M_{\text{Pl}}$, a value in perfect agreement with the exact, numerical, value given above. In the heavy phase, when $\phi_{\text{h}} \gg \phi_{\ell}$, $\cos^2 \theta$ is a small quantity (for the initial conditions studied here this is admittedly not very accurate since one “only” has $\cos^2 \theta_{\text{ini}} = 4/13 \simeq 0.31$ but it could be smaller if the difference between $\phi_{\text{h}}|_{\text{ini}}$ and $\phi_{\ell}|_{\text{ini}}$ were chosen to be larger) and

$$s \simeq C (\cos^2 \theta)^{-R^2/(R^2-1)} \left(1 - \frac{\cos^2 \theta}{R^2 - 1} + \dots \right) \simeq \frac{C}{\cos^2 \theta}, \quad (5.25)$$

where (in the last expression only) we have also assumed $R \gg 1$. As a consequence, $\theta \simeq \arccos[(C/s)^{1/2}]$ and one obtains

$$\phi_{\ell} = M_{\text{Pl}}\sqrt{4s} \cos[\theta(s)] \simeq 2M_{\text{Pl}}C^{1/2} \simeq \phi_{\ell}|_{\text{ini}}, \quad (5.26)$$

which is a constant, in agreement with what we observe in Fig. 1 during the domination of the heavy field. Notice that this approximation also leads to a simplified expression for the constant C , namely

$$C \simeq \frac{\phi_{\ell}^2|_{\text{ini}}}{4M_{\text{Pl}}^2}. \quad (5.27)$$

Regarding the heavy field, in the regime discussed here, its slow-roll trajectory can be approximated by $\phi_{\text{h}} = M_{\text{Pl}}\sqrt{4s} \sin[\theta(s)] \simeq M_{\text{Pl}}\sqrt{4(s-C)}$, or

$$\phi_{\text{h}}^2(N) = -\phi_{\ell}^2|_{\text{ini}} - 4M_{\text{Pl}}^2(N - N_{\text{end}}) = \phi_{\text{h}}^2|_{\text{ini}} - 4M_{\text{Pl}}^2(N - N_{\text{ini}}), \quad (5.28)$$

where, in the last expression, we have made use of Eq. (5.20). This last expression corresponds to the single-field trajectory for a large field model (with a quadratic potential) which, of course, makes sense since, in this regime, the heavy field completely dominates the energy budget of the Universe. It is also easy to calculate the evolution of the Hubble parameter, and the results reads

$$H^2 \simeq -\frac{1}{6}m_{\text{h}}^2 \frac{\phi_{\ell}^2|_{\text{ini}}}{M_{\text{Pl}}^2} - \frac{2}{3}m_{\text{h}}^2 = H^2|_{\text{ini}} - \frac{2}{3}m_{\text{h}}^2(N - N_{\text{ini}}), \quad (5.29)$$

where, again, we have used Eq. (5.20). As expected, one also recovers the single-field expression of the Hubble parameter.

Finally, making use of Eq. (5.20) yet another time, with the fiducial parameters chosen before, one has $N_{\text{tot}} \simeq 52$ to be compared with the exact, numerical, value $N_{\text{tot}} = 53.6$.

The regime described above lasts until the energy density of the heavy field (which decreases with time) equals that of the light field (which stays approximatively constant). This transition occurs when $m_{\text{h}}\phi_{\text{h}} = m_{\ell}\phi_{\ell}$ or $\theta_{\text{trans}} = \arctan(1/R)$. Let us notice that, at the transition $\cos \theta_{\text{trans}} = R/\sqrt{R^2 + 1}$ and, in the limit $R \gg 1$, we see that $\cos \theta_{\text{trans}}$

is not small (but rather of order one) and, therefore, one expects to observe deviations from the above trajectories already at the transition (or even before). Using Eq. (5.18), which is valid even if $\cos \theta$ is not small, one can evaluate the time of transition quite precisely. One obtains

$$s_{\text{trans}} = -N_{\text{trans}} + N_{\text{end}} = CR^{2R^2/(1-R^2)}(1+R^2) \simeq \frac{\phi_{\ell}^2|_{\text{ini}}}{4M_{\text{Pl}}^2} R^{2R^2/(1-R^2)}(1+R^2), \quad (5.30)$$

where we have used the simplified expression of C , see Eq. (5.27). For the fiducial parameters used before, one finds $N_{\text{trans}} - N_{\text{end}} \simeq -14.6$, in perfect agreement with the exact, numerical, value $N_{\text{trans}} - N_{\text{end}} = -14.49$. Notice that, in Fig. 1, the crossing between the blue and orange lines corresponds to the time at which the vacuum expectation value of the heavy field becomes smaller than the expectation value of the light field. This time has clearly nothing to do with the transition mentioned before and is not associated with any change in the physical properties of the system. In fact, the passage from the phase dominated by the heavy field to the phase dominated by the light field manifests itself by the small dropout in the evolution of the Hubble parameter that can be seen in Fig. 1 and which occurs around N_{trans} . At this time, using Eq. (5.21), the Hubble parameter is given by

$$H_{\text{trans}}^2 = \frac{2}{3}s_{\text{trans}}m_{\ell}^2[1 + (R^2 - 1)\sin^2 \theta_{\text{trans}}] = \frac{4}{3}s_{\text{trans}}m_{\ell}^2 \frac{R^2}{R^2 + 1} \quad (5.31)$$

$$\simeq \frac{1}{3} \frac{\phi_{\ell}^2|_{\text{ini}}}{M_{\text{Pl}}^2} m_{\text{h}}^2 R^{2R^2/(1-R^2)}, \quad (5.32)$$

that is to say $H_{\text{trans}} \simeq 4.3 \times 10^{-5} M_{\text{Pl}}$ to be compared with the value observed in Fig. 1, namely 4.27×10^{-5}

After the transition, the contribution from the heavy field becomes negligible and the universe is dominated by the light field which is no longer frozen (as can be checked in Fig. 1) and starts to move. In this regime $\theta \ll 1$ [we have seen before that, already at the transition, $\theta_{\text{trans}} = \arctan(1/R) \ll 1$] and, as a consequence, we can write

$$s \simeq C \theta^{2/(R^2-1)} \left[1 + \frac{3R^2-1}{3(R^2-1)} \theta^2 + \dots \right] \simeq C \theta^{2/R^2} (1 + \theta^2 + \dots), \quad (5.33)$$

where, in the last equality, we have used $R \gg 1$. This implies that $\theta \simeq (s/C)^{R^2/2}$ and this phase corresponds to values of s/C such that $s/C \ll 1$. Then, using the slow-roll trajectory (5.16) where we neglect the cosine term given that $\theta \ll 1$, one obtains

$$\phi_{\ell}^2 \simeq 4M_{\text{Pl}}^2(N_{\text{end}} - N). \quad (5.34)$$

In a similar way, using Eq. (5.21), one finds that

$$H^2 \simeq \frac{2}{3}m_{\ell}^2 s = \frac{2}{3}m_{\ell}^2(N_{\text{end}} - N). \quad (5.35)$$

Notice that, at the end of inflation, by definition, $s = 0$ and, therefore, one finds $\phi_\ell|_{\text{end}} = H_{\text{end}} = 0$. It is easy to see that this is a consequence of the fact that we chose $N_p = N_{\text{end}}$. If, instead, as discussed above, we had chosen $N_p = N_{\text{end}} + 1/2$ then we would have found $H^2 = 2m_\ell^2(N_{\text{end}} - N + 1/2)/3$ and, therefore, $H_{\text{end}}^2 = m_\ell^2/3$. This is completely consistent with the fact that, during the epoch dominated by the light field, $\epsilon_1 \simeq 2M_{\text{Pl}}^2/\phi_\ell^2$ implying that $\phi_\ell|_{\text{end}} \simeq \sqrt{2}M_{\text{Pl}}$ and $H_{\text{end}} \simeq m_\ell/\sqrt{3} \simeq 5.8 \times 10^{-6}$, to be compared with the exact numerical value $H_{\text{end}} = 4.97 \times 10^{-6}$.

5.2.3 Matter and radiation energy densities during slow-roll

Let us now study how matter and radiation behave in the regime described above. The conservation equation for matter (5.8) can be re-written

$$\frac{d}{dt}(a^3 \rho_m) = \frac{\Gamma_{\text{hm}}}{2} a^3 \dot{\phi}_h^2, \quad (5.36)$$

and the solution reads

$$a^3(t) \rho_m(t) - a^3(t_{\text{ini}}) \rho_m(t_{\text{ini}}) = \frac{\Gamma_{\text{hm}}}{2} \int_{t_{\text{ini}}}^t a^3(\tau) \dot{\phi}_h^2(\tau) d\tau. \quad (5.37)$$

A rough approximation consists in assuming that, since the heavy field is in slow-roll, the quantity $\dot{\phi}_h^2$ can be brought outside the integral. Then, using an exponential (de Sitter) scale factor, we arrive at

$$\rho_m(t) \simeq \left(\frac{a_{\text{ini}}}{a}\right)^3 \left[\rho_m(t_{\text{ini}}) - \frac{\Gamma_{\text{hm}}}{6H} \dot{\phi}_h^2 \right] + \frac{\Gamma_{\text{hm}}}{6H} \dot{\phi}_h^2 \longrightarrow \frac{\Gamma_{\text{hm}}}{6H} \dot{\phi}_h^2 \simeq \frac{\Gamma_{\text{hm}} m_h^4}{54H^3} \phi_h^2(t). \quad (5.38)$$

This expression is valid as long as the heavy field is in slow-roll that is to say, roughly speaking, until the transition time. Similar considerations lead to a solution for the radiation energy density, namely

$$\rho_\gamma(t) \simeq \left(\frac{a_{\text{ini}}}{a}\right)^4 \left[\rho_\gamma(t_{\text{ini}}) - \frac{\Gamma_{\ell\gamma}}{8H} \dot{\phi}_\ell^2 \right] + \frac{\Gamma_{\ell\gamma}}{8H} \dot{\phi}_\ell^2 \longrightarrow \frac{\Gamma_{\ell\gamma}}{8H} \dot{\phi}_\ell^2 \simeq \frac{\Gamma_{\ell\gamma} m_\ell^4}{72H^3} \phi_\ell^2(t). \quad (5.39)$$

Since the light field is in slow-roll until the end of inflation, this solution is valid until that time. The two solutions (5.38) and (5.39) are represented in Fig. 2 and compared to the corresponding exact, numerical, solutions. Evidently, they match very well the numerical results.

5.2.4 Decays of inflaton fields

Let us now discuss the decays of the heavy and light fields. The decay of the heavy field happens first. Predicting, with good accuracy, the time at which it happens turns out to be a central issue in this article since we will see in the following sections that, in fact, this quantity determines the level of non-adiabatic perturbations in the post-inflationary universe. Usually, the criterion that allows us to identify when the decay starts is $H \simeq \mathcal{O}(1)\Gamma_{\text{hm}}$ or, dimensionally, $t_{\text{decay,h}} \simeq \mathcal{O}(1)/\Gamma_{\text{hm}}$. This criterion can be

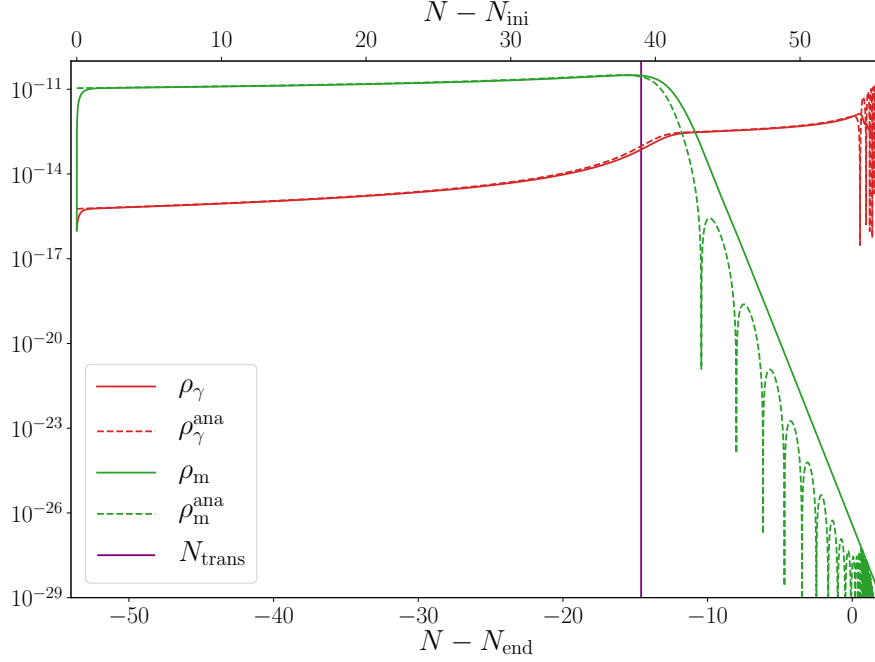


Figure 2: Behaviour of the fluids’ energy densities during multifield inflation. Exact numerical results (solid lines) as well as the analytical approximations “ana” (dashed lines) given by Eqs. (5.38)–(5.39), are represented both for radiation (red) and matter (green). The agreement is nearly perfect until the time when the scalar field to which the fluid is coupled, leaves the slow-roll regime and begins to oscillate. The vertical purple line indicates the transition between the regime dominated by the heavy field and the regime dominated by the light field.

quite accurate especially in the context of single-field models where H evolves rapidly towards the end of inflation. However, it is interesting to notice that this is no longer true in the present context, a fact that, to our knowledge, has not been fully appreciated in the existing literature. The reason for this difficulty is that the Hubble parameter changes very slowly in this regime (recall that H still obeys the slow-roll approximation since the light field is now dominant). As a consequence, a substantial error in the determination of the decay time can easily be made resulting in a large error in the predicted level of non-adiabatic perturbations in the post-inflationary Universe [and in the value of $\rho_h(t)$ at the end of inflation]. Therefore, it is important to track the behaviour of the background during the heavy field decay with some accuracy. We now turn to this question.

In order to further motivate the need for an accurate (hence, unfortunately, more complicated) treatment of the question, which is given in Appendix A, we start with a treatment which is both intuitive and simple. As argued in this section, it will turn out

that this approach is not enough in order to reach our goal, namely calculate analytically, with good accuracy, the non-adiabatic perturbations after inflation.

Soon after the transition between the phase dominated by the heavy field and the phase dominated by the light field, the heavy field oscillates and decays. In order to study the detailed behaviour of $\phi_h(t)$, one writes $\phi_h(t) = (a/a_p)^{-3/2} \phi_{h,p} e^{-\Gamma_{hm}(t-t_p)/4} g_h(t)$, where we recall that t_p is a particular time and $g_h(t)$ is a function defined by the previous equation. Let us also emphasize here that this particular time needs not to be chosen as before. In the present context, it should be thought as the time from which the above writing of $\phi_h(t)$ is relevant, see below for more discussions about this point, which turns out to be quite important. Then, using Eq. (5.7) the function $g_h(t)$ obeys the equation

$$\ddot{g}_h(t) + m_h^2 \left(1 - \frac{3}{2} \epsilon_1 \frac{H^2}{m_h^2} - \frac{9}{4} \frac{H^2}{m_h^2} - \frac{1}{16} \frac{\Gamma_{hm}^2}{m_h^2} - \frac{3}{4} \frac{H}{m_h} \frac{\Gamma_{hm}}{m_h} \right) g_h(t) = 0. \quad (5.40)$$

This is the equation of a parametric oscillator with its time-dependent frequency given by

$$\omega_h^2(t) = m_h^2 - \frac{3}{2} \epsilon_1 H^2 - \frac{9}{4} H^2 - \frac{1}{16} \Gamma_{hm}^2 - \frac{3}{4} H \Gamma_{hm}. \quad (5.41)$$

Unfortunately, the exact time dependence of $\omega_h^2(t)$ is too complicated to permit an explicit integration of Eq. (5.40). A plot of ω_h^2 is given in Appendix A, see Fig. 24. One of the main feature of this plot is to show that ω_h^2 is negative during the heavy field slow-roll regime. In fact, it remains negative until a time t_{osc} such that $\omega_h^2(t_{osc}) = 0$ (which is, therefore, a turning point) after which $\omega_h^2 > 0$ and it is only in this regime that $\phi_h(t)$ starts oscillating. It is also important to notice that the transition time lies in the region where $\omega_h^2 < 0$, that is to say $t_{trans} < t_{osc}$.

During the decay of the heavy field, the background is still in slow-roll and, therefore, the Hubble parameter evolves slowly. As a first approximation, we can thus assume that ω_h^2 remains constant in this regime. Then, it is straightforward to write the solution of Eq. (5.40) which reads $g_h(t) = \cos[\omega_h(t - t_p)] + B \sin[\omega_h(t - t_p)]$, where B is an integration constant. Notice that $g_h(t_p) = 1$ (as appropriate given the definition of g_h) and $B = \dot{g}_h(t_p)/\omega_h$. From the above considerations, it is clear that t_p must be chosen such that $t_p > t_{osc}$ (and, as a consequence, t_p cannot be chosen to be t_{trans}). For times $t \gg t_p$, $\phi_h(t)$ has undergone several oscillations and we can calculate the time average of the solution (denoted by $\langle \cdot \rangle$ in the following). This leads to

$$\langle \phi_h^2 \rangle = \phi_p^2 \frac{1}{2} (1 + B^2) \left(\frac{a_p}{a} \right)^3 e^{-\Gamma_{hm}(t-t_p)/2}, \quad (5.42)$$

and

$$\langle \dot{\phi}_h^2 \rangle = m_h^2 \phi_p^2 \frac{1}{2} (1 + B^2) \left(\frac{a_p}{a} \right)^3 e^{-\Gamma_{hm}(t-t_p)/2}. \quad (5.43)$$

We see that the two above equations imply equipartition between kinetic and potential energy. Notice that the term $\propto \epsilon_1 H^2/m_h^2$ has been neglected in order to be consistent

with the assumption that the Hubble parameter is constant. This gives an expression for the heavy field energy density, $\rho_h \simeq m_h^2 \langle \phi_h^2 \rangle$.

The expression of the field derivative (5.43) could also be used to calculate the evolution of the matter energy density, see Eq. (5.37). Indeed, contrary to the slow-roll case, the evolution of the heavy field is no longer slow and, as a consequence, the term $\dot{\phi}_h^2$ cannot be brought outside the integral. However, using the above analytical formula (5.43), it can be calculated explicitly. Indeed, inserting Eq. (5.43) in Eq. (5.37), one arrives at

$$\rho_m(t) = m_h^2 \phi_p^2 \frac{1}{2} (1 + B^2) \left(\frac{a_p}{a} \right)^3 \left[1 - e^{-\Gamma_{hm}(t-t_p)/2} \right] + \rho_m^p \left(\frac{a_p}{a} \right)^3. \quad (5.44)$$

Pushing the solution (5.38) up to t_p , we have $\rho_m^p \sim \Gamma_{hm} m_h^4 \phi_p^2 / (54H^3)$, hence the second term is negligible as soon as $1 - e^{-\Gamma_{hm}(t-t_p)/2} > \Gamma_{hm} m_h^2 / [27(1+B^2)H^3]$ which is very quickly true, roughly $\Gamma_{hm}(t-t_p) > 0.05$. Therefore, the second term can be neglected and, following the considerations presented above, we have thus obtained simple expressions for $\rho_h(t)$ and $\rho_m(t)$.

Then, the time of decay of the heavy field, $t_{\text{decay,h}}$ is defined by the condition $\rho_h(t_{\text{decay,h}}) = \rho_m(t_{\text{decay,h}})$ and, using the above expressions, we arrive at

$$t_{\text{decay,h}} - t_p = \frac{2}{\Gamma_{hm}} \ln 2. \quad (5.45)$$

We see it has the form predicted above (namely, inversely proportional to the decay rate) with the factor $\mathcal{O}(1)$ being simply $2 \ln 2 \simeq 1.39$.

Finally, if one wants to express the time of decay not in terms of cosmic time but in terms of the number of e-folds, one can use the fact that the oscillatory behaviour of the heavy field takes place during the phase dominated by the light field during which $H^2 = 2m_\ell^2(N_{\text{end}} - N)/3$, see Eq. (5.35). As a consequence, given that $dN = Hdt$, one finds

$$t - t_p = -\frac{\sqrt{6}}{m_\ell} \left[(N_{\text{end}} - N)^{1/2} - (N_{\text{end}} - N_p)^{1/2} \right], \quad (5.46)$$

which allows us to relate t and N . This relation is a simplified version of the exact (5.24). It follows that the number of efolds at which the heavy field decay occurs would be given by the expression

$$N_{\text{end}} - N_{\text{decay,h}} = \left[(N_{\text{end}} - N_p)^{1/2} - \frac{m_\ell}{\Gamma_{hm}} \frac{2}{\sqrt{6}} \ln 2 \right]^2. \quad (5.47)$$

At this stage, we would need to choose the particular time t_p . As already mentioned, this cannot be t_{trans} because it lies in the region where $\omega_h^2 < 0$. It cannot be t_{osc} either since $\omega(t_{\text{osc}}) = 0$ and the solution for $g_h(t)$ in terms of trigonometric functions presented before becomes ill-defined. In fact, the trigonometric solution for $g_h(t)$ introduced before is nothing but the WKB solution of Eq. (5.40) in the regime where ω_h^2 is constant and

positive. The WKB approximation becomes valid if $\dot{\omega}_h/(2\omega_h^2) < 1$. Therefore, a natural definition of t_p would be the time such that $\dot{\omega}_h = 2\mathcal{C}\omega_h^2$ where $\mathcal{C} \leq 1$ is a constant which quantifies how restrictive the WKB criterion is chosen (namely, for instance, $\mathcal{C} = 1$ or $0.1, \dots$). This time will be noted $t_p = t_{\text{wkb}}$ in the following. In the vicinity of the turning point (since we expect $t_p = t_{\text{wkb}}$ to be close to t_{osc}) a good approximation for the time-dependent frequency is $\omega_h^2 \simeq m_h^2 - 9H^2/4$, which implies that $\dot{\omega} = 9\epsilon_1 H^3/(4\omega)$. As a consequence t_{wkb} (or rather θ_{wkb}) is a solution of the following equation

$$\frac{H^2}{m_h^2} = \left[\frac{9}{4} + \left(\frac{9\epsilon_1}{8\mathcal{C}} \right)^{2/3} \right]^{-1}, \quad (5.48)$$

where H is given by Eq. (5.21) [with s defined by Eq. (5.18)] and ϵ_1 by Eq. (A.14). For $\mathcal{C} = 1$, one finds $\tan \theta_{\text{wkb}} \simeq 0.076$ and for $\mathcal{C} = 0.1$, $\tan \theta_{\text{wkb}} \simeq 0.031$ that is to say $N_{\text{end}} - N_{\text{wkb}} \simeq 12.98$ ($\mathcal{C} = 1$) or $N_{\text{end}} - N_{\text{wkb}} \simeq 11.99$ ($\mathcal{C} = 0.1$). Using Eq. (5.47), this leads to $N_{\text{end}} - N_{\text{decay,h}} \simeq 9.22$ ($\mathcal{C} = 1$) or $N_{\text{end}} - N_{\text{decay,h}} \simeq 8.39$ ($\mathcal{C} = 0.1$). At the time t_{wkb} , the Hubble parameter is equal to $H_{\text{wkb}} \simeq 3.13 \times 10^{-5} M_{\text{Pl}}$ ($\mathcal{C} = 1$) or $H_{\text{wkb}} \simeq 2.86 \times 10^{-5} M_{\text{Pl}}$ ($\mathcal{C} = 0.1$). If the WKB criterion is more stringent, then, since H decreases during inflation, it is satisfied later in the history of the Universe which explains the previous results. The corresponding values for the effective frequency are $\omega_{\text{wkb}} \simeq 1.7 \times 10^{-5} M_{\text{Pl}}$ ($\mathcal{C} = 1$) or $\omega_{\text{wkb}} \simeq 2.5 \times 10^{-5} M_{\text{Pl}}$ ($\mathcal{C} = 0.1$). These are the values of the frequency to be used in the expression of $g_h(t)$ introduced above. Finally, making use of Eq. (A.12), one has $\dot{g}(t_{\text{wkb}})/\omega_h(t_{\text{wkb}}) = B \simeq 1.34$ ($\mathcal{C} = 1$) and $\dot{g}(t_{\text{wkb}})/\omega_h(t_{\text{wkb}}) = B \simeq 0.65$ ($\mathcal{C} = 0.1$). The last ingredient is $\phi_p = \phi_h(t_{\text{wkb}})$. Here, one can use the slow-roll expression even if, strictly speaking, we are already outside its domain of validity. However, since t_{wkb} lies close to the transition between slow-roll and the onset of the oscillations, this estimate should be reasonable, see Fig. 1. One obtains $\phi_h(t_{\text{wkb}}) \simeq 0.54 M_{\text{Pl}}$ ($\mathcal{C} = 1$) or $\phi_h(t_{\text{wkb}}) \simeq 0.21 M_{\text{Pl}}$ ($\mathcal{C} = 0.1$). We now have everything to plot $\rho_h = m_h^2 \langle \phi_h^2 \rangle$, see Eq. (5.42) and ρ_m , see Eq. (5.44). They are represented and compared to the exact, numerical, solutions in Fig. 3. The above considerations lead to $N_{\text{decay,h}} \simeq -8.39$ to be compared with the exact result $N_{\text{decay,h}} \simeq -10.81$.

Unfortunately, we notice that the precision of this result is not enough to predict with good accuracy the behaviours of $\rho_h(t)$ and $\rho_m(t)$ and, therefore, the final level of non-adiabatic perturbations after the end of inflation. Therefore, if one wants an analytical result for $N_{\text{decay,h}}$, one needs better approximations for the behaviour of $\rho_h(t)$ and $\rho_m(t)$ around the time of decay of the heavy field. Such a calculation (which is more involved at the technical level) is carried out in great details in Appendix A.

