Quantum and thermodynamic windows into the Universe

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Als meus pares

No olvidemos que el libro ha sido nuestro aliado, desde hace muchos siglos, en una guerra que no registran los manuales de historia. La lucha por preservar nuestras creaciones valiosas: las palabras, que son apenas un soplo de aire; las ficciones que inventamos para dar sentido al caos y sobrevivir en él; los conocimientos verdaderos, falsos y siempre provisionales que vamos arañando en la roca dura de nuestra ignorancia.

Irene Vallejo, *El infinito en un junco* (2019).

Abstract

Cosmology is the branch of physics that deals with the study of the universe as a whole. At first glance our understanding of the universe seems to be solely anchored in classical gravity. Indeed, general relativity is a powerful tool that provides a successful geometric description of the cosmos. However, if one scratches beneath the surface, the universe becomes a fascinating playground for thermal and quantum phenomena.

On the one hand, the quantum origin of primordial fluctuations and, ultimately, the structure of the universe, is a spectacular and unavoidable prediction of the inflationary paradigm. The universe may look classical, but it is certainly quantum at a fundamental level. On the other hand, in an expanding universe many out-of-equilibrium thermodynamic processes take place, which allows us to introduce an arrow of time: the very concepts of past and future. The aim of the research collected in this thesis is to provide results and insight regarding phenomena that transcend the bare geometric cosmic description and are true quantum and thermodynamic windows into the universe.

On the quantum window we explore topics that merge quantum information techniques in real space and physics of the early universe. One can view the amplification of quantum fluctuations during inflation as a process of particle creation. We argue that due to this process distant regions share long-range correlations, as opposed to the standard short-range entanglement present in the Minkowski vacuum. We elaborate on this by showing the enhancement of the perturbative mutual information between two arbitrary regions of an inflating or radiation-dominated universe. Unlike the fast power decay found in the Minkowski vacuum, in a cosmological setup the decay is logarithmic and long-range share of information is possible. Furthermore, we study Bell inequalities in real space, showing that they are not violated by the Bunch-Davies vacuum of de Sitter spacetime, despite several hints on the existence of genuine quantum correlations in the quantum state of the Mukhanov-Sasaki field.

On the thermodynamic window, we develop a framework that allows to formulate non-equilibrium thermodynamics within general relativity in a consistent way. The Einstein field equations or, equivalently, the Hamilton equations in the (3+1)-formalism are modified in compliance with the laws of thermodynamics. One immediate and fundamental

consequence of this is the breaking of symmetry under time inversion and the emergence of the arrow of time. Furthermore, the Raychaudhuri equation is also modified and, thus, the way in which gravitational collapse takes place. When applied to cosmology, the Friedmann equations include an entropic force, which is always of accelerating nature when the universe is expanding. Even though most of the expansion history of the universe is isentropic, such a force may become relevant in out-of-equilibrium cosmic phenomena: for instance (p)reheating, phase transitions and gravitational collapse.

Moreover, we propose an explanation to the current accelerated expansion of the universe as a sustained entropic force coming from the growth of the causal horizon in an open inflation scenario. We name this the general relativistic entropic acceleration (GREA) theory. Cosmological data in absence of priors on H_0 strongly favours GREA in comparison with ΛCDM. Future cosmological surveys will further constrain cosmological parameters and may clearly support one model over the other.

Resumen

La cosmología es la rama de la física que se encarga del estudio del universo en su conjunto. A simple vista parece que nuestra comprensión del universo se fundamental únicamente en gravedad clásica. En efecto, la relatividad general es una potente herramienta que ofrece con éxito una descripción geométrica del universo. Sin embargo, si nos adentramos bajo la superficie, el universo se convierte en un escenario fascinante de fenónmenos térmicos y cuánticos.

Por un lado, el origen cuántico de las fluctuaciones primordiales y, en última instancia, de la estructura del universo, es una predicción espectacular e inevitable del paragima inflacionario. El universo puede parecer clásico, pero es sin duda cuántico a nivel fundamental. Por otro lado, en un universo en expansión ocurren muchos procesos termodinámicos fuera del equilibrio, lo cual nos permite introducir una flecha del tiempo: los propios conceptos de pasado y futuro. El objetivo de la investigación recogida en esta tesis es aportar resultados y una mayor percepción de los fenómenos que trascienden la mera descripción geométrica y son auténticas ventanas cuánticas y termodinámicas al universo.

En la ventana cuántica exploramos temas que combinan técnicas de información cuántica en espacio real y física del universo temprano. Podemos entender la amplificación de fluctuaciones cuánticas durante inflación como un proceso de creación de partículas. Argumentamos que, debido a este proceso, existen correlaciones de gran alcance entre regiones distantes, en contraste con el entrelazamiento de corto alcanze presente en el vacío de Minkowski. Continuamos mostrando el aumento de la información mutua perturbativa entre dos regiones arbitrarias de un universo inflacionario o dominado por radiación. A diferencia del vacío de Minkowski, en el que esta cantidad decrece rápidamente como una potencia, en un contexto cosmológico el decrecimiento es logarítimico, por lo que se comparte información a grandes distancias. Además, estudiamos las desigualdades de Bell en espacio real, mostrando que el vacío de Bunch-Davies del espaciotiempo de de Sitter no las viola, a pesar de que la existencia de correlaciones cuánticas genuinas en el estado del campo Mukhanov-Sasaki parecería indicar lo contrario.

En la ventana termodinámica, desarrollamos un marco teórico que permite formular la termodinámica fuera del equilibrio en relatividad general de modo congruente. Las

ecuaciones de campo de Einstein o, de manera equivalente, las ecuaciones de Hamilton en el formalismo (3+1) se modifican de acuerdo con la segunda ley de la termodinámica. Una consecuencia inmediata y fundamental es la ruptura de la simetría bajo inversión temporal y la emergencia de la flecha del tiempo. Además, la ecuación de Raychaudhuri se ve modificada, así como la manera en la que ocurre el colapso gravitacional. En aplicaciones a cosmología, las ecuaciones de Friedmann incluyen una fuerza entrópica, que siempre tiende a acelerar un universo en expansión. A pesar de que expansión del universo es isoentrópica durante la mayor parte de su historia, dicha fuerza podría ser relevante en fenómenos cósmicos fuera del equilibrio, por ejemplo: el (p)recalentamiento, las transiciones de fase y el colapso gravitacional.

Además, proponemos una explicación para la actual expansión acelerada del universo en forma de una fuerza entrópica sostenida, debido al crecimiento del horizonte causal en un escenario de inflación abierta. Llamamos a esta idea la teoría de la aceleración entrópica relativista general (GREA[1]). Los datos de observaciones cosmológicas, exluyendo probabilidades *a priori* de H_0, muestran una preferencia fuerte de GREA en comparación con ΛCDM. Será tarea de los estudios cosmológicos futuros el constreñir todavía más los parámetros cosmolgógicos y ofrecer un claro veredicto sobre uno u otro modelo.

[1]Por sus siglas en inglés, *general relativistic entropic acceleration.*

Declaration

This thesis collects original results obtained during the last four years at the Instituto de Física Teórica UAM-CSIC. Most of them have been published in collaboration with other colleagues in the following articles:

[1] L. Espinosa-Portalés and J. García-Bellido, *Entanglement entropy of Primordial Black Holes after inflation*, *Phys. Rev. D* **101** (2020) 043514 [1907.07601]

[2] L. Espinosa-Portalés and J. García-Bellido, *Long-range enhanced mutual information from inflation*, *Phys. Rev. D* **103** (2021) 043537 [2007.02828]

[3] L. Espinosa-Portales and J. Garcia-Bellido, *Covariant formulation of non-equilibrium thermodynamics in General Relativity*, *Phys. Dark Univ.* **34** (2021) 100893 [2106.16012]

[4] J. Garcia-Bellido and L. Espinosa-Portales, *Cosmic acceleration from first principles*, *Phys. Dark Univ.* **34** (2021) 100892 [2106.16014]

[5] R. Arjona, L. Espinosa-Portales, J. García-Bellido and S. Nesseris, *A GREAT model comparison against the cosmological constant*, *Phys. Dark Univ.* **36** (2022) 101029 [2111.13083]

[6] L. Espinosa-Portalés and V. Vennin, *Real-space Bell inequalities in de Sitter*, 2203.03505

These results have also been presented in several international conferences, some of which lead to the following conference proceedings:

[7] L. Espinosa-Portalés, *Entropy in the early universe*, *PoS* **EPS-HEP2021** (2022) 123

[8] L. Espinosa-Portalés and J. García-Bellido, "Entropy and irreversible processes in gravity and cosmology." Contribution to MG16. In press.

In particular, chapter 3 is based on ref. [1], chapter 4 is based on ref. [2], chapter 5 is based on ref. [6], chapter 6 is based on ref. [3] and chapter 7 is based on refs. [4] and [5]. The contents of chapters 6 and 7 are also reviewed to some extent in refs. [7,8]. Chapters

1 and 2 are introductory reviews based on multiple references cited therein and no claim of originality is made on them. Chapters 8 and 9 give concluding remarks and recapitulate the results presented in the rest of the thesis. Finally, appendix A is based on the appendices of refs. [2,3], while appendix B contains additional figures from refs. [5,6].

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Llorenç Espinosa Portalés
Madrid, May 2022

Acknowledgements

This thesis is not only a collection of my scientific work during the last four years, but also, and perhaps more importantly, is the pinnacle of a personal voyage in the realm of physics, a part of my life driven by curiosity and fascination for the world around me and a will to understand it. As the time of closure and retrospection has come, I realize how much I owe to the people that have accompanied me.

It is only fair to begin by expressing my gratitude to my supervisor Juan García-Bellido. His guidance, deep knowledge and intuition has been invaluable. I owe to his firm support the freedom in developing my project. I am likewise thankful to Vincent Vennin for his hospitality and for sharing his expertise with me during my research stay at the Laboratoire Astroparticule et Cosmologie in Paris.

It is impossible to disentangle the purely scientific work from the atmosphere of friendship and peer support I enjoyed at the Instituto de Física Teórica. I am convinced there is no better path to foster scientific progress. Everyone is responsible for this in some way, but I would like to thank specially my office mates Xurxo, José and Walter, for we know our office is the true social room, and my friends Fran, Sergio, Judit, Max, Alessandro, Joan and Rubén, who were often guests within our four walls. Our friendship has survived the harsh isolation of the pandemic and I hope it will last much longer.

Living in Madrid has also given me the opportunity of sharing an appartment and countless good moments with Andrés and Débora. Feeling at home is a necessary condition for happiness. I am also grateful for enjoying this city and its wonders with my friends Javi, Filips, Carmen, Miriam, Sonia, Miryam, Sara, Luis and Yaiza. I cannot forget my link with València, my dear friends Belén, Raquel and Blas, whom I (re)discovered years later in the Spanish capital.

I turn my head to both sides of the Atlantic Ocean and thank Silvia and Robert for sharing unique moments of science, laughter and supportive desperation. I want to thank Isa for equally fun and profound conversations on physics and life. I am also in debt with all the *lacaixitos*, who have made this endeavour a bit easier and certainly more fun, and specially Olga for her friendship in the hardest of times.

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I cannot overstate the lifelong support and love received from all my family. I think every day of my grandma María, who saw the beginning but not the end of this thesis project, and my grandma Rosita, who makes sure everyone in Nules is aware of my steps. I'll always treasure the memories with my grandpa Batiste and my great aunt Carmen, who I know believed in me since I took my first steps in this pale blue dot. To my great uncle Luis and my great aunt María Teresa I thank their love and tireless vitality. In a certain way, the road leading here started in a bench in central Castelló de la Plana, where my uncle Paco taught me the concept of infinity, as he'd done to countless students before. To my cousin David I owe insightful conversations on science, life and their splendid overlap. The rest of my family I keep likewise in a special part of my heart and my identity.

I conclude this foreword by thanking my parents. To my father Llorenç I owe the discovery of physics and the endless wonders of the universe. To my mother Lourdes, the opening the gates of the world and the toolkit to explore and thrive in it. To both, their unconditional support and love, a highly non-trivial gift. Gràcies.

Introduction

Cosmology is the science that studies the universe as a whole, aiming to answer some of the oldest questions raised by humanity. Being a branch of modern physics since the early 20th century, it is now equipped with the proper tools to pose and tests hypotheses about the origin, evolution, destiny and fundamental properties of the universe.

On the one hand, current technology allows to study cosmic structure in great detail, even the so called large scale structure, forming a true cosmic cartography which allow us to know that the universe is expanding and, at present, this expansion is accelerating. In order to do so it analyzes visible light and other parts of the electromagnetic spectrum coming from distant objects, such as galaxies and groups and clusters thereof. Furthermore, studying the cosmic microwave background, a remnant of the early universe, allows one to reconstruct the so called thermal history of the universe, back to the time when matter was concentrated in a particle plasma. In contrast with other branches of physics, whose empirical side rests on reproducible and standarizable experiments, cosmology has the challenge of building knowledge and verifying or falsifying hypotheses solely from observations, for it is impossible to create a new universe or repeat cosmic history.

On the other hand, theoretical physics offers a firm ground, a logical construct within which cosmological observations can fit. The theory of general relativity, the theoretical framework of spacetime as geometry and the gravitational interaction between systems with energy and momentum, is a fundamental tool to understand the universe, its shape and expansion rate at any of its stages. Quantum mechanics and quantum field theory are also required to understand key aspects of the universe, in particular its evolution during its earliest stages and even the origin of its structure. It is only natural, therefore, that the birth of physical cosmology is a relatively recent happening, needing both advanced observational instrumentation and the revolutions of phyiscs of the 20th century. Thanks to its billions-of-years-lasting expansion, cosmology establishes a beautiful connection between the tiniest of elementary particles to the immensity of the entirety of the observable universe. Thermodynamics plays a determinant role in the connection between the microscopic and the macroscopic worlds. Most of the expansion of the universe takes place in equilibrium, although certain key events take place out of equilibrium.

The goal of this thesis is to deal with some aspects of the crossroad of gravity and cosmology with quantum mechanics and thermodynamics.

The standard model of cosmology, ΛCDM[2], is based precisely on these theoretical and observational pillars. It proposes that the expansion of the universe is dominated by the cosmological constant Λ, which determines its current acceleration, and dark matter. Ordinary matter and radiation are less abundant ingredients, but allow us to perform the observations themselves.

Despite the success of ΛCDM, the universe has some quite particular properties, such as its homogeneity and isotropy on large scales, which require fine-tuned initial conditions. Inflation is the theory that currently counts with greater support as an explanation for these initial conditions. It proposes the existence of an accelerated expansion of the universe before the creation of the matter we observe. In addition to determining the geometry and basic symmetries of the universe, inflation offers a quantum origin for the deviations of homogeneity and isotropy that we observe by the very existence of structure in the universe, the matter that clusters in galaxies and groups thereof instead of being completely homogeneous, as well as the anisotropies of the cosmic microwave background. During inflation microscopic quantum fluctuations arise and are stretched out due to the accelerated expansion until reaching macroscopic scales. These fluctuations turn then into curvature perturbations of the universe and, later, into matter density perturbations.

These fluctuations of quantum origin can be studied with modern quantum information techniques. The goal is to understand the nature of the classical and quantum correlations between distant regions of the observable universe due to this common origin of structure. It is possible to distinguish between classical and the so called genuinely quantum correlations, given the fact that quantum mechanics violate the upper bound to correlations between two subsystems established by classical physics. Quantum entanglement, which prevents us from describing a given quantum subsystem with certainty without its complementary, is perhaps one of the most novel phenomena in quantum mechanics and it is responsible of the possibility of violating this bound.

The concept of entropy is key to study a quantum system. Entropy quantifies the lack of information of a quantum system or subsystem and it is the first step to understand the existence of entanglement and genuinely quantum correlations with other subsystems. In other words, the lack of information suggests that it can be obtained if the interaction with another subsystem is known. This quantity and others derived from it are to be studied in this thesis, in the context of primordial perturbations as a quantum system.

Entropy plays yet another role in cosmology, as a key quantity in thermodynamics. As a measure of the lack of information, the evolution of entropy distinguishes between process in- and out-of-equilibrium in the thermodynamic sense. When it is conserved, the

[2] CDM stands for cold dark matter.

system is in quasi-equilibrium and the dynamics is reversible, whereas it grows out of it and the dynamics becomes irreversible. In other words, the deviation from thermodynamic quasi-equilibrium implies irreversibility and information loss. Once reached, strict thermodynamic equilibrium sets an upper bound on the entropy of the system and an exit from it is exponentially unlikely.

Thermodynamics in general and entropy in particular are unexpectedly relevant in the consistency between gravity and quantum mechanics, as well as in its potential unification in a theory of quantum gravity. This is thanks to black holes, physical objects with such a high density that they can trap light with their gravitational field. The discovery that black holes satisfy the laws of thermodynamics points towards the existence of a quantum microscopic description, from whose statistics emerges thermodynamics, as it happens in any other many-particle quantum system. A greater logical connection between thermodynamics and gravity, both in- and out-of-equilibrium, may help deepening its link with quantum physics.

This thesis is organized in four parts and nine chapters as follows. In part I the foundations of theoretical physics on which the thesis is based are reviewed: in chapter 1 several aspects of cosmology are introduced, with emphasis on inflation, while chapter 2 collects selected topics on quantum mechanics. In part II quantum properties of primordial perturbations in real space are discussed: chapter 3 deals with the entropy of entanglement, chapter 4 presents a perturbative computation of the mutual information and chapter 6 deals with Bell inequalities. In part III a change in the usual treatment of out-of-equilibrium thermodynamics in cosmology is proposed: in chapter 6 a covariant and variational formulation of gravity and thermodynamics is presented, while chapter 7 deals with achieving an accelerated expansion of the universe as an out-of-equilibrium process. Finally, the conclusions of the thesis are collected in part IV, chapters 8 and 9.

Introducción

La cosmología es la ciencia que estudia el universo en su conjunto, con el objetivo de responder algunas de las preguntas más antiguas planteadas por el ser humano. Como rama de la física moderna desde principios del siglo XX, cuenta por primera vez con las herramientas adecuadas para plantear y comprobar hipótesis sobre su origen, evolución, destino y propiedades fundamentales.

Por un lado, la tecnología actual permite estudiar la estructura cósmica en gran detalle, incluso la llamada estructura a gran escala, constituyendo una auténtica cartografía cósmica que nos permite saber que el universo se expande y que, en la actualidad, lo hace de manera acelerada. Para ello analiza la luz visible y otras partes del espectro electromagnético que nos llegan de objetos distantes, como galaxias y grupos y cúmulos de estas. Además, el estudio la radiación de fondo de microondas, un remanente del universo antiguo, permiten reconstruir la llamada historia térmica del universo, hasta cuando la materia estaba concentrada en un plasma de partículas. A diferencia de otras ramas de la física, cuyo lado empírico descansa sobre experimentos repetibles y estandarizables, la cosmología tiene el reto de construir conocimiento y verificar o falsar hipótesis a partir únicamente de observaciones, pues es imposible crear un nuevo universo o repetir la historia cósmica.

Por otro lado, la física teórica ofrece un fundamento firme, un constructo lógico en el que encajar las observaciones cosmológicas. La teoría de la relatividad general, el marco teórico del espacio-tiempo como geometría y de la interacción gravitatoria entre sistemas físicos dotados de energía y momento, es una herramienta fundamental para comprender el universo, su forma y su ritmo de expansión en cualquiera de sus estadíos. La mecánica cuántica y la teoría cuántica de campos también son necesarias para comprender aspectos clave del universo, en particular su evolución en las etapas más tempranas e incluso el origen de su estructura. Es natural, por tanto, que el nacimiento de la cosmología física sea relativamente reciente, al necesitar tanto de instrumentación observacional avanzada como de las revoluciones de la física del siglo XX. Gracias a su expansión durante miles de millones de años, la cosmología establece una bella conexión entre lo minúsculo de las partículas elementales a la inmensidad de la totalidad del universo observable. En la conexión entre lo microscópico y lo macroscópico juega un papel determinante la termodinámica. La mayor parte de la expansión del universo ocurre en equilibrio, pero ciertos momentos clave ocurren fuera del equilibrio.

El objetivo de esta tesis es tratar algunos aspectos de la encrucijada de la gravedad y cosmología con la mecánica cuántica y la termodinámica.

El modelo estándar de la cosmología, llamado ΛCDM[3], se basa precisamente en estos pilares teóricos y observacionales. Propone que la expansión del universo está dominado por la constante cosmológica Λ, que determina su aceleración actual, y la materia oscura. La materia ordinaria y la radiación son ingredientes menos abundantes, pero permiten la propia realización de observaciones.

A pesar del éxito de ΛCDM, el universo tiene algunas propiedades muy particulares, por ejemplo su homogeneidad e isotropía a grandes escalas, que requieren de unas condiciones iniciales ajustadas. Inflación es la teoría que actualmente cuenta con mayor respaldo para explicar esas condiciones iniciales. Propone la existencia de una expansión acelerada del universo antes de la creación de la materia que observamos. Además de determinar la geometría y las simetrías básicas del universo, inflación ofrece un origen cuántico para las desviaciones de homogeneidad e isotropía que observamos por la misma existencia de estructura en el universo, la materia se concentra en galaxias y agrupaciones de estas en lugar de ser totalmente homogénea, así como las anisotropías en el fondo de radiación de microondas. Durante inflación se producen fluctuaciones cuánticas a nivel microscópico que son estiradas debido a la expansión acelerada hasta alcanzar escalas macroscópicas. Estas fluctuaciones se traducen en perturbaciones de la curvatura del universo y, más adelante, en perturbaciones de la densidad de materia.

Estas fluctuaciones de origen cuántico se pueden estudiar mediante técnicas modernas de información cuántica. El objetivo es comprender la naturaleza de las correlaciones clásicas y cuánticas entre regiones distantes del universo debido a este origen común de la estructura. Es posible distinguir entre correlaciones clásicas y las llamadas genuinamente cuánticas, ya que la mecánica cuántica viola la cota superior a las correlaciones entre dos subsistemas establecida por la física clásica. El entrelazamiento cuántico, que impide describir un subsistema cuántico determinado con seguridad sin su complementario, es quizá uno de los fenómenos más novedosos de la mecánica cuántica y es responsable de la posibilidad de violar dicha cota.

El concepto de entropía es clave en el estudio de un sistema cuántico. La entropía cuantifica la falta información de un sistema o subsistema cuántico y es el primer paso para entender la existencia de entrelazamiento y correlaciones genuinamente cuánticas con otros subsistemas. Es decir, la falta de información sugiere que esta puede ser obtenida si es conocida la interacción con otro subsistema. Esta cantidad y otras derivadas de ella

[3]CDM significa *cold dark matter* o materia oscura fría

son objeto de estudio de esta tesis, en el contexto de las perturbaciones primordiales como sistema cuántico.

La entropía juega además otro papel en cosmología, como cantidad clave en termodinámica. Como medida de la falta de información, la evolución de la entropía permite distinguir entre procesos dentro y fuera del equilibrio en el sentido termodinámico. Cuando esta se conserva, el sistema se encuentra en cuasi equilibrio y la dinámica es reversible, mientras que crece cuando sale de él y la dinámica se vuelve irreversible. Es decir, la desviación del cuasi equilibrio termodinámico conlleva irreversibilidad y pérdida de información. El equilibrio termodinámico estricto, una vez alcanzado, supone una cota superior a la entropía del sistema y una salida de él es exponencialmente improbable.

La termodinámica en general y la entropía en particular tienen una relevancia sorprendente *a priori* en la coherencia entre la gravedad y la mecánica cuántica, así como en su potential unión en una teoría de gravedad cuántica. Esto se debe a los agujeros negros, objetos físicos con una densidad tan alta que son capaces de atrapar la luz mediante su campo gravitatorio. El descubrimiento de que los agujeros negros cumplen con las leyes de la termodinámica es señal de la existencia de una descripción microscópica cuántica, de cuya estadística emerge la termodinámica, al igual que en cualquier otro sistema cuántico de muchas partículas. Una mayor conexión lógica entre la termodinámica y la gravedad, tanto dentro como fuera del equilibrio, podrían ayudar a profundizar su vínculo con la cuántica.

Esta tesis se organiza en cuatro partes y nueve capítulos de la siguiente manera. En la parte I se revisan los fundamentos de física teórica en los que se basa la tesis: en el capítulo 1 se introducen varios aspectos de cosmología con enfásis en inflación, mientras que en el capítulo 2 se seleccionan temas relevantes de mecánica cuántica. Los resultados de la tesis se presentan en las partes II y III. En la parte II se discuten propiedades cuánticas de las perturbaciones primordiales en espacio real: en el capítulo 3 se estudia la entropía de entrelazamiento, en el capítulo 4 se realiza un cálculo perturbativo de la información mutua y en el capítulo 5 se estudian las desigualdades de Bell. En la parte III se propone un cambio en el tratamiento de la termodinámica fuera del equilibrio en cosmología: en el capítulo 6 se elabora una formulación covariante y variacional que auna gravedad y termodinámica, mientras que en el capítulo 7 se plantea cómo lograr una expansión acelerada del universo como un proceso fuera del equilibrio. Finalmente, en la parte IV, capítulos 8 y 9, se exponen las conclusiones de la tesis.

Contents

Part I

Foundations

Chapter 1

Inflationary cosmology

> "Este palacio es fábrica de los dioses", pensé primeramente. Exploré los inhabitados recintos y corregí: "Los dioses que lo edificaron han muerto". Noté sus peculiaridades y dije: "Los dioses que lo edificaron estaban locos"
>
> Jorge Luis Borges, *El Aleph* (1943)

1.1 Spacetime, relativity and geometry

Cosmology, understood as the pursue of knowledge about the whole of existing phenomena, is an ancient discipline. Religions throughout the world provided a plethora of beliefs about the origin, purpose, nature and destiny of the universe. Metaphysics still addresses some of these questions today from a rational point of view.