Finally, as can also be observed in Fig. 1, the light field starts to oscillate and decays when $H \simeq \Gamma_{\ell\gamma}$, that is to say

$$s_{\ell,\text{decay}} = -N_{\ell,\text{decay}} + N_{\text{end}} \simeq \frac{3}{2} \mathcal{O}(1) \frac{\Gamma_{\ell\gamma}^2}{m_\ell^2}. \quad (5.49)$$

Numerically, for the parameters considered here, this gives $N_{\ell,\text{decay}} \simeq N_{\text{end}}$, namely around the end of inflation in agreement with Fig. 1. This estimate is better than the

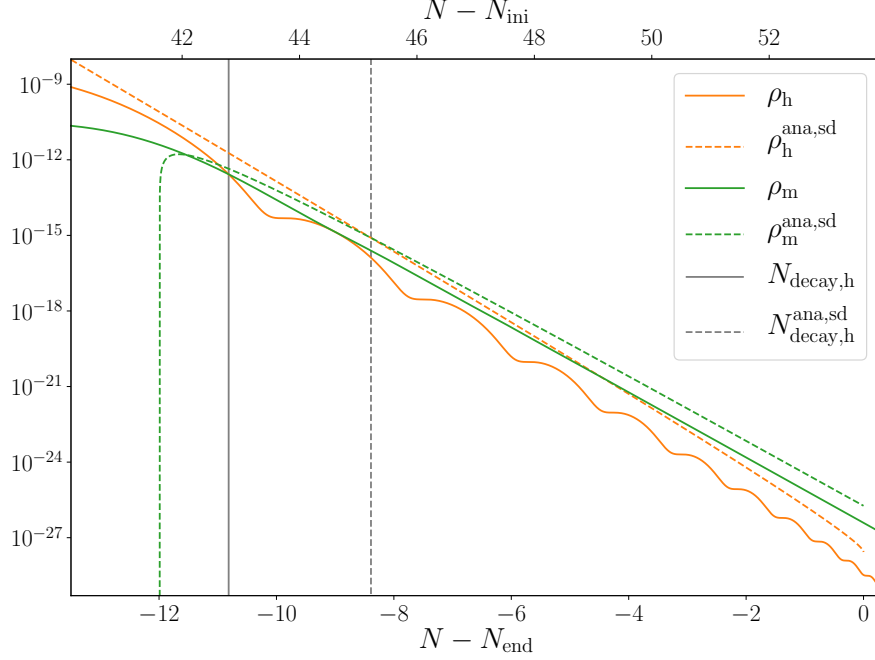
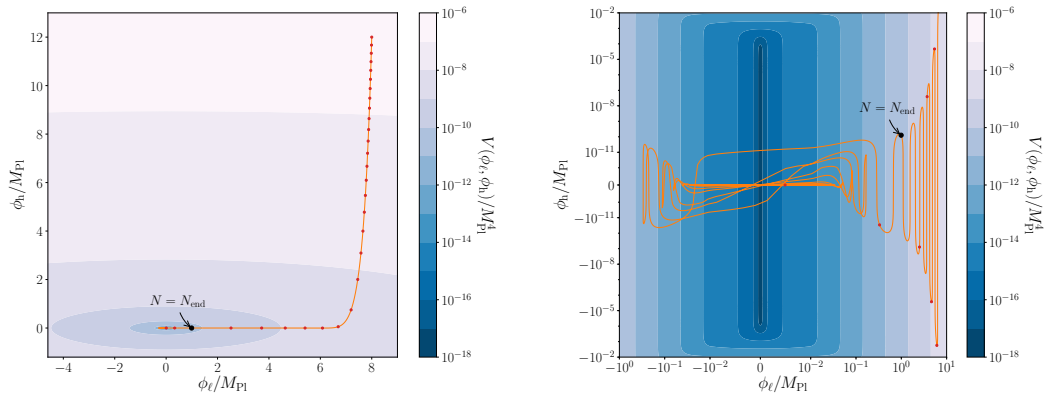


Figure 3: Behaviour of ρ_h and ρ_m during the decay of the heavy field. Here we show both their exact numerical values (respectively the orange and green solid lines), and their analytical formulas inferred from the simple decay approximation presented in this section, “ana,sd” (respectively the orange and green dashed lines) as given by Eqs. (5.42)–(5.43) and Eq. (5.44). Moreover the time of decay of the heavy field, defined as the time when $\rho_h = \rho_m$ is shown with the vertical grey lines both from the numerical approach (solid line, $N_{\text{decay,h}} = -10.81$) and the simple decay analytical approximation (dashed line, $N_{\text{decay,h}}^{\text{ana,sd}} = -8.39$). Clearly, this simple formalism is not sufficient to encapsulate the physics of the decay of the heavy field: a more rigorous approach is proposed in the Appendix A, see in particular Fig. 26.

estimate of the heavy field decay time because, around the end of inflation, the Hubble parameter evolves much more abruptly than when the heavy field starts oscillating. This also leads to an estimate of the reheating temperature of this model. Given that, just after the end of inflation, the universe is dominated by radiation, one can write $3M_{\text{Pl}}^2 H_{\ell,\text{decay}}^2 \simeq 3M_{\text{Pl}}^2 \Gamma_{\ell\gamma}^2 = \pi^2 g_* T_{\text{rh}}^4 / 30$ or

$$g_*^{1/4} T_{\text{rh}} \simeq \left(\frac{90}{\pi^2} \right)^{1/4} \sqrt{\Gamma_{\ell\gamma} M_{\text{Pl}}}, \quad (5.50)$$

where g_* is the number of relativistic degrees of freedom just after the fields decay. With our fiducial parameters, one finds $g_*^{1/4} T_{\text{rh}} \simeq 0.0023 M_{\text{Pl}} \simeq 5.53 \times 10^{15} \text{ GeV}$.



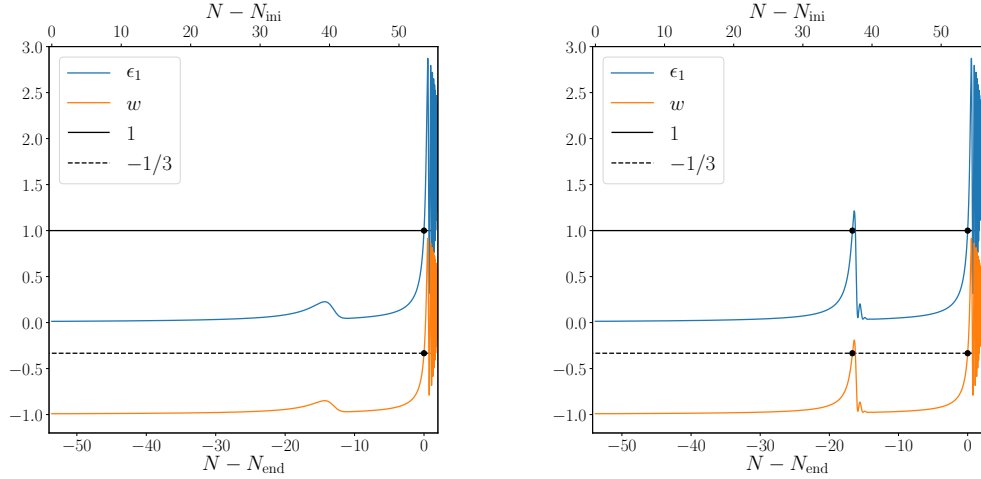
(a) Linear scaling for the whole trajectory: the field-space turn is clearly visible. (b) Logarithmic scaling for the last e -folds of inflation: the fields' oscillations are resolved.

Figure 4: Field-space (ϕ_ℓ, ϕ_h) background trajectory from the numerical evolution (orange line) superimposed on the two-field potential contour levels. The instantaneous direction of the trajectory is aligned with the potential gradient and is therefore effectively single-field like, except around the turn which is a truly multifield feature. Red dots along the trajectory are equally spaced by $\Delta N = 2$ e -folds of expansion and the black dot denotes the end of inflation.

5.2.5 Evolution in field space

In Fig. 4, we have again represented the trajectory of the system but, now, in the two-dimensional space (ϕ_ℓ, ϕ_h) superimposed on the potential contour levels. On the left panel, we have focused on the slow-roll regime and the two phases, dominated respectively by the heavy and light fields, are clearly visible. The sharp turn separating these two epochs is also easy to identify. On the right panel, we have zoomed in on the vicinity of the minimum of the potential in order to see the oscillations of the fields occurring after the end of inflation. In those two panels, the “non-isotropic” character of the contour levels is of course a consequence of the fact that the two fields do not have the same mass.

In Fig. 5, we have represented the evolution of the first Hubble-flow parameter (blue line) and the equation of state parameter, namely the pressure to energy density ratio (orange line), during inflation. The left panel corresponds to the fiducial parameters already used in Fig. 1 (and used throughout this article). We see that it represents a situation where inflation is never interrupted. The time at which the heavy field (or, rather, the energy density associated to this field) becomes subdominant manifests itself as a small bump around $N - N_{end} \simeq -14.6$ (already identified as a small dropout in the evolution of the Hubble parameter in Fig. 1) but we notice that ϵ_1 never reaches one (horizontal solid black line) and w is never greater than $-1/3$ (horizontal dashed black line). The end of inflation occurs when the light field starts to oscillate and is represented by the black dot. The right panel represents the evolution of the same quantities with the



(a) Set of parameters presented in the main text and used in all other figures. (b) Same set of parameters, except for the ratio of masses taken to be $R = 15$ here.

Figure 5: First Hubble-flow parameter $\epsilon_1 = -\dot{H}/H^2$ and total equation of state of the universe $w = p/\rho$, for two sets of parameters differing only by the value of R . The solid (respectively dashed) black line represents the maximal value for ϵ_1 (respectively w) in order for inflation to proceed: 1 (respectively $-1/3$). Black dots represent times at which inflation is stopped, either temporarily or permanently. For $R = 5$ (left panel), inflation slows down but does not stop when the heavy field reaches the minimum of its potential around $N - N_{\text{end}} \simeq -14.6$, while for $R = 15$ (right panel) its oscillations are so strong that inflation is transiently violated. In this work, we choose to focus on a region of parameter space such that inflation is not transiently violated, and keep $R = 5$ in our fiducial model. At the end of inflation, the fast oscillations of the light field at the bottom of its quadratic potential around $N \simeq N_{\text{end}}$, are responsible for an equation of state w which averages to zero over a few oscillations, the Universe thus behaving, on average and on large scales, effectively as if it was dominated by a pressure-less fluid.

same initial conditions for the fields and the same values of the parameters except that, now, $R = 15$. In that case, the physical situation is very different from the one depicted on the left panel. In particular, around $N - N_{\text{end}} \simeq -16.4$ (“first” black dot), we notice that inflation temporarily comes to an end at the transition between the heavy and light phases. Indeed, ϵ_1 becomes larger than one and w becomes larger than $-1/3$. This can be understood as follows. At the transition, $R\phi_h = \phi_\ell$ and, therefore, from Eq. (5.12), $\epsilon_1 \simeq M_{\text{Pl}}^2(1+R^2)/(2\phi_\ell^2)$. Using the crude approximation that the light field stays constant during the heavy phase, this can also be written as $\epsilon_1 \simeq M_{\text{Pl}}^2(1+R^2)/(2\phi_\ell|_{\text{ini}}^2)$. As a consequence, inflation stops at the transition only if $R \gtrsim \sqrt{2}\phi_\ell|_{\text{ini}}/M_{\text{Pl}}$, which gives in our case $R \gtrsim 11.3$ (exploring the parameter space numerically, we rather find this threshold value to be $R \gtrsim 12.9$). Therefore, the left panel of Fig. 5 ($R = 5$) corresponds

to a case where inflation does not stop since R is slightly below the threshold. On the contrary, the situation on the right panel corresponds to $R = 15$ and one expects a transient violation of inflation which is what is observed.

We see that, despite its *a priori* simplicity, the solutions for the fields in the double inflation model possess a rich variety of different behaviours. In order to simplify the discussion, in the following, we will always assume that inflation never stops before both fields have reached the bottom of their potential. In practice, as already mentioned, we will always work with the fiducial parameters corresponding to Fig. 1.

5.2.6 Evolution of the fractional energy densities

Yet another way to understand the evolution of the system is to plot the quantities $\Omega_i \equiv \rho_i/\rho_{\text{tot}}$ where ρ_i is the energy density of the fluid “ i ” and ρ_{tot} is the total energy density. By definition, one has $\sum_i \Omega_i = 1$. The corresponding plot is presented in Fig. 6 where Ω_{ϕ_ℓ} corresponds to the solid blue line, Ω_{ϕ_h} to the solid orange line, Ω_γ (radiation) to the solid red line and, finally, Ω_m (pressureless matter) to the solid green line. Let us emphasize that it is possible to plot Ω_{ϕ_ℓ} and Ω_{ϕ_h} because, in the particular case of double inflation, it is possible to define separately a fluid associated with the heavy and light fields since the potential is separable. As already mentioned when Fig. 1 was described, at the beginning of inflation, the energy density associated to the heavy field dominates the energy budget of the universe. At $N_{\text{trans}} - N_{\text{end}} \simeq -14.6$, estimated in Eq. (5.30), the contribution of the light field takes over and the blue and orange lines intersect. At this time, the decay of the heavy field is apparent as the quantity Ω_{ϕ_h} sharply drops out (while oscillating). Then, the phase dominated by the light field starts until inflation comes to an end. During inflation, we also remark that the contributions originating from radiation and/or pressureless matter remain negligible except, of course, when the end of the inflationary phase is approached.

Having described how inflation proceeds, let us now extend our analysis to the post-inflationary universe. In Fig. 7, we have plotted the evolution of the fictitious “kinetic fluids” associated to the light field, Ω_{K_ℓ} (solid blue line), to the heavy field, Ω_{K_h} (solid orange line) and to the “potential fluid”, Ω_V (solid grey line). We have also represented the contribution of the “real fluids”, namely radiation (solid red line) and pressureless matter (solid green line). As expected, during inflation, we see that the “potential fluid” dominates over all the other components. At $N = N_{h,\text{decay}}$, the heavy field decays and one sees Ω_{K_h} sharply dropping as $\rho_{K_h} \propto a^{-3}e^{-\Gamma_{\text{hm}}t/2}$, see the considerations around Eqs. (5.40) and (5.41). Starting from the same time, the pressure-less matter that has been produced by the heavy field decay behaves as $\Omega_m \propto a^{-3}$ (the orange curve envelope has, initially, namely before the exponential term in ρ_{K_h} takes over, the same slope as the solid green line). At the end of inflation, all fluids associated to the scalar fields quickly become subdominant and radiation becomes the main component in the universe, $\Omega_\gamma \simeq 1$. Then, during the subsequent radiation-dominated epoch, pressureless matter is subdominant but its relative contribution grows as $\Omega_m \propto a$ given that $\rho_\gamma \propto 1/a^4$ and $\rho_m \propto 1/a^3$. Eventually, around $N - N_{\text{end}} \simeq 40$ e -folds after the end of inflation, pressure-less matter becomes dominant and the matter dominated era starts. Equality

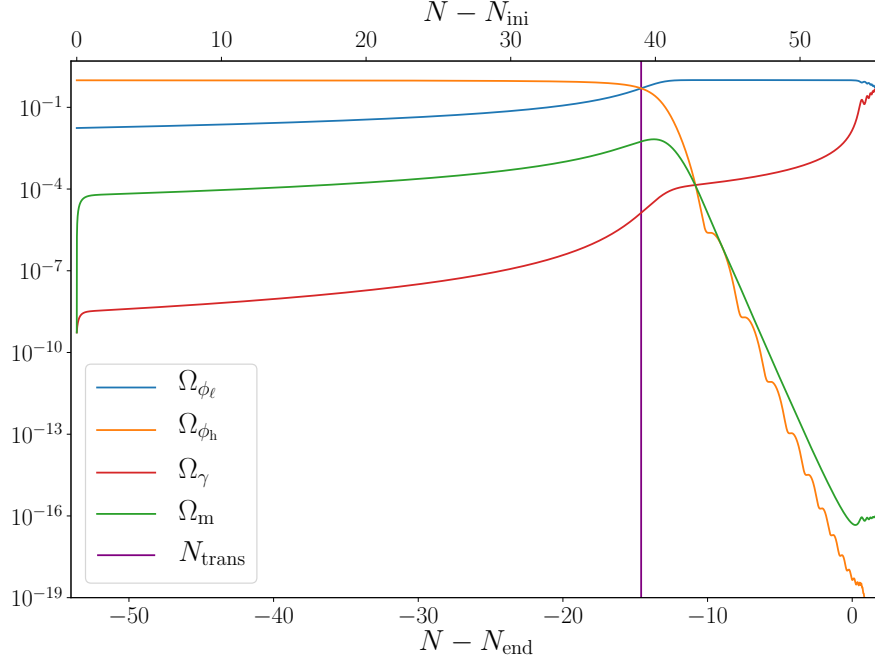


Figure 6: Numerical evolution of the energy budget in the universe during inflation. The four fundamental components of matter are represented: the light scalar field (blue line) and the heavy one (orange line), as well as the radiation fluid (red line) and the pressure-less, matter one (green line). The scalar field that is driving inflation is the one that is dominating the energy budget (by definition), and the contributions from the cosmological fluids are overall negligible but not astonishingly small. The vertical purple line indicates the transition between the regime dominated by the heavy field and the regime dominated by the light field, a time around which the energy from the heavy field is transferred to the matter fluid. Inflation stops at $N = N_{\text{end}}$ after a total of 53.61 e -folds of expansion from the initial time of the simulation, and the energy from the light scalar fields completes its transition to the radiation fluid, thus setting the stage for the radiation-dominated era.

occurs at the temperature

$$T_{\text{eq}} \simeq 2.43 \times 10^{18} \left(\frac{90}{\pi^2} \right)^{1/2} \left(\frac{\Gamma_{\ell\gamma}}{M_{\text{Pl}}} \right)^{1/2} \Omega_{\text{m}}|_{\text{rh}} \text{ GeV}. \quad (5.51)$$

This gives $T_{\text{eq}} \simeq 0.73 \text{ GeV}$, where we have used $\Omega_{\text{m}}|_{\text{rh}} \simeq 10^{-16}$ as can be checked in Fig. 7. Notice that we do not use an analytical approximation for the quantity $\Omega_{\text{m}}|_{\text{rh}}$ due to the remarks made before, namely the fact that the decay of the heavy field is difficult to predict with good accuracy in the approximate framework used here (although it could

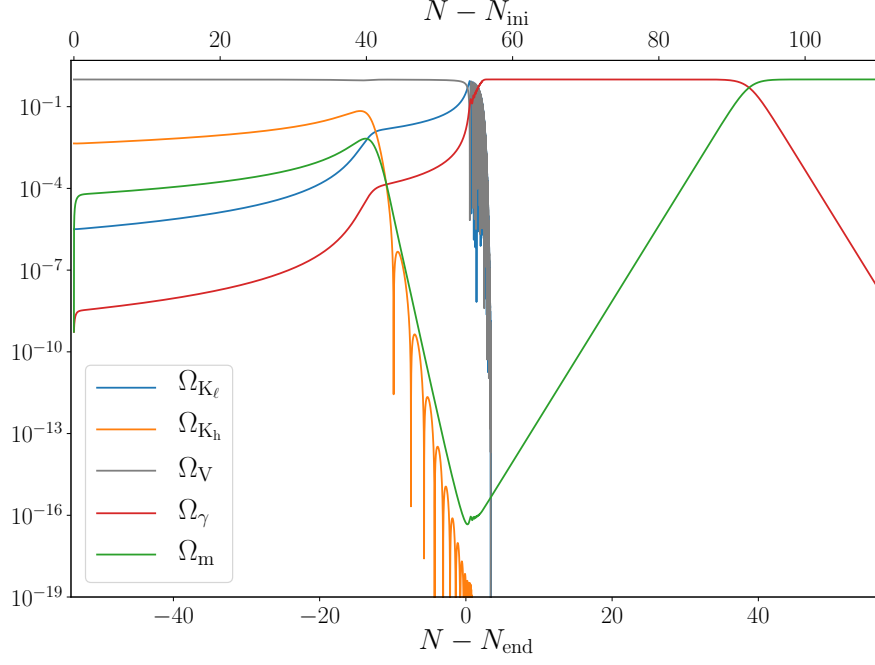


Figure 7: Energy budget $\Omega_{(\alpha)} = \rho_{(\alpha)}/\rho$ between the “fictitious” and “real” fluids in the universe during inflation, reheating, radiation domination and matter domination. During inflation, the potential fluid is always dominating, and the second most important contribution comes from the kinetic fluid corresponding to the scalar field that is driving inflation at that time. As already mentioned, the contributions from the cosmological fluids are then negligible but not extremely small. Clearly, when the heavy field reaches the minimum of its potential, it begins to oscillate and redshift, and completes its transfer of energy to the matter fluid (however the latter quickly begins to decay a bit less rapidly than a^{-3} because it is then only sustained by the exponentially decreasing kinetic energy of the heavy field). At the end of inflation, both the kinetic energy of the light scalar field and the potential energy oscillate with opposite phases but equal amplitudes, and the universe therefore behaves on average and on large scales as in a matter-dominated epoch. This large kinetic energy of the light scalar field is efficiently transferred to the radiation fluid, whose contribution rapidly grows during reheating. Around 3 e -folds after the end of inflation, reheating is complete and it is the onset of the radiation-dominated era, which lasts until radiation has so much redshifted (as a^{-4}) that the small remaining quantity of matter at the end of reheating (that redshifts slower as a^{-3}) eventually dominates, thus setting the stage for the radiation-dominated era.

be attempted using considerations presented in App. A). The temperature obtained before is a temperature higher than the BBN scale. This means that the parameters chosen before are not very realistic and, in order to be realistic, one should change them, for instance lower the value of $\Gamma_{\ell\gamma}$. However, in the following, we will nevertheless continue to work with the fiducial parameters for various reasons. First, considering smaller values of the decay rates can introduce severe numerical problems and, second, since we have analytical estimates that are well-verified in the regime where numerical calculations are available, it would be easy to derive useful predictions in situations of physical interest simply by using these estimates. Here, our main goal is not to build a fully realistic multifield scenario but to investigate and test the accuracy of the tools that have been developed to study these models.

The last figure of this section is Fig. 8 in which we have represented the “trajectories” of the system in the two-dimensional space $(\Omega_\gamma, \Omega_m)$ for different initial conditions. The main conclusion is that the late time behaviour of Ω_γ and Ω_m is not sensitive to the choice of these initial conditions. Indeed, after $\simeq 3$ e-folds, the system joins an attractor as can be seen in Fig. 8. Therefore, we have established that our results do not depend on what we assume about the initial energy densities stored in radiation and pressure-less matter.

5.3 Solutions for the perturbations

5.3.1 Adiabatic and non-adiabatic modes during inflation

In this section, we investigate the solutions for the perturbations during the phase of inflation. Here, and for the remainder of this work, we focus on a single wavenumber k , chosen such that $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$, which therefore features approximately 4.6 e-folds of sub-Hubble evolution before crossing the Hubble radius. Actually, our numerical simulation enables to follow its evolution until it re-enters the Hubble radius in the matter dominated era (though remember that the radiation-matter equality is not realistic in our fiducial model). The cosmic history of this mode, stretched by inflation to super-horizon scales and then re-entering our observable Universe, is represented in Fig. 9.

We neglect, at least for the moment, the contributions of matter and radiation. As a consequence, the perturbed quantities that remain to be studied are the Bardeen potential and the two (heavy and light) field fluctuations. The equations of motion of these quantities are given by Eqs. (4.32), (4.33) and (4.34). During inflation, on large scales, we can also use the slow-roll approximation which transforms the equations of motion, which are second order differential equations, into first order differential equations. These considerations lead to simplified versions of Eqs. (4.32), (4.33) and (4.34)

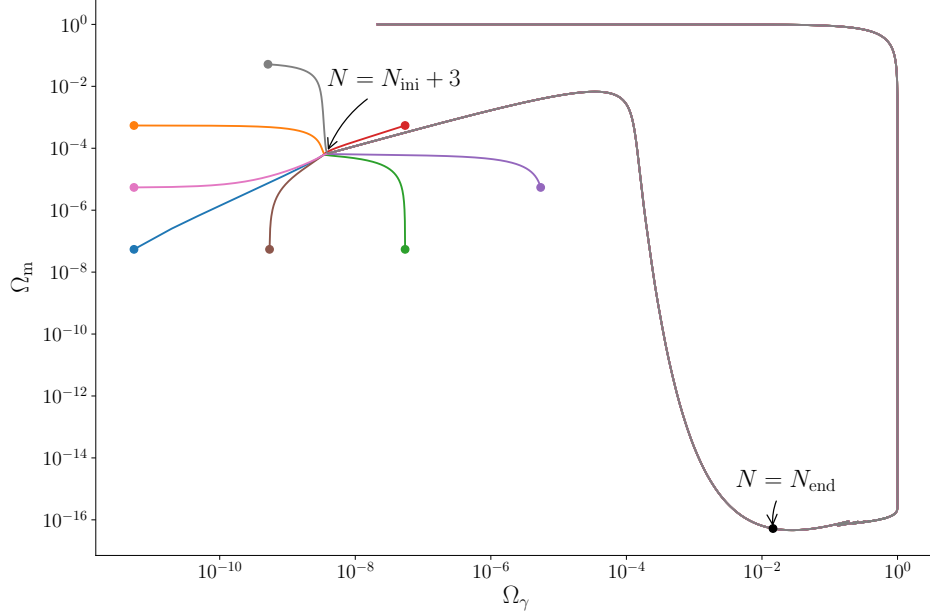


Figure 8: This figure shows the independence of the dynamics of the cosmological fluids on their initial conditions, as found with numerical simulations. Different colors correspond to different initial conditions for ρ_γ and ρ_m and the colorful dots indicate these initial conditions. During inflation, the energy densities of the fluids clearly reach an attractor dynamics along which they are negligible, independently on their initial conditions, as can be understood with the investigation of Eqs. (5.38)–(5.39). The first turn in this $(\Omega_\gamma, \Omega_m)$ two-dimensional space corresponds to the decay of the heavy scalar field, during which the contribution of the matter fluid is rapidly decaying, and the second turn coincides with the end of inflation, denoted by the black dot. Afterward, the radiation fluid dominates the energy budget until the time of equality, from which the matter fluid is dominating.

which, on large scales, can be expressed as

$$\Phi_A = \frac{1}{2M_{\text{Pl}}^2 H} \left(\dot{\phi}_\ell \delta\phi_{\ell,A} + \dot{\phi}_h \delta\phi_{h,A} \right), \quad (5.52)$$

$$3H\dot{\phi}_{\ell,A} + \frac{\partial^2 V_\ell}{\partial \phi_\ell^2} \delta\phi_{\ell,A} + 2\frac{\partial V_\ell}{\partial \phi_\ell} \Phi_A = 0, \quad (5.53)$$

$$3H\dot{\phi}_{h,A} + \frac{\partial^2 V_h}{\partial \phi_h^2} \delta\phi_{h,A} + 2\frac{\partial V_h}{\partial \phi_h} \Phi_A = 0. \quad (5.54)$$

Notice that, for the moment, we have not used the specific form of the potential (namely

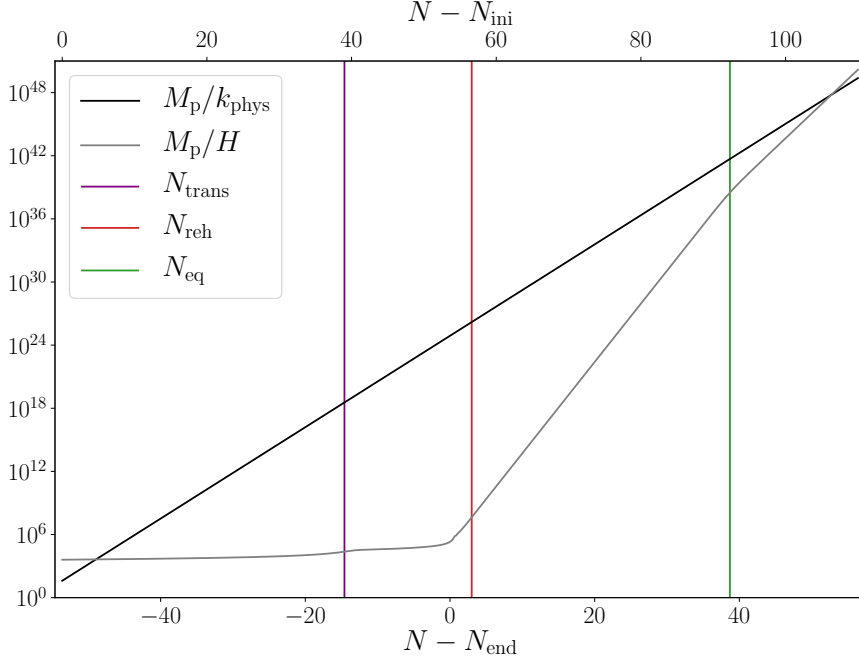


Figure 9: Cosmic history for the representative physical scale k_{phys}^{-1} (black line) corresponding to the mode $k_{\text{phys}} = k/a$ with $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$. This physical wavelength is stretched from sub-Hubble scales where it behaves as in the Bunch-Davies vacuum, to super-horizon ones (the transition happens when the physical scale $k_{\text{phys}}^{-1} = H^{-1}$, where H^{-1} is the Hubble radius and is represented in grey), where crucially non-trivial dynamics may happen due to the multi-species nature of the model at hand. Then it re-enters the horizon of our observable Universe during the matter era. Particular times of interest are represented with vertical lines, such as the transition between the two regimes of inflation (purple line), the end of reheating and beginning of the radiation-dominated era (red line), and the time of equality from which matter is dominating (green line).

the fact that it is quadratic). The only property utilized above is that the potential is separable.

Then, it turns out that this system of equations can be solved exactly. The solution for the Bardeen potential reads [15]

$$\Phi_A = -C_{1,A} \frac{\dot{H}}{H^2} - H \frac{d}{dt} \left(\frac{d_{\ell,A} V_\ell + d_{h,A} V_h}{V} \right) \quad (5.55)$$

$$= C_{1,A} \epsilon_1 + \frac{(d_{\ell,A} - d_{h,A})}{3(V_\ell + V_h)^2} \left[\left(\frac{\partial V_\ell}{\partial \phi_\ell} \right)^2 V_h - \left(\frac{\partial V_h}{\partial \phi_h} \right)^2 V_\ell \right], \quad (5.56)$$

where we recall that ϵ_1 is the first Hubble flow parameter, while the solutions for the field fluctuations take the form

$$\frac{\delta\phi_{\ell,A}}{\dot{\phi}_\ell} = \frac{C_{1,A}}{H} - 2H(d_{h,A} - d_{\ell,A})\frac{V_h}{V_\ell + V_h}, \quad (5.57)$$

$$\frac{\delta\phi_{h,A}}{\dot{\phi}_h} = \frac{C_{1,A}}{H} + 2H(d_{h,A} - d_{\ell,A})\frac{V_\ell}{V_\ell + V_h}. \quad (5.58)$$

In these expressions, $C_{1,A}$, $d_{h,A}$ and $d_{\ell,A}$ are integration constants.