The scientific study of the universe, what one may call physical cosmology, is a relatively modern branch of physics. It wasn't until the development of a mathematically rigorous and experimentally tested dynamical theory of spacetime, general relativity (GR) that one was able to scientifically pose the questions mentioned above.

Space and time were considered separate and absolute entities for centuries. This means that distances would look the same and clocks would tick at the same rate for any observer. Albert Einstein challenged this view in 1905, proposing that space and time are actually observer-dependent [9]: those that move faster experience time dilation and length contraction. This striking statement was a logical consequence of the postulates of special relativity (SR): all physical laws look the same to and the speed of light is measured to be the same constant by any inertial observer, where an inertial observer moves at constant speed. Later in 1908, Hermann Minkowski interpreted this relative nature of space and time as a single geometric entity: *spacetime* [10].

This geometric way of thinking can be seen as a true paradigm shift and allowed Einstein to make the postulates of gravity consistent with the gravitational interaction.

- Principle of general covariance. The laws of physics are the same for all observers. They admit a mathematical formulation in terms of tensors defined on a differentiable manifold that make this invariance explicit. In other words, the laws of physics are invariant under an arbitrary change of coordinates.
- The equivalence principle. The laws of physics reduce locally to those of SR, that is, no local experiment can determine the existence of the gravitational interaction.

Based on these physical principles and their mathematical implementation, Einstein proposed the gravitational field equations [11]

$$\text{Geometry} = \text{Matter} \tag{1.1}$$

or, more concretely

$$G_{\mu\nu} = \kappa T_{\mu\nu} \,. \tag{1.2}$$

This equation relates a geometric quantity, the Einstein tensor $G_{\mu\nu}$ with a description of matter, the stress-energy tensor $T_{\mu\nu}$, by the gravitational coupling κ.

The description of gravity in terms of geometry ammounts to the replacement of flat spacetime with the Minkowski metric $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$ by a more general spacetime manifold equipped with a metric tensor $g_{\mu\nu}$ with Lorentzian signature.

GR passed its first experimental tests by explaining the perihelion precession of Mercury and predicting the correct value of the gravitational deflection of light [12], which doubled the Newtonian prediction. It is considered today to be a successful physical theory, able to explain all observed gravitational phenomena: celestial orbits [12], cosmic evolution [13], black holes [14], gravitational waves [15–17], etc.

Einstein's equations are compatible with yet another backbone of physics: the variational or extremal action principle. The gravitational part can be obtained from the Einstein-Hilbert action [18]

$$\mathcal{S}_{EH} = \frac{1}{2\kappa} \int d^4x \sqrt{-g}\, R \,, \tag{1.3}$$

where $R = g^{\mu\nu} R_{\mu\nu}$ is the Ricci scalar, the trace of the Ricci tensor $R_{\mu\nu}$. The variation of the Einstein-Hilbert action ($\delta \mathcal{S}_{EH} = 0$) gives the vacuum Einstein field equations $R_{\mu\nu} = 0$. Including matter, the whole action takes the form

$$\mathcal{S} = \mathcal{S}_{EH} + \mathcal{S}_m \,, \tag{1.4}$$

so that one defines the stress-energy tensor associated to a matter action as

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta \mathcal{L}_m}{\delta g^{\mu\nu}}\,, \tag{1.5}$$

where $\mathcal{L}_m$ is the matter Lagrangian given by $\mathcal{S}_m = \int d^4x \mathcal{L}_m$. GR is then a fully-fledged theory, which is consistent with or generalizes the principles of classical physics.

Somewhat simultaneously to the development of relativity, another revolution of modern physics took place: the birth of quantum physics, required to explain the behavior of microscopic phenomena, such as atoms and elementary particles. To put it in short: quantum mechanics is revolutionary because it requires giving up one of the following two physical principles: locality or realism. This will be discussed in more detail in chapter 2.

Strictly speaking, GR can be quantized within the framework of quantum field theory (QFT) as an effective field theory (EFT) [19]. This means that its validity is restricted below a certain energy scale, the Planck scale, which is way above the reach of any feasible experiment performed with current and foreseeable technology. However, significant departures from the classical theory, i.e., quantum corrections, are also expected to arise around the Planck scale. Hence, classical gravity suffices in principle to explain observable gravitational phenomena. There are proposals, however, as to how the logical and physical consistency of quantum gravity may constraint the range of low-energy effective field theories of gravity and other fields that can be consistently completed at high energies by it [20–22].

Furthermore, even if a classical theory suffices for observational purposes, it may as well be that the correct one is not GR. Indeed, many modified gravity theories have been proposed as alternatives to GR [23]. Reasons to do so vary, but phenomenologically can be linked to two physical phenomena not fully-satisfactory described by GR: dark matter and dark energy, which we will briefly discuss in sec. 1.2.

1.2 FLRW cosmology

As a physical theory of spacetime, GR provided for the first time the required tools to describe the universe as a whole. Besides the physical principles included in the theory, there is a crucial additional one: the Copernican principle. Loosely speaking, it is the statement that humans, Earth or the Solar System are not privileged observers of the universe. Put more rigorously: the universe is homogeneous and isotropic, i.e., the universe looks the same everywhere and looking in any direction. This principle is named after Nicolaus Copernicus, who argued in 1543 that Earth was orbiting the Sun, and thus had no privileged position over the other planets.

Mathematically, the copernican principle is translated into a particular ansatz for the spacetime metric of the universe. In spherical coordinates (t, r, θ, φ) this takes the form

$$ds^2 = -dt^2 + a^2(t) \left(\frac{dr^2}{1 - kr^2} + r^2 \left(d\theta^2 + \sin^2 \theta d\varphi^2 \right) \right) . \tag{1.6}$$

This is the Friedmann-Lemaître-Robertson-Walker (FLRW) metric, named after the four scientists that contributed more generally to the foundation of homogeneous and isotropic cosmology in the 1920s and 30s [24–27], also named FLRW cosmology after them. This metric describes a spacetime geometry whose constant-time hypersurfaces are spatially homogeneous and isotropic. There exist three such hypersurfaces, labelled by $k = \{-1, 0, 1\}$, corresponding to hyperbolic, Euclidian or elliptic space. They describe, respectively, an open, flat or closed universe.

Of uttermost relevance is the scale factor $a(t)$, a function of time that describes the expansion or contraction of physical distances within the hypersurfaces. A universe with constant scale factor is said to satisfy the perfect Copernican principle, but this is not the case of our universe. In fact, galaxies observed from Earth recede at a velocity proportional to its distance [28]

$$v = Hd \, , \tag{1.7}$$

where H is the Hubble parameter, which is actually time-dependent $H = H(t)$. This relation, called the Hubble law, can be shown to be the only one that can make galactic recession consistent with spatial homogeneity and isotropy.

The time-dependent value of $H(t)$ is a consequence of the dynamical expansion of the universe and can be obtained by applying the Einstein field equations. In fact

$$H(t) = \frac{\dot{a}}{a} \tag{1.8}$$

Let us asume that the universe is filled by a perfect fluid, characterized by the following stress-energy tensor

$$T_{\mu\nu} = (\rho + p) u_\mu u_\nu + p g_{\mu\nu} \tag{1.9}$$

where $\rho = \rho(t)$ and $p = p(t)$ are, respectively, the energy density and pressure of the perfect fluid as measured by a comoving observer who finds the universe around it to be homogeneous and isotropic and, thus, ρ and p only can depend on cosmic time. The covariant conservation of this tensor implies the continuity equation

$$D_\mu T^{\mu\nu} = 0 \quad \Rightarrow \quad \dot{\rho} + 3H(\rho + p) = 0 \, . \tag{1.10}$$

The Einstein field equations with the FLRW metric ansatz and the stress-energy tensor of a perfect fluid become the Friedmann equations for the scale factor

$$\begin{aligned} H^2 &= \frac{8\pi G}{3} \rho - \frac{k}{a^2} \\ \frac{\ddot{a}}{a} &= -\frac{4\pi G}{3} (\rho + 3p) \, . \end{aligned} \tag{1.11}$$

Note that the continuity equation and the Friedmann equations are interdependent.

Hence, FLRW cosmology predicts a decelerating expansion of the universe. In the distant past, the universe was filled with a plasma, much denser and hotter than it is today. Since then it has expanded and cooled down in a procedure called the thermal history of the universe. This framework, sometimes called *Big Bang* cosmology, can correctly predict many present observations, such as the abundance of light elements in the universe [29], due to *Big Bang* nucleosynthesis, or the cosmic microwave background (CMB) [30], redshifted isotropic radiation coming from the last scattering between photons and free protons and electrons before their recombination into hydrogen atoms.

One firstly observes two kinds of matter in the universe: baryonic matter[1] and photons. Baryonic matter is a particular case of dust, i.e., it has negligible pressure ($p = 0$) due to its non-relativistic nature. Photons, on the other hand, are a particular case of radiation, i.e., their pressure is that of an ultra-relativistic particle ($p = \rho/3$).

These, however, cannot account for all phenomena observed in the universe. Frank Zwicky proposed in the 1930s the existence of additional dust, called dark matter due to its lack of electromagnetic interaction, motivated by the observed motion of galaxies in clusters and the virial theorem [31]. This proposal was strengthened later by the study of galactic rotation curves by Vera Rubin [32]. Since then, many other astronomical observations require the inclusion of dark matter in the cosmic fluid. Whether it requires an extension of the standard model of particle physics (SM) or can be explained by conventional physics, such as black holes, is still up to debate. This dark matter is said to be cold, since it behaves as dust.

Furthermore, the expansion of the universe is not decelerating today, contrary to predictions of FLRW cosmology. It was discovered in 1998 by observing Type Ia supernovae [33, 34] that, instead, it started accelerating recently. The current accepted explanation for this observation is the existence of a non-vanishing cosmological constant Λ. This means that the universe will asymptotically converge to de Sitter spacetime, thus finishing emptied out and causally disconnected. A plethora of alternatives to the cosmological constant has been proposed. These can be put into to categories: modified gravity (MG) at large scales and dark energy (DE) [35]. However, so far none of them provides a statistically favored explanation in comparison with the cosmological constant.

Finally, we should mention that, although the universe is homogeneous and isotropic at large scales, this feature is not exact and certainly does not hold at small scales due to existence of large scale structure (LSS) in the universe[2]. Observations of the CMB anisotropies

[1] The term baryonic matter as widely used in cosmology is somewhat inconsistent with the concept of baryon in particle physics, since atomic nuclei are made up of baryons (protons and neutrons), but electrons are certainly not. Since atomic nuclei make up most of the atomic mass, this inaccuracy is usually tolerated.

[2] LSS is large compared to Earth, the Solar System or even the Milky Way galaxy, but small compared to the size of the universe.

are consistent with a spectrum of scale-invariant and small density perturbations [36], which eventually grow due to gravitational collapse and form the large inhomogeneities observed at small scales, thus explaining LSS [37].

The key ingredients outlined here: FLRW cosmology with baryonic matter, radiation (photons and neutrinos), cold dark matter, the cosmological constant and a Gaussian and scale-invariant spectrum of primordial perturbations constitute the concordance model of cosmology, usually labelled Λ - cold dark matter (ΛCDM). This is the currently accepted model to describe the universe as a whole. Despite the remaining uncertainties and the unknown fundamental nature of some of its components, it is a remarkable achievement that one can obtain such a consistent and accurate physical description of the universe with 1) an underlying physical theory of spacetime and a model within it built from first principles and 2) observations from Earth that are able to fit the parameters of the model up to $\mathcal{O}(1\%)$ or even better precision [38].

There remains the question of the initial conditions that deliver a universe such as the one we observe and is accurately described by ΛCDM. As a matter of fact, these initial conditions need to be finely tuned due to the dynamical behavior of the Friedmann equation. A solution to this and other problems is provided by inflation.

1.3 The idea of inflation

Big Bang cosmology, as the logical consequence of GR, the Copernican principle and the observed expansion of the universe is remarkably successful. Nevertheless, it suffers from several theoretical issues [13, 39]:

- The flatness problem. It can be summarized as the paradox of observing an almost spatially flat universe, despite gravity tending to increase curvature. Let us rewrite the first Friedmann equation as

$$1 = \Omega + \Omega_K \,, \tag{1.12}$$

  where $\Omega = 8\pi G\rho/(3H^2)$ is the density parameter of the universe and $\Omega_K = -k/(aH)^2$ is the curvature parameter. During most of the known expansion history and before the begin of its current accelerated state (dark energy domination), time evolution tends to rapidly increase the value of Ω_K, at rates $\Omega_K \sim t^{2/3}$ during matter domination and $\Omega_K \sim t$ during radiation domination. Hence, for the current observational bounds on $|\Omega_K| \lesssim 10^{-3}$, the matter content of the very early universe must be precisely balanced as to give an extremely tiny value of the curvature parameter.