Following Ref. [23], it is interesting to split the above solutions in adiabatic and non-adiabatic modes. Concretely, for the adiabatic components, we define

$$\Phi_A^{\text{ad}} = C_{1,A}\epsilon_1, \quad \delta\phi_{\ell,A}^{\text{ad}} = \frac{C_{1,A}}{H}\dot{\phi}_\ell, \quad \delta\phi_{h,A}^{\text{ad}} = \frac{C_{1,A}}{H}\dot{\phi}_h. \quad (5.59)$$

The justification for these definitions is as follows. One can use these solutions to calculate the corresponding curvature perturbations. This means that we consider the standard expression for curvature perturbation in terms of the Bardeen potential and the field fluctuations but when the concrete forms of Φ_A and $\delta\phi_{h,\ell,A}$ are used in this expression, only the adiabatic modes are taken into account. Explicitly, we have

$$\zeta_{\ell,A}^{\text{ad}} = -\Phi_A^{\text{ad}} - H\frac{\delta\rho_{\ell,A}^{\text{ad}}}{\dot{\rho}_\ell} \simeq -C_{1,A}, \quad (5.60)$$

where $\delta\rho_{\ell,A}^{\text{ad}} = \dot{\phi}_\ell\delta\dot{\phi}_{\ell,A}^{\text{ad}} - \dot{\phi}_\ell^2\Phi_A^{\text{ad}} + (\partial V_\ell/\partial\phi_\ell)\delta\phi_{\ell,A}^{\text{ad}}$. Of course, one also has $\zeta_{h,A}^{\text{ad}} \simeq -C_{1,A}$ since the same calculation holds for the heavy field. This implies that $\zeta_{h,A}^{\text{ad}} - \zeta_{\ell,A}^{\text{ad}} = 0$, which, therefore, indeed, corresponds to an adiabatic perturbation, justifying the split (and the notation) introduced before.

In a similar way, the non-adiabatic components of the full solution can be defined by the following formulas

$$\Phi_A^{\text{nad}} = \frac{(d_{\ell,A} - d_{h,A})}{3(V_\ell + V_h)^2} \left[\left(\frac{\partial V_\ell}{\partial\phi_\ell} \right)^2 V_h - \left(\frac{\partial V_h}{\partial\phi_h} \right)^2 V_\ell \right], \quad (5.61)$$

$$\delta\phi_{\ell,A}^{\text{nad}} = -2H\dot{\phi}_\ell(d_{h,A} - d_{\ell,A})\frac{V_h}{V_\ell + V_h}, \quad (5.62)$$

$$\delta\phi_{h,A}^{\text{nad}} = -2H\dot{\phi}_h(d_{\ell,A} - d_{h,A})\frac{V_\ell}{V_\ell + V_h}. \quad (5.63)$$

Using these results, one can establish the corresponding expressions for curvature perturbations. For the light field, one arrives at

$$\begin{aligned} \zeta_{\ell,A}^{\text{nad}} = & -\frac{2}{9(V_\ell + V_h)^2}(d_{h,A} - d_{\ell,A}) \left[\left(\frac{\partial V_h}{\partial\phi_h} \right)^2 V_\ell - \left(\frac{\partial V_\ell}{\partial\phi_\ell} \right)^2 V_h \right] \\ & + 2H^2(d_{h,A} - d_{\ell,A})\frac{V_h}{V_\ell + V_h}, \end{aligned} \quad (5.64)$$

and a similar equation for the quantity $\zeta_{h,A}^{\text{nad}}$, where the indices ℓ and h are permuted. It follows that $\zeta_{h,A}^{\text{nad}} - \zeta_{\ell,A}^{\text{nad}} \neq 0$ which justifies why these branches of the full solutions are called non-adiabatic. In fact, using the above expressions, it is straightforward to show that

$$S_{\ell h,A} = \zeta_{\ell,A}^{\text{nad}} - \zeta_{h,A}^{\text{nad}} = 2C_{3,A}H^2, \quad (5.65)$$

where we have defined the constant $C_{3,A}$ by $C_{3,A} = d_{h,A} - d_{\ell,A}$. We emphasize again that the above considerations are valid for any potential provided this one is separable.

5.3.2 Fixing the initial conditions

To go further and have a complete knowledge of the large scales solutions (5.56), (5.57) and (5.58), we must fix the constants $C_{1,A}$ and $C_{3,A}$. Inverting Eqs. (5.57) and (5.58), one obtains

$$C_{1,A} = -\frac{1}{M_{\text{Pl}}^2} \left(\frac{V_\ell}{\partial V_\ell / \partial \phi_\ell} \delta \phi_{\ell,A} + \frac{V_h}{\partial V_h / \partial \phi_h} \delta \phi_{h,A} \right), \quad (5.66)$$

$$C_{3,A} = \frac{3}{2} \left(\frac{\delta \phi_{\ell,A}}{\partial V_\ell / \partial \phi_\ell} - \frac{\delta \phi_{h,A}}{\partial V_h / \partial \phi_h} \right), \quad (5.67)$$

and, therefore, it is sufficient to evaluate the time-dependent quantities that appear in the above formulas at a specific time to find the two constants $C_{1,A}$ and $C_{3,A}$ once and for all. This can be achieved with the help of the following considerations. The exact equations for field fluctuations are Eqs. (4.33) and (4.34). By plotting all the terms appearing in those equations, see Figs. 10 and 11, one can see that it is a good approximation to assume that, on sub-Hubble scales, both field fluctuations behave as

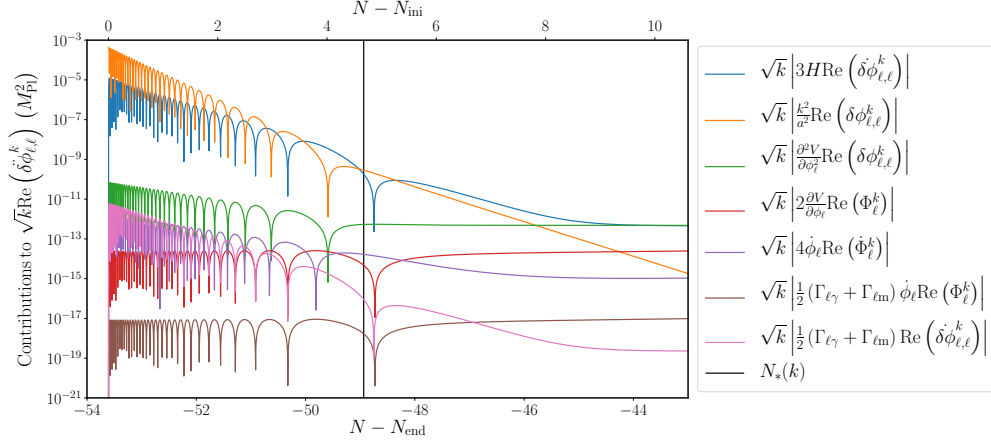
$$\delta \phi_{\ell,h,A}'' + 2\mathcal{H}\delta \phi_{\ell,h,A}' + [k^2 + m_{\ell,h}^2 a^2(\eta)] \delta \phi_{\ell,h,A} \simeq 0, \quad (5.68)$$

where all terms proportional to the Bardeen and to the decay constants $\Gamma_{\text{hm}}, \Gamma_{\ell\gamma}$ were neglected. In fact, and this is going to play an important role in the following, one can show that the approximation discussed above should be valid not only on sub-Hubble scales, but also up to a time slightly after Hubble radius crossing. This is because, until that time, the terms that we have neglected in Eqs. (4.33) and (4.34) remain sub-dominant⁴.

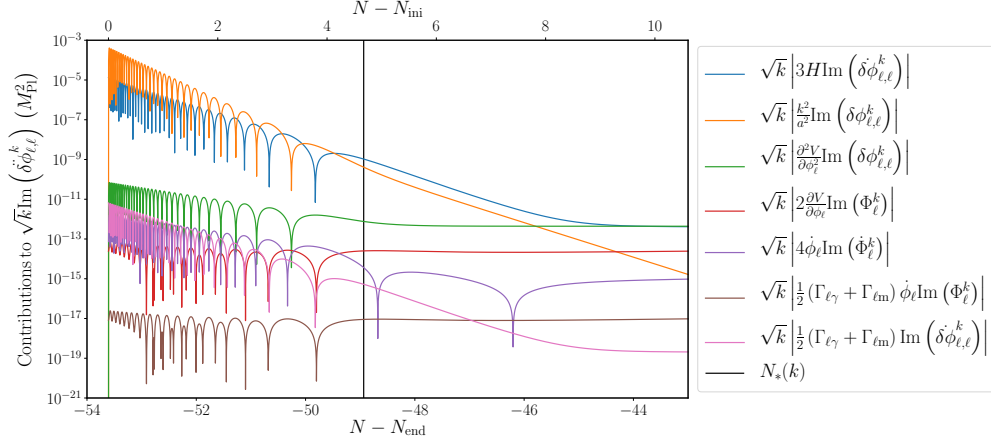
Eq. (5.68) can be rewritten in a way which is more suitable to discuss its solutions, namely

$$f_{\ell,h,A}'' + \left[k^2 - \frac{a''}{a} + m_{\ell,h}^2 a^2(\eta) \right] f_{\ell,h,A} = 0, \quad (5.69)$$

⁴Note from Figs. 10 and 11 that this approximation seems better verified for the perturbations of the light scalar field than the ones of the heavy one. And indeed one can see in Figs. 12 and 13 a better accuracy for the light fluctuations than for the heavy ones for times after Hubble crossing.



(a) Real part



(b) Imaginary part

Figure 10: Absolute values of the contributions to the equation of motion of the perturbations of the light scalar field, for the mode that is initially aligned with the oscillator $A = \ell$: $\delta\phi_{\ell,\ell}^k$. The Hubble-crossing time for the mode k of interest is represented by the vertical black line. Before and around Hubble crossing, the two dominant terms are the Hubble friction $\propto H$ (blue line) and the quantum oscillations $\propto k^2/a^2$ (orange line). The mass term $\propto m_1^2$ (green line) comes as a third, small contribution around and just after Hubble crossing. Note that for the times represented here, the Bardeen contributions (red, purple and brown lines) remain sub-dominant even on super-Hubble scales. This is because the light field is not driving inflation and therefore the component of the Bardeen along the oscillator $A = \ell$, Φ_ℓ , is negligible until the transition time $N_{\text{trans}} - N_{\text{end}} = -14.6$ which happens dozens of e -folds after Hubble crossing. The decay terms (brown and pink lines) also play a negligible role in the dynamics of $\delta\phi_{\ell,\ell}^k$ before and around Hubble crossing. The picture is shared both by the real part (upper panel) and the imaginary one (lower panel).

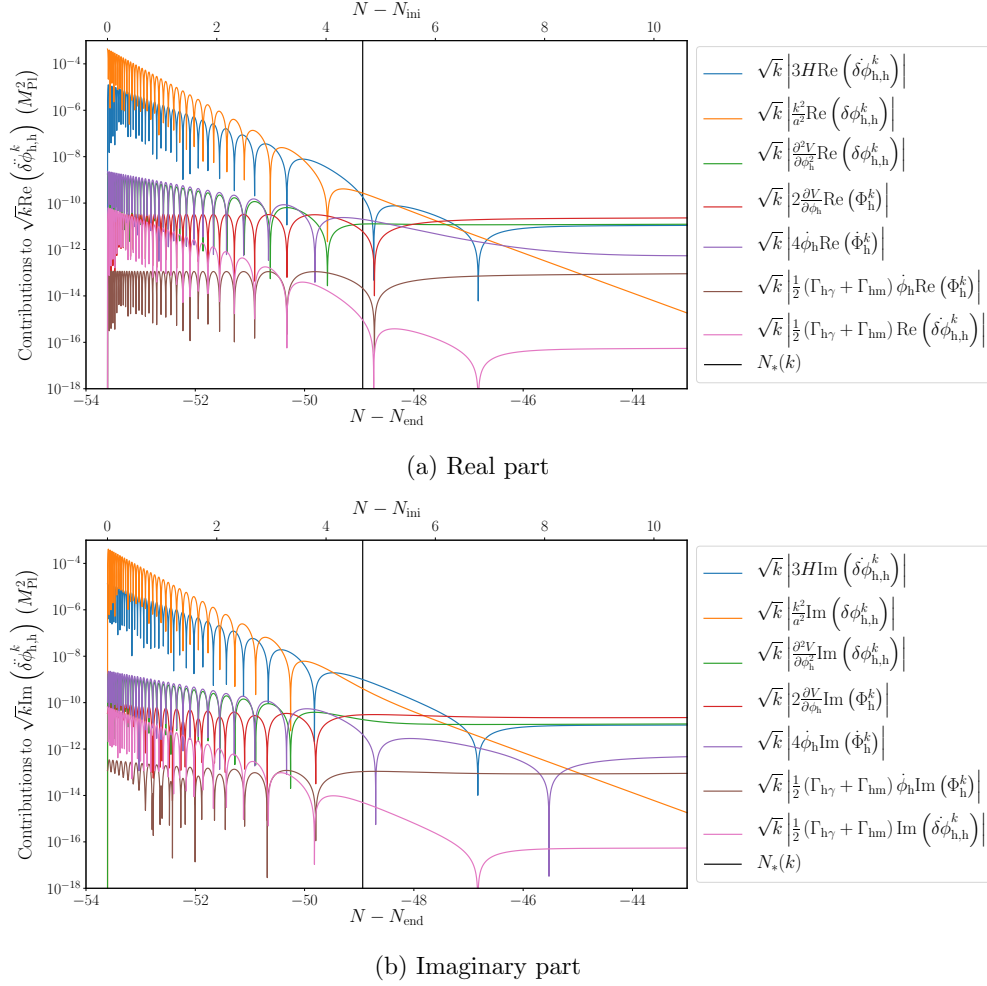


Figure 11: Absolute values of the contributions to the equation of motion of the perturbations of the heavy scalar field, for the mode that is initially aligned with the oscillator $A = h$: $\delta\phi_{h,h}^k$. Before and around Hubble crossing, the two dominant terms are the Hubble friction $\propto H$ (blue line) and the quantum oscillations $\propto k^2/a^2$ (orange line). The mass term $\propto m_2^2$ (green line) comes as a third, small contribution around and just after Hubble crossing. In contrast to the situation with the light scalar field, the heavy scalar field is driving inflation and therefore the Bardeen contributions are not always negligible. First, on super-Hubble scales, the Bardeen contribution $\propto m_2^2$ (red line) becomes the dominant one and therefore it can not be neglected at all. More importantly (because the current section aims at finding approximations on sub-Hubble scales), both the Bardeen contributions $\propto m_2^2$ and to $\dot{\phi}_h$ (red and purple lines) are small but not completely negligible around Hubble crossing (in particular, they are of the same order than the mass term), and therefore neglecting them is a source of small inaccuracy in this treatment. The decay terms (brown and pink lines) also play a negligible role in the dynamics of $\delta\phi_{\ell,\ell}$ before and around Hubble crossing. The picture is similar for the real part (upper panel) and the imaginary one (lower panel).

where one has defined $\delta\phi_{\ell,h,A}(\eta) \equiv f_{\ell,h,A}(\eta)/a(\eta)$. As expected, we obtain an equation which is in fact similar to the equation of a test massive field in an expanding spacetime. Eq (5.69) should be solved with the following, Bunch-Davies, initial conditions

$$f_{\ell,A}(\eta_{\text{ini}}) = \frac{1}{\sqrt{2k}}\delta_{\ell,A}, \quad f_{h,A}(\eta_{\text{ini}}) = \frac{1}{\sqrt{2k}}\delta_{h,A}, \quad (5.70)$$

$$f'_{\ell,A}(\eta_{\text{ini}}) = -i\sqrt{\frac{k}{2}}\delta_{\ell,A}, \quad f'_{h,A}(\eta_{\text{ini}}) = -i\sqrt{\frac{k}{2}}\delta_{h,A}, \quad (5.71)$$

with, in principle, $k\eta_{\text{ini}} \rightarrow -\infty$. These conditions are such that, initially, each mode function labelled by A only possesses a non-vanishing component along that direction. Of course, this is equivalent to the initial conditions already discussed in Eq. (4.64) and in the text after Eq. (4.70).

Let us now discuss the solutions of Eq. (5.69). If the physical wavelength of the Fourier mode under consideration is much smaller than the Hubble radius, namely $k\eta \ll -1$, then the two terms a''/a and $m_{\ell,h}^2 a^2(\eta)$ are negligible. In this regime, one does not need to know the form of the scale factor explicitly in order to solve the equation. The corresponding solution, satisfying the initial conditions (5.70) and (5.71) reads

$$f_{\ell,h,A}(\eta) = \frac{1}{\sqrt{2k}} e^{-ik(\eta-\eta_{\text{ini}})} \delta_{\ell,h,A}, \quad (5.72)$$

where the symbol $\delta_{\ell,h,A}$ means either $\delta_{\ell,A}$ or $\delta_{h,A}$ depending of whether the mode functions $f_{\ell,A}(\eta)$ or $f_{h,A}(\eta)$ are considered. Again, equivalent considerations have already been presented around Eq. (4.64).

As the Universe expands, the physical wavelength of the Fourier mode increases and the above solution ceases to be valid: around Hubble horizon crossing (in principle, before since we deal with an equation valid on small scales only), namely $k/(a_* H_*) = 1$, the two terms mentioned before are indeed no longer negligible. In that case, in order to solve Eq. (5.69) in this regime, the form of the scale factor is needed. Since the background is undergoing inflation, this can be obtained by means of the slow-roll approximation. At first order, $a(\eta) \propto a_*(\eta/\eta_*)^{-1-\epsilon_{1*}}$, where ϵ_{1*} is the first slow-roll parameter (evaluated at Hubble radius crossing), which can also be expanded as $a(\eta) \simeq -(H_*\eta)^{-1}(1 + \epsilon_{1*} - \epsilon_{1*} \ln \eta/\eta_* + \dots)$. This approximation for the scale factor is expected to be valid only around Hubble radius crossing. Notice that, in the regime of validity of Eq. (5.72), the background should also be inflationary and, as a consequence, the slow-roll approximation should also be satisfied. However, if the number of e-folds separating this epoch to the epoch of Hubble radius crossing is too large, the assumption that ϵ_1 is always constant becomes questionable. In other words, one has two epochs where slow-roll is valid, each one having its own slow-roll parameter, $\epsilon_{1\text{ini}}$ and ϵ_{1*} . Within each regimes, the slow-roll parameter can indeed be considered constant but these constants are *a priori* not the same in different epochs. With the scale factor given above, Eq (5.69) takes the form

$$f''_{\ell,h,A} + \left[k^2 - \frac{1}{\eta^2} \left(2 + 3\epsilon_{1*} - \frac{m_{\ell,h}^2}{H_*^2} \right) \right] f_{\ell,h,A} = 0. \quad (5.73)$$

Notice that, in the present context, it is justified to go beyond a simple de Sitter approximation (namely $\epsilon_{1*} = 0$). Indeed, it is well-known that this one is not very accurate for a background which resembles Large Field Models (LFI) [12]. It would certainly be better in a small field/Starobinsky (SFI/HI, see Ref. [12]) context where, to a very good accuracy, the Hubble parameter remains constant. It is also interesting to remark that, in order to have a better (more accurate) solution, what is needed is not to consider the impact of the terms neglected in Eqs. (4.33) and (4.34), since, anyway, we showed before that they remain negligible in the range of e-folds we are interested in. Rather a better description of the evolution of the background is what matters in order to improve the description of the system. Then, Eq (5.73) can be solved in terms of Bessel function

$$f_{\ell,h,A}(\eta) = (-k\eta)^{1/2} \left[A_{\ell,h,A} H_{\nu_{\ell,h}}^{(1)}(-k\eta) + B_{\ell,h,A} H_{\nu_{\ell,h}}^{(2)}(-k\eta) \right], \quad (5.74)$$

where $\nu_{\ell,h} = 3/2 + \epsilon_{1*} - m_{\ell,h}^2/(3H_*^2)$ and $H_\nu^{(1,2)}$ are Hankel functions of the first and second kind. The quantities $A_{\ell,h,A}$ and $B_{\ell,h,A}$ are integration constants.

The next step consists in matching the solutions (5.72) and (5.74) at a time η_m , where “m” stands for matching, which is such that $\eta_{\text{ini}} < \eta_m < \eta_*$ (that is to say before Hubble radius crossing). Requiring the continuity of the mode function and of its derivative, one finds

$$A_{\ell,h,A} = \frac{\pi z_m^{1/2}}{4i} \frac{1}{\sqrt{2k}} e^{iz_m + ik\eta_{\text{ini}}} \left[\left(-\frac{1}{2z_m} + \frac{\nu_{\ell,h}}{z_m} + i \right) H_{\nu_{\ell,h}}^{(2)}(z_m) - H_{\nu_{\ell,h}-1}^{(2)}(z_m) \right] \delta_{\ell,h,A}, \quad (5.75)$$

$$B_{\ell,h,A} = -\frac{\pi z_m^{1/2}}{4i} \frac{1}{\sqrt{2k}} e^{iz_m + ik\eta_{\text{ini}}} \left[\left(-\frac{1}{2z_m} + \frac{\nu_{\ell,h}}{z_m} + i \right) H_{\nu_{\ell,h}}^{(1)}(z_m) - H_{\nu_{\ell,h}-1}^{(1)}(z_m) \right] \delta_{\ell,h,A}, \quad (5.76)$$

where $z_m \equiv -k\eta_m$. Since the matching time is chosen to be before Hubble radius crossing, one has $z_m \gg 1$ and the large argument limit of the Hankel functions can be used. As a result, one obtains

$$A_{\ell,h,A} \simeq \frac{1}{2} \sqrt{\frac{\pi}{k}} e^{ik\eta_{\text{ini}} + i\pi\nu_{\ell,h}/2 + i\pi/4} \left[1 + \mathcal{O}\left(\frac{1}{z_m}\right) \right] \delta_{\ell,h,A}, \quad (5.77)$$

$$B_{\ell,h,A} \simeq \mathcal{O}\left(\frac{1}{z_m^2}\right) \delta_{\ell,h,A}. \quad (5.78)$$

It can be noticed that, in the limit $z_m \rightarrow \infty$, $B_{\ell,h,A} \rightarrow 0$. This case is formally identical to the situation where the solution (5.74) is assumed to be valid all the way from η_{ini} to Hubble radius crossing and where the constants $A_{\ell,h,A}$ and $B_{\ell,h,A}$ are obtained by requiring the function (5.74) to tend towards (5.72).

Using Eqs. (5.77) and (5.78), the solution around Hubble radius crossing for the field fluctuation can be written as

$$a_{\text{ini}}^{3/2} \delta\phi_{\ell,h,A}(\eta) \simeq \frac{a_{\text{ini}}}{a(\eta)} (-k\eta)^{1/2} \frac{1}{\sqrt{2k/a_{\text{ini}}}} \sqrt{\frac{\pi}{2}} e^{i\pi(\nu+1/2)/2} e^{ik\eta_{\text{ini}}} H_\nu^{(1)}(-k\eta) \delta_{\ell,h,A}. \quad (5.79)$$

Again, as explained above, although this expression is formally equivalent to the solution that one would obtain assuming that (5.74) is valid from η_{ini} to Hubble radius crossing (since, formally, we took the limit $z_m \rightarrow \infty$), we emphasize again that we will consider that Eq. (5.79) describes the behaviour of $\delta\phi_{\ell,h,A}(\eta)$ only in the vicinity of Hubble radius crossing. This will allow us to consider that ϵ_{1*} and $\epsilon_{1\text{ini}}$ are not necessary equal, which leads to more accurate expressions.

The above solution is expressed in terms of conformal time. In order to make the connection with numerical calculations, it is necessary to express it in terms of the number of e-folds. From the exact expression

$$dN = -\mathcal{H}d\left(\frac{1+\epsilon_1}{\mathcal{H}}\right) + \frac{\mathcal{H}}{a}d\left(\frac{\epsilon_1}{H}\right), \quad (5.80)$$

one obtains, at first order in slow-roll, $dN \simeq -(1+\epsilon_1)\mathcal{H}d(1/\mathcal{H})$ which can be integrated to $\mathcal{H} = \mathcal{H}_p e^{(N-N_p)/(1+\epsilon_{1p})}$ where “p” just denotes a peculiar time. Integrating this relation leads to $\eta = -(1+\epsilon_{1p})/\mathcal{H}_p e^{-(N-N_p)/(1+\epsilon_{1p})}$ where we have chosen an integration constant to match the standard de Sitter limit. In the following, we will choose the initial time to be the peculiar time for the first regime [namely the regime where the solution is given by Eq. (5.72)], meaning

$$k\eta = -(1+\epsilon_{1\text{ini}})\frac{k}{a_{\text{ini}}H_{\text{ini}}}e^{-(N-N_{\text{ini}})/(1+\epsilon_{1\text{ini}})}, \quad (5.81)$$

and the Hubble radius crossing time for the second regime [namely the regime where the solution is given by Eq. (5.74)] implying

$$k\eta = -(1+\epsilon_{1*})e^{-(N-N_*)/(1+\epsilon_{1*})}, \quad (5.82)$$

where we have used $k/(a_*H_*) = 1$.

In Fig. 12, we have compared the exact, numerical, real and imaginary parts of $\delta\phi_{\ell,h,A}$ with the analytical solution (5.79) from the initial time η_{ini} to a time slightly after Hubble radius crossing (indicated by the black solid vertical line). Evidently, the two solutions match very well. It is especially interesting to remark that the analytical solution is still a very good approximation even a few e-folds after Hubble radius crossing even if the equation used is, in principle, only valid before Hubble radius crossing. In Fig. 13, we have represented the same quantities but zoomed out. It shows the limitations of the previous remark: one indeed notices that the agreement between the small scale solution and the exact solution after Hubble radius crossing is only valid a few e-folds. Then, as expected, the two functions split. Moreover, note that the analytical approximation neglects the mixing of perturbations: indeed $\delta\phi_{\ell,A} \propto \delta\ell_A$ and $\delta\phi_{h,A} \propto \delta\phi_{h,A}$.

Given the previous considerations, our final move will be to use the solution (5.79) evaluated at a time slightly after Hubble radius crossing; in this regime we can consider that $-k\eta \ll 1$ and one can take the small argument limit in the Hankel function. This

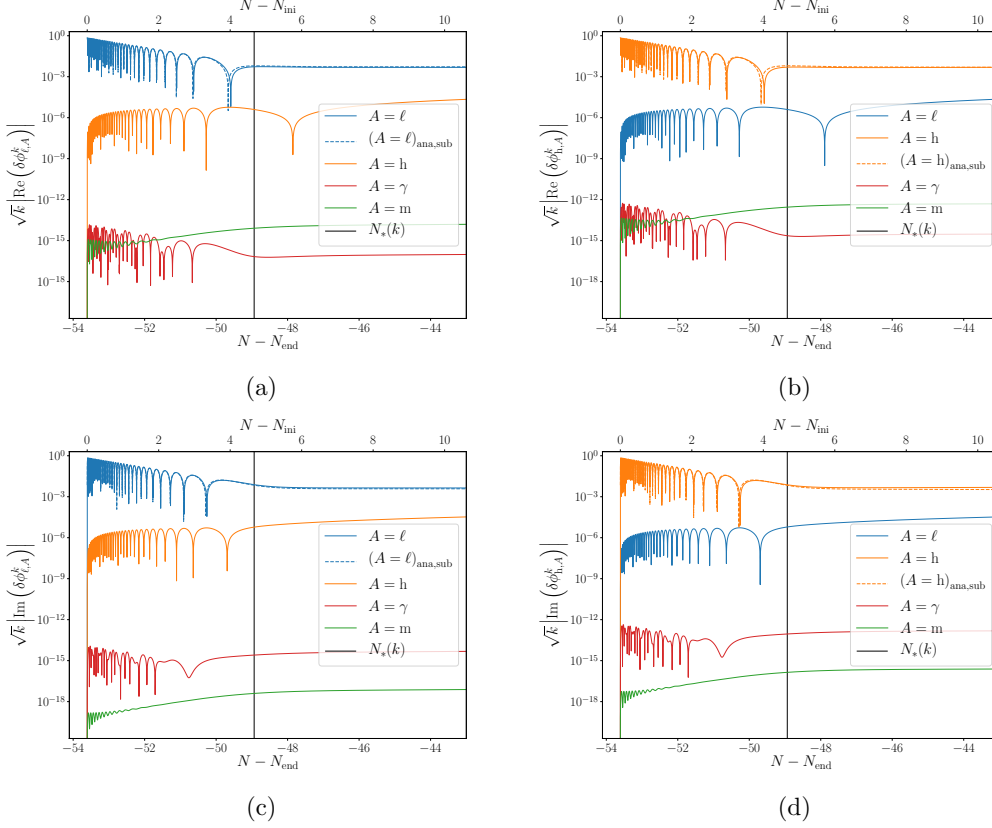


Figure 12: Real (upper panels) and imaginary parts (lower panels) of the fields’ perturbations $\delta\phi_{\ell,A}$ (left panels) and $\delta\phi_{h,A}$ (right panels), including the exact numerical solutions for the different components $A = \ell, h, 1, 2$ along the four fundamental oscillators (respectively blue, orange, red and green solid lines), and the sub-Hubble, slow-roll analytic approximations “ana,sub” with Hankel functions for the diagonal mode functions $\delta\phi_{\ell,\ell}$ and $\delta\phi_{h,h}$ (respectively blue and orange dashed lines). Evidently, the analytical approximations are extremely accurate, even though slightly better for the light field than for the heavy one. Note that the analytic approximation used on sub-Hubble scales neglects the non-diagonal mode functions such as $\delta\phi_{\ell,h}$ and $\delta\phi_{h,\ell}$, which seems indeed to be accurate again. Note that the oscillators $A = \gamma, m$ of the scalar fields remain negligible in this regime. The vertical black line corresponds to the time of horizon crossing for the mode $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$ represented in these plots.

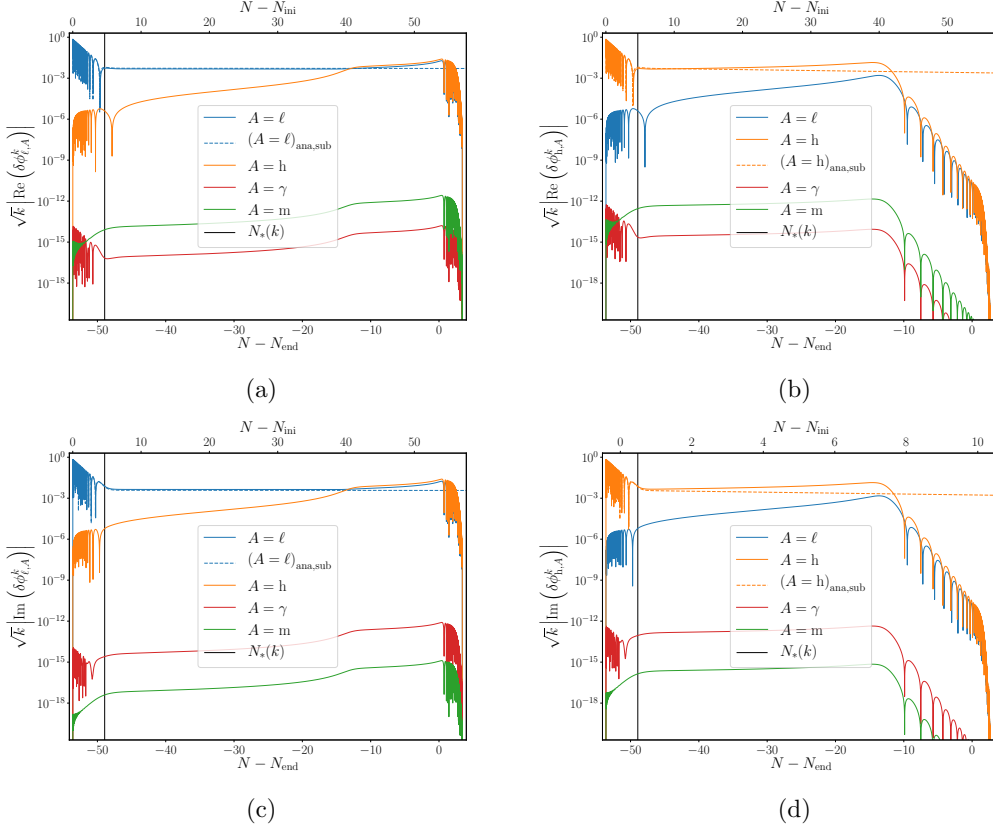


Figure 13: Same figures than the one represented in Fig. 12, but unzoned until the end of inflation. Clearly, the sub-Hubble approximations become inaccurate after horizon crossing, for mainly two reasons. First, the diagonal mode functions eventually become inaccurate. For the heavy field that is first driving inflation, we have understood that the Bardeen contribution, neglected in the above treatment, is actually not negligible and therefore results in the departure observed on the right panels between the orange solid and dashed lines representing $\delta\phi_{h,h}$. The same phenomenon happens on the left panels for $\delta\phi_{\ell,\ell}$ (departure between the blue solid and dashed lines) after the light field begins to drive inflation. Secondly, the non-diagonal mode functions cease to be negligible, in particular the mode function $\delta\phi_{\ell,h}$ (orange line in the left panels) receives an important contribution from the heavy field during the transition between the two regimes of inflation. This is also true, although in a less striking manner, for the other non-diagonal function $\delta\phi_{h,\ell}$ (blue line in the right panels). It is crucial to understand this super-horizon interaction in order to model correctly the physics of non-adiabatic perturbations in multifield inflation. Clearly, it is not encapsulated by the approximations made in this section, and it is the aim of Sec. 5.3.3 to address this question. Note that the oscillators $A = \gamma, m$ of the scalar fields remain negligible throughout the whole inflationary epoch.

leads to the following expressions for the field fluctuations:

$$a_{\text{ini}}^{3/2} \delta\phi_{\ell,h,A}(N) = H_{\text{ini}}^{-1/2} \frac{H_*}{H_{\text{ini}}} \left(\frac{k}{a_{\text{ini}} H_{\text{ini}}} \right)^{-3/2} \exp \left[-\frac{m_{\ell,h}^2}{3H_*^2} (N - N_*) \right] \mathcal{F}(\nu_{\ell,h}) \delta_{\ell,h,A}, \quad (5.83)$$

with

$$\mathcal{F}(\nu) = \frac{2^{\nu-1}}{\sqrt{\pi}} \Gamma(\nu) (1 + \epsilon_*)^{1/2-\nu} e^{i[\frac{\pi}{2}(\nu-1/2) + k\eta_{\text{ini}}]}. \quad (5.84)$$

We see that the mode functions still possess a mild time dependence because of the exponential term $[m_{\ell,h}^2/(3H_*^2)]$ is a small factor. This dependence vanishes in the limit of massless fields. This makes sense because, in this limit, on large scales, $f_{\ell,h,A}(\eta) \propto a(\eta)$ and, as a consequence, $\delta\phi_{\ell,h,A}(\eta) = f_{\ell,h,A}(\eta)/a(\eta)$ is frozen.

Finally, in order to be in a position where the constants $C_{1,A}$ and $C_{3,A}$ can be calculated according to Eqs. (5.66) and (5.67), we also need to evaluate the quantities $V_{\ell,h}$ and $\partial V_{\ell,h}/\partial\phi_{\ell,h}$. Since we need to calculate those quantities just after Hubble horizon crossing and since this happens in the epoch dominated by the heavy field, ϕ_ℓ and ϕ_h (and H as well as the first slow-roll parameter) can be replaced with their slow-roll trajectory during the epoch dominated by the heavy field. First, using Eqs. (5.66) and (5.67), one arrives at

$$C_{1,A}(N_m) = -\frac{H_{\text{ini}}^{-1/2}}{2M_{\text{Pl}}^2} \frac{H_*}{H_{\text{ini}}} \left(\frac{k}{a_{\text{ini}} H_{\text{ini}}} \right)^{-3/2} \left[\phi_\ell(N_m) e^{-\frac{m_\ell^2}{3H_*^2}(N_m - N_*)} \mathcal{F}(\nu_\ell) \delta_{\ell,A} + \phi_h(N_m) e^{-\frac{m_h^2}{3H_*^2}(N_m - N_*)} \mathcal{F}(\nu_h) \delta_{h,A} \right], \quad (5.85)$$

$$C_{3,A}(N_m) = \frac{3H_{\text{ini}}^{-1/2}}{2} \frac{H_*}{H_{\text{ini}}} \left(\frac{k}{a_{\text{ini}} H_{\text{ini}}} \right)^{-3/2} \left[\frac{\mathcal{F}(\nu_\ell) \delta_{\ell,A}}{m_\ell^2 \phi_\ell(N_m)} e^{-\frac{m_\ell^2}{3H_*^2}(N_m - N_*)} - \frac{\mathcal{F}(\nu_h) \delta_{h,A}}{m_h^2 \phi_h(N_m)} e^{-\frac{m_h^2}{3H_*^2}(N_m - N_*)} \right]. \quad (5.86)$$

In the above expressions, N_m should be understood as the e-fold number at which the coefficient $C_{1,A}$ is calculated. As already discussed before, N_m should be chosen such that it corresponds to a time slightly after Hubble crossing time. In the following, we use the fiducial parameters already considered before, namely $m_\ell = 10^{-5} M_{\text{Pl}}$ and $m_h = 5 \times 10^{-5} M_{\text{Pl}}$ with the initial conditions $\phi_\ell|_{\text{ini}} = 8M_{\text{Pl}}$, $\phi_h|_{\text{ini}} = 12M_{\text{Pl}}$. We recall that this implies that $H_{\text{ini}} \simeq 2.5 \times 10^{-4} M_{\text{Pl}}$ and $\epsilon_{1\text{ini}} \simeq 0.01388$. We take the e-fold number at which we evaluate the constants $C_{1,A}$ and $C_{3,A}$ to be 3 e-folds after the Hubble radius crossing, namely $N_m - N_{\text{ini}} \sim 7.67$ given that $N_* - N_{\text{ini}} \sim 4.67$. Then, we can make use of the slow-roll approximation to evaluate the other quantities. We take $\phi_\ell(N_m) \simeq \phi_\ell|_{\text{ini}} = 8M_{\text{Pl}}$, see Eq. (5.26) and $\phi_h(N_m) = \sqrt{\phi_h^2|_{\text{ini}} - 4M_{\text{Pl}}^2(N_m - N_{\text{ini}})} \simeq 10.64M_{\text{Pl}}$, see

Quantity / Value	Numeric	Analytic	Relative error
$\Re C_{1,\ell}$	-0.122	-0.124	1.4%
$\Im C_{1,\ell}$	-0.112	-0.113	0.9%
$\Re C_{1,h}$	-0.159	-0.159	< 0.1%
$\Im C_{1,h}$	-0.157	-0.138	12.1%
$\Re C_{3,\ell} M_{\text{Pl}}^2 \times 10^{-7}$	5.77	5.79	0.3%
$\Im C_{3,\ell} M_{\text{Pl}}^2 \times 10^{-7}$	5.26	5.27	0.1%
$\Re C_{3,h} M_{\text{Pl}}^2 \times 10^{-7}$	-0.158	-0.169	7.2%
$\Im C_{3,h} M_{\text{Pl}}^2 \times 10^{-7}$	-0.142	-0.146	3.1%

Table 1: Analytical predictions versus exact numerical results for the constants $C_{1,3,A}$ evaluated at the matching time $N_{\text{m}} = N_*(k) + 3$, where $N_*(k)$ corresponds to the time of Hubble crossing for the mode k under investigation. These values are only very mildly dependent on the exact choice of N_{m} . The relative error = $|\text{analytic} - \text{numeric}|/|\text{numeric}|$ is also displayed.

Eq. (5.28). Given that Hubble radius crossing occurs during the phase dominated by the heavy, we can consider that $\epsilon_1 = 2M_{\text{Pl}}^2/\phi_{\text{h}}^2$, see the arguments presented after Eq. (5.12), implying $\epsilon_{1*} \simeq 0.0159$. We also have, see Eq. (5.29), $H^2 = H_{\text{ini}}^2 - 2m_{\text{h}}^2(N - N_{\text{ini}})/3$, which means $H_* \simeq 0.00228M_{\text{Pl}}$. From these numerical values, it follows that $\nu_{\ell} \simeq 1.515$ and $\nu_{\text{h}} \simeq 1.500$. Using these numbers, we analytically find the values of $C_{1,A}$ and $C_{3,A}$ collected in the column “Analytic” of Table 1, which should be compared to the exact, numerical values in column “Numeric”; the relative errors between those estimates are summarized in the last column “Relative error”.

Therefore, we have obtained accurate (except, maybe, for the imaginary part of $C_{1,h}$), analytical, expressions for the constants $C_{1,A}$ and $C_{3,A}$ which allow us to follow the perturbations during inflation on large scales. In particular, note the interesting ratio between the constants $C_{1,A}$ and $C_{3,A}$:

$$\frac{C_{3,\ell}}{C_{1,\ell}} = - \frac{3M_{\text{Pl}}^2}{2V_{\ell}} \Big|_{N_{\text{m}}}, \quad \frac{C_{3,h}}{C_{1,h}} = \frac{3M_{\text{Pl}}^2}{2V_{\text{h}}} \Big|_{N_{\text{m}}}. \quad (5.87)$$

Finally, let us mention that other expressions of the two constants C_1 and C_3 (the “standard” expressions that have been used in the literature so far) will be obtained in Sec. 6.

5.3.3 Large scale solutions during inflation

Having determined the constants $C_{1,A}$ and $C_{3,A}$, we now have a complete knowledge of the solutions (5.56), (5.57) and (5.58). This also gives the adiabatic part of curvature

perturbations, see Eq. (5.60) and, moreover, using the relations between $C_{1,A}$ and $C_{3,A}$, see Eq. (5.87), the non-adiabatic parts of curvature perturbations can be re-written as

$$\zeta_{\ell,\ell}^{\text{nad}} = -C_{1,\ell} \frac{V_h}{V_\ell|_{N_m}} \left[1 - \frac{2V_\ell}{9V} \frac{m_\ell^2}{H^2} (R^2 - 1) \right] \quad (5.88)$$

$$\zeta_{\ell,h}^{\text{nad}} = C_{1,h} \frac{V_h}{V_h|_{N_m}} \left[1 - \frac{2V_\ell}{9V} \frac{m_\ell^2}{H^2} (R^2 - 1) \right] \quad (5.89)$$

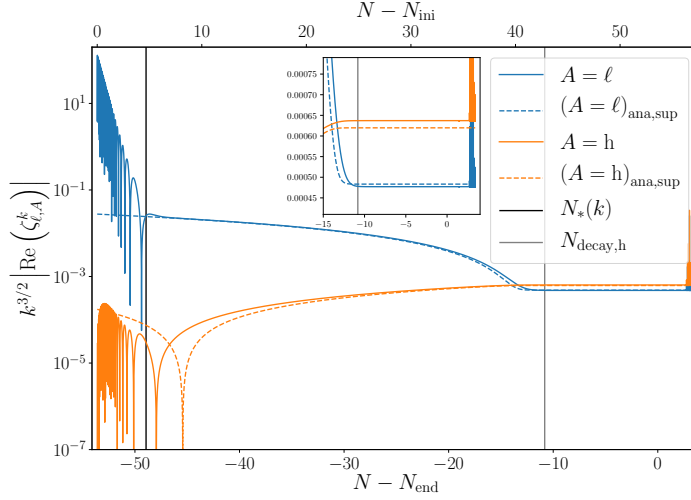
$$\zeta_{h,h}^{\text{nad}} = -C_{1,h} \frac{V_\ell}{V_h|_{N_m}} \left[1 + \frac{2V_h}{9V} \frac{m_\ell^2}{H^2} (R^2 - 1) \right] \quad (5.90)$$

$$\zeta_{h,\ell}^{\text{nad}} = C_{1,\ell} \frac{V_\ell}{V_\ell|_{N_m}} \left[1 + \frac{2V_h}{9V} \frac{m_\ell^2}{H^2} (R^2 - 1) \right]. \quad (5.91)$$

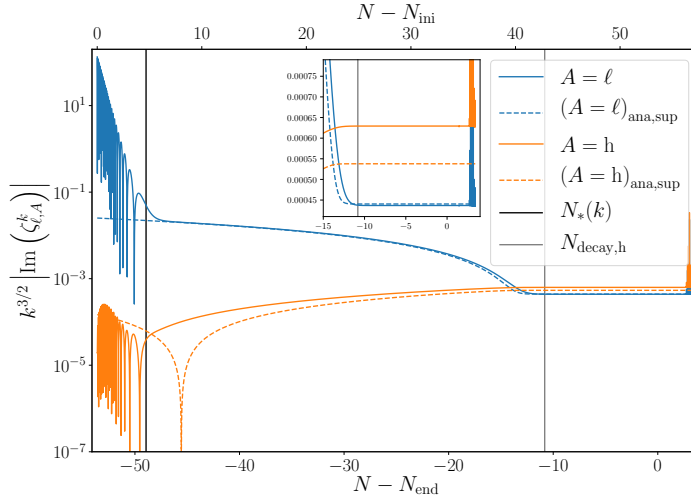
In Fig. 14, we have represented the exact (numerical) real and imaginary parts of $\zeta_{\ell,A}$ together with the (super-Hubble) analytical expression, $\zeta_{\ell,A} = \zeta_{\ell,A}^{\text{ad}} + \zeta_{\ell,A}^{\text{nad}} = -C_{1,A} + \zeta_{\ell,A}^{\text{nad}}$, where we have used Eq. (5.60) and where $\zeta_{\ell,A}^{\text{nad}}$ are given by Eqs. (5.88) and (5.89). We see that, after Hubble radius crossing, the analytical and numerical curves match very well, thus confirming that our analytical approximations are very good. In Fig. 15, we have again represented the analytical $\zeta_{\ell,\ell}$ and $\zeta_{\ell,h}$ but we have split these quantities into their adiabatic and non-adiabatic components. We see that $\zeta_{\ell,\ell}$ is initially dominated by its non-adiabatic part, $\zeta_{\ell,\ell} \simeq \zeta_{\ell,\ell}^{\text{nad}}$, which makes sense since, prior to the heavy field decay, one has $V_h \gg V_\ell|_{N_m}$, see Eq. (5.88). After the decay, the non-adiabatic part strongly decreases and the adiabatic part takes over, $\zeta_{\ell,\ell} \simeq \zeta_{\ell,\ell}^{\text{ad}}$. For $\zeta_{\ell,h}$, initially, there is no clear hierarchy between the adiabatic and non-adiabatic contributions [see Eq. (5.89) where the overall amplitude of $\zeta_{\ell,h}^{\text{nad}}$ is proportional to $V_h/V_h|_{N_m}$] but, after the decay of the heavy field, the adiabatic component largely dominates and $\zeta_{\ell,h} \simeq \zeta_{\ell,h}^{\text{ad}}$.

In Fig. 16, we have plotted the numerical and analytical (super-Hubble) real and imaginary parts of $\zeta_{h,A}$. We see that, after Hubble radius crossing, both types of solution match well, the agreement being much better for the component $\zeta_{h,h}$ than for $\zeta_{h,\ell}$. After the decay of the heavy field, both exact components start to oscillate while the analytical $\zeta_{h,h}$ and $\zeta_{h,\ell}$ continue to monotonically evolve. We think that those oscillations are numerical artefacts: during the oscillations of the heavy field, there are exact cancellations of $\delta\rho_h/\rho_h$ that are not exactly reproduced at the numerical level and, therefore, result in these oscillations. In Fig. 17, we have represented the real and imaginary parts of the analytical components $\zeta_{h,\ell}$ and $\zeta_{h,h}$ as well as their adiabatic and non-adiabatic contributions. Before the heavy field decay, $\zeta_{h,\ell}^{\text{ad}}$ and $\zeta_{h,\ell}^{\text{nad}}$ are constant and almost equal. After the decay, the non-adiabatic part starts to decrease and we are left with $\zeta_{h,\ell} \sim \zeta_{h,\ell}^{\text{ad}}$. For $\zeta_{h,h}$, the non-adiabatic part is always subdominant (and is constant before the decay and then decreases) and, as a consequence, we always have $\zeta_{h,h} \sim \zeta_{h,h}^{\text{ad}}$.

Finally, in Fig. 18, we have represented the real and imaginary parts of the amplitude of non-adiabatic perturbations during inflation, $S_{\ell h,A}$, compared to the analytical approximation given by Eq. (5.65). Again, after Hubble radius crossing, we observe a very good agreement between the two. After the heavy field decay, the numerical solu-

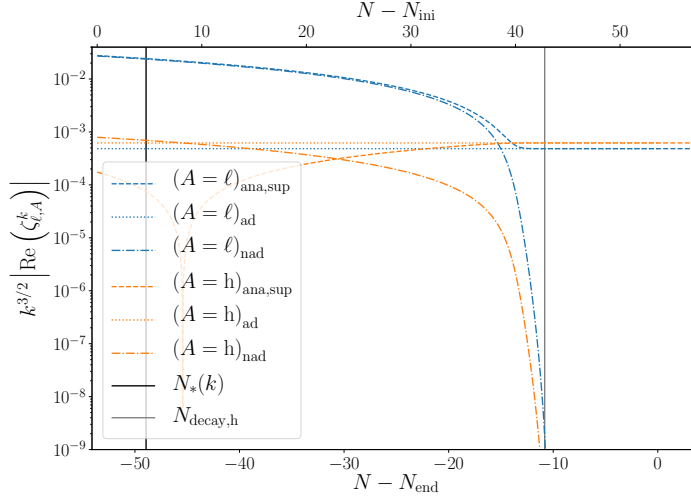


(a) Real part

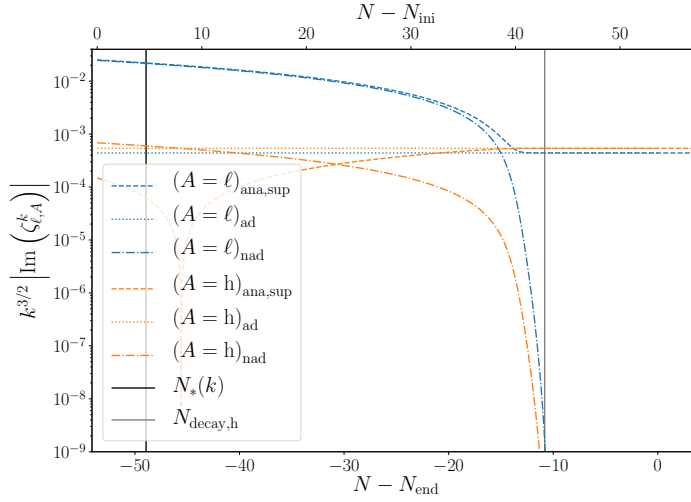


(b) Imaginary part

Figure 14: Real (upper panel) and imaginary (lower panel) parts of the light field's curvature perturbations $\zeta_{\ell,\ell}$ and $\zeta_{\ell,h}$ during inflation, including the exact numerical solutions (respectively blue and orange solid lines) and their analytical approximations on super-Hubble scales “ana,sup” (respectively blue and orange dashed lines). The vertical black line corresponds to the time of horizon crossing for the mode $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$ represented in these plots, and the vertical grey one to the time of decay of the heavy field, slightly after the transition time from which inflation is driven by the light field rather than the heavy one. After sub-Hubble oscillations and horizon crossing, these curvature perturbations are well approximated by the super-Hubble formulas inferred from Eqs. (5.57)–(5.58). Clearly, both the diagonal mode function $\zeta_{\ell,\ell}$ the non-diagonal one $\zeta_{\ell,h}$ are now accurately described (there is of course a residual error, see the inset, that will be quantified in the final result).

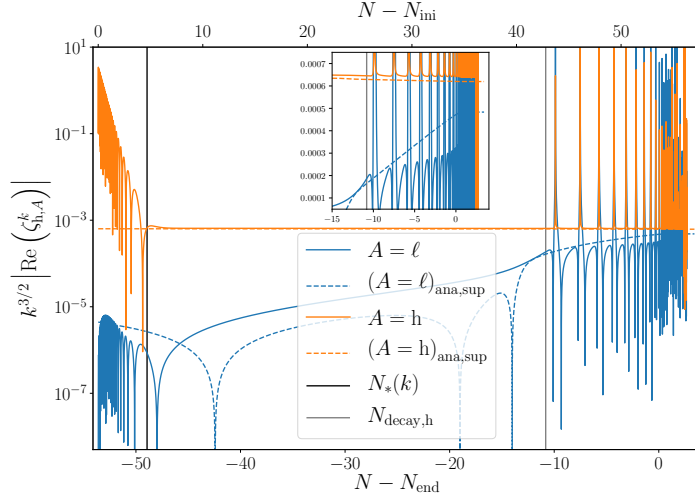


(a) Real part

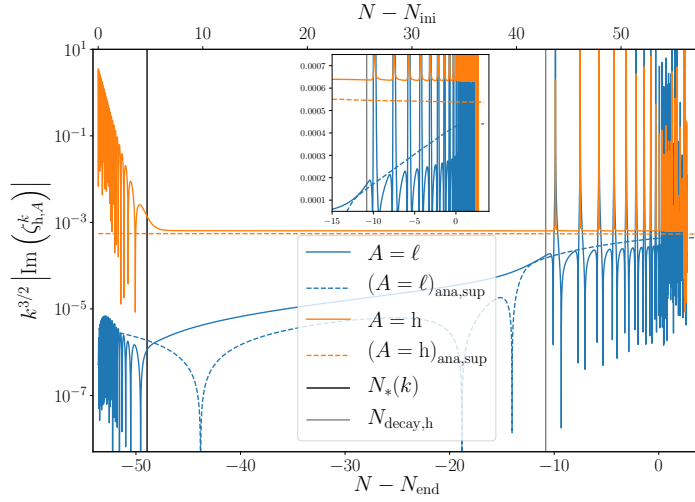


(b) Imaginary part

Figure 15: Real and imaginary parts of the analytical approximations “ana, sup” of the light field’s curvature perturbations $\zeta_{\ell,\ell}$ and $\zeta_{\ell,h}$ (respectively blue and orange dashed lines) during inflation, decomposed into their adiabatic parts $\zeta_{\ell,A}^{\text{ad}}$ (respectively blue and orange dotted lines) defined in Eq. (5.60) and non-adiabatic ones $\zeta_{\ell,A}^{\text{nad}}$ (respectively blue and orange dotted-dashed lines) defined in Eq. (5.64). The vertical black line corresponds to the time of horizon crossing for the mode $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$ represented in these plots, and the vertical grey one to the time of decay of the heavy field, slightly after the transition time from which inflation is driven by the light field rather than the heavy one. In the phase of inflation driven by the heavy scalar field, the light field’s curvature perturbations possess a non-negligible non-adiabatic component, which then decays around the transition time, and eventually these perturbations are well described by their adiabatic components only.

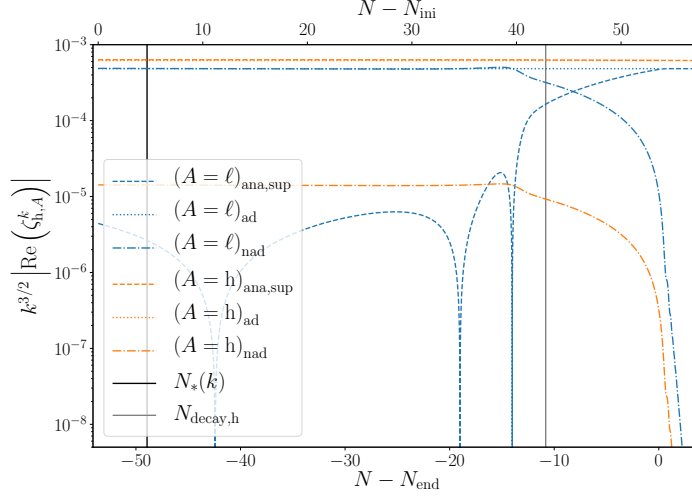


(a) Real part

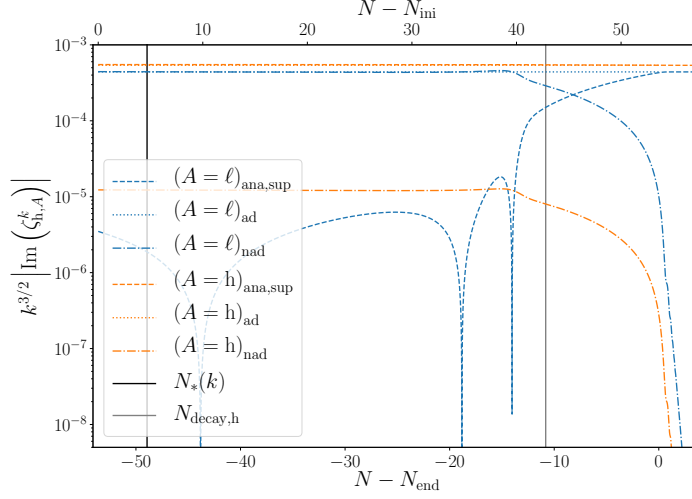


(b) Imaginary part

Figure 16: Real (upper panel) and imaginary (lower panel) parts of the heavy field’s curvature perturbations $\zeta_{h,\ell}$ and $\zeta_{h,h}$ during inflation, including the exact numerical solutions (respectively blue and orange solid lines) and their analytical approximations on super-Hubble scales “ana,sup” (respectively blue and orange dashed lines). The vertical black line corresponds to the time of horizon crossing for the mode k , and the vertical grey one to the time of decay of the heavy field. On large scales, these curvature perturbations are well approximated by the super-Hubble formulas inferred from Eqs. (5.57)–(5.58). Both the non-diagonal mode function $\zeta_{h,\ell}$ and the diagonal one $\zeta_{h,h}$ are now accurately described (there is of course a residual error, see the inset, that will be quantified in the final result). During the oscillations of the heavy scalar field after the time of decay, its curvature perturbations seem to oscillate, but this is a numerical artefact (see how the analytical approximation follows accurately the envelop of these oscillations).