- The homogeneity problem. Similarly to the flatness problem, gravity tends to bring together matter, and a paradox arises between the Copernican principle at large scales and the dynamical evolution of the universe, which would again require deviations from homogeneity in the very early universe to be extremely tiny.

- The horizon problem. Because of the finite speed of light and the finite age of the universe, at any given time there exist causally disconnected patches. The CMB photons we observe now arise from 10^5 causally disconnected regions at recombination time, yet they have the same average temperature and correlated deviations from it. This seems extremely unlikely, unless there was indeed a common causal origin.

One may argue that these problems do not actually exist, for they do not arise as actual contradictions between FLRW cosmology and cosmological observations. Indeed, these issues, which we could summarize as the initial conditions problem, are not really concerned with the dynamical evolution of the universe nor the physical principles behind our description for it. However, the goal of theoretical physics as a scientific discipline is not merely to *describe* observations, but also to *explain* them. In a modern application of Occam's razor, a physical explanation can be regarded to be preferred if its requires a smaller amount of free parameters[3].

Therefore, one may aim to explain the universe without such fine-tuned initial conditions or, at least, in terms of parameters that do not require them. This is achieved by adding a cosmological era before radiation domination that has a very different dynamical behavior. In order to suppress inhomogeneities and curvature and make tiny scales cross outside the horizon (i.e. $d/dt(a/d_H) > 0$), the expansion of the universe needs to be accelerated

$$\ddot{a} > 0\,, \tag{1.13}$$

very much like it is today. An explanation in terms of the cosmological constant is, however, inadequate, since such an accelerated expansion would not end. Instead, the theory of inflation was developed in the early 1980s. First, Andrei Starobinsky realized that higher curvature contributions to the action could set de Sitter spacetime as the initial state of the universe [41]. Shortly after, Alan Guth realized that an exponential expansion would solve the problems of FLRW cosmology [42]. Finally, Andrei Linde proposed a fully viable model to start and end this exponential expansion [43].

During this new cosmological era, the universe is dominated by a scalar field ϕ, the inflaton, whose action is given by

$$\mathcal{S}_\phi = \int d^4x\sqrt{-g}\left(\frac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi)\right) \tag{1.14}$$

and $V(\phi)$ is the inflaton potential. Under the so called slow-roll conditions, an inflaton-dominated universe undergoes an exponential expansion that quickly suppresses any inho-

[3] Occam's razor is not only a traditional philosophical statement, but has also a modern implementation in statistical model comparison [40].

mogeneity or deviation from flatness and, hence, sets up the right initial conditions for our universe to be consistent with our observations [13].

The main argument in favor of inflation is not, however, the solution of the initial conditions problem *per se*. Rather, it is that it provides, at the same time, a quasi scale-invariant spectrum of primordial Gaussian perturbations [44, 45], as required by CMB and LSS observations. Most models predict both scalar perturbations, responsible for curvature and subsequent density perturbations, and yet-to-be-observed tensor ones. The mechanism behind this will be reviewed in the next subsection.

The paramount role played by inflation in modern Cosmology can be understood from its ability to explain these features of the universe from minimal assumptions. Its observational drawback its, consequently, that it seems to be hard to determine which particular inflationary model is the right one [13]. Not only it's hard to determine $V(\phi)$, but one may even have additional scalar fields (multi-field inflation), giving a much richer phenomenology. CMB anisotropies provide the best tool today to constraint inflationary models [38], precisely due to the differences between the spectra of primordial perturbations. These are mainly characterized by the deviation from scale invariance (spectral index) for scalar perturbations n_s and the tensor-to-scalar ratio r. Future observations will provide tighter constraints. Furthermore, the potential observation of primordial tensor perturbations could be the definite observational test for inflation if the consistency relation $r = -8n_t$ is measured, where n_t is the tensor spectral index [39]. This could be measured either directly as a contribution to the stochastic gravitational wave background (SGWB) or, more likely, indirectly as B-modes in the CMB photons.

1.4 Cosmological perturbation theory

The Copernican principle does not hold exactly in our universe, as it is obvious from the existence of galaxies, stars, planets or life. It is estimated to break down at around scales of order ~ 100 Mpc[4], see for instance ref. [46], so that structures form at smaller scales and the metric from eq. (1.6) is no longer valid. Therefore, it is important to understand how the spacetime geometry in GR behaves in the presence of these deviations from homogeneity and isotropy. The loss of symmetry implies that there are no preferred spatial hypersurfaces. Instead, one performs a (3+1)-splitting of spacetime, a foliation that parametrizes the 4-dimensional metric $g_{\mu\nu}$ by means of a 3-dimensional metric h_{ij} and the lapse and shift functions N and N^i. Spacetime dynamics is treated as the evolution of space-like hypersurfaces Σ_t, parametrized by some parameter t, which is usually taken to be the time coordinate. This is called the Arnowitt-Deser-Misner (ADM) formalism of GR [47] and allows for a Hamiltonian formulation of the equations of motion. See

[4] $1\text{pc} \simeq 3.26$ ly $\simeq 3.09 \cdot 10^{16}$ m is a common unit of length in Astronomy.

refs. [39, 48] for a modern review. An arbitrary[5] metric takes the form

$$ds^2 = -(Ndt)^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt)\,. \tag{1.15}$$

We will denote as Σ the 3-dimensional hypersurface and n its normal vector

$$n_\alpha = (-N, 0, 0, 0)\,, \tag{1.16}$$

which is a unit vector, i.e., $n_\alpha n^\alpha = -1$. Spacetime indices are lowered and raised as usual by $g_{\mu\nu}$. Spatial indices, however, are lowered and raised by h_{ij}, which furthermore satisfies $h_{ij}h^{jk} = \delta_i^k$.

Equivalently, one can write the splitting of the metric as

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu\,, \tag{1.17}$$

so that it is clear that $h_{\mu\nu}$ is purely tangential to the hypersurface. Then its spatial part h_{ij} is equal to the pull-back of the 4-dimensional metric $g_{\mu\nu}$ onto Σ and is a legitimate 3-dimensional metric.

The Einstein-Hilbert action, given by eq. (1.3), for this parametrization of the metric is given by the following gravitational Lagrangian

$$\mathcal{L}_G = \sqrt{-g}R = N\sqrt{h}\left({}^{(3)}R + K_{ij}K^{ij} - K^2\right)\,, \tag{1.18}$$

where K_{ij} is the extrinsic curvature of the 3-hypersurface Σ and is given by the Lie derivative along the normal vector n

$$K_{ij} = \frac{1}{2}\pounds_n h_{ij} = \frac{1}{2N}\left(\partial_0 h_{ij} - \nabla_i N_j - \nabla_j N_i\right)\,. \tag{1.19}$$

where ∇ denotes the covariant derivative on Σ with respect to the 3-metric h_{ij}. Its trace and traceless part are

$$\begin{aligned} K &= h^{ij}K_{ij} = \frac{1}{N}\left(\partial_0 \ln\sqrt{h} - \nabla_i N^i\right) \\ \bar{K}_{ij} &= K_{ij} - \frac{1}{3}K h_{ij}\,. \end{aligned} \tag{1.20}$$

Unlike the intrinsic curvature, described by the Riemann tensor $R^\rho_{\mu\nu\lambda}$ and its contractions, the extrinsic curvature is a quantity that depends on the embedding of a surface in a larger manifold.

The extrinsic curvature can be a complicated function of the parameters. Therefore, it is convenient to shift to the Hamiltonian formulation of the stationary-action principle.

[5] The manifold must actually satisfy a causality requirement called called global hyperbolicity, which we will not discuss in detail, but is basically related to admitting the foliation itself.

Note that the only quantity whose time derivative appears in the gravitational Lagrangian is the 3-spatial metric h_{ij} and, thus, it is the only dynamical or propagating degree of freedom (d.o.f.). Correspondingly, one defines its conjugate momentum as:

$$\Pi^{ij} = \frac{\partial \mathcal{L}_G}{\partial \dot{h}_{ij}} = \sqrt{h}\left(K^{ij} - K h^{ij}\right) . \tag{1.21}$$

With this, the gravitational Lagrangian can be rewritten as

$$\begin{aligned} \mathcal{L}_G &= N\sqrt{h}\,^{(3)}R - \frac{N}{\sqrt{h}}\left(\Pi_{ij}\Pi^{ij} - \frac{1}{2}\Pi^2\right) - 2\Pi^{ij}\nabla_i N_j \\ &= \Pi^{ij}\dot{h}_{ij} - N\mathcal{H} - N_i\mathcal{H}^i - 2\nabla_i\left(\Pi^{ij}N_j\right) , \end{aligned} \tag{1.22}$$

where $\Pi = h_{ij}\Pi^{ij}$ and we introduced the functions

$$\begin{aligned} \mathcal{H} &= -\sqrt{h}\,^{(3)}R + \frac{1}{\sqrt{h}}\left(\Pi_{ij}\Pi^{ij} - \frac{1}{2}\Pi^2\right) \\ \mathcal{H}^i &= -2\nabla_j\left(h^{-1/2}\Pi^{ij}\right) . \end{aligned} \tag{1.23}$$

Since N and N_i are not dynamical variables, they merely enter the gravitational Lagrangian as Lagrange multipliers. One defines the gravitational Hamiltonian as

$$\begin{aligned} \mathcal{H}_G &= \Pi^{ij}\dot{h}_{ij} - \mathcal{L}_G \\ &= N\mathcal{H} + N_i\mathcal{H}^i + \nabla_i\left(\Pi^{ij}N_j\right) , \end{aligned} \tag{1.24}$$

with the Hamiltonian and momentum constraints

$$\begin{aligned} \frac{\delta\mathcal{H}_G}{\delta N} &= \mathcal{H} = 0 \\ \frac{\delta\mathcal{H}_G}{\delta N_i} &= \mathcal{H}^i = 0 . \end{aligned} \tag{1.25}$$

The Hamiltonian evolution equations are obtained from the variations of the action with respect to the metric and conjugate momentum

$$\delta\mathcal{S} = \int d^4x \left[\left(-\dot{\Pi}^{ij} - \frac{\delta\mathcal{H}_G}{\delta h_{ij}} + 2\kappa\frac{\partial\mathcal{L}_m}{\partial h_{ij}}\right)\delta h_{ij} + \left(\dot{h}_{ij} - \frac{\delta\mathcal{H}_G}{\delta\Pi^{ij}}\right)\delta\Pi^{ij}\right] , \tag{1.26}$$

By setting the variation to 0 we obtain the two Hamilton equations

$$\begin{aligned} \frac{\delta\mathcal{H}_G}{\delta h_{ij}} &= -\dot{\Pi}^{ij} - +2\kappa\frac{\partial\mathcal{L}_m}{\partial h_{ij}} \\ \frac{\delta\mathcal{H}_G}{\delta\Pi^{ij}} &= \dot{h}_{ij} . \end{aligned} \tag{1.27}$$

These equations are equivalent to the Einstein field equations and, as such, describe the dynamical evolution of the spacetime metric.

As discussed previously, inflation makes the universe highly homogeneous, isotropic and flat. Simultaneously, it amplifies quantum fluctuations and sources small metric perturbations in a process that will described in more detail later. The general dynamics of perturbations can be rather complicated due to the equivalence principle: they couple to all kinds of matter which, in turn, couple again to the gravitational field. However, sufficiently small perturbations are said to be linear, i.e., so small compared to the background metric that do not significantly act as sources of gravitational field by these higher order effects.

Perturbations can be of scalar, vector and tensor nature. The most general metric at linear order perturbation theory that includes all of them is [13, 39, 45]

$$\begin{aligned} ds^2 =& a^2(\eta)\{ - (1+2\phi)d\eta^2 + 2(B_{|i} - S_i)dx^i d\eta \\ &+ \left[(1+2\psi)\gamma_{ij} + 2E_{|ij} + 2F_{(i|j)} + \delta h_{ij}\right] dx^i dx^j \,, \end{aligned} \tag{1.28}$$

where γ_{ij} is the metric induced on the constant-time hypersurfaces in the FLRW metric and $|i$ denotes a covariant derivative with respect to that metric. Note that the vector perturbations are transverse, i.e., $\gamma^{ij}S_{i|j} = 0$ and $\gamma^{ij}F_{i|j} = 0$, while the tensor perturbation is symmetric and transverse traceless, i.e., $\gamma^{ij}\delta h_{ij} = 0$. We also introduced here a new time coordinate called conformal time

$$\eta = \int \frac{dt}{a(t)} \,, \tag{1.29}$$

which is particularly convenient, as it allows to factor out the scale factor $a(\eta)$ in the metric. We will make this choice quite often. Derivatives with respect to η are denoted by $'$.

According to the principle of general covariance, there is freedom in choosing a set of coordinates for a given spacetime manifold. In cosmological perturbation theory, this freedom is translated into gauge redundancy. Under changes of coordinates, the set of scalar, vector and tensor perturbations introduced in eq. (1.28) transform in such a way that physical quantities remain invariant. Thus, it is useful to build gauge-invariant quantities.