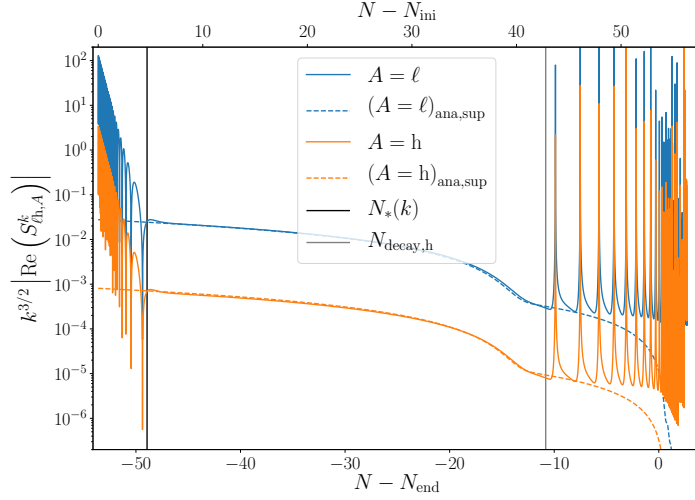


(a) Real part

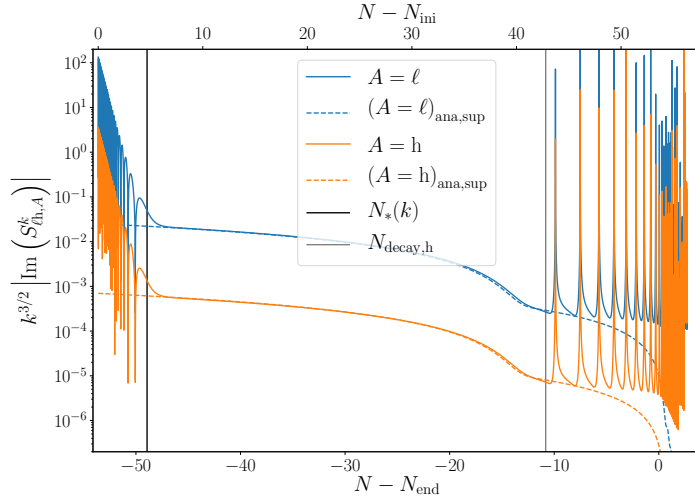


(b) Imaginary part

Figure 17: Real and imaginary parts of the analytical approximations “ana, sup” of the heavy field’s curvature perturbations $\zeta_{h,\ell}$ and $\zeta_{h,h}$ (respectively blue and orange dashed lines) during inflation, decomposed into their adiabatic parts $\zeta_{h,A}^{\text{ad}}$ (respectively blue and orange dotted lines) defined in a way similar to Eq. (5.60) and non-adiabatic ones $\zeta_{h,A}^{\text{nad}}$ (respectively blue and orange dotted-dashed lines) defined in a way similar to Eq. (5.64). The vertical black line corresponds to the time of horizon crossing for the mode k , and the vertical grey one to the time of decay of the heavy field. Strikingly, the non-adiabatic component plays an important role for the curvature perturbation $\zeta_{h,\ell}$ until the decay of the heavy field and it will be the main source of final non-adiabatic perturbations.



(a) Real part



(b) Imaginary part

Figure 18: Real (upper panel) and imaginary (lower panel) parts of the non-adiabatic fluctuations $S_{\ell,h,\ell}$ and $S_{\ell,h,h}$, including the exact numerical solutions (respectively blue and orange solid lines) and their analytical approximations on super-Hubble scales “ana,sup” (respectively blue and orange dashed lines). The vertical black line corresponds to the time of horizon crossing for the mode $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$ represented in these plots, and the vertical grey one to the time of decay of the heavy field, slightly after the transition time from which inflation is driven by the light field rather than the heavy one. The approximations are again very accurate, at least until the time of decay for the heavy field from which any way the non-adiabatic component is transferred to the “real” cosmological fluids as we will see in the following.

tions start to oscillate and the presence of those oscillations is due to the same reason given above.

We conclude this section by stating that, during inflation and on super Hubble scales, we have a good analytical control on the behaviour of the various individual curvature perturbation components.

5.3.4 Matching to the radiation-dominated era

We are now in a position where we can turn to one of the main question studied in this paper, namely the calculation of non-adiabatic perturbations in the post-inflationary Universe. Clearly this requires another matching, this time between quantities defined in the inflationary phase and quantities defined in the radiation-dominated era. Since our assumption is that the heavy field decays in pressure-less matter and the light field in radiation, the fundamental assumption used in order to relate inflationary and post-inflationary quantities will be the continuity of the corresponding (individual) curvature perturbations at the time of decay. Concretely, this means

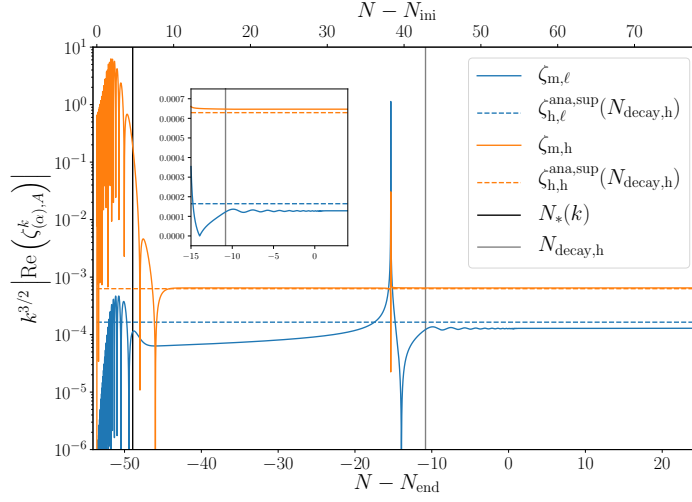
$$\zeta_{m,A} = \zeta_{h,A}(t_{\text{decay},h}), \quad \zeta_{\gamma,A} = \zeta_{\ell,A}(t_{\text{decay},\ell}), \quad (5.92)$$

and, using Eq. (3.32), it follows that

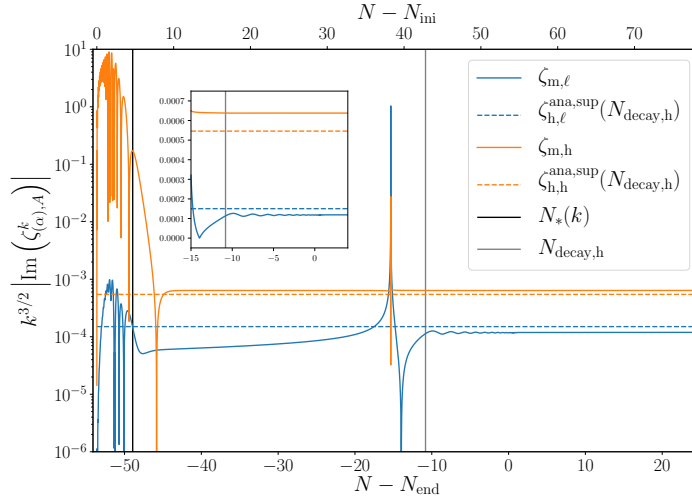
$$S_{m\gamma,A} = 3 [\zeta_{h,A}(t_{\text{decay},h}) - \zeta_{\ell,A}(t_{\text{decay},\ell})]. \quad (5.93)$$

In Figs. 19 and 20, we have represented the evolution, during and after inflation, of matter and radiation curvature perturbations in order to check the conditions (5.92). In Fig. 19, we have represented the real and imaginary parts of $\zeta_{m,\ell}$ and $\zeta_{m,h}$ as functions of the number of e-folds during inflation. The two horizontal dotted blue and orange lines corresponds to the values of $\zeta_{h,\ell}$ and $\zeta_{m,h}$ (respectively) at the time of the heavy field decay. We see that, after this time (and, for $\zeta_{m,h}$, it is even true after Hubble radius crossing), we indeed have $\zeta_{m,\ell}(N) \rightarrow \zeta_{h,\ell}^{\text{ana,sup}}(N_{\text{decay},h})$ and $\zeta_{m,h}(N) \rightarrow \zeta_{h,h}^{\text{ana,sup}}(N_{\text{decay},h})$. We also notice that the agreement is better for the second limit than for the first one. In Fig. 20, we have plotted the real and imaginary parts of $\zeta_{\gamma,\ell}$ and $\zeta_{\gamma,h}$ and studied how they tend towards $\zeta_{\ell,\ell}^{\text{ana,sup}}(N_{\text{decay},\ell})$ and $\zeta_{\ell,h}^{\text{ana,sup}}(N_{\text{decay},\ell})$, respectively. As can be seen in the figures (and in the insets), these limits are well-verified. We conclude that Figs. 19 and 20 validate Eqs. (5.92).

In order to calculate the inflationary curvature perturbations, $\zeta_{h,A}$ and $\zeta_{\ell,A}$, we make use of Eqs. (5.88), (5.89), (5.90) and (5.91). A first remark is that the quantities $\zeta_{\ell,\ell}^{\text{nad}}(t_{\text{decay},\ell})$ and $\zeta_{\ell,h}^{\text{nad}}(t_{\text{decay},\ell})$ are proportional to $V_h|_{N_{\text{decay},\ell}}/V_\ell|_{N_m}$ and $V_h|_{N_{\text{decay},\ell}}/V_h|_{N_m}$, respectively, see Eqs. (5.88), and (5.89), which implies that they are in fact sub-dominant quantities since, by the time of the light field decay, the contribution of the heavy field is highly suppressed. This can be easily checked by inspection of Figs. 14, 15, 16 and 17. Indeed, if one compares Fig. 14 and 16 (in particular the insets), we notice that the quantities $\zeta_{\ell,\ell}$, $\zeta_{\ell,h}$, $\zeta_{h,\ell}$ and $\zeta_{h,h}$ are, very roughly speaking, all of the same order of magnitude at the end of inflation. However, what matters are in fact the non-adiabatic components since (by the definition) the adiabatic ones cancel

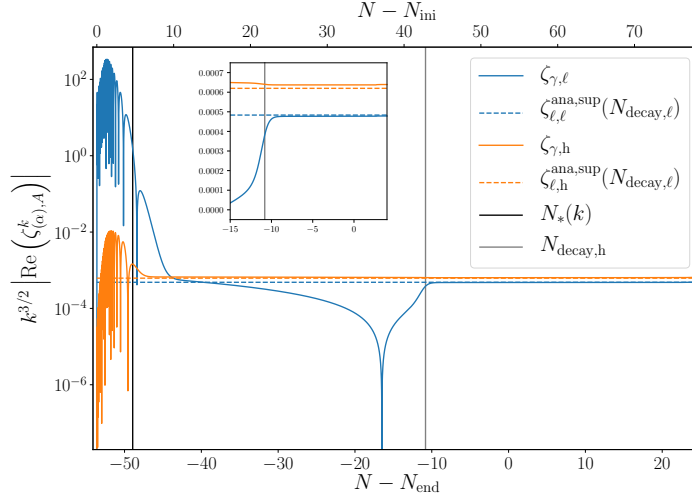


(a) Real part

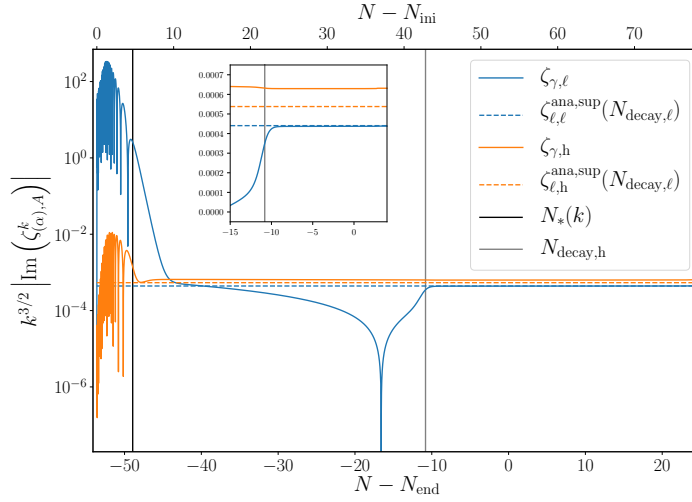


(b) Imaginary part

Figure 19: Real (upper panel) and imaginary (lower panel) parts of the matter fluid's curvature fluctuations $\zeta_{m,\ell}$ and $\zeta_{m,h}$ (respectively blue and orange solid lines) and their analytical approximations $\zeta_{h,A}^{\text{ana,sup}}(N_{\text{decay,h}})$ valid after the decay of the heavy field (respectively blue and orange dashed lines), as given by Eq. (5.92). The vertical black line corresponds to the time of horizon crossing for the mode $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$ represented in these plots, and the vertical grey one to the time of decay of the heavy field, slightly after the transition time from which inflation is driven by the light field rather than the heavy one. The asymptotic solutions for the fluid's curvature perturbations in the radiation era are very accurate again (there is of course a residual error, see the inset, that will be quantified in the final result).

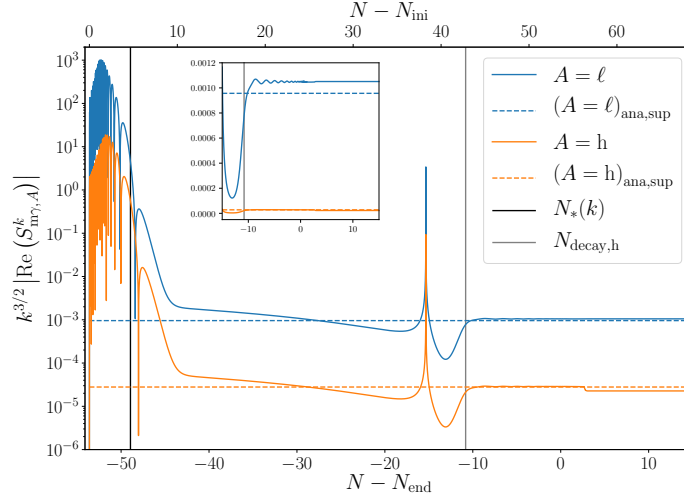


(a) Real part

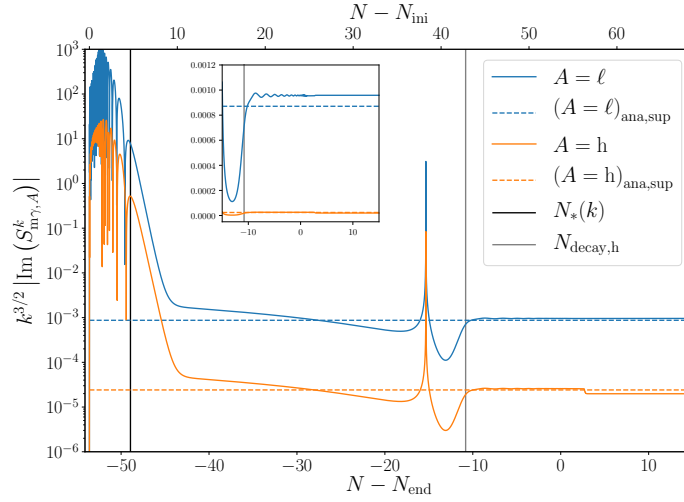


(b) Imaginary part

Figure 20: Real (upper panel) and imaginary (lower panel) parts of the radiation fluid's curvature fluctuations $\zeta_{\gamma,\ell}$ and $\zeta_{\gamma,h}$ (respectively blue and orange solid lines) and their analytical approximations $\zeta_{\ell,A}^{\text{ana,sup}}(N_{\text{decay},\ell})$ valid after the decay of the light field corresponding to the end of inflation $N = N_{\text{end}}$ (respectively blue and orange dashed lines), as given by Eq. (5.92). The vertical black line corresponds to the time of horizon crossing for the mode $k = 100 \times a_{\text{ini}} H_{\text{ini}} \simeq 0.025 M_{\text{Pl}}$ represented in these plots, and the vertical grey one to the time of decay of the heavy field, slightly after the transition time from which inflation is driven by the light field rather than the heavy one. The asymptotic solutions for the fluid's curvature perturbations in the radiation era are very accurate again (there is of course a residual error, see the inset, that will be quantified in the final result).



(a) Real part



(b) Imaginary part

Figure 21: Real (upper panel) and imaginary (lower panel) parts of the non-adiabatic fluid's fluctuations $S_{m\gamma,\ell}$ and $S_{m\gamma,h}$ (respectively blue and orange solid lines) and their analytical approximations valid respectively after the decay of the heavy and respectively light fields (respectively blue and orange dashed lines). The asymptotic solutions for the fluid's non-adiabatic perturbations in the radiation era are very accurate again, and the residual errors of $\sim 5\%$ for the component $A = \ell$ and visible in the inset, correspond to the ones of the final result. Note that the small drop around $N - N_{\text{end}} = 2.7$ (only visible by eye in a logarithmic scale and for the smallest component $A = h$) is a numerical artefact due to the fact that the heavy field is abandoned from the numerical evolution at that time because its tiny oscillations are computationally expensive to follow (we have checked that by changing the time at which the heavy field is abandoned, the position and the height of the drop changes accordingly, but always remains negligible).

out in the expression of $S_{m,\gamma}$; and if one now looks at Figs. 15 and 17, we notice that there is a clear hierarchy between the quantities $\zeta_{\ell,\ell}^{\text{nad}}$, $\zeta_{\ell,h}^{\text{nad}}$ on one hand and $\zeta_{h,\ell}^{\text{nad}}$, $\zeta_{h,h}^{\text{nad}}$ on the other hand, namely $\zeta_{h,\ell}^{\text{nad}}, \zeta_{h,h}^{\text{nad}} \gg \zeta_{\ell,\ell}^{\text{nad}}, \zeta_{\ell,h}^{\text{nad}}$. As a consequence, $\zeta_{\ell,\ell}^{\text{nad}}, \zeta_{\ell,h}^{\text{nad}}$ can be neglected in Eq. (5.93) which, therefore, reduces to the following expression

$$S_{m\gamma,A} \simeq 3\delta_{A,\ell}\zeta_{h,\ell}^{\text{nad}}(N_{\text{decay},h}) + 3\delta_{A,h}\zeta_{h,h}^{\text{nad}}(N_{\text{decay},h}) . \quad (5.94)$$

We see that the non-adiabatic perturbations in the post-inflationary Universe is in fact completely determined by what happens at the time of decay of the heavy field.

Then, in order to calculate $\zeta_{h,\ell}^{\text{nad}}$ and $\zeta_{h,h}^{\text{nad}}$, we use Eqs. (5.90) and (5.91). Since the decay of the heavy field happens during the phase of inflation dominated by the light field, the slow-roll approximation for the background can be used, which leads to the following results: $\phi_\ell^2 \simeq 4M_{\text{Pl}}^2(N_{\text{end}} - N)$ and $V_h/V \ll 1$. As a consequence, from Eqs. (5.90) and (5.91), one obtains

$$S_{m\gamma,\ell} \simeq C_{1\ell} \frac{12M_{\text{Pl}}^2}{\phi_{\ell,\text{ini}}^2} (N_{\text{end}} - N_{\text{decay},h}) , \quad (5.95)$$

$$S_{m\gamma,h} \simeq -C_{1h} \frac{1}{R^2} \frac{12M_{\text{Pl}}^2}{\phi_h^2(N_m)} (N_{\text{end}} - N_{\text{decay},h}) . \quad (5.96)$$

In Fig. 21, we have represented the real and imaginary parts of $S_{m\gamma,A}$ as a function of the number of e-folds compared to the numerical estimates given by Eqs. (5.95) and (5.96). We see that, after the decay of the heavy field, the numerical exact curves freeze out to a value which match well the analytical approximations.

Then, we calculate the non-adiabatic power spectrum of $S_{m\gamma}$, $P_{S_{m\gamma}}$, which involves the different components of $S_{m\gamma,A}$. It can be expressed as

$$P_{S_{m\gamma}} \propto |S_{m\gamma,\ell}|^2 + |S_{m\gamma,h}|^2 \simeq |S_{m\gamma,\ell}|^2 \left\{ 1 + \left| \frac{C_{1,h}}{C_{1,\ell}} \right|^2 \frac{1}{R^4} \left[\frac{\phi_{\ell,\text{ini}}^2}{\phi_h(N_m)} \right]^4 \right\} . \quad (5.97)$$

From Eqs. (5.95), (5.96) and (5.97), we see that the crucial quantity that needs to be calculated in order to evaluate the amplitude of the non-adiabatic perturbations is $N_{\text{decay},h}$ or $N_{\text{end}} - N_{\text{decay},h}$. As discussed in Sec. 5.2.4, the decay time of the heavy field is the time before which the amount of cold dark matter should be negligible, and after which the heavy field should be negligible. Therefore, in Sec. 5.2.4, this time was taken to be $\rho_h(N_{\text{decay},h}) = \rho_m(N_{\text{decay},h})$. In this paper, given the importance of calculating $N_{\text{decay},h}$, we have developed different methods to estimate it. First, there are of course numerical calculations leading to a semi-analytical determination of $P_{S_{m\gamma}}$, namely $P_{S_{m\gamma}}$ is found analytically according to Eq. (5.97) but, in this equation, $N_{\text{decay},h}$ is evaluated numerically. A second way is to use the simple considerations presented in Sec. 5.2.4, which leads to Eq. (5.45). Finally, we have also worked out a more precise approach in App. A, based on the WKB approach, which leads to a third estimate of the non-adiabatic perturbations. These results are summarized in Table. 2. We see that the first method leads to an error of $\sim 10\%$, the WKB-based one to an error of $\sim 20\%$ and,

Quantity / Value	Numeric	Analytic ($N_{\text{decay,h}}$)	error	Analytic ($N_{\text{decay,h}}^{\text{WKB}}$)	error	Analytic ($N_{\text{decay,h}}^{\text{ana,sd}}$)	error
$\Re S_{\text{m}\gamma,\ell}$	-0.269	-0.251	6.5%	-0.241	10.5%	-0.195	27.4%
$\Im S_{\text{m}\gamma,\ell}$	-0.245	-0.229	6.6%	-0.219	10.6%	-0.177	27.5%
$\Re S_{\text{m}\gamma,\text{h}} \times 10^3$	7.35	7.29	0.9%	6.98	5.1%	5.66	23.1%
$\Im S_{\text{m}\gamma,\text{h}} \times 10^3$	6.60	6.33	4.2%	6.06	8.3%	4.91	25.7%
$P_{S_{\text{m}\gamma}}$	0.132	0.116	12.7%	0.106	20.0%	0.070	47.4%

Table 2: Numerical results versus analytical approximations following different treatments to find the time of decay of the heavy field, for the non-adiabatic fluctuations $S_{\text{m}\gamma,A}$ and its power spectrum $P_{S_{\text{m}\gamma}} = |S_{\text{m}\gamma,\ell}|^2 + |S_{\text{m}\gamma,\text{h}}|^2$ at the end of reheating and beginning of the radiation-domination era. The analytical approximations crucially depend on the value of the time of the decay for the heavy field, so three possibilities are shown: $N_{\text{decay,h}} = -10.81$ for the value from the numerical evolution of the background, $N_{\text{decay,h}}^{\text{WKB}} = -10.35$ for the analytical treatment with the WKB approximation presented in the App. A (see Fig. 26) and $N_{\text{decay,h}}^{\text{ana,sd}} = -8.39$ with the simple analytical treatment that was shown in Sec. 5.2.4 not to be very precise (see Fig. 3).

finally, the estimate of Eq. (5.45) to a $\sim 50\%$ error. In the case of the first method, since $N_{\text{decay,h}}$ is calculated exactly, the 10% error originates from the condition (5.92). Since it is difficult to see how other analytical approximations could be designed, it represents, to some extent, the incompressible error of any analytical approach.

6 Comparison with the standard approach

In this section, we compare our (numerical and analytical) calculations of the non-adiabatic perturbations to the calculations of Refs. [15, 16] and Ref. [17], which also derive an analytical formula for $P_{S_{\text{m}\gamma}}$ in the double inflation scenario.

Before carrying out this comparison, we first recall, very briefly, how the results of Refs. [15, 16] and Ref. [17] are obtained. Since the details of reheating and of the decay process are neglected in those references, each fluid is always individually conserved and the amplitude of the non-adiabatic modes can be defined by Eq. (3.33), namely

$$S_{\text{m}\gamma} = \frac{\delta\rho_{\text{m}}}{\rho_{\text{m}}} - \frac{3}{4} \frac{\delta\rho_{\gamma}}{\rho_{\gamma}} \simeq \frac{\delta\rho_{\text{m}}}{\rho_{\text{m}}}, \quad (6.1)$$

where the last expression is again the fact, discussed in the previous section, that the amplitude of the non-adiabatic perturbation is dominated by what happens at the heavy field decay. The question is then to relate $\delta\rho_{\text{m}}/\rho_{\text{m}}$ to $\delta\rho_{\text{h}}/\rho_{\text{h}}$. In the literature, $\delta\phi_{\text{h}}/\phi_{\text{h}}$ is taken to be constant during the oscillations of the heavy field (because $\delta\phi_{\text{h}}$ and ϕ_{h}

obey the same equation of motion in this regime) which covers the phase between the heavy field decay and the end of inflation. At the end of inflation, one can thus write

$$\frac{\delta\rho_{\text{m}}}{\rho_{\text{m}}} \sim \frac{\delta\rho_{\text{h}}}{\rho_{\text{h}}} \sim 2\frac{\delta\phi_{\text{h}}}{\phi_{\text{h}}}, \quad (6.2)$$

which comes from the continuity of energy density and $\rho_{\text{h}} \sim m_{\text{h}}^2 \langle \phi_{\text{h}} \rangle^2 / 2$.

Then, our next goal is to make the connection between the previous considerations and the super Hubble slow-roll solution given by Eq. (5.58), which can be written as

$$\delta\phi_{\text{h}} = \frac{C_1}{H} \dot{\phi}_{\text{h}} + 2HC_3 \frac{V_{\ell}}{V_{\ell} + V_{\text{h}}} \dot{\phi}_{\text{h}} = -2C_1 \frac{M_{\text{Pl}}^2}{\phi_{\text{h}}} \frac{V_{\text{h}}}{V_{\text{h}} + V_{\ell}} - \frac{2}{3} C_3 \frac{\partial V_{\text{h}}}{\partial \phi_{\text{h}}} \frac{V_{\ell}}{V_{\text{h}} + V_{\ell}}. \quad (6.3)$$

From this expression, we conclude that, if the light field dominates ($V_{\ell} \gg V_{\text{h}}$), then the first branch of the solution $\propto C_1$ can be ignored and one has

$$\frac{\delta\phi_{\text{h}}}{\phi_{\text{h}}} \simeq -\frac{2}{3} C_3 m_{\text{h}}^2. \quad (6.4)$$

As a consequence, the quantity $\delta\phi_{\text{h}}/\phi_{\text{h}}$ also remains constant once the light field has started to dominate, which occurs slightly before the decay of the heavy field (if one can really define a time of decay for the heavy field, see the discussion in the previous sections). In some sense, these considerations allow us to fix the value of the constant $\delta\phi_{\text{h}}/\phi_{\text{h}}$ at the end of inflation in Eq. (6.2) and one can write

$$S_{\text{m}\gamma} \simeq \frac{\delta\rho_{\text{m}}}{\rho_{\text{m}}} \simeq -\frac{4}{3} m_{\text{h}}^2 C_3. \quad (6.5)$$

One recovers the fact that non-adiabatic perturbations solely depend on the constant C_3 .

Then, the constant C_3 is evaluated with the help of Eq. (5.67). In this formula, the quantities $\delta\phi_{\ell}$ and $\delta\phi_{\text{h}}$ are written

$$\delta\phi_{\ell} = \frac{H_*}{\sqrt{2k^3}} e_{\ell}, \quad \delta\phi_{\text{h}} = \frac{H_*}{\sqrt{2k^3}} e_{\text{h}}, \quad (6.6)$$

where we recall that H_* denotes the value of the Hubble parameter at horizon crossing and e_i ($i = \ell, \text{h}$) are classical random Gaussian processes with $\langle e_i(\mathbf{k}) \rangle = 0$ and $\langle e_i(\mathbf{k}) e_j^*(\mathbf{k}') \rangle = \delta_{ij} \delta(\mathbf{k} - \mathbf{k}')$. It follows that Eq. (5.67) can be re-written as

$$S_{\text{m}\gamma} = \sqrt{\frac{2}{k^3}} H_* \left(\frac{e_{\text{h}}}{\phi_{\text{h}}} - R^2 \frac{e_{\ell}}{\phi_{\ell}} \right). \quad (6.7)$$

As a consequence, using Eqs. (5.16), (5.18) and (5.21), one arrives at

$$P_{S_{\text{m}\gamma}} = |S_{\text{m}\gamma}|^2 = \frac{1}{3k^3} \frac{m_{\ell}^2}{M_{\text{Pl}}^2} [1 + (R^2 - 1) \sin^2 \theta_*] \left(\frac{1}{\sin^2 \theta_*} + \frac{R^4}{\cos^2 \theta_*} \right), \quad (6.8)$$

an equation that should be compared to Eq. (5.97). Numerically, this equation gives (we use $\theta_* = 0.962$ from $N_* = 4.67$ determined numerically and $-N_* + N_{\text{end}} \simeq C/\cos^2\theta_*$) $P_{S_{m\gamma}} = 0.072$, to be compared with the numerical result $P_{S_{m\gamma}} = 0.132$ and the analytical approximations presented in this work: the relative error found with Eq. (6.8) is 45.5%, which is comparable to our worst analytical estimate with $N_{\text{decay,h}}^{\text{ana,sd}}$, see Table. 2.

Therefore, we conclude that modeling the reheating mechanism is crucial in order to get an accurate prediction for non-adiabatic perturbations after the end of multifield inflation, in the post-inflationary Universe. Ignoring the details of reheating can indeed lead to an error as big as $\sim 50\%$.

It is also interesting to compare the amplitude of adiabatic and non-adiabatic perturbations. In the radiation-dominated era, we have $\zeta_\gamma \simeq \zeta_\ell^{\text{ad}} = -C_1$, see Eq. (5.60). Using Eq. (5.66), one has

$$\zeta_\gamma = \frac{1}{2M_{\text{Pl}}^2} \frac{H_*}{\sqrt{2k^3}} (\phi_h e_h + \phi_\ell e_\ell), \quad (6.9)$$

from which we deduce

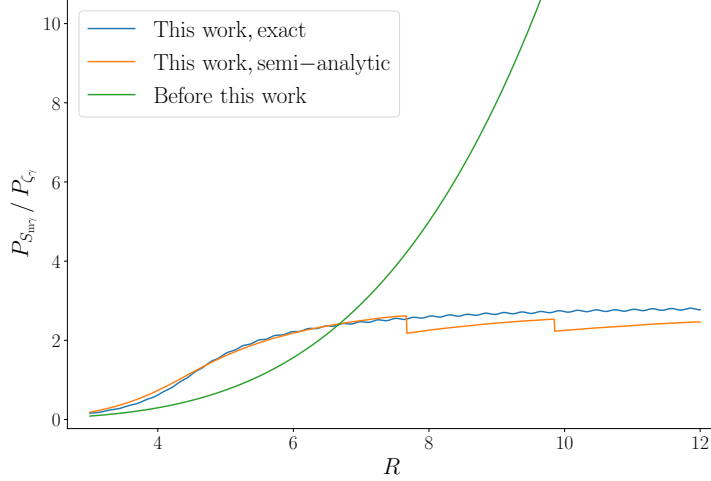
$$P_{\zeta_\gamma} = \frac{C^2}{3k^3} \frac{m_\ell^2}{M_{\text{Pl}}^2} [1 + (R^2 - 1) \sin^2 \theta_*] \frac{(\tan \theta_*)^{4/(R^2-1)}}{\cos^4 \theta_*}. \quad (6.10)$$

It follows, using the expression (5.27) of the constant C , that the non-adiabatic to adiabatic power spectrum ratio can be expressed as

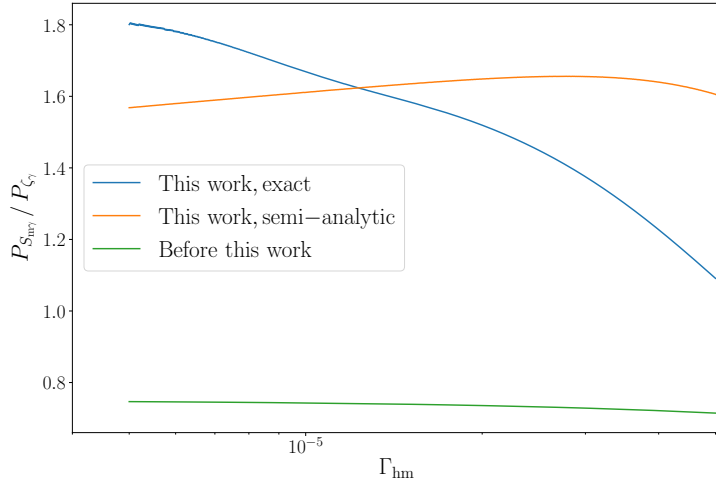
$$\frac{P_{S_{m\gamma}}}{P_{\zeta_\gamma}} = \frac{16M_{\text{Pl}}^4}{\phi_\ell^4|_{\text{ini}}} (\tan \theta_*)^{4/(1-R^2)} \left(\frac{\cos^4 \theta_*}{\sin^2 \theta_*} + R^4 \cos^2 \theta_* \right). \quad (6.11)$$

For our fiducial parameters used above (leading to $\theta_* \simeq 0.962$), one finds $P_{S_{m\gamma}}/P_{\zeta_\gamma} \simeq 0.75$. This should be compared to our results, $P_{S_{m\gamma}}/P_{\zeta_\gamma} \simeq 1.65$ numerically and $P_{S_{m\gamma}}/P_{\zeta_\gamma} \simeq (1.60, 1.46, 0.96)$ analytically with the three possible choices of $N_{\text{decay,h}}$ as explained in Sec. 5.3.4. Notice that the precision on the non-adiabatic power spectrum to adiabatic power spectrum ratio seems better than the numbers quoted in Tables. 1 and 2 (for instance, it is 3% with an exact $N_{\text{decay,h}}$). This is due to the fact that both quantities are underestimated and, as a consequence, the error in their ratio is smaller than the error in each of them.

In Fig. 22, we have represented the ratio $P_{S_{m\gamma}}/P_{\zeta_\gamma}$ versus R , for a fixed Γ_{hm} (taken at its fiducial value $\Gamma_{\text{hm}} = 1.0 \times 10^{-5} M_{\text{Pl}}$) and versus Γ_{hm} for a fixed R (also taken at its fiducial value $R = 5$) for three cases: the blue curve corresponds to the exact (numerical) result, the orange curve corresponds to the semi-analytical result obtained in this paper and the green curve is obtained from Eq. (6.11). In panel (a), we see that our semi-analytical result reproduces well the exact result while the standard formulation poorly performs, especially for $R \gtrsim 8$. The two drops that can be seen on the orange curve are due to the way $N_{\text{decay,h}}$ is calculated. $N_{\text{decay,h}}$ is obtained by determining when ρ_h and ρ_m intersect. Since these two quantities oscillate in this regime, the intersection can occur around one specific oscillation and then, suddenly, when the value of R changes,



(a) Ratio $P_{S_{m\gamma}}/P_{\zeta\gamma}$ as a function of R



(b) Ratio $P_{S_{m\gamma}}/P_{\zeta\gamma}$ as a function of Γ_{hm}

Figure 22: Ratio $P_{S_{m\gamma}}/P_{\zeta\gamma}$ as a function of the parameter R , panel (a), and as a function of the parameter Γ_{hm} , panel (b). The blue line represents the exact result, obtained by means of numerical calculations. The orange line corresponds to the analytical approach developed in this paper with $N_{\text{decay,h}}$ determined numerically. Finally, the green line corresponds to the standard formulation, see Eq. (6.11).

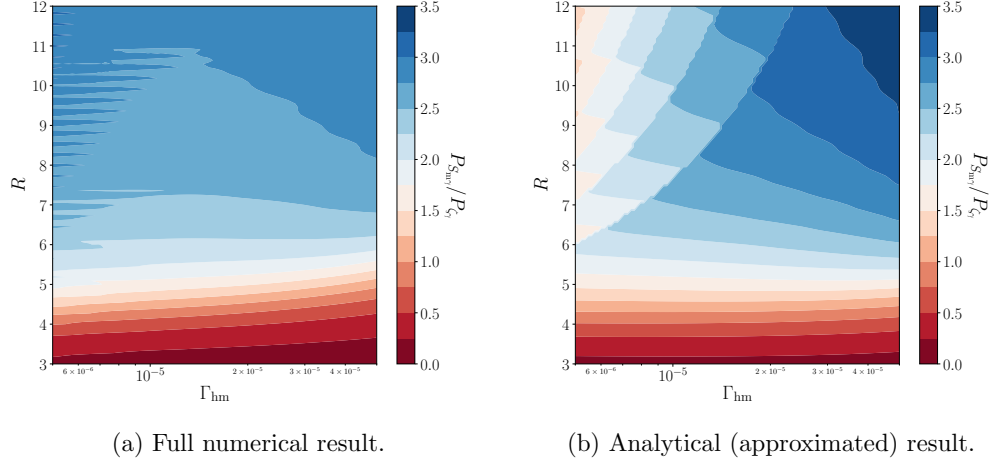


Figure 23: Contour levels of the ratio $P_{S_{m\gamma}}/P_{\zeta_\gamma}$ as a function of R and Γ_{hm} . The figure in the left panel is obtained by numerical calculations and is the results of 10000 simulations (namely 100 values for R and 100 values for Γ_{hm}). The right panel is obtained by means of the analytical approximations discussed in this work.

jumps to another oscillation resulting in the behaviour observed in Fig. 22. In panel (b), we notice that the agreement between the exact and analytical results (blue and orange lines) is still quite good but, admittedly, less good than in panel (a). On the other hand, the standard formula (green line) still poorly performs. Notice that the latter is almost independent of Γ_{hm} , a slight dependence being nevertheless present through the value of θ_* . We also remark that the agreement between the numerical and analytical results deteriorates when Γ_{hm} increases compared to our fiducial value $\Gamma_{hm} = 1.0 \times 10^{-5} M_{Pl}$. However, when this is the case, one enters a regime where, in the Klein-Gordon equation, the contribution of the term proportional to Γ_{hm} is no longer negligible compared to H_{ini} at the onset of inflation. This means that we are in a situation which is reminiscent of warm inflation where the considerations presented in this work are no longer valid. Moreover, although the departure is less visible, it seems also that the analytical approximation is less accurate when Γ_{hm} decreases too much. But again, this can be understood: if Γ_{hm} is very small, then the instantaneous decay approximation for the heavy field is even less justified, and even though one can still define the time $N_{decay,h}$ as the time when $\rho_h = \rho_m$, it becomes less relevant to use it as a particularly interesting time. This shows once more that, in the general case, the system should be solved numerically in order to derive reliable predictions for the cosmological observables.

In Fig. 23, we present a comparison of the ratios $P_{S_{m\gamma}}/P_{\zeta_\gamma}$, as a function of the parameters R and Γ_{hm} , obtained numerically and analytically. This confirms that our analytical approximations correctly reproduce the exact results, especially for $R \lesssim 7$.

For larger values of R , the agreement is less good and we observe a complicated structure in parameter space. As already mentioned above, this structure is due to difficulties in handling $N_{\text{decay,h}}$. This structure is the two-dimensional manifestation of the drops observed in the orange line in Fig. 22, panel (a). Fig. 23 also confirms that the dependence of $P_{S_{m\gamma}}/P_{\zeta_\gamma}$ is stronger in the R -direction than in the Γ_{hm} , a property which can also be noticed in Fig. 22. However, numerical calculations indicate that this dependence is less flat than suggested by analytical approximations.

We conclude by stressing again that a detailed modelling of the reheating epoch can affect the predictions of multifield scenarios and in a regime in which non-adiabatic perturbations represent a non-negligible fraction of the adiabatic ones.

7 Conclusions

In multifield inflation, because curvature perturbations are not necessarily conserved on large scales, one expects the predictions of a model to depend on what happens during reheating, and the main goal of this article was to investigate whether this effect can indeed be relevant. Moreover, beyond being a question of principle, this issue is also important, and timely, because future, high-accuracy, experiments could maybe, open up a new window on the micro-physics of inflation.

In order to carry out the aforementioned task at the practical level, we have introduced a detailed description of reheating which explicitly takes into account the interactions between the inflaton fields and their decay products. As an illustration of a property that can be affected by the physical processes at play during reheating, we have chosen to consider the amplitude of non-adiabatic perturbations in the post-inflationary Universe.

We have then developed new numerical codes, and new analytical techniques, allowing us to track the behaviour of the perturbations throughout reheating. Concretely, these tools were used in the context of a specific model, namely double inflation.

The main result of this study is that, indeed, in the context of multifield inflation, the predictions can be quite sensitive to the details of what is going on during reheating. In the case studied here, we have estimated that different modellings of the reheating phase can result in predictions that differ by almost $\sim 50\%$. Of course, this number is to be taken with a grain of salt given that it was obtained for a particular model and for a particular observable. However, we think it illustrates well the main conclusion of this article. Another conclusion is that it is possible to develop analytical techniques which can reasonably approximate the exact calculations, at the $\sim 10\%$ level. However, for a more realistic and, therefore, more complicated model (with, for instance, interaction between the inflaton fields, more complicated potentials, more decay channels $\dots$), it is very likely that no analytical approach will be able to reach a good level of accuracy. In this respect, the codes that we have developed for this paper should be very useful for future investigations in multifield inflation.

As a final remark, let us notice that it would be interesting to test the robustness of the above mentioned lessons by exploring whether other effects in double inflation,

new models and/or new observables are also dependent on the details of reheating at the level found before. We hope to return to these questions soon.

A Background evolution at heavy field decay

In this appendix, we consider again the problem of modelling the behaviour of the background around the decay time of the heavy field. This question was already treated in Sec. 5.2.4 and our aim in this appendix is to improve this treatment. Here, we study in details the behaviour of the system when the heavy field leaves the slow-roll regime and starts to oscillate and to decay. As argued before, see Sec. 5.3.4, this is important because tracking what happens to the background in this regime with good accuracy turns out to be crucial in order to predict the level of non-adiabatic perturbations that remains after the end of inflation.

A.1 Time-dependent frequency

Since we know that the heavy field decays and oscillates, as it was already done in Sec. 5.2.4, it is especially convenient to write this quantity as

$$\phi_h(t) = \phi_{h,p} \left(\frac{a_p}{a} \right)^{3/2} e^{-\Gamma_{hm}(t-t_p)/4} g_h(t), \quad (\text{A.1})$$

with “p” meaning evaluated at a particular time. The quantity $\phi_{h,p}$ is the vacuum expectation value of the heavy field at this particular time. This particular time will be specified soon. Eq. (A.1) defines the new function $g_h(t)$. Then, using Eq. (5.7), it is straightforward to show that $g_h(t)$ obeys the equation [see also Eqs. (5.40) and (5.41) where these quantities were already discussed in the main text],

$$\ddot{g}_h(t) + \omega_h^2(t) g_h(t) = 0, \quad (\text{A.2})$$

with

$$\omega_h^2(t) = m_h^2 \left(1 - \frac{3}{2} \epsilon_1 \frac{H^2}{m_h^2} - \frac{9}{4} \frac{H^2}{m_h^2} - \frac{1}{16} \frac{\Gamma_{hm}^2}{m_h^2} - \frac{3}{4} \frac{H}{m_h} \frac{\Gamma_{hm}}{m_h} \right). \quad (\text{A.3})$$

This effective frequency is represented in Fig. 24 (blue solid line). Analytically, viewed as a function of cosmic time, the explicit form of $\omega_h^2(t)$ is complicated and, as a consequence, Eq. (A.2) cannot be integrated exactly. We see that, at the beginning of inflation, $\omega_h^2(t)$ is negative, vanishes at a time that we denote in the following by t_{osc} , which is a turning point, and then becomes positive which entails the presence of oscillations in the solution.

The position of the turning point can be determined with the help of the following considerations. In the neighbourhood of the turning point, one can use an approximation for $\omega_h(t)$ and write $\omega_h^2 \simeq m_h^2 - 9H^2/4$. The turning point is therefore located at a time when $H_{\text{osc}} \simeq 2m_h/3$ and using the expression (5.21), it occurs at a value of $\tan \theta_{\text{osc}}$ which is a solution to the following equation

$$(\tan \theta_{\text{osc}})^{2/(R^2-1)} (1 + R^2 \tan^2 \theta_{\text{osc}}) = \frac{2R^2}{3C}. \quad (\text{A.4})$$

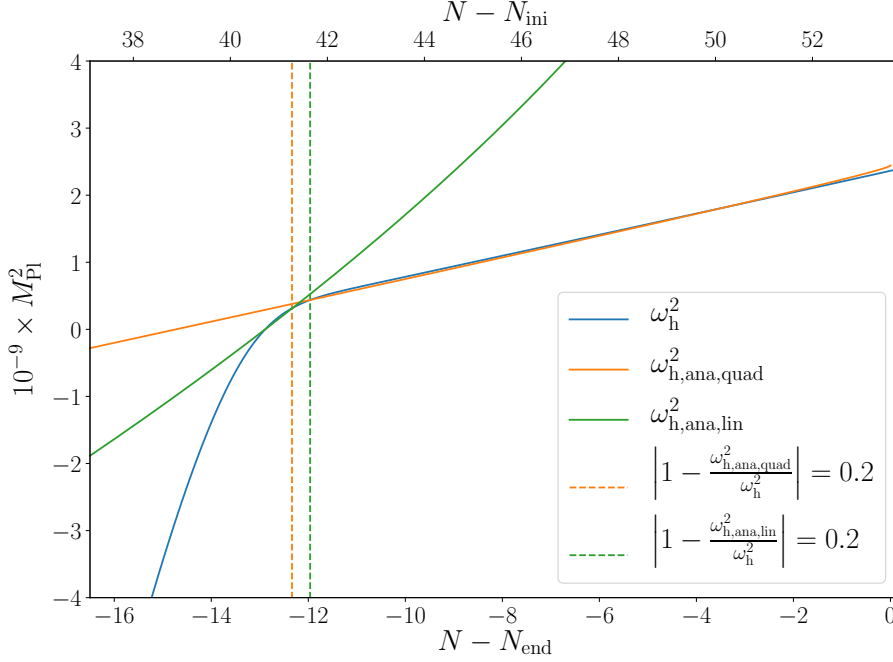


Figure 24: Squared pulsation ω_h^2 , defined in Eq. (A.3), versus number of e-folds: exact numerical result (blue line), quadratic approximation $\omega_{h,\text{ana},\text{quad}}^2$ (orange line) given by Eq. (A.7) and that becomes roughly valid after the time represented by the orange vertical dashed line, and linear approximation $\omega_{h,\text{ana},\text{lin}}^2$ (green line) given by Eq. (A.13) and that is roughly valid until the time represented by the green vertical dashed line. Both approximations are faithful in the time domain between the two vertical dashed lines, which also coincides roughly with the time at which the WKB solution becomes correct (see the next figure).

This equation is a polynomial equation in $\tan^2 \theta_{\text{osc}}$ which, unfortunately, cannot be solved exactly. However, one can use Newton's method to find an approximate solution. Starting from the initial guess $\tan^2 \theta_{\text{osc}} \sim R^{-2}$, the first iteration leads to

$$\tan^2 \theta_{\text{osc}} \simeq \frac{3 - R^2 + 2R^2(R^2 - 1)R^{2/(R^2-1)}/(3C)}{R^2(1 + R^2)}. \quad (\text{A.5})$$

The exact (numerical) solution to Eq. (A.4), for the fiducial parameters, is $\tan^2 \theta_{\text{osc}} \simeq 0.0101$ to be compared with the solution (A.5), $\tan^2 \theta_{\text{osc}} \simeq 0.0104$, and corresponding to $N_{\text{osc}} - N_{\text{end}} = -13.3$, to be compared with the exact time found numerically, $N_{\text{osc}} - N_{\text{end}} = -12.89$.

As noticed above, the form of $\omega_h^2(t)$ is complicated. However, depending on the regimes considered, some useful approximations can be found. For instance, in the

regime dominated by the light field, the Hubble parameter simplifies and is given by Eq. (5.35), $H^2 = 2m_\ell^2(N_{\text{end}} - N)/3$. Moreover, given that $dN = Hdt$, the relationship between the number of e-folds and the cosmic time can be expressed as [This equation was already derived, see Eq. (5.46), and we reproduce it here for convenience]

$$t - t_p = -\frac{\sqrt{6}}{m_\ell} \left[(N_{\text{end}} - N)^{1/2} - (N_{\text{end}} - N_p)^{1/2} \right]. \quad (\text{A.6})$$

As a consequence, inserting those equations in Eq. (A.3), one finds that $\omega_h^2(t)$ reduces to a quadratic polynomial in time, namely

$$\omega_h^2(t) \simeq \bar{c} + \bar{b} m_\ell (t - t_p) + \bar{a} m_\ell^2 (t - t_p)^2, \quad (\text{A.7})$$

with

$$\bar{a} = -\frac{1}{4} m_\ell^2, \quad (\text{A.8})$$

$$\bar{b} = \frac{1}{4} m_\ell \Gamma_{\text{hm}} + \sqrt{\frac{3}{2}} m_\ell^2 \sqrt{N_{\text{end}} - N_p}, \quad (\text{A.9})$$

$$\bar{c} = m_h^2 - \frac{1}{2} m_\ell^2 - \frac{\Gamma_{\text{hm}}^2}{16} - \sqrt{\frac{3}{8}} \Gamma_{\text{hm}} m_\ell \sqrt{N_{\text{end}} - N_p} - \frac{3}{2} m_\ell^2 (N_{\text{end}} - N_p). \quad (\text{A.10})$$

This approximation is represented and compared to the exact $\omega_h^2(t)$ in Fig. 24 (solid orange line).

A.2 The WKB approximation for the heavy field

As discussed earlier, Eq. (A.2) cannot be solved exactly due to the complex analytical time dependence of $\omega_h^2(t)$. However, the WKB approximation can be used to find an approximate solution. Indeed, if one represents the WKB criterion, Q/ω_h^2 , where

$$Q = \frac{3}{4} \frac{\dot{\omega}_h^2}{\omega_h^2} - \frac{\ddot{\omega}_h}{2\omega_h}, \quad (\text{A.11})$$

versus time, see Fig. 25, we notice that, quite quickly, on the left and right hand sides of the turning point (where, by definition, Q blows up), this quantity tends to zero, signalling that WKB should be a very good approximation. Usually, the WKB approximation is used in the following way. It is first used on the left side of the turning point (region I) where the initial conditions are specified and, as consequence, where the solution is completely specified. The WKB approximation is also used on the right side (region III) where the solution, being a solution of a second order differential equation, depends on two arbitrary integration constants. These two constants can be fixed if the solution in region III is matched to the solution in region I. However, as noticed above, the solution in between (region II) is *a priori* not known since the WKB approximation fails in this region. What is usually done to deal with this problem is to linearize the effective frequency in region II which allows us to find an approximation of the solution

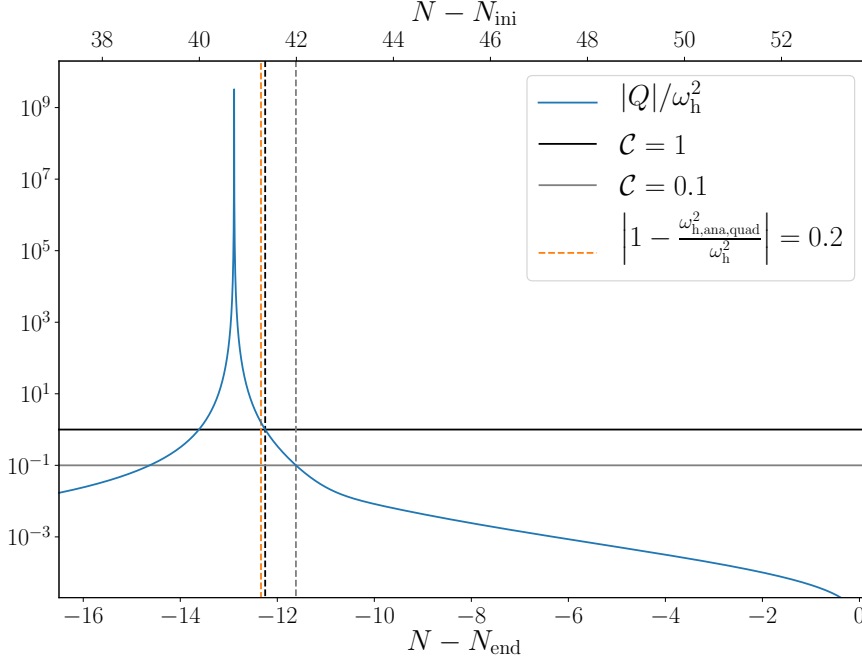


Figure 25: Time evolution of the quantity Q/ω_h^2 (blue line) with Q defined in Eq. (A.11), before, around and after the time “osc”. The smallness of this quantity represents a criterion for the regime of validity of the WKB approximation, whose strictness is parameterised by the number $\mathcal{C}$ which is either 1 (horizontal black line) or 0.1 (horizontal grey line) in this work. The corresponding time from which the WKB approximation becomes valid are represented by vertical dashed lines (respectively black and grey ones). The time from which the quadratic approximation for the pulsation ω_h^2 becomes roughly valid is also represented by the orange vertical dashed lines.

in this regime which, then, permits to connect the solution in region I to the solution in region III. In this way, one can specify the two unknown integration constants in region III and have a complete knowledge of the solution.

Here, we closely follow this WKB procedure with, however, some differences in order to adapt our method to the problem at hand. In region I, the solution is known and is given by the slow-roll approximation. So we do not need to employ the WKB approximation in this regime (although it might be interesting to study how WKB is connected to slow-roll in this regime, see also Ref. [82]). As a consequence, we will “start the evolution” not deep in region I (on the left) but at the onset of region II. In fact, the time of transition, t_{trans} turns out to be located precisely at the beginning of this region and, therefore, we fix the “initial conditions” (those relevant for our problem here; they have obviously nothing to do with the physical initial conditions, discussed before, and

chosen at the onset of inflation) at this time. In addition, they are completely known from the previously studied slow-roll solution and read

$$g_h(t_{\text{trans}}) = 1, \quad \dot{g}_h(t_{\text{trans}}) = -\frac{m_h^2}{3H(t_{\text{trans}})} + \frac{3H(t_{\text{trans}})}{2} + \frac{\Gamma_{\text{hm}}}{4}, \quad (\text{A.12})$$

where we used the slow-roll expression of $\dot{\phi}_h$. Numerically, with our fiducial parameters, given that $H_{\text{trans}} = 4.3 \times 10^{-5}$ (obtained analytically within the slow-roll approximation), we find that $\dot{g}_{\text{trans}} = 4.8 \times 10^{-5}$. Moreover, one can compute the difference in cosmic time between the transition ($\theta_{\text{trans}} = \arctan(1/R)$) and the onset of the oscillations ($\theta_{\text{osc}} = \arctan(\sqrt{0.0104})$), with use of Eq. (5.24) which is indeed relevant around the transition time, and one finds $m_\ell(t_{\text{osc}} - t_{\text{trans}}) = 0.32$.