First, the gauge-invariant scalar quantities are the Bardeen potentials

$$\begin{aligned} \Phi &= \phi + \mathcal{H}(B - E') + (B - E)' \,, \\ \Psi &= \psi - \mathcal{H}(B - E') \,. \end{aligned} \tag{1.30}$$

Similarly, one can build the gauge-invariant vector quantity

$$\Sigma_i = S_i + F_i' \,. \tag{1.31}$$

Tensor perturbations, on the other hand, are automatically gauge-invariant.

From now on, we will pick the longitudinal or Newtonian gauge. For this particular gauge fixing, the two scalar metric perturbations coincide with the Bardeen potentials, i.e., $\phi = \Phi$ and $\psi = \Psi$. Furthermore, vector perturbations vanish. Hence, the perturbed metric takes the form

$$ds^2 = -a^2(\eta)\left[(1 + 2\Phi(t, \vec{x}))d\eta^2 + (1 - 2\Psi(t, \vec{x}))\gamma_{ij}dx^i dx^j\right], \tag{1.32}$$

where we do not include tensor perturbations, i.e., gravitational waves, because they decouple from scalar perturbations at linear order.

Connecting with the ADM formalism, this metric is parametrized by the quantities

$$N = 1 + \Phi\,, \quad N^i = 0 \quad \text{and} \quad h_{ij} = (1 - 2\Psi)\gamma_{ij}\,. \tag{1.33}$$

This metric is particularly suitable to describe the evolution of scalar perturbations during inflation for two reasons: i) the spatial isotropy of the metric is manifest right away (gauge-invariant vector perturbations decay quickly anyway) and ii) constant-time hypersurfaces are orthogonal to geodesic curves.

Furthermore, it can be shown that, in GR and for isotropic stress-energy tensors, $\Phi = \Psi$, so that there is really only one scalar gravitational perturbation.

Up to this point we considered solely perturbations of the metric. However, the inflaton field fluctuates as well and deviates from spatial homogeneity and isotropy

$$\varphi(\eta, \vec{x}) = \varphi_0(t) + \delta\varphi(\eta, \vec{x})\,. \tag{1.34}$$

Note that in this subsection we denote the inflaton field as φ in order to avoid confusion with the scalar metric perturbation ϕ. One can also build a gauge invariant perturbation of the inflaton field

$$\delta\bar{\varphi} = \delta\varphi + \varphi'(B - E') \tag{1.35}$$

Finally, one can summarize the scalar gravitational and inflaton perturbations into a single scalar perturbation called the Mukhanov-Sasaki variable [13, 39, 44, 49, 50]

$$v = a\delta\varphi + z\Phi\,, \tag{1.36}$$

where

$$z = a\frac{\varphi_0'}{\mathcal{H}}\,. \tag{1.37}$$

It is indeed remarkable that one can reduce cosmological perturbations from inflation to just one scalar d.o.f. plus gravitational waves. Furthermore, the Mukhanov-Sasaki variable

v is of uttermost importance to understand the quantum origin of these perturbations. It is a dynamical variable whose action is

$$\mathcal{S}_v = \frac{1}{2}\int d\eta d^3x \left((v')^2 - \delta^{ij}\partial_i v \partial_j v + \frac{z''}{z}v^2 \right) . \tag{1.38}$$

This is the action of a scalar field in flat spacetime with time-dependent mass $m_{\text{eff}} = -z''/z$. One can obtain the equation of motion of the field right away, but it is more instructive to introduce first the Fourier modes

$$v_{\vec{k}}(\eta) = \int d^3x e^{i\vec{k}\cdot\vec{x}} v(\eta, \vec{x}) . \tag{1.39}$$

The equation of motion for each mode reads

$$v''_{\vec{k}} + \left(k^2 - \frac{z''}{z}\right) = 0 . \tag{1.40}$$

This equation has two quite distinct regimes:

- Sub-horizon regime, i.e., $k^2 \gg z''/z$ or $k^2 \gg (aH)^{-2}$. These are modes whose wavelength is much smaller than the Hubble scale and, thus, are not significantly affected by the spacetime geometry. They behave as a collection of harmonic oscillators, i.e., plane waves.
- Super-horizon regime, i.e., $k^2 \ll z''/z$ or $k^2 \ll (aH)^{-2}$. These are modes whose wavelength is much larger than the Hubble scale and, thus, are significantly affected by the spacetime geometry. In fact, they are sourced by it. Solutions are not interpreted as plane waves. Instead, each Fourier mode contains a growing and a decaying mode. The growing mode is responsible for perturbations of cosmological relevance, but the decaying mode is still related to their quantum nature.

1.5 Quantum fields in curved spacetime

Quantum fields are the theoretical fundament of particle physics. According to the mathematical framework of QFT, every elementary particle known in the SM is understood as the excitation of an underlying field [51, 52]. A quantum field is an operator function of spacetime points and usual particle physics is defined on Minkowski spacetime, where gravity is absent. It is possible, as mentioned earlier, to quantize gravity as an EFT on top of Minkowski spacetime, so that the quantized gravitational field is actually the difference $h_{\mu\nu} = g_{\mu\nu} - \eta_{\mu\nu}$. Again, quantum gravitational effects are not expected at energy scales below the Planck scale. This does not mean, however, that gravity does not have an effect on other quantum fields. In fact, by virtue of the equivalence principle, gravity couples to any quantum field. QFT in curved spacetime addresses the quantization of a field in geometric backgrounds different of Minkowski spacetime, i.e., in presence of gravity [53].

In Minkowski spacetime, quantum states associated to elementary particles can be understood as irreducible representations of the Lorentz group. In this case the vacuum state, the absence of particles, can be safely defined as the quantum state invariant under Lorentz transformations or, in other words, equal to all the inertial observers of SR [13,51]. Particle states, excitations of the vacuum states, have an (inertial) observer-independent particle number, even if energy and momentum are observer-dependent. As we will see, this is no longer the case for an arbitrary gravitational background.

Let us consider a scalar field $v(t,\vec{x})$, which can be the Mukhanov-Sasaki variable described previously. Its classical dynamics is described in terms of an equation of motion that can be obtained by varying the action. In order to perform its canonical quantization, which we will describe shortly, we need to derive its Hamiltonian dynamics. It is convenient to modify the scalar field action by adding the total derivative [6]

$$\Delta\mathcal{S}_v = -\left(\frac{z'}{z}v^2\right)' , \tag{1.41}$$

which does not alter its dynamics. Then the canonically conjugated momentum and the Hamiltonian are defined as

$$p(t,\vec{x}) \equiv \frac{\partial\mathcal{L}}{\partial v'} = v' - \frac{z'}{z}v \quad \text{and} \quad \mathcal{H} = pv' - \mathcal{L}\,. \tag{1.42}$$

Canonical quantization is then performed by promoting v and p to quantum operators and imposing the canonical quantization relation

$$[v(\eta,\vec{x}), p(\eta,\vec{y})] = i\delta^{(3)}(\vec{x}-\vec{y})\,, \tag{1.43}$$

so that creation and annihilation operators, $\hat{a}_{\vec{k}}$ and $\hat{a}^{\dagger}_{\vec{k}}$, can be built from suitable linear combinations of the Fourier transforms of v and p. Equivalently, one can perform the operator mode expansion

$$\hat{v}(\eta,\vec{x}) = \int\!\!\!\int\!\!\!\!\int \frac{d^3k}{(2\pi)^{3/2}}\frac{1}{\sqrt{2}}\left(e^{i\vec{k}\cdot\vec{x}}v_k^*(\eta)\hat{a}_{\vec{k}} + e^{-i\vec{k}\cdot\vec{x}}v_k(\eta)\hat{a}^{\dagger}_{\vec{k}}\right) , \tag{1.44}$$

where the mode functions $v_k(\eta)$ satisfy the equations of motion. A quantum field can be then seen as an infinite collection of harmonic oscillators, one for each Fourier mode. For

[6]See ref. [54] for a discussion on how both actions are equivalent not only at the classical level, but also at the quantum one.

a given operator mode expansion, the vacuum state is defined implicitly as the eigenstate of all annihilation operators with eigenvalue 0

$$a_{\vec{k}} |0\rangle = 0 \quad \forall \vec{k} \in \mathbb{R}^3 \,, \tag{1.45}$$

while $(n, m...)$-particle states are defined as

$$\left| n_{\vec{k}_1}, m_{\vec{k}_2} ... \right\rangle = \frac{1}{\sqrt{n!m!...}} \left[\left(a^\dagger_{\vec{k}_1} \right)^n \left(a^\dagger_{\vec{k}_2} \right)^m ... \right] |0\rangle \,. \tag{1.46}$$

In principle, infinitely many choices of mode functions $v_{\vec{k}}(\eta)$ can be done, corresponding to the infinite choice of basis of two-dimensional set of solutions of the equation of motion [53]. Then, in order for the quantum field to be correctly reproduced regardless of this choice, the nature of the creation and annihilation operators must depend on it. Hence, the very definition of the vacuum and particle states depends on the choice of mode functions. Different choices of mode functions v_k and u_k are related by Bogolyubov transformations

$$v_k^*(\eta) = \alpha_k u_k^*(\eta) + \beta_k u_k(\eta), \quad |\alpha_k|^2 + |\beta_k|^2 = 1 \,. \tag{1.47}$$

Annihilation operators $\hat{a}_k$ and $\hat{b}_k$ are related similarly by

$$\hat{b}_{\vec{k}} = \alpha_k \hat{a}_{\vec{k}} + \beta_k^* a^\dagger_{-\vec{k}} \,. \tag{1.48}$$

As mentioned above, this arbitrariness is settled in Minkowski spacetime by demanding the vacuum state to be invariant under Lorentz transformations. This means also that the expected value of the Hamilton operator takes its minimum value for the vacuum state at all times. In an arbitrary spacetime, Lorentz transformations are only valid locally but not globally, and such a preferred choice is not available.

During inflation, the universe undergoes an exponential expansion, which can be approximated by a de Sitter-like expansion. In that case, the scale factor is

$$a = -\frac{1}{H\eta} \,, \quad \eta = -\frac{1}{H} e^{-Ht} \tag{1.49}$$

where $\eta \in (-\infty, 0^-)$ for de Sitter spacetime, although, in practice, it ranges until the end of inflation at $\eta = \eta_* < 0$.

Intuitively, one would expect short-distance to be unaffected by the expansion of the universe or, in other words, the recession of relatively distant objects. This statement is supported by the equivalence principle. This motivates the Bunch-Davies prescription for the vacuum state of de Sitter spacetime, which states that the mode functions of the vacuum reduce to those of Minkowski spacetime in the sub-horizon limit or, equivalently, in the infinite past [55]. For a quasi-de Sitter expansion these mode functions are [13]

$$v_k(\eta) = \sqrt{\frac{\pi|\eta|}{2}} H_n^{(2)}(k|\eta|) \,. \tag{1.50}$$

where $H_n^{(2)}$ is a Hankel function of second kind. For quasi - de Sitter expansion one has $n = 3/2$, but in general it depends on the dynamics of the inflaton field. For instance, for an inflaton potential $V(\phi) = m^2\phi^2/2$ one has $n = \sqrt{9/4 - m^2/H^2}$.

The Bunch-Davies vacuum has 0 particles only in the limit where it matches the Minkowski vacuum. This can be checked by inspecting the Hamiltonian in Fourier space

$$\hat{H} = \int d^3k \left[\frac{k}{2} \left(\hat{a}_{\vec{k}} \hat{a}^{\dagger}_{\vec{k}} \right) - \frac{i}{2} \frac{z'}{z} \left(\hat{a}_{\vec{k}} \hat{a}_{-\vec{k}} - \hat{a}_{-\vec{k}} \hat{a}_{\vec{k}} \right) \right] \tag{1.51}$$

and performing the time-evolution in the Schrödinger picture[7] of the Bunch-Davies vacuum

$$\Omega(\eta') = e^{i\hat{H}(\eta'-\eta)} \left|\Omega(\eta)\right\rangle \tag{1.52}$$

where the time evolution operator is actually a squeezing operator. The resulting 2-mode squeezed state is a high-occupation number quantum state that entangles particles with momenta $\vec{k}$ and $-\vec{k}$. The physical picture here is that, as time evolution proceeds during inflation, particle pair production takes place. This is sourced by the gravitational field, which acts as a classical source for the quantum field.

The 2-mode squeezed state can be parametrized as [56–58]

$$\Omega(\eta') = \frac{1}{\cosh^2 \tau_k} \sum_{n=0}^{\infty} e^{2in\varphi_k} (-1)^n \tanh^n \tau_k \;\; n_{\vec{k}}, n_{-\vec{k}} \Big\rangle, \tag{1.53}$$

where τ_k and φ_k are, respectively, the squeezing parameter and phase. They satisfy suitable coupled differential equations, which can be solved analytically for quasi - de Sitter

$$\tau_k(\eta) = -\mathrm{arcsinh}\left(\frac{1}{2k\eta}\right), \quad \varphi_k = \frac{\pi}{4} - \frac{1}{2}\arctan\left(\frac{1}{2k\eta}\right). \tag{1.54}$$

The squeezing formalism is rather useful for characterizing the properties of the quantum state. It can be applied to other models of single-field inflation. Furthermore, it can be used to compute physical quantities such as the particle number per mode

$$n_k = \sinh^2 \tau_k = \left(\frac{1}{2k\eta}\right)^2, \tag{1.55}$$

where the second equality holds for quasi - de Sitter inflation only. Cosmological observables are usually obtained as correlation functions of the Mukhanov-Sasaki variable or quantities

[7] One can, alternatively, perform the time-evolution of the creation and annihilation operators in the Heisenberg picture, which leads to a time-dependent Bogolyubov transformation.

derived from it. Hence, it is useful to compute the 2-point correlation functions in the squeezing formalism [59, 60]

$$\begin{aligned}\langle v(\eta,\vec{x})v(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})} \frac{1}{2k} \left(2\sinh^2 r_k + 1 - \sinh 2r_k \cos 2\varphi_k\right) \\ \langle p(\eta,\vec{x})p(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})} \frac{k}{2} \left(2\sinh^2 r_k + 1 + \sinh 2r_k \cos 2\varphi_k\right) \\ \langle v(\eta,\vec{x})p(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})} \frac{i}{2} \left(1 - i\sinh 2\tau_k \sin 2\varphi_k\right) .\end{aligned} \tag{1.56}$$

Plugging eq. 1.55 into eq. 1.56, one can check that scalar perturbations have a scale-invariant spectrum, as required by cosmological observations. It is in this way that inflation combines quantum field theory and gravity in order to provide a simple but deep origin to the structure of the universe.

1.6 Quantum perturbations after inflation

We can conclude from the discussion in the two previous sections that there exist a single scalar gauge-invariant quantity in cosmological perturbation theory, the Mukhanov-Sasaki variable v. This quantity carries information from the Bardeen potential and the gauge invariant perturbations of the inflaton in a single variable. Another relevant gauge-invariant scalar quantity is the gauge-invariant curvature perturbation [60]

$$\zeta(\vec{x},\eta) = \frac{v(\eta,\vec{x})}{z}, \quad \zeta'(\vec{x},\eta) = \frac{p(\eta,\vec{x})}{z}. \tag{1.57}$$

The direct quantization of this magnitude is more complicated than that of the Mukhanov-Sasaki variable, which has a simple action. Still, it is perhaps of greater physical meaning.

At the end of inflation, the inflaton field decays into ultra-relativistc particles in a process called reheating [61, 62]. This cosmic era offers rich phenomenology, which we will, however, not explore here. It is sufficient for our purposes to asume instantaneous reheating, which means for cosmic history that the conformal time jumps $\eta_* \to -\eta_* > 0$, while $a(-\eta_*) = a(\eta_*)$. It is at this point (or, more generally, at the end of reheating), that the universe is filled with these ultra-relativistic particles and the radiation era starts. The universe continues expanding, albeit at a decelerating rate, so that the scale factor increases then as $a \sim \eta$. As the expansion proceeds, the universe cools down at a rate $T \sim a^{-1}$, while the energy density of radiation and dust scale, respectively, as $\rho_r \sim a^{-4}$ and $\rho_m \sim a^{-3}$ for most of the expansion history[8]. Hence, the matter density eventually overtakes the

[8]The scalings are true during the radiation era as long as the number of relativistic species is constant. As the universe cools down, this number decreases, which affects the temperature in a non-trivial way. For instance, when electrons and positrons become non-relativstic, at $T \simeq m_e$, they are annihilated into photons and increase the temperature of the plasma.

radiation density at the matter-radiation equality, which takes place at $\eta = \eta_{\text{eq}}$, and the matter era begins. Then the scale factor increases as $a \sim \eta^2$.

During inflation, perturbations are said to be stretched-out and exit the horizon when their wave-length becomes larger than the event horizon $d_H = 1/H$. This happens because the scale factor $a(t)$ grows faster than d_H, which, in fact, remains almost constant. During the radiation and matter eras, on the contrary, d_H grows faster than $a(t)$, which means that given wavelengths re-enter the horizon. Now, as long as they are in the super-horizon mode, curvature perturbations are said to freeze, i.e., to be unaffected by cosmic evolution until they cross the horizon again. This can be understood as follows: take the equation of motion for the Mukhanov-Sasaki equation in the super-horizon limit $k^2 \ll z''/z$. Then there is a solution $v \sim z$, which is called the growing mode, for which $\zeta \sim$ constant and so perturbations can be said to be frozen[9]. Likewise, there is a decaying mode, which is quickly suppressed and becomes irrelevant classically. The entanglement between the growing and the decaying mode is, however, relevant to some quantum features of cosmological perturbations.

Many relevant phenomena take place during these eras, in particular those related to cosmological perturbations: they leave their imprint in the CMB anisotropies and seed structure formation [13,39]. This is due to the coupling between the Bardeen potential and the matter content of the universe via the Einstein field equations. Current observations are in excellent agreement with the generic predictions of inflation and are compatible with many particular models [38]. They are, however, unable to resolve the quantum properties of the Mukhanov-Sasaki field. Detecting genuine quantum phenomena associated with cosmological observables would rule out classical origins of primordial perturbations, such as thermal excitations [63]. Furthermore, it would be a powerful statement on the validity of quantum mechanics and quantum field theory up to scales close to the Planck scale. We will deal with the distinctive features of quantum mechanics as a theory and how to quantify quantumness in the next chapter.

1.7 Primordial Black Holes

We finish this chapter by reviewing another potential observable consequence of cosmological perturbations. Sufficiently large curvature perturbations may cause matter to undergo gravitational collapse upon reentry and eventually form a black hole during the radiation era [64, 65]. To distinguish these black holes from astrophysical black holes, created by the gravitational collapse of a star in the late universe, they are named primordial black holes

[9]This argument does not hold as it is for a radiation dominated universe, for which $z'' = 0$. Instead, solutions of the equations of motion are plane waves regardless of the wave-length of the mode. However, initial conditions from inflation put all super-horizon modes in the growing part of the oscillation, and remain so as long as they are super-horizon, for an oscillation takes around $\sim k^{-1}$ in conformal time.

(PBH). Density contrasts of order $\delta\rho/\rho \sim \mathcal{O}(0.1)$ [66] or large non-Gaussianities induced by quantum diffusion [67] are required. Gravitational collapse takes place once the perturbation re-enters the horizon due to causality, and produces a black hole with mass of the order of the mass inside the Hubble radius, with negligible angular momentum. Thus, these black holes are well described with the Schwarzschild metric[10].

Although the first proposals go back to the 1970s [69, 70], PBHs have regained interest in the last year due to the black hole merger observations by the gravitational wave observatories LIGO and VIRGO [17, 71–73]. The origin of these black holes, with rather large masses, is advocated by many cosmologists to be of primordial origin, although the question is not settled yet. The Chandrasekhar limit sets a lower bound on the astrophysical black hole mass of about $M \simeq 1.4 M_\odot$. Hence, a detection of a black hole below a solar mass would be a definite signal of its primordial origin.

If they exist and are abundant, PBH could constitute a notable fraction of the dark matter of the universe. Indeed, they only interact gravitationally with ordinary matter and their equation of state is $p = 0$. This would allow to explain dark matter without invoking physics beyond GR and the SM. PBH have sustained an extensive search and many observational bounds have been set. Assuming a monochromatic mass distribution for PBH, they could only constitute all of dark matter if their mass is in the asteroid range, i.e., somewhat between $10^{-10} M_\odot$ and $10^{-15} M_\odot$, but the existence and size of these windows are updated often [74]. For more general mass functions and spatially clustered PBH, they could still constitute the whole of the dark matter.

These PBH would form during the radiation era. Hence, they require a sufficiently large perturbation, which can trigger gravitational collapse and, furthermore, overcome radiation pressure. Large curvature perturbations are scarce in single-field slow-roll inflation and, thus, require in principle enhancements of the power spectrum of the Mukhanov-Sasaki variable, linked to non-trivial inflationary dynamics. Another alternative is the non-perturbative enhancement of large fluctuations due to quantum diffusion, which is a generic feature of inflation.

A distinct feature of PBH formation is that the relevant scale is precisely the Hubble radius R_H at formation time. In a radiation-dominated universe the scale factor grows as $a \sim t^{1/2}$ and therefore the Hubble scale grows as $R_H = H^{-1} = 2t$. With this scaling at hand, we can extract the evolution of the energy density from the second Friedmann equation

$$H^2 = \frac{8\pi G}{3}\rho = \frac{1}{4t^2} \quad \text{and so} \quad \rho = \frac{3}{32\pi G t^2}\,. \tag{1.58}$$

[10] Despite fulfilling the criterion of having vanishing angular momentum, it must be noted that the Schwarzschild metric is a vacuum solution of the Einstein field equations. Its embedding into a cosmological solution is non-trivial and there is no consensus as to how this should be done and how it affects the dynamics of the event horizon of the black hole [68].

Then it is possible to compute the mass contained inside the Hubble scale as

$$M = \frac{4\pi}{3}\rho(2t)^3 = \frac{t}{G}\,. \tag{1.59}$$

The Schwarzschild radius of a black hole of this mass corresponds precisely to the Hubble radius

$$R_S = 2GM = 2t = R_H\,. \tag{1.60}$$

It is clear then that, up to a $\mathcal{O}(1)$ factor due to the efficiency of the gravitational collapse, the PBH will be of the size of the Hubble scale, i.e. $M_{\mathrm{PBH}} = \gamma M$ and so actually $R_S = \gamma R_H$. This can obtained from estimates [69, 70], but is also confirmed by numerical simulations [66, 75].

Should PBH exist due to primordial perturbations of quantum origin, it is natural to reflect on the quantum properties these PBH may have. In particular, there may exist quantum entanglement between them. Dealing with this intriguing possibility is one of the main goals of this thesis. Furthermore, quantum entanglement between black holes has been proposed to be equivalent to wormholes, i.e., geometric links between them [76]. This is the ER = EPR proposal[11].

[11] This proposal is named after two influential 1935 papers by Einstein and Rosen [77] and Einstein, Podolsky and Rosen [78]. The latter will be briefly discussed in chapter 2.

Chapter 2

Quantum Mechanics

Our revels now are ended. These our actors,
As I foretold you, were all spirits, and
Are melted into air, into thin air;
And, like the baseless fabric of this vision,
The cloud-capp'd towers, the gorgeous palaces,
The solemn temples, the great globe itself,
Yea, all which it inherit, shall dissolve,
And, like this insubstantial pageant faded,
Leave not a rack behind. We are such stuff
As dreams are made on; and our little life
Is rounded with a sleep.

Prospero in *The Tempest* (ca. 1610) by William Shakespeare.

2.1 The postulates of Quantum Mechanics

Physics as a science progresses in a continuous interplay between theory and experiment. Theoretical arguments, based on well-rooted principles and logical arguments, have led to powerful predictions later confirmed by experiment. An example of this are gravitational waves (GW), propagating excitations of the gravitational field. They were predicted in 1916 by Albert Einstein as a logical consequence of GR [15, 16], but not directly detected until 2015 [17]. GW constitute now one of the most active fields of research, both at the fundamental level and for their role as astronomical messengers. On the other hand, experimental results lacking a satisfactory theoretical explanation have historically fostered theoretical breakthroughs. This has meant, sometimes, abandoning deep physical principles. A paradigmatic example of this is the birth of quantum mechanics (QM), motivated by the puzzling experimental results such as the black-body radiation [79] or the photoelectric effect [80].

QM is considered to be one of the two revolutions of the 20th century in physics, the other being relativity. SR meant rejecting the notion of absolute space and time of Newtonian mechanics, and redefining them in a way consistent with the postulates of relativity [9]. Likewise, GR led to the reformulation of a basic element of physics: the inertial observer [11]. In sum, relativity destroyed the very concept of an absolute observer.

The postulates of QM have a profound impact on the description of Nature and its observation. Let us briefly go over the its postulates to see this [81, 82]

- An isolated physical system is described by a unit *state vector* $|\psi\rangle$ belonging to a Hilbert space.

- The time-evolution of an isolated physical system is unitary and described by the Schrödinger equation [83]

$$i\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle \tag{2.1}$$

- Quantum measurements are described by a collection $\{M_n\}$ of *measurement operators*, so that the probability of obtaining the measure outcome m is

$$p(m) = \left\langle \psi \;\; M_m^\dagger M_m \;\; \psi \right\rangle \Big(\tag{2.2}$$

  and the state vector subsequently becomes

$$|\psi\rangle \to \frac{M_m|\psi\rangle}{\sqrt{\left\langle \psi \Big(\;\; M_m^\dagger M_m \;\; \psi \right\rangle \Big(}}. \tag{2.3}$$

Hence, by its very postulates, QM makes a clear distinction between isolated time evolution and measurements, which constitute an interaction and a departure from unitary evolution. According to the mainstream Copenhagen interpretation [84, 85], the wave function described by $|\psi\rangle$ is said to *collapse* as a consequence of this interaction. It must be noted, however, that the postulates assume that the measurement is performed by a classical observer, which is not a quantum system. How the collapse of the wave function occurs (or whether it happens at all) is still a matter of debate in the field of foundations of QM and the heart of the so called measurement problem [85].