Let us now turn to the question of calculating $g_h(t)$ in region II. As explained before, in this region, the WKB approximation breaks down and we need to use another technique which consists in linearizing the effective frequency around the turning point. Concretely, we write

$$\omega_h^2 = -\alpha(t - t_{\text{osc}}) + \dots \quad (\text{A.13})$$

with $\alpha \equiv -d\omega_h^2(t = t_{\text{osc}})/dt$. In our case, α is negative. The linear approximation (A.13) is represented in Fig. 24, see the solid green line. We have seen before that, in the vicinity of the turning point, $\omega_h^2 \simeq m_h^2 - 9H^2/4$, and this implies that $\alpha = -9/2 \times (\epsilon_1 H^3)_{\text{osc}}$. With the fiducial parameters, we find analytically $\alpha = -3.0 \times 10^{-14}$ in M_{Pl}^3 units, where one has used the slow-roll formula for ϵ_1 , namely

$$\epsilon_1 = \frac{1}{2s} \frac{1 + R^4 \tan^2 \theta}{\cos^2 \theta (1 + R^2 \tan^2 \theta)^2}. \quad (\text{A.14})$$

Then, plugging the expression (A.13) into the equation (A.2), and introducing a new variable y defined by the expression $y \equiv \alpha^{1/3}(t - t_{\text{osc}})$, the equation for $g_h(t)$ takes the form

$$\frac{d^2 g_h}{dy^2} - y g_h = 0. \quad (\text{A.15})$$

The solution to this equation is well-known and can be expressed in terms of the Airy functions of first and second kind, Ai and Bi [80, 81]. As a consequence, one can write

$$g_h(t) = B_1 \text{Ai}(y) + B_2 \text{Bi}(y), \quad (\text{A.16})$$

where B_1 and B_2 are two integration constants. These constants can be determined using the values of g_h and its derivative at the transition point, see Eqs. (A.12). This leads

$$B_1 = \pi \left[\frac{d}{ds} \text{Bi}(y_{\text{trans}}) - \frac{1}{\alpha^{1/3}} \dot{g}_{\text{trans}} \text{Bi}(y_{\text{trans}}) \right], \quad (\text{A.17})$$

$$B_2 = -\pi \left[\frac{d}{ds} \text{Ai}(y_{\text{trans}}) - \frac{1}{\alpha^{1/3}} \dot{g}_{\text{trans}} \text{Ai}(y_{\text{trans}}) \right]. \quad (\text{A.18})$$

Numerically, with our fiducial parameters, one finds, $B_1 \simeq 1.98 + 3.90i$ and $B_2 \simeq 3.75 - 2.26i$. An intermediate step has been to use $y_{\text{trans}} = e^{i\pi/3}|\alpha|^{1/3}(t_{\text{trans}} - t_{\text{osc}})$, with the value of $(t_{\text{trans}} - t_{\text{osc}})$ that was found in the previous section.⁵ This completes our calculation of g_{h} (and, therefore, of ϕ_{h}) in region II which is now completely known.

The final step consists in writing the solution in region III. This region is the most interesting one for us since it corresponds to the phase dominated by the light field. Obtaining the solution for $g_{\text{h}}(t)$ in this regime allows us to track the behaviour of $\phi_{\text{h}}(t)$ when the light field drives inflation and the heavy field oscillates and decays. As explained before, in this region, $Q/\omega_{\text{h}}^2 \ll 1$ and the WKB approximation is satisfied. As a consequence, the solution can be written as

$$g_{\text{h}}(t) = \frac{C_+}{\omega_{\text{h}}^{1/2}} e^{i \int_{t_{\text{osc}}}^t \omega_{\text{h}}(\tau) d\tau} + \frac{C_-}{\omega_{\text{h}}^{1/2}} e^{-i \int_{t_{\text{osc}}}^t \omega_{\text{h}}(\tau) d\tau}, \quad (\text{A.19})$$

where C_+ and C_- are two integration constants. This solution is valid only in region III, namely only for times t where $Q/\omega_{\text{h}}^2 \ll 1$ (on the right hand side of the turning point). Notice, however, that the lower bounds in the integrals have been taken at the turning point. We first remark that changing the lower bound is in fact equivalent to redefining the constants C_+ and C_- . So choosing the lower bound to be the turning point is not in contradiction with the WKB approximation and just amounts to a particular (convenient) definition of C_+ and C_- . At this stage, our first goal is to determine these two quantities. In order to carry out this calculation, we must check that there is an overlap between region II and region III, that is to say a patching region where the linear approximation of the effective frequency is not too bad and where, at the same time, the WKB regime is satisfied. The linear approximation is acceptable if the second order term remains smaller than the first order one which means $t - t_{\text{osc}} \lesssim 2(d\omega_{\text{h}}^2/dt)/(d^2\omega_{\text{h}}^2/dt^2)$ or

$$m_{\ell}(t - t_{\text{osc}}) \lesssim \frac{3}{R(\epsilon_1 - 3\epsilon_2)|_{\text{osc}}}. \quad (\text{A.20})$$

On the other hand, if the linear approximation is accurate, the WKB approximation is satisfied provided $|\dot{\omega}_{\text{h}}/\omega_{\text{h}}^2| < 1$, namely

$$m_{\ell}(t - t_{\text{osc}}) \gtrsim \left(\frac{m_{\ell}^3}{4|\alpha|} \right)^{1/3}. \quad (\text{A.21})$$

This is possible if

$$|\alpha| > \frac{m_{\text{h}}^3}{108} (\epsilon_1 - 3\epsilon_2)^3|_{\text{osc}}, \quad (\text{A.22})$$

⁵These results and the following ones (until the numerical determination of the constants $C_{\pm}$) are derived with the choice of a complex cubic root for the negative number $\alpha = |\alpha|e^{i\pi}$ which is $\alpha^{1/3} = e^{i\pi/3}|\alpha|^{1/3}$. Note that in this case the time coordinate y has a constant phase $\pi/3$, as indeed $y = e^{i\pi/3}|\alpha|^{1/3}(t - t_{\text{osc}})$, a fact that is crucial in order to derive consistently the asymptotic limit shown in Eq. (A.23). This choice should not matter as long as it is consistent during the whole calculation, and indeed we have checked that using the different cubic root $\alpha^{1/3} = -|\alpha|^{1/3}$, leads to the same final results (but intermediate ones like the values for y_{trans} or $B_{1,2}$ are therefore obviously different).

which is satisfied since, numerically, one finds $|\alpha| > 2.5 \times 10^{-14}$ to be compared with the value found here, $|\alpha| = 3.0 \times 10^{-14}$. In this patching region, one can use at the same time the solution (A.16) and the WKB solution (A.19). Since both formula must lead to the same solution, this allows us to identify the coefficients C_+ and C_- in terms of B_1 and B_2 . Concretely, if one goes away from the turning point, Eq. (A.16) leads to

$$g_h(t) \simeq \frac{1}{2\sqrt{\pi}} e^{-i\pi/12} |\alpha|^{-1/12} (t - t_{\text{osc}})^{-1/4} \left[(B_1 + iB_2) e^{-\frac{2i}{3}|\alpha|^{1/2}(t-t_{\text{osc}})^{3/2}} + 2B_2 e^{\frac{2i}{3}|\alpha|^{1/2}(t-t_{\text{osc}})^{3/2}} \right], \quad (\text{A.23})$$

while the WKB solution (A.19) in the linear part of the time-dependent frequency can be written as

$$g_h(t) \simeq |\alpha|^{-1/4} (t - t_{\text{osc}})^{-1/4} \left[C_+ e^{\frac{2i}{3}|\alpha|^{1/2}(t-t_{\text{osc}})^{3/2}} + e^{-\frac{2i}{3}|\alpha|^{1/2}(t-t_{\text{osc}})^{3/2}} \right]. \quad (\text{A.24})$$

Requiring these two expressions to represent the same solution, this immediately leads to the relationship

$$C_+ = \frac{B_2}{\sqrt{\pi}} |\alpha|^{1/6} e^{-i\pi/12}, \quad C_- = \frac{B_1 + iB_2}{2\sqrt{\pi}} |\alpha|^{1/6} e^{-i\pi/12}, \quad (\text{A.25})$$

Numerically, one finds $C_+ \simeq 0.0096 - 0.01i$ and $C_- = C_+^*$, as required since $g_h(t)$ is a real function. Therefore, one has reached our goal, namely expressing $g_h(t)$ in the region where inflation is driven by the light field. The solution is *a priori* entirely specified since the constants C_+ and C_- are now related to what happens at the transition time. However, we must also calculate the WKB phase which requires the integration of $\omega_h(t)$. It can be expressed as

$$\int_{t_{\text{osc}}}^t \omega(\tau) d\tau = \int_{t_{\text{osc}}}^{t_{\text{match}}} \omega(\tau) d\tau + \int_{t_{\text{match}}}^t \omega(\tau) d\tau = \Phi + \int_{t_{\text{match}}}^t \omega(\tau) d\tau, \quad (\text{A.26})$$

where we have introduced the time t_{match} . This time is a time at which the quadratic approximation of $\omega_h^2(t)$, see Eq. (A.7), becomes valid. In principle, the phase Φ can be calculated but, in our case, this would require the integration of the exact time-dependent frequency which is complicated given its form (A.3) (and which would undermine the interest of having an analytical approximation). A rough approximation is to use the linear expression in the vicinity of the turning point which results in

$$\Phi \simeq \frac{2}{3} |\alpha|^{1/2} (t_{\text{match}} - t_{\text{osc}})^{3/2}. \quad (\text{A.27})$$

However, this result does not give a very accurate estimation of the phase while the accuracy of the WKB approximation quite sensitively depends on Φ . A more careful calculation, using $\omega_h^2 \simeq m_h^2 - 9H^2/4$ gives, after the change of variable defined in

Eq. (5.22)

$$\Phi = -\sqrt{6C} \frac{R}{R^2 - 1} \int_{\theta_{\text{osc}}}^{\theta_{\text{match}}} \frac{\sqrt{1 + R^2 \tan^2 \theta}}{\sin \theta \times \cos \theta} (\tan \theta)^{\frac{1}{R^2 - 1}} \left[1 - \frac{3C}{2R^2} \frac{(\tan \theta)^{\frac{2}{R^2 - 1}}}{\cos^2 \theta} \right]^{1/2} d\theta. \quad (\text{A.28})$$

Unfortunately, this integral cannot be computed analytically, but it is straightforward to compute it numerically. It gives $\Phi = 1.093$ for the fiducial parameters of the model, a value that should be compared with the numerical result $\Phi = 2.039$. Admittedly, the result is still not very accurate and, therefore, the determination of Φ constitutes an additional source of error. Nevertheless, taking into account the phase determined according to the considerations presented above significantly improves the agreement between the exact and WKB solutions.

Let us now turn to the calculation of the second term in Eq. (A.26). As already discussed above, this can be carried out with the help of the quadratic approximation for $\omega_h^2(t)$, see Eq. (A.7). It is especially convenient to redefine the coefficients $\bar{a}$, $\bar{b}$ and $\bar{c}$ according to $a = -\bar{a}/m_\ell = 1/4$, $b = \bar{b}/m_\ell^2$ and $c = \bar{c}/m_\ell^2$. In fact, since $c = R^2 - 1/2 - b^2$, there remains only one free coefficient which can be chosen to be b , a positive definite quantity. Then, defining

$$u = \frac{m_\ell(t - t_{\text{trans}}) - 2b}{2\sqrt{R^2 - 1/2}}, \quad (\text{A.29})$$

the frequency $\omega_h^2(t)$ takes the form

$$\omega_h(t) = m_\ell \left(R^2 - \frac{1}{2} \right)^{1/2} (1 - u^2)^{1/2}. \quad (\text{A.30})$$

Notice that, in the regime we are interested in, u^2 is always smaller than one since $\omega_h^2(t)$ is always real and positive. Then, it follows that

$$\int_{t_{\text{match}}}^t \omega(\tau) d\tau = 2 \left(R^2 - \frac{1}{2} \right) \int_{u_{\text{match}}}^u du \sqrt{1 - u^2} = \left(R^2 - \frac{1}{2} \right) G(u), \quad (\text{A.31})$$

with

$$G(u) = \left[u \sqrt{1 - u^2} + \arcsin(u) \right]_{u_{\text{match}}}^u. \quad (\text{A.32})$$

This completes the calculation of $g_h(t)$ since all the terms of Eq. (A.19) are now explicitly known.⁶

The result of the WKB approximation is represented in Fig. 26 where the evolution of the heavy field energy density

$$\rho_h(t) = \frac{1}{2} \dot{\phi}_h^2 + \frac{1}{2} m_h^2 \phi_h^2 \quad (\text{A.40})$$

is represented and compared to the numerical solution. Evidently, the result is excellent and the WKB solution follows quite accurately the exact result.

⁶It is also interesting to notice that, in region III, if the quadratic approximation for the effective frequency is used, then an exact solution is available. Let us indeed define $z = 2^{1/2} a^{1/4} [x - b/(2a)]$ and

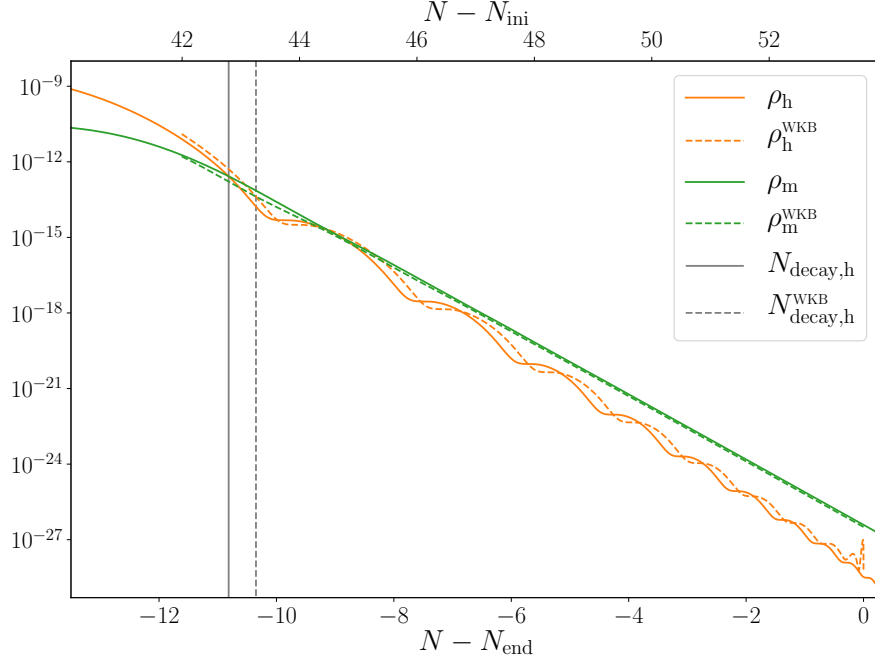


Figure 26: Comparison of ρ_h and ρ_m during the oscillations and decays of the heavy field, between their exact numerical results (respectively the orange and green solid lines), and their analytical approximations inferred from the WKB approach (respectively the orange and green dashed lines), see Eq. (A.40) and Eq. (A.55). The time of decay of the heavy field, defined as the time when $\rho_h = \rho_m$ is shown with the vertical grey lines both from the numerical approach (solid line, $N_{\text{decay,h}} = -10.81$) and the analytical one (dashed, $N_{\text{decay,h}}^{\text{WKB}} = -10.35$). This approach clearly gives much better results than the one presented in body of the paper, compared to Fig. 3 and the previous estimate $N_{\text{decay,h}}^{\text{sd}} = -8.39$, and enables one to derive reliably and analytically the time of decay $N_{\text{decay,h}}$.

$A = -1/(2\sqrt{a})[b^2/(4a) + c] = 1/2 - R^2$. Concretely, z can be expressed as

$$z = -\frac{1}{2} \frac{\Gamma_{\text{hm}}}{m_\ell} - \sqrt{6}(N_{\text{end}} - N)^{1/2}. \quad (\text{A.33})$$

Then, it follows that Eq. (A.2) can be written as

$$\frac{d^2 g}{dz^2} - \left(\frac{z^2}{4} + A \right) g = 0, \quad (\text{A.34})$$

which is the canonical form of the equation defining the Parabolic cylinder functions [80, 81]. As a consequence, the solution in region III takes the following form [80, 81]

$$g(z) = C_1 U(A, z) + C_2 V(A, z), \quad (\text{A.35})$$

A.3 The evolution of the matter energy density

Having calculated the evolution of the heavy field, we now turn to the behaviour of the matter energy density ρ_m whose equation of motion is Eq. (5.8). As it was already noticed before, its solution can be expressed as

$$a^3(t)\rho_m(t) = a^3(t_{\text{ini}})\rho_m(t_{\text{ini}}) + \frac{\Gamma_{\text{hm}}}{2} \int_{t_{\text{ini}}}^t a^3(\tau)\dot{\phi}_h^2(\tau)d\tau. \quad (\text{A.41})$$

We see that this requires the calculation of the integral of the kinetic energy density of the field, $\mathcal{I} = \int_{t_{\text{ini}}}^t a^3(\tau)\dot{\phi}_h^2(\tau)d\tau$. In the slow-roll regime, $\dot{\phi}_h^2(t)$ evolves slowly and could be put outside the integral, immediately leading to an explicit solution, see Sec. 5.2.3. Here, however, it is no longer possible to use this trick and we must insert the WKB expression of $\phi_h(t)$ in the above integral and calculate it explicitly. This leads to

$$\begin{aligned} \mathcal{I} = & a_p^3 \phi_p^2 \int_{t_{\text{match}}}^t d\tau e^{-\Gamma_{\text{hm}}(\tau-t_p)/2} \left(\frac{9}{4} H^2 g_h^2 + \frac{3}{4} H \Gamma_{\text{hm}} g_h^2 - 3H g_h \dot{g}_h - \frac{\Gamma_{\text{hm}}}{2} g_h \dot{g}_h \right. \\ & \left. + \frac{\Gamma_{\text{hm}}^2}{16} g_h^2 + \dot{g}_h^2 \right). \end{aligned} \quad (\text{A.42})$$

In the present case, the initial time has been taken to be t_{match} , the time from which the quadratic assumption becomes satisfied. Using the WKB solution (A.19) for $g_h(t)$, the above integral takes the form

$$\begin{aligned} \mathcal{I} = & \phi_p a_p^3 \int_{t_{\text{match}}}^t d\tau e^{-\Gamma_{\text{hm}}(\tau-t_p)/2} \left[C_+^2 \left(\frac{\mathcal{C}}{\omega_h} - i \right)^2 \omega_h e^{2i \int_{t_{\text{osc}}}^{\tau} \omega_h d\tau} \right. \\ & \left. + C_-^2 \left(\frac{\mathcal{C}}{\omega_h} + i \right)^2 \omega_h e^{-2i \int_{t_{\text{osc}}}^{\tau} \omega_h d\tau} + 2C_+ C_- \omega_h \left(\frac{\mathcal{C}}{\omega_h} - i \right) \left(\frac{\mathcal{C}}{\omega_h} + i \right) \right], \end{aligned} \quad (\text{A.43})$$

with

$$U(A, z) = D_{-A-1/2}(z), \quad (\text{A.36})$$

$$V(A, z) = \frac{1}{\pi} \Gamma \left(\frac{1}{2} + A \right) [D_{-A-1/2}(-z) + \sin(\pi A) D_{-A-1/2}(z)] \quad (\text{A.37})$$

where C_1 and C_2 are two integration constant and $D_\nu(z)$ are parabolic functions. Notice that another canonical form which is also convenient is [80, 81]

$$\frac{d^2 g}{dz^2} + \left(\nu + \frac{1}{2} - \frac{z^2}{4} \right) g = 0, \quad (\text{A.38})$$

where $A = -\nu - 1/2$ or $\nu = R^2 - 1$. In that case, the solution can be written as

$$g(z) = C_1 D_\nu(z) + C_2 D_\nu(-z), \quad (\text{A.39})$$

since $D_\nu(\pm z)$ are linearly independent provided $\nu \neq 0, \pm 1, \dots$ (we have used the same notations for the integration constants but obviously they differ from the ones already introduced before).

with

$$\frac{\mathcal{C}}{\omega_h} = \frac{3}{2} \frac{H}{\omega_h} + \frac{1}{4} \frac{\Gamma_{hm}}{\omega_h} + \frac{\dot{\omega}_h}{2\omega_h^2} \simeq \frac{3}{2} \frac{H}{\omega_h} + \frac{1}{4} \frac{\Gamma_{hm}}{\omega_h}. \quad (\text{A.44})$$

We see that we have three terms to calculate and we write them as $\mathcal{I} = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3$. The next step consists in inserting the form of $\omega_h(t)$ in the above expression. Since we are interested in the behaviour of ρ_m in region III, one can use the quadratic approximation of $\omega_h^2(t)$, see Eq. (A.30) expressed in terms of the variable u , see Eq. (A.29). Then, the first term reads

$$\mathcal{I}_1 = a_p^3 \phi_p C_+^2 e^{i2\Phi} (2R^2 - 1) e^{-b\Gamma_{hm}/m_\ell} \int_{u_{\text{match}}}^u du F(u) e^{i(2R^2-1)G(u)}, \quad (\text{A.45})$$

with

$$F(u) = e^{-\Gamma_{hm}(R^2-1/2)^{1/2}u/m_\ell} (1-u^2)^{-1/2} \left[u - i(1-u^2)^{1/2} \right]^2, \quad (\text{A.46})$$

and where the calculation of the WKB phase (A.31) has been used, see Eq. (A.32) for the definition of the function $G(u)$. The second term is then trivially found since this is just the complex conjugate of the first one, $\mathcal{I}_2 = \mathcal{I}_1^*$. Unfortunately, the integral (A.45) cannot be performed analytically. However, we notice that the integrand has the form of a smooth function $F(u)$ multiplied by an *a priori* rapid oscillatory phase (since $2R^2 - 1$ is *a priori* quite a large number). As is well-known, several techniques (Filon method, Levin collocation method etc., see Ref. [83]) have been developed to deal with this type of integrals. The simplest one just consists in integrating by part leading to

$$\begin{aligned} \int_{u_{\text{match}}}^u du F(u) e^{i(2R^2-1)G(u)} &= \frac{1}{i(2R^2-1)} \left[\frac{F(u)}{G'(u)} e^{i(2R^2-1)G(u)} \right. \\ &\quad \left. - \frac{F(u_{\text{match}})}{G'(u_{\text{match}})} e^{i(2R^2-1)G(u_{\text{match}})} \right] \\ &\quad - \frac{1}{i(2R^2-1)} \int_{u_{\text{match}}}^u du \frac{d}{du} \left(\frac{F}{G'} \right) e^{i(2R^2-1)G(u)}. \end{aligned} \quad (\text{A.47})$$

In terms of the (inverse of the) large parameter $2R^2 - 1$, the second term is of higher order and, therefore, can be neglected thus leading to an approximation of the integral. If one uses this approximation to estimate $\mathcal{I}_1$, this gives

$$\mathcal{I}_1 \simeq -a_p^3 \phi_p i C_+^2 e^{i2\Phi} e^{-b\Gamma_{hm}/m_\ell} \left[\frac{F(u)}{G'(u)} e^{i(2R^2-1)G(u)} - \frac{F(u_{\text{match}})}{G'(u_{\text{match}})} e^{i(2R^2-1)G(u_{\text{match}})} \right]. \quad (\text{A.48})$$

In principle, additional (successive) integrations by parts could lead to an even more accurate approximation but, here, we will restrict ourselves to first order.

Finally, the third term remains to be calculated. Straightforward manipulations show that it can be written as

$$\mathcal{I}_3 = 2a_p^3 \phi_p C_+ C_- (2R^2 - 1) e^{-b\Gamma_{hm}/m_\ell} \int_{u_{\text{match}}}^u du e^{-\Re u} (1-u^2)^{-1/2}. \quad (\text{A.49})$$

with

$$\aleph = \frac{\Gamma_{\text{hm}}}{m_\ell} \left(R^2 - \frac{1}{2} \right)^{1/2}. \quad (\text{A.50})$$

The integral (A.49) $\mathcal{J} = \int_{u_{\text{match}}}^u du e^{-\aleph u} (1 - u^2)^{-1/2}$ cannot be performed exactly. But it is however relatively easy to derive an accurate analytical approximation of $\mathcal{J}$. One can proceed as follows. Let us first introduce the new variable ψ such that $u = \cos \psi$. Then the integral to be calculated reduces to

$$\mathcal{J} = - \int_{\psi_{\text{match}}}^{\psi} e^{-\aleph \cos \Omega} d\Omega. \quad (\text{A.51})$$

The integrand can easily be written as Fourier series, namely

$$e^{-\aleph \cos \Omega} = I_0(-\aleph) + 2 \sum_{n=1}^{+\infty} I_n(-\aleph) \cos(n\Omega), \quad (\text{A.52})$$

where I_n is a modified Bessel function [80, 81]. Each term of the series (A.52) can easily be integrated exactly and it follows that the integral $\mathcal{J}$ can be expressed as

$$\mathcal{J} = \left[-I_0(-\aleph)\psi - 2 \sum_{n=1}^{+\infty} \frac{1}{n} I_n(-\aleph) \sin(n\psi) \right]_{\psi_{\text{match}}}^{\psi} \quad (\text{A.53})$$

In practice, in order to reach a good accuracy, it is sufficient to keep only the first two or three terms in the above sum. We conclude that

$$\begin{aligned} \mathcal{I}_3 = & -2a_{\text{p}}^3 \phi_{\text{p}} C_+ C_- (2R^2 - 1) e^{-b\Gamma_{\text{hm}}/m_\ell} \left[I_0(-\aleph) \arccos u \right. \\ & \left. + 2 \sum_{n=1}^{+\infty} \frac{1}{n} I_n(-\aleph) \sin(n \arccos u) \right]_{u_{\text{match}}}^u. \end{aligned} \quad (\text{A.54})$$

The final step consists in collecting the three terms calculated before in the final expression of the matter energy density. One obtains the rather lengthy, but explicit, following equation [using the fact that $G(u_{\text{match}}) = 0$ by definition]

$$\begin{aligned} \rho_{\text{m}}(t) \simeq & \rho_{\text{m}}^{\text{match}} \left[\frac{a_{\text{match}}}{a(t)} \right]^3 + \phi_{\text{p}} \left[\frac{a_{\text{p}}}{a(t)} \right]^3 \frac{\Gamma_{\text{hm}}}{2} e^{-b\Gamma_{\text{hm}}/m_\ell} \\ & \times \left(2\text{Re} \left\{ -iC_+^2 e^{i2\Phi} \left[\frac{F(u)}{G'(u)} e^{i(2R^2-1)G(u)} - \frac{F(u_{\text{match}})}{G'(u_{\text{match}})} \right] \right\} \right. \\ & \left. - 2|C_+|^2 (2R^2 - 1) \left[I_0(-\aleph) \arccos u + 2 \sum_{n=1}^{+\infty} \frac{1}{n} I_n(-\aleph) \sin(n \arccos u) \right]_{u_{\text{match}}}^u \right). \end{aligned} \quad (\text{A.55})$$

This expression is represented in Fig. 26 together with the exact (numerical) solution of ρ_{m} . Obviously, it matches quite well the numerical result.

A.4 Determination of the time of decay

Having determined the WKB form of $\rho_h(t)$, see Eq. (A.40) and $\rho_m(t)$, see Eq. (A.55), we can now calculate the time of decay. Recall that it is defined by the condition $\rho_h(t_{\text{decay},h}) = \rho_m(t_{\text{decay},h})$. Given the complexity of Eqs. (A.40) and (A.55), it is clear that it is hopeless to solve $\rho_h(t_{\text{decay},h}) = \rho_m(t_{\text{decay},h})$ analytically. Here, we solve this transcendental equation numerically and the solution is denoted $N_{\text{decay},h}^{\text{WKB}}$. For the fiducial parameters, one finds $N_{\text{decay},h}^{\text{WKB}} = -10.35$ to be compared with the exact value $N_{\text{decay},h} = -10.81$. The quantity $N_{\text{decay},h}^{\text{WKB}}$ is used in Table. 2 for the analytical estimation of the amplitude of non-adiabatic perturbations after double inflation.

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9.2 Going further: a few possibilities

The general formalism presented above can be used to investigate different scenarios, and extended to even more generic cases and interactions. Of course, the multiscalar model could be changed for another one with a more complicated potential, and to many-fields and many-fluids cases. But more fundamentally, it misses a few ingredients that could substantially extend the range of physical phenomena that it encapsulates.

A first interesting generalisation would be the one of multi-scalar models with non-canonical kinetic terms, as it is the case for non-linear sigma models of inflation; indeed the current formalism relies on the separation between the individual kinetic terms allowing to define independent kinetic fluids with constant eos, and adding kinetic interactions seems a non-trivial task: is there an observational effect of reheating on a curved field space? Moreover, it currently only handles perturbations to linear order, and cannot grasp interesting non-linear physics during perturbative reheating, such as a potential production of primordial non-Gaussianities due to the multi-species interactions. References on this topic include Refs. [287–290], but they do not allow fluid–fluid interactions nor do they follow the statistics of isocurvature modes, nor do they take into account velocity perturbations: many interesting phenomena remain to be explored. For example, it would be interesting to predict the initial bispectrum of the cosmological fluids’ energy densities and velocities, on top of their power spectra that the current formalism can compute.

Actually, even with the current version of the formalism, we could study in details the linear dynamics of velocity isocurvature fluctuations, a physical perturbation that seems to have been somehow overlooked in the past, and that could be used to constrain micro-physical models of inflation and reheating by comparing their predictions with actual CMB data. Moreover, there could be interactions amongst the real cosmological fluids as described by decay rates $\Gamma_{(\alpha)\rightarrow(\beta)}$, which could also substantially affect the physics of isocurvature modes in general. These are projects that we have already started to work on, and a general program that I wish to complete in the near future.

Conclusion and prospects

In this thesis, I have studied how the presence of multiple degrees of freedom in the early Universe, can affect the theoretical predictions of cosmological and astrophysical observables, which in turn sharpens our understanding of the physics of cosmic inflation and reheating.