The postulates can be generalized to open quantum systems, i.e., those that constitute a subsystem of a larger quantum system. In that case, the postulates are reformulated as

- An isolated physical system is described by a positive *density matrix*[1] $\hat{\rho}$ which acts on a Hilbert space and satisfies $\mathrm{Tr}\rho = 1$.

- The Time-evolution of an isolated physical system is unitary and described by the Schrödinger equation.

$$i\frac{d}{dt}\hat{\rho} = \left[\hat{H}, \hat{\rho}\right] \tag{2.4}$$

- Quantum measurements are described by a collection $\{M_n\}$ of *measurement operators*, so that the probability of obtaining the measure outcome m is

$$p(m) = \mathrm{Tr}\left(M_m^\dagger M_m \rho\right) \tag{2.5}$$

  and the state subsequently becomes

$$\rho \to \frac{M_m \rho M_m^\dagger}{\mathrm{Tr}\left(M_m \rho M_m^\dagger\right)}\,. \tag{2.6}$$

The density matrix formulation reduces to the state vector one when there exists a state vector such that $\hat{\rho} = |\psi\rangle\langle\psi|$. Otherwise, the density matrix is said to describe an ensemble of vector states $|\psi_i\rangle$ with probability p_i, so that

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|\,. \tag{2.7}$$

for a suitable basis choice. For an arbitrary basis, however, $\hat{\rho}$ need not be diagonal.

2.2 Locality and realism

Once we have set up the basics of QM, we are ready to understand some of its implications for our understanding of fundamental physics. As mentioned earlier, relativity meant giving up the notion of absolute space and time and, furthermore, the redefinition of what inertial observers are. Classical physics, in the sense of non-quantum physics, regardless of whether relativistic or not, lies on the principle of *local realism*:

- Locality. Physical interactions take place locally, i.e., only occur between nearby physical systems. Furthermore, interactions mediated by a third system cannot travel faster than the speed of light.

[1] A more appropriate name would perhaps be density operator, as the state space may be infinite dimensional. However, we will follow the historical and usual convention and call it density matrix.

- Realism. Physical magnitudes have well-defined values at all times, prior and irrespective of measurements.

In QM, the knowledge of a physical quantity precludes the knowledge of of another one if their corresponding operators are non-commuting. This would not be the case if they were linked to physical properties which are intrinsic and independent from measurement. Thus, QM is not a local realist theory. However, this does not mean *a priori* that QM cannot be reformulated as a local realist theory, which contains *hidden* variables to be discovered or understood.

Local realism is not, however, a mere matter of interpretation of a physical theory, but rather has precise phenomenological predictions. They can be tested. John Bell showed in 1964 that local realism sets an upper bound on the correlations shared by the constituents of a bi-partite system [86]. This system can be, for instance, made of two subsystems A and B, each of which is a spin-1/2 particle. According to the Stern-Gerlach experiment, measurements of spin in a given direction $\hat{S}_{\vec{a}}$ always return a result aligned or anti-aligned with it. We consider four measurement directions $\vec{a}$, $\vec{a}'$, $\vec{b}$, $\vec{b}'$. Upon repeated measurements, one can reconstruct the correlation function

$$E(\vec{a},\vec{b}) = \left\langle \hat{\mathcal{S}}_{\vec{a}}\hat{\mathcal{S}}_{\vec{b}} \right\rangle . \tag{2.8}$$

Then it can be shown that, under the assumption of locality and realism, the following inequality is satisfied

$$B = E(\vec{a},\vec{b}) + E(\vec{a},\vec{b}') + E(\vec{a}',\vec{b}) - E(\vec{a}',\vec{b}') \leq 2\,. \tag{2.9}$$

This is the Bell inequality in the Clauser-Horne-Shimony-Holt (CHSH) form [87]. As a matter of fact, there exist quantum states which violate it. Consider, for instance, the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) . \tag{2.10}$$

This is one of the so-called Bell states. If the spin is measured in the z-axis for both subsystems, the outcome of one automatically predicts the outcome of the other one. Such a state is said to be maximally entangled. Upon a suitable choice of axes, this state clearly violates the Bell inequality

$$B = 2\sqrt{2}\,. \tag{2.11}$$

This value actually saturates the Tsirelson bound, which is the maximal value attainable by B without further assumption. Hence, it can be concluded that QM is not a local realist theory. Experimental results clearly confirm this prediction [88].

The breakdown of local realism due to quantum entanglement is a profound statement. Einstein, Podolsky and Rosen (EPR) were the first to point out the contradiction between entanglement and local realism, which they used to argue against QM being a complete description of reality [78], a viewed not shared by Bohr [89]. We now understand that this is not the case. QM is a valid physical theory and it cannot be replaced by a more complete local realist physical theory[2].

The key message to convey here is that QM allows for correlations that cannot be explained within a classical theory (again, in the sense of a local realist theory). We saw in chapter 1 that, according to the inflationary paradigm, cosmological perturbations are of quantum-mechanical origin. Therefore, one may in principle be able to detect genuinely[3] quantum features in cosmological observables. In later chapters we deal with this idea and study quantum properties of the Mukhanov-Sasaki field, including Bell inequalities.

2.3 Measures of entanglement and information

Entanglement is probably the most distinctive feature of QM. It is behind phenomena considered to be counter-intuitive and the reason behind enhanced correlations that can lead to the violation of Bell inequalities. Even if its role is qualitatively clear and so is its mathematical form in certain quantum states, it is not trivial to quantify it in general. Here, we review some relevant quantities[4]. In doing so we will characterize a quantum state by its density matrix ρ.

First, let us define the *purity* of a quantum state as

$$\mathfrak{p} = \mathrm{Tr}\rho^2 \leq 1\,. \tag{2.12}$$

If the inequality is saturated, the state is said to be *pure*. Such a state can be written as a vector state as $\hat{\rho} = |\psi\rangle\langle\psi|$. Otherwise, the state is said to be *mixed*. Another way of quantifying this is by its von Neumann entropy [91]

$$S = -\mathrm{Tr}\left(\hat{\rho}\log\hat{\rho}\right)\,. \tag{2.13}$$

A pure quantum state has $S = 0$, while a mixed quantum state has $S \neq 0$. Later we shall introduce other measures of entropy and distinguish them by labelling the von Neumann entropy as S_N.

Quantum states describe a physical system which may be composed of many degrees of freedom. Let us now asume that it can be split into complementary subsystems A and B.

[2]QM is still a falsifiable scientific theory. One may eventually find experimental results that contradict it and require its replacement by another or more complete physical theory. Such theory would still be inconsistent with local realism.

[3]In spirit of the Bell inequalities, by genuine we mean non-reproducible by classical systems. Nevertheless, systems with correlations consistent with classicality or local realism may still be well accommodated within QM.

[4]See refs. [81, 90] for a more general discussion.

The quantum state $\hat{\rho}_A$ describing subsystem A can be obtained by tracing over the degrees of freedom of B, i.e., $\hat{\rho}_A = \mathrm{Tr}_B \hat{\rho}$. The state $\hat{\rho}_B$ is likewise defined. The von Neumann entropy of a subsystem is given by

$$S_A = -\mathrm{Tr}\left(\hat{\rho}_A \log \hat{\rho}_A\right) . \tag{2.14}$$

If ρ is pure, then $S_A = S_B$ and is called the *entanglement entropy*. This quantity is a good measure of the quantum entanglement between the A and B.

In general, a mixed state can be purified by embedding its state space into a larger state space, so that the state is entangled with the complementary subspace [92]. Hence, ensembles of states can be understood as quantum subsystems.

We are ready now to see the first link between entanglement and information. If the basis is chosen so that $\hat{\rho}$ is diagonal, then the von Neumann entropy has the form of the Shannon information entropy as defined for a probability distribution [93]. Hence, an increase in entanglement between subsystems leads to a decrease in the information each of them carry. Recall the example of a maximally entangled Bell state. Before measurement, the state of each subsystem can be either $|\downarrow\rangle$ or $|\uparrow\rangle$ with probability $1/2$ and so provides no information. After measurement of one subsystem, however, the outcome of a measurement on the complementary is fully determined. Both subsystems clearly share information.

The information thus shared by two subsystems is characterized by their *mutual information*, defined as the difference

$$\mathcal{I}(A, B) = S_A + S_B - S_{A\cup B} . \tag{2.15}$$

This quantity is non-negative, symmetric and extensible to multi-partite systems, where A and B need not be complementary. Mutual information is a quantification of total correlations between two subsystems: both classical and genuinely quantum. However, one would aim at achieving a measure of quantum correlations only. Mutual information as defined in eq. (2.15) is a quantum-mechanical extension of an equivalent definition in probability theory, in which S_i label the Shannon information entropy associated with random variables and their probability distributions. Nevertheless, this extension is not unique. Another one is provided by the expression

$$\mathcal{J}(A, B) = S_A - S_{A|B} , \tag{2.16}$$

where $A|B$ refers to subsystem A conditioned on a measurement on subsystem B.

When applied to probability distributions, the functions introduced in eqs. (2.15) and (2.16) are equal. However, they differ when applied to quantum states. First, the measurement on B needs to be specified with a complete set of measurements $\{M_n\}$. Second, due to the entanglement between A and B, measurements on B have an effect on A that may be larger than what one may expect when dealing with probability distributions. In practice, ρ_A collapses according to eq. (2.6). In other words, quantum measurement destroys correlations that were present due to quantum entanglement.

This departure due to the particular nature of quantum measurement allows one to quantify genuine quantum correlations by means of the *quantum discord* [94, 95]

$$\mathcal{D}(A, B) = \min_{\{M_n\}} \left[\mathcal{I}(A, B) - \mathcal{J}(A, B)\right] , \tag{2.17}$$

where the minimum is taken over any possible complete set of measurements $\{M_n\}$. Note that, unlike mutual information, quantum discord is not symmetric. Furthermore, it vanishes if and only if there exist a quantum measurement on B that does not disturb the state of A, confirming the key role played by quantum measurement.

Quantum discord is a widespread proposal to quantify quantum entanglement. However, its validity is unsettled. If the system $A \cup B$ is in a pure state, then discord $\mathcal{D}$ trivially equal to mutual information $\mathcal{I}$ and to twice the entanglement entropy S. In this case, discord is a clear measurement of entanglement, but is not more useful than S or $\mathcal{I}$ in that respect. This happens because all correlations between A and B are genuinely quantum due to the purity of the whole state. The power of discord would come when $A \cup B$ is a in a mixed state. In that case, correlations between A and B can also be classical, and one needs a way to tell classical and quantum correlations apart. As we will later argue in the context of QFT and cosmology, see chapter 5, quantum discord does not seem to be a good proxy of Bell inequality violations, at least when the quantum state is highly mixed.

For completeness, let us comment that there exist other measures of quantum entanglement. Some of them are similar to quantum discord, but based on the distance between the quantum states rather than on measurement [90]. Others follow different approaches.

As mentioned earlier, the quantification of entanglement is interesting to us in order to probe the quantum origin of cosmological perturbations. Still, there are many other reasons why the broader scientific community is interested in the quantification of entanglement. Perhaps most crucially, 2-level quantum systems can be used to store quantum bits of information (qubits), which are the basis of quantum computation [81]. Logical gates are then applied by means of unitary operators in order to build quantum circuits, which end with certain measurements that deliver the result of the computation. Quantum computing has a promising future: it is known that quantum algorithms beat classical ones in certain problems, such as the factorization of prime numbers or search algorithms.

Entanglement is a main resource in quantum computing, as it allows speed-ups due to simultaneous computation. A wave function can store a number of parameters that is exponential in the number of qubits, while quantum gates operate simultaneously on them. Their extraction by quantum measurement is, however, highly non-trivial. Furthermore, entanglement may not be the only valuable quantum resource, as there seems to be non-trivial quantum correlations even in absence of entanglement and discord [96].

2.4 Entanglement in QFT

We have seen how QM allows for the possibility of correlations between physical subsystems that exceed those permitted by the requirements of locality and realism. It is natural to ask ourselves if quantum entanglement is present in the fundamental interactions. Indeed, in the framework of QFT, elementary particles or even the vacuum are full-fledged quantum states.