The first part of this manuscript, part [I](#), is about the current cosmological paradigm, that encompasses the largest scales at which the Universe is homogeneous, as well as the smaller ones where it develops the inhomogeneities that we observe. After summarising shortly the successes of relativity, first in the absence of gravity with special relativity and then incorporating it in general relativity, I reviewed in [Chapter 1](#) the foundations of modern cosmology on large scales: the Λ CDM model was explained, and the current most probable history of the Universe was taught. What I call the “early Universe” refers to the cosmological history before the onset of the radiation-dominated era, as early as approximately 10^{-32} seconds after the Big Bang, and the leading paradigm to describe it is the theory of cosmic inflation. But before digging into the details of inflation, I explained in [Chapter 2](#) how to extend the description of the Universe to finite scales at which the cosmological principle does not apply and perturbations can develop, both at the level of the geometry of spacetime and of the matter content of the Universe. The gauge ambiguity was carefully investigated and various popular gauges as well as gauge-invariant perturbations were defined, thus setting the stage for the remainder of this manuscript.

The second part, part [II](#), introduces the theory of cosmic inflation, both in the context of single-field and multifield models, but always according to the canonical treatment: the background is supposed to be homogeneous and well described by general relativity only, while fluctuations appear in a perturbative way but require a more careful quantum treatment. [Chapter 3](#) motivates the introduction of cosmic inflation as an era of decreasing comoving Hubble radius, or equivalently accelerated expansion of space, in order to solve the puzzles of the standard Hot Big Bang scenario; the horizon and the flatness problems are particularly investigated. The dynamics of single-field inflation are shown, both at the level of the background scalar field whose equation of motion may be solved in a slow-roll approximation, and of its fluctuations. The quantisation of linear perturbations is carefully explained and the Bunch-Davies vacuum is defined, I moreover show how to approximate the power spectrum of the comoving curvature perturbation, and of test scalar fields, in an quasi-de Sitter Universe. Then, I summarised how CMB

observations in the (n_s, r) -plane constrain the single-field models of inflation. In order to show that model-independent conclusions can be drawn in single-field inflation, I also reviewed the Effective Field Theory of Inflation that encapsulates the leading-order effects of many single-field models at the level of fluctuations, highlighting the crucial differences with the more canonical case where the inflaton has standard kinetic terms and putting emphasis on the use of (broken) symmetries. In Chapter 4, I introduced the most general multifield theory of inflation at lowest order in derivatives, so-called non-linear sigma models of inflation, where the scalar fields may interact both via a scalar potential and through their kinetic terms. Motivation is given for their study, both in a bottom-up approach and a top-down one: not only single-field inflation suffers from conceptual difficulties, but multifield models seem easier to embed in a UV completion encapsulating quantum gravity effects. The multifield dynamics are studied, and particular emphasis is put on the use of covariant derivatives and perturbations, both at the level of the background and of linear fluctuations. After generalising the quantisation procedure to these multifield models, I showed that the power spectra may be computed in a massless approximation, though encapsulating at first order the geometrical effects coming from the curved internal field space. The adiabatic-entropic decomposition is explained and used in the study of how entropic fluctuations can source the growth of the comoving curvature perturbation on large scales in two-field inflation. I closed this general chapter by discussing possible multifield instabilities due to a tachyonic entropic mass, either on sub-Hubble or super-Hubble scales. Eventually, the long Chapter 5 presents in detail the computation of primordial non-Gaussianities, as encapsulated by the cumulants of the comoving curvature perturbation, of order larger than or equal to three. I explained how to compute non-Gaussianities with the quantum in-in formalism, as well as with the classical δN -formalism, and I have put them to good use in both single-field and multifield examples of various kinds, discussing both the amplitude and the shape of the bispectrum, and sometimes the trispectrum. Then, I dug into the details of my research about primordial non-Gaussianities: amplification of perturbations and thus large non-Gaussianities in flattened configurations due to a transient tachyonic instability in two-field models with a strongly bent background trajectory, computation of the cubic action of two-field and N_{field} -inflation in the comoving gauge and corresponding single-field effective theories, careful treatment of the boundary terms and investigation of the geometrical effects in the bispectrum of multifield inflation, etc.

The third part, part III, proposes a different formalism to follow the dynamics of inflation, the so-called stochastic formalism that enables one to derive non-perturbative results for the largest scales during inflation. Chapter 6 introduces the formalism in a heuristic way, explaining the emergence of stochasticity and the simplest Langevin equation that may be derived in the single-field case. I explained how the corresponding Fokker-Planck equation for the Probability Density Function of the inflaton may be used to infer its correlation functions, as well as the power spectrum of the comoving curvature perturbation thanks to the stochastic δN -formalism, or used to derive interesting non-perturbative Quantum Field Theory results in de Sitter space. The stochastic formalism is extended to the multifield case in Chapter 7, with my two published articles on the

topic: it is explained how we unveiled the presence of inflationary stochastic anomalies, ultimately due to the ambiguity in the time discretisation of the path integral, and that we understood how to solve them with a careful investigation of the quantum nature of the sub-Hubble perturbations. We also showed how to properly derive the multifield Langevin equations with the use of the Schwinger-Keldysh formalism borrowed from out-of-equilibrium statistical field theories, and precisely investigated the boundary conditions when a small-scale mode joins the infrared regime.

The fourth part, part [IV](#), deals with the end of inflation, and more particularly with the decays of the scalar field(s) responsible for inflation into other degrees of freedom that must ultimately describe the Standard Model and dark matter particles that we observe in our Universe, a multifaceted mechanism dubbed cosmic reheating because those decays products eventually thermalise and thus enable one to define for the first time the temperature of the Universe. The details of reheating only mildly impact cosmological observables on CMB scales in single-field inflation. Clearly, an interesting physical system that is not encapsulated by this statement consists in the small scales. Chapter [8](#) proposes both an introduction to the general theory of reheating and a direct application with an article on the topic of metric preheating which consists in an amplification of the inflaton's fluctuations at the end of inflation, when the scalar field is oscillating at the bottom of its potential. Importantly, we showed that this instability is not spoiled but simply dynamically stopped by the couplings of the inflaton to another degree of freedom, described as a cosmological fluid with any equation of state in this work. This has important astrophysical implications, such as a copious production of Primordial Black Holes due to collapsing overdensities during and after the instability. In order to do this, we had to use a particular formalism to couple a scalar field with a cosmological fluid, and such formalism is presented in great details in Chapter [9](#) in the context of multifield–multi-fluid interactions as can be the case in multifield inflation when the scalars fields all decay at the end of inflation into different kinds of cosmological fluids, such as radiation and dark matter that must constitute the dominant part of the energy budget of the Universe in the subsequent cosmological eras. The example of double quadratic inflation is extensively studied, both analytically and with a careful numerical treatment, each important approximation and analytical formula being checked against the exact numerical result. In particular, we showed how to describe the evolution of energy density isocurvature perturbations through reheating in two-field inflation, and concluded that a numerical treatment is necessary in most realistic cases, therefore sharpening our understanding of the physics of isocurvature perturbations and possibly revisiting how CMB observations constrain their values at the end of inflation.

In the future, I would like to further investigate a few of these topics that I have been studying during my thesis, as well as begin to work on new ones. Regarding primordial non-Gaussianities, my collaborators and I are currently trying to extend the

Quasi-Single-Field Inflation setup presented in Sec. 5.1.3 to the case of many-field inflation, building up on the general multifield action that I have presented in the article presented in Sec. 5.3.2. In particular, the squeezed limit of the many-field bispectrum could interestingly feature modulated oscillations depending on the eigenvalues of the multi-dimensional entropic mass matrix, therefore further extending the cosmological collider program to more degrees of freedom, and to the case of kinetic interactions. As for stochastic inflation, I think that the generic multifield formalism that we have developed during my thesis and that is presented in Sec. 7.2, could be applied to interesting physical cases, such as the computation of non-perturbative results in de Sitter space for non-linear sigma models, or the production of PBH in multifield setups, etc. Reheating at the end of inflation can also feature fascinating phenomena, and as a first step we have begun to think about the generation of a different kind of isocurvature fluctuation in multifield setups, an analysis that requires not only a theoretical description, but also a numerical resolution and possibly a comparison with actual data: this is a promising and concrete program that I wish to carry in the near future.

But my future research will also be pointing in different, new directions. In particular, the study of primordial gravitational waves, generated during extreme phenomena in the early Universe, seems both timely and motivated. It would be an opportunity for me to keep working on early Universe physics, but directed towards the prediction of different observables: stochastic gravitational wave background, chirality of the signal, etc., in a time when cosmological gravitational-waves physics has become an ubiquitous topic of research. Moreover, this interesting phenomenology can be due to the presence of extra degrees of freedom beyond the inflaton, but not necessarily bosonic, spin-0 scalar fields as in multifield inflation: gauge fields and fermions seem to be playing an important role, and I am eager to learn new techniques and formalisms that are needed to describe them. But of course, research can not be too much anticipated, and I will obviously remain open to new interests and curious about any advance of theoretical cosmology and observational discoveries.

The early Universe is an exciting playground for theoretical physicists, for it necessitates the understanding of many diverse physical phenomena, ranging from astrophysics to Quantum Field Theory, mixing perturbative theories with non-perturbative ones, statistical physics and gravitational aspects, most often using classical equations but studying quantum phenomena, with the possibility of an analytical description in the simple cases but however requiring numerical assistance in the more involved ones, and with cosmological and astrophysical data of excellent quality that enables one to test theories against actual observations, therefore making it a natural science deeply rooted into experiments. I hope to keep working on such a thrilling topic of research.

Compte-rendu en français

Introduction

Ce court chapitre résume en français et en quelques pages, les résultats obtenus dans le cadre de ma thèse de doctorat, et présentés en anglais et en détail dans le reste de ce manuscrit. Ces travaux peuvent se scinder en trois parties différentes bien que reliées par le même but : étudier les signatures observationnelles permettant de distinguer les modèles multichamps de l'univers primordial. Après une introduction générale dans la première partie de cette thèse, on s'intéresse dans la partie II aux non-Gaussianités primordiales qui permettent en effet de sonder ce contenu en particules. Ensuite, la partie III traite du formalisme stochastique pour l'inflation multichamps et de comment cette thèse a permis de révéler une lacune, ainsi que de la combler, dans la description habituelle. Pour finir, la partie IV est dédiée à l'étude du (p)réchauffement à la fin de l'inflation à un champ et à plusieurs champs. Ces trois parties sont résumées dans la suite de ce chapitre.

Non-gaussianités primordiales : des signatures du contenu en particules dans l'univers primordial

Les modèles inflationnaires les plus simples, dits à un champ, à roulement lent, et avec des termes cinétiques canoniques, prédisent de manière universelle que les non-gaussianités primordiales possèdent une amplitude infime qu'on ne peut espérer observer dans les quelques prochaines années. Bien que ceci ne soit plus vrai pour des dynamiques non-attracteurs ou pour des théories d'ordre supérieur en dérivées, la présence de multiples degrés de liberté peut laisser une trace particulière dans ces déviations des perturbations cosmologiques à une statistique gaussienne.

Dans notre article [1], publié dans *Physical Review Letters* (PRL) et sur lequel l'INSU-CNRS a choisi de communiquer ([voir ici](#)), nous avons montré que lorsque la dynamique de l'inflation est "fortement non-géodésique", c'est-à-dire lorsque la trajectoire dans l'espace multichamps est particulièrement courbée (par rapport aux géodésiques qui généralisent les lignes droites aux espaces courbés), une instabilité particulière se développe au niveau des fluctuations. En effet, la masse effective des fluctuations orthogonales à la trajectoire (dites entropiques), et pour les modes sous l'horizon (petites échelles), en unités du facteur de Hubble H , est $m_s^2/H^2 = V_{;ss}/H^2 + \epsilon R_{fs} M_{Pl}^2 - \eta_\perp^2$, où $V_{;ss}$

est la contribution habituelle venant de la matrice hessienne covariante du potentiel, où $\epsilon R_{\text{fs}} M_{\text{Pl}}^2$ est un terme lié à la géométrie de l'espace des champs (dont R_{fs} est la courbure scalaire) et où $\eta_{\perp}$ est un nombre sans dimension mesurant l'amplitude de la déviation à une trajectoire géodésique. Lorsque la trajectoire dans l'espace des champs est fortement non-géodésique, $\eta_{\perp}^2 \gg 1$ et $m_s^2 < 0$, signalant une instabilité tachyonique pour les fluctuations concernées. Heureusement, cette instabilité est seulement transitoire car lorsque ces modes sortent de l'horizon dû à l'expansion de l'Univers, leur masse effective est modifiée par une nouvelle contribution qui les stabilise : $m_{s,\text{eff}}^2 = m_s^2 + 4\eta_{\perp}^2 > 0$. Cependant, cette violente dynamique, bien que passagère, laisse une trace caractéristique dans les non-gaussianités primordiales. En effet, tous les cumulants d'ordre supérieur ou égal à trois ont une amplitude grande dictée par la durée de l'instabilité et pour une configuration particulière des nombres d'ondes $\vec{k}_i$ des modes concernés, appelée "aplatie" et pour laquelle $\exists i_0, k_{i_0} = \sum_{i \neq i_0} k_i$. Les modèles où l'instabilité dure trop longtemps et où les non-gaussianités sont donc trop importantes, sont par conséquent exclus. À l'inverse, la possible détection future de non-gaussianités de ce type distinctif donnerait une indication très forte en faveur de ceux de ces modèles où l'instabilité est présente mais de manière modérée.

Ces découvertes nous ont poussé à explorer de manière plus systématique les non-gaussianités dans les modèles d'inflation à deux champs, et dans l'article [2] publié dans *Journal of High Energy Physics* (JHEP) nous avons étendu le fameux calcul de Maldacena du bispectre de l'inflation à un champ, au cas de deux champs scalaires avec des termes cinétiques non-canoniques et un potentiel scalaire quelconques. Tout d'abord, les questions de jauge sont discutées en détail, les perturbations sont paramétrées dans la base adiabatique-entropique permettant de calculer les observables physiques directement, et le lagrangien à deux champs est développé à l'ordre cubique en prenant en compte tous les couplages avec l'espace-temps. Il est alors nécessaire de travailler ce résultat brut afin d'éliminer les opérateurs redondants et expliciter l'amplitude de chacune des interactions de manière unique, de nombreuses annulations entre elles les rendant effectivement plus petites que ce qui serait attendu naïvement. Un traitement détaillé des termes de bord temporels est présenté, où il est expliqué pourquoi ils sont *a priori* importants pour le calcul du bispectre, et quels sont-ils dans le résultat final obtenu. Enfin, du lagrangien cubique à deux champs complètement générique calculé, nous avons obtenu les interactions cubiques effectives pour la perturbation de courbure adiabatique lorsque le mode entropique est très lourd et peut être intégré hors de la théorie. De manière très intéressante, le résultat est le même que celui des théories à un champ les plus générales, où le lagrangien du champ scalaire peut avoir des dérivées d'ordre supérieur, et dans une certaine limite nous retrouvons les interactions dominantes prédites par la théorie effective de l'inflation, mais cette fois avec une prédiction pour leur amplitude en terme des paramètres du modèle à deux champs sous-jacent.

J'ai ensuite étendu ce résultat dans l'article [3], publié dans *Journal of Cosmology and Astroparticle Physics* (JCAP), au cas de non plus seulement deux, mais n'importe quel nombre N_{field} de champs scalaires, une situation plus générale pertinente au vu des prédictions pour l'inflation des théories quantiques de la gravité. Outre la difficulté

technique, ce travail est aussi conceptuel. Par exemple, j’ai proposé dans le cas général, une décomposition pertinente du tenseur de Riemann qui rentre dans le terme de masse des perturbations entropiques, incluant non seulement la courbure scalaire de l’espace des champs, R_{fs} , mais aussi ses composantes données par le tenseur de Ricci sans trace (pour $N_{\text{field}} \geq 3$) et le tenseur de Weyl (pour $N_{\text{field}} \geq 4$). Le lagrangien cubique dans la base adiabatique-entropique et avec des interactions dont l’amplitude est explicite est calculé dans ce cas multichamps le plus général (à cet ordre en dérivées), et permet de déduire les interactions effectives de la perturbation de courbure lorsque tous les modes entropiques sont lourds et peuvent être intégrés hors de la théorie. Ce travail ouvre de nombreuses perspectives, telles que l’implémentation de la méthode transport pour le calcul des non-gaussianités primordiales multichamps, directement en termes de la perturbation adiabatique, ou bien le calcul perturbatif *a la quasi-single-field* du bispectre dans le cas de $N_{\text{field}} - 1$ fluctuations entropiques.

En somme, mon travail de thèse a permis de renforcer et de détailler l’idée selon laquelle les non-gaussianités primordiales peuvent être utilisées comme des indicateurs clairs et distinctifs de la présence de plusieurs champs scalaires durant l’inflation, au-delà du paradigme actuel à un champ.

Formalisme stochastique pour l’inflation multichamps, et l’ambiguïté de la discrétisation temporelle

Il est un régime où les effets des perturbations quantiques s’accumulent au point de mettre à mal la validité du formalisme perturbatif le plus couramment utilisé. En effet, si le potentiel scalaire est très plat, la dynamique classique qui en dérive peut devenir négligeable par rapport à la diffusion résultant des fluctuations de nature quantique. Le formalisme stochastique pour l’inflation est justement dédié à la description de tels phénomènes dits non-perturbatifs, en traitant de manière effectivement classique, bien que stochastique, les effets des modes quantiques sur les échelles cosmologiques.

Dans notre article [4] publié dans *Classical and Quantum Gravity* (CQG), nous avons proposé d’appliquer le formalisme stochastique au cas général de l’inflation multichamps avec des termes cinétiques non-canoniques, et en tenant compte de toute la dynamique dans l’espace des phases. Au-delà des équations de Langevin et de Fokker-Planck généralisées que nous avons trouvées, nous y expliquons la présence d’une ambiguïté dans le formalisme stochastique en général, et particulièrement mis en exergue dans le contexte multichamps, liée aux problèmes usuels de discrétisation temporelle des équations différentielles stochastiques. La discrétisation dite *de Itô* rompt la covariance des équations décrivant le modèle, dû au fait que la règle de dérivée des fonctions composées n’est vérifiée que pour une autre discrétisation, appelée *de Stratonovich*. Cependant, la discrétisation de Stratonovich ne semblait alors pas non plus pertinente, car la résolution de l’équation différentielle stochastique associée nécessite la spécification arbitraire d’une racine carrée de la matrice de covariance du bruit. Dans le cas de deux champs scalaires spectateurs dans un univers de Sitter, une situation idéalisant le paradigme inflationnaire mais néanmoins conceptuellement intéressante, cette ambiguïté

de discrétisation disparaît et nous avons été en mesure de calculer de manière perturbative les premiers moments décrivant la statistique d'un de ces champs, étendant de fait au cas multichamps des résultats difficiles à obtenir dans le cadre de la théorie quantique des champs en espace-temps courbe.

Nous avons ensuite compris dans notre article [3] et publié dans *Journal of Cosmology and Astroparticle Physics* (JCAP), que les anomalies stochastiques mentionnées ci-haut et reliées à l'ambiguïté de la discrétisation temporelle des équations de Langevin, pouvaient être résolues par la prise en compte de la nature quantique des perturbations qui nécessite la spécification d'une base "privilégiée" d'oscillateurs quantiques indépendants, et qui permet de définir de manière naturelle la racine carrée de la matrice de covariance du bruit. La discrétisation de Stratonovich ne nécessitant donc plus de choix arbitraire, et permettant de décrire le modèle multichamps de manière covariante, apparaît donc comme la solution la plus satisfaisante conceptuellement. Une fois celle-ci choisie, nous montrons comment obtenir l'équation de Langevin correspondante mais écrite dans la discrétisation de Itô, modifiée donc par la présence d'une nouvelle contribution permettant de définir des dérivées covariantes compatibles avec les règles de calcul de Itô. De plus, ce travail propose de trouver les équations de Langevin dans ce cadre très général de plusieurs champs scalaires avec des termes cinétiques non canoniques et en espace des phases, à partir d'une approche basée sur les intégrales de chemin fermées du formalisme dit *de Schwinger-Keldysh*, ou *in-in*, une méthode empruntée aux théories cinétiques hors équilibre de la physique statistique. Un soin tout particulier est porté à la description de la transition des modes quantiques de petite longueur d'onde vers le système classique aux échelles bien plus grandes que l'horizon, démontrant le lien entre les détails fins de cette transition et l'absence d'un terme de dissipation ainsi que d'une partie imaginaire dans la statistique du bruit, deux effets parfois présents de manière indue dans la littérature. Enfin, nous montrons dans cet article comment estimer la statistique du bruit dans le cas multichamps, dans une approximation lentement variable et pour des champs scalaires sans masse ou légers ; nous y montrons aussi comment le formalisme cesse d'être valide pour des champs massifs, comme attendu de manière intuitive.

Il est donc légitime de dire que mon travail de thèse a permis d'étendre le formalisme stochastique aux théories multichamps de l'univers primordial les plus générales (à cet ordre en dérivées), en considérant la dynamique complète dans l'espace des champs et en tenant compte des détails de la discrétisation temporelle qui doivent nécessairement être stipulés pour de telles équations différentielles stochastiques. Ceci a par ailleurs permis de révéler une ambiguïté généralement présente dans tous les théories d'inflation stochastique, même à un champ, et d'en proposer une résolution pratique et conceptuellement satisfaisante.

Fin de l'inflation et réchauffement : impact sur les observables astrophysiques et cosmologiques

Pour que la théorie de l'inflation soit vraiment prédictive, il faut en principe spécifier les détails de la transition entre un univers en expansion quasi-exponentielle, et les ères

cosmologiques plus classiques dominées par la radiation et la matière. Cette transition possède nécessairement un mécanisme dit *de réchauffement*, pendant lequel l'énergie potentielle du ou des champs scalaires responsable(s) de l'inflation, doit être transférée à des particules du Modèle Standard ou d'un secteur sombre (matière noire, énergie noire) de la physique des particules, qui finiront par atteindre un équilibre thermique et donc par définir, pour la première fois, la température de l'Univers.

Dans le cadre standard de l'inflation de roulement lent à un seul champ scalaire, il existe un théorème qui stipule la constance des perturbations cosmologiques une fois qu'elles ont été étirées au-dessus du rayon du Hubble par l'expansion de l'univers. Celles de ces perturbations qui sont observées dans le fond diffus cosmologique, sont sorties de l'horizon bien avant la fin de l'inflation et le réchauffement, et ne sont, en conséquence de théorème, que peu sensibles aux détails de la transition vers les ères de radiation et matière. Cependant, les fluctuations à des échelles bien plus petites (sous l'horizon pendant le réchauffement) peuvent être affectées. Dans notre article [6] et publié dans *Journal of Cosmology and Astroparticle Physics* (JCAP), nous avons étudié en détail le mécanisme de réchauffement de l'univers par désintégration de l'inflaton en un fluide cosmologique d'équation d'état quelconque et pouvant représenter radiation, matière noire froide, ou autre. Ceci se produit lorsque l'inflaton arrive au minimum de son potentiel, se met à osciller et donc termine l'inflation. En effet, son énergie cinétique est alors en moyenne égale à son énergie potentielle, et donc l'équation d'état de l'univers, bien qu'oscillante, est de moyenne nulle et l'expansion de l'univers ne peut plus être accélérée aux temps longs. Les oscillations du champ scalaire résultent en une instabilité paramétrique, appelée *préchauffement de métrique*, pour ses propres perturbations dans une bande de nombres d'onde dictée par l'étude des équations de Mathieu, et correspondant à des modes sous l'horizon, au point que leur croissance exponentielle est responsable de la production de nombreux trous noirs primordiaux. Ce résultat était déjà connu, mais négligeait les détails du mécanisme de réchauffement qui est pourtant nécessaire pour terminer l'instabilité et éviter que notre univers entier ne soit englouti en un immense trou noir... De manière intéressante, notre formalisme permet de suivre de manière dynamique comment l'instabilité se développe et se termine, sans stipuler sa fin de manière *ad hoc*. Les trous noirs primordiaux constituent des signaux astrophysiques prometteurs et présents de manière générique d'après ce mécanisme de (p)réchauffement minimaliste. Les contraintes actuelles sur leur spectre de masse peuvent donc être utilisées pour comprendre les détails du (p)réchauffement, tels que la durée de l'instabilité sus-mentionnée, permettant donc de mieux comprendre l'univers primordial à l'aide d'échelles astrophysiques relativement petites, en complément des observations du fond diffus cosmologique aux très grandes échelles.

Mais les effets du réchauffement sont encore plus spectaculaires dans le cadre de théories de l'inflation multichamps, et en considérant la production de différentes espèces en équilibre thermique à la fin de l'inflation, une situation plus réaliste tant d'un point de vue de physique des hautes énergies (plusieurs champs scalaires pendant l'inflation) que d'observations cosmologiques (plusieurs espèces visibles dans le fond diffus cosmologique). Nous avons donc développé dans [7] et soumis pour publication à *Journal*

of Cosmology and Astroparticle Physics (JCAP), un formalisme permettant de suivre l'évolution de l'univers homogène ainsi que de toutes les perturbations linéaires, à la fois pendant l'inflation multichamps, le réchauffement et les époques subséquentes dominées par la radiation et la matière. En particulier, nous utilisons la propriété que N_{field} champs scalaires avec des termes cinétiques canoniques, peuvent être traités comme $N_{\text{field}} + 1$ fluides cosmologiques parfaits en les décomposant en leur parties cinétiques et potentielle, à condition que ces fluides “fictifs” soient en interaction. Leurs tenseurs énergie-impulsion ne sont donc pas individuellement conservés, bien que leur somme le soit évidemment par cohérence avec les équations d'Einstein et les identités de Bianchi. Il est alors possible de rajouter au modèle de “vrais” fluides cosmologiques, tels que matière noire froide et radiation, ou autre, et de paramétriser de nouvelles interactions avec les fluides “fictifs”. De cette manière, le mécanisme de réchauffement n'est pas rajouté à la main à la fin de l'inflation, mais devient simplement dynamiquement de plus en plus pertinent à mesure que les champs scalaires responsables de l'inflation arrivent vers le minimum de leur potentiel. Le formalisme permet de traiter la partie homogène de la cosmologie, mais aussi les fluctuations linéaires des champs scalaires et des “vrais” fluides cosmologiques (leurs densités d'énergie et vitesses). Pour illustrer l'intérêt du formalisme très général que nous présentons, nous étudions en détail le mécanisme de réchauffement à la fin du modèle d'inflation multichamps le plus simple, durant lequel deux champs scalaires de masse différente mais sans interactions sont responsables de deux phases d'inflation séparées par un virage dans l'espace des champs. Le champ scalaire lourd est couplé à un secteur sombre de la physique des particules représenté par un fluide cosmologique de matière noire froide, et le champ léger est couplé à un fluide de radiation pouvant représenter le bain de photons de l'univers primordial. Ces fluides restent négligeables jusqu'à ce que le champ avec lequel ils sont respectivement en interaction se mette à osciller autour du minimum de son potentiel ; leurs perturbations sont également excitées à cette époque. En particulier, nous montrons de manière analytique et numérique le transfert de la perturbation non-adiabatique des champs scalaires vers celle, observable, des fluides de matière et de radiation, durant le réchauffement. Le résultat principal de cet étude, outre le formalisme général qui y est présenté, est que les détails du mécanisme de désintégration affectent de manière importante la quantité de modes non-adiabatiques dans l'ère de radiation. Par ailleurs, nous montrons que les approximations analytiques décrites dans la littérature et ne se souciant pas de ces détails, présentent une erreur relative de l'ordre de 50%. Bien que nous proposons une analyse plus détaillée avec “seulement” 10% d'erreur relative, nous argumentons que, dans le cas général, seule une résolution numérique (que nous utilisons pour définir ces erreurs relatives) permet de tirer des conclusions suffisamment précises pour les comparer aux données cosmologiques. Nous pensons que ce formalisme peut être utilisé dans différents contextes pour déterminer les conséquences observationnelles du réchauffement à plusieurs espèces.

En conclusion, mon travail de thèse sur la fin de l'inflation à un champ et multichamps, a permis de sonder avec davantage de précision les effets du mécanisme détaillé de (p)réchauffement pour diverses observables astrophysiques et cosmologiques, à la fois

aux petites échelles qui peuvent s'effondrer et former des trous noirs primordiaux, ainsi qu'aux grandes échelles que le fond diffus cosmologique permet de contraindre. En comparant ces nouvelles prédictions théoriques aux observations astronomiques, nous parvenons donc à une meilleure compréhension de la physique de l'univers primordial, et en particulier de cette période de transition à la fois si cruciale et si peu comprise.

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