It is hard, in general, to exactly characterize the state of a quantum field. This task is simpler when the state is Gaussian. Let $|\phi\rangle$ be the eigenvector of the quantum field operator $\hat{\phi}$ with eigenvalue ϕ. In this basis, the components of an arbitrary Gaussian density matrix are given by [97]

$$\begin{aligned}\rho(\phi^+,\phi^-) = \exp\Big\{ & -\frac{1}{2}\phi_+^\dagger h\phi_+ - \frac{1}{2}\phi_-^\dagger h^\dagger \phi_- + \frac{i}{2}\left(\phi_+^\dagger - \phi_-^\dagger\right)\lambda \\ & + \frac{i}{2}\lambda^\dagger\left(\phi_+ - \phi_-\right) + \frac{1}{2}\left(\phi_+^\dagger + \phi_-^\dagger\right)\kappa + \frac{1}{2}\kappa^\dagger\left(\phi_+ + \phi_-\right)\Big\}\end{aligned} \tag{2.18}$$

where the operators h, λ and κ depend on the spatial coordinates and products are understood to be performed in the operator sense as

$$\phi_+^\dagger h\phi_+^\dagger = \iint d^3x\, d^3y\, \phi_+^\dagger(\vec{x})h(\vec{x},\vec{y})\phi_+(\vec{y}) \tag{2.19}$$

and so on.

A similar expression can be obtained for Gaussian mixed states by integrating over the state ensemble, appropriately weighted by a Gaussian probability distribution. Likewise, reduced density matrices can be obtained by integrating over some d.o.f. or, equivalently, by projecting the fields onto the subspace of choice. Given these expressions, one is ready to compute the von Neumann entropy of an arbitrary Gaussian state. Furthermore, the resulting formula can be expressed in terms of the 1- and 2-point correlation function of the Gaussian field, see refs. [97–99]

An essential example of Gaussian states are thermal states, which describe the state of a field within a fluid at finite temperature T. Such states describe, for instance, Hawking [100] or Unruh [101] radiation. However, not all relevant quantum states are Gaussian. Primordial non-Gaussianities are relevant in Cosmology [67, 102], but we will not include them in our analysis.

The first computation of entanglement entropy in QFT was performed by Bombelli et al [103] by characterizing the vacuum state similarly to the way outlined above. They showed that entanglement entropy in vacuum of a scalar field in a spherical region is formally divergent. If a UV-regulator ϵ is introduced, the entropy scales as the area

$$S \sim \frac{A}{\epsilon^2}\,. \tag{2.20}$$

This result was also found independently by Srednicki [104]. This is a crucial result for at least two reasons. First, it shows that the entanglement entropy of a quantum field is extensive, but not with the number of d.o.f. If that were the case, the entropy would scale as the volume of the sphere, not as its surface. This can be understood by viewing entanglement as a UV-phenomenon, i.e., the dominant contribution to the entanglement entropy of a quantum field comes from the entanglement of neighbor d.o.f. across the boundary of the sphere. Second, it has a potentially deep connection with black hole physics. Indeed, the Bekenstein entropy of a black hole scales as its area [105], not its volume, and is regulated by the Planck scale. Hence, it has been proposed that black hole entropy may be due to quantum entanglement [103]. This idea has led to numerous works connecting gravity with quantum entanglement [76, 106–109].

It must be noted, however, that there also exist proposals to explain black hole entropy as regular micro-state entropy and not entanglement entropy, for instance in ref. [110].

Other quantum-information properties of the vacuum state of a scalar field in Minkowski space-time have been computed. For instance, it was shown by Shiba in [111, 112] that the mutual information between two spheres of radii R_1 and R_2 is given at first order in perturbation theory by

$$\mathcal{I} \simeq \frac{1}{4}\frac{R_1^2 R_2^2}{r^4}\,. \tag{2.21}$$

We will apply the same method in sec. 4 to compute the mutual information of cosmological perturbations. Two comments are in order regarding this finding. First, unlike entanglement entropy, mutual information is UV-finite. This suggests that the local entanglement is no longer the one involved. This makes sense, since the spheres are actually far apart. Second, the quantity is rapidly decreasing with distance. This is consistent with the picture obtained from entanglement entropy. If the entanglement between far apart d.o.f. is much smaller than that of nearby d.o.f. and the former dominates the expression for the mutual information, then this will be comparatively small.

2.5 Phase space formulation

Bell inequality violations make clear the departure of QM from classical physics. This was perhaps expected from the very construction of the theory in terms of the postulates. Indeed, classical and quantum physics look formally very distinct, and so do the mathematical objects associated with them. Physical states in classical Hamiltonian mechanics are points in phase space $(\vec{x}, \vec{p})$, while quantum states are represented either by state vectors or density matrices. A first link between them can be seen in canonical quantization, a procedure already seen in sec. 1.5, which promotes phase space variables to quantum operators $\vec{x} \to \hat{\vec{x}}$ and $\vec{p} \to \hat{\vec{p}}$ and imposes the commutation relation

$$\left[\hat{x}^i, \hat{p}^j\right] = i\delta^{ij}\,, \quad \left[\hat{x}^i, \hat{x}^j\right] = 0\,, \quad \left[\hat{p}^i, \hat{p}^j\right] = 0\,, \tag{2.22}$$

which replaces the Poisson bracket relation of Hamiltonian dynamics. If the phase space variables are fields, then the Kronecker delta is replaced by a Dirac delta.

This link can be deepened by switching from the operator formulation to the phase space formulation of QM[5]. It is a completely equivalent mathematical formalism that makes no use of the Hilbert space structure. Instead, phase-space variables are assigned quasi-probabilistic distributions. We will briefly discuss how the phase space formulation can be derived from the operator formulation, but it must be noted that the former may be postulated independently from the latter.

First, let us introduce the *Wigner function* as

$$W_{\hat{\rho}}(\vec{q},\vec{p}) = \int_{\mathbb{R}} \frac{d^n z}{(2\pi)^n} e^{-i\vec{p}\cdot\vec{z}} \left\langle \vec{q} + \frac{1}{2}\vec{z} \right| \hat{\rho} \left| \vec{q} - \frac{1}{2}\vec{z} \right\rangle , \tag{2.23}$$

where $|\vec{q}\rangle$ is a simultaneous eigenvector of the operators $\{\hat{x}^i\}$ with eigenvalues $\{q^i\}$[6].This is a real scalar function in phase space that fully characterizes the quantum state of the physical system. Note that there is a one-to-one correspondence between a density matrix and its Wigner function. Other quantum operators are similarly mapped to real scalar functions in phase space by replacing $\hat{\rho}$ with the operator $\hat{O}$ in eq. (2.23). This map is invertible and generically referred to as *Wigner-Weyl transform*. Expected values of observables in a given state are then computed as integrals over phase space

$$\langle O|O\rangle_{\rho} = \mathrm{Tr}\left(\hat{\rho}\hat{O}\right) = (2\pi)^n \int d^n q d^n p W_{\hat{\rho}}(q,p) W_{\hat{O}}(q,p) \,. \tag{2.24}$$

At this point, one is tempted to make an analogy between probability theory and QM, interpreting $W_{\hat{\rho}}(q,p)$ as a probability distribution and $W_{\hat{O}}(q,p)$ as a random variable. This can be done at the expense of discarding one of the axioms of probability theory, since $W_{\hat{\rho}}(q,p)$ can take negative values. Therefore, it is called a *quasi-probability* distribution, which still satisfies

$$\int d^n q d^n p W_{\hat{\rho}}(q,p) = \mathrm{Tr}\left(\hat{\rho}\right) = 1 \,. \tag{2.25}$$

The possibility of the Wigner function taking negative values implies that expected values of physical observables might be inconsistent with classical mechanics. In fact, they can lead to Bell inequality violations. Even if the Wigner function is positive, as it is the case of the one associated to a Gaussian state, Bell inequalities can be violated if it is constructed with improper operators [117]. A *proper* operator admits a spectral decomposition as

$$\hat{O} = \int d^n q \, |\vec{q}\rangle \, O(\vec{q}) \, \langle \vec{q}| \; , \tag{2.26}$$

[5] See ref. [113] for a review and [114–116] for the original formulation.

[6] Note that commuting operators are simultaneously diagonalizable.

where $O(\vec{q})$ is a bounded function. It's Wigner-Weyl transformation is then

$$W_{\hat{O}}(\vec{q},\vec{p}) = O(\vec{q})\,, \tag{2.27}$$

which takes all and only the eigenvalues of $\hat{O}$. An operator not satisfying this condition is called *improper*.

The probabilistic nature of microscopic phenomena (and, at a deep fundamental level, all physical phenomena) is a key building block of QM. It is supported by experimental results such as the Stern-Gerlach experiment. As we have seen, this randomness is intrinsic, i.e., not due to experimental error or uncertainties in the initial conditions. Here there is a key discrepancy with classical mechanics: a point in phase space has a deterministic future evolution. Observables in QM, on the contrary, are always probabilistic, even if the evolution of the quantum state is deterministic.

Furthermore, it cannot be reproduced by usual probability theory. This sounds surprising at first, since one can have probabilistic outcomes if the classical state is not a point in phase space, but rather a probability distribution representing a statistical ensemble. Still, QM allows for Wigner functions which may take negative values and strongly deviate from the classical result. This can lead to Bell inequality violations (although it is not the only way [118]). In the usual operator formulation of QM, this discrepancy is due to states having complex amplitudes in general, which leads to well-known genuinely quantum phenomena such as interference. Probabilities are then computed as the square of the amplitudes.

2.6 Quantum Statistical Mechanics

Large quantum systems are hard to describe exactly, to the extent that they might be completely intractable at the microscopical level. Recall that the parameters describing a quantum state vector scale exponentially in the dimension of the Hilbert space. It is for this reason that, when dealing with a large system, microphysical details need to be coarse-grained and one must focus instead on its macrophysical properties. This is the task of statistical mechanics [119]. Emergent physical laws, such as the laws of thermodynamics, ultimately have a microphysical origin.

We will not attempt here a comprehensive review of statistical mechanics. Still, it is relevant to us to understand the role played by statistical mechanics in the definition of concepts like entropy or information, and its connection with quantum mechanics. Indeed, as we saw in sec. 2.3, entropy can be understood as an inverse measure of information, either in a probability distribution or in a quantum state. Mixed states, which have a non-vanishing von Neumann entropy, can be understood as an ensemble of pure states. Ensembles of states are precisely the subject of study in statistical mechanics. On the other hand, according to the laws of thermodynamics, entropy is a non-decreasing function of time and a macrophysical property of a large system.

Hence, statistical ensembles are described by means of a quantum density matrix. In equilibrium, i.e., when $\dot{\rho} = 0$, it can be built right away according to three set-ups: microcanonical (total energy and particle number are fixed), canonical (only total particle number is fixed) and grand-canonical (neither total energy nor particle number are fixed). In all those ensembles, the entropy can be computed by the von Neumann formula in eq. (2.13). It typically grows logarithmic in the size of the phase space consistent with the macrophysical variables, i.e., it grows linearly with the number of particles or the dimension of the Hilbert space. Thus, entropy quantifies the lack of information due to the coarse-grain over a region of phase space, which is described by emergent microphysical quantities.

Quantum Statistical Mechanics ultimately leads to the laws of thermodynamics. We provide them here in its axiomatic formulation first introduced by Stückelberg [120].

- First law. For every system Σ, there exists an extensive scalar state function E, called energy, which is conserved unless external forces are applied on it (work is done) or there is heat or matter transfer with the exterior.

$$\frac{dE}{dt} = P^W + P^H + P^M \tag{2.28}$$

- Second law. For every system Σ, there exists an extensive scalar state function S, called entropy, which is a non-decreasing function of time.

$$\frac{dS}{dt} \geq 0 \,. \tag{2.29}$$

  The equality is only saturated in equilibrium.

The laws of thermodynamics are useful when dealing with systems that satisfy the local equilibrium condition, even if strictly speaking are out of equilibrium. More precisely, when dealing with a fluid changes of entropy are given by

$$dS = \frac{1}{T}\left(dU + pdV\right) \,, \tag{2.30}$$

where U is the internal energy of the system, T is its temperature, p its pressure and V its volume. If the system is isolated, transitions between these quasi-equilibrium states can only take place with an increase in entropy, i.e., with a loss of information about the system.

It is not easy to reconcile the laws of thermodynamics, which allow for an increase in the entropy, with the fact that the von Neumann entropy S_N is invariant under unitary transformations and, thus, invariant under unitary evolution [81]. Let us briefly discuss solutions to this issue. First, due to interactions with an environment, a quantum system may undergo non-unitary evolution in a process called *decoherence* [121], which can certainly change S_N. Still, the total von Neumann entropy should remain constant. In thermodynamics, the von Neumann entropy is also called Gibbs entropy S_G and has a classical analog [119]. Again, the classical S_G does not grow as a consequence of the Liouville's theorem, which states that phase space distribution functions are conserved by classical Hamiltonian evolution [122].

It must be noted, however, that this entropy is microscopic and relies on the validity of the statistical ensembles mentioned above, which is lost out of equilibrium. In this situation, the entropy of a macrostate M is given by the Boltzmann entropy [119, 122]

$$S_B = k_B \log |\Gamma_M| \,, \tag{2.31}$$

where $|\Gamma_M|$ is the volume of phase space with microstates consistent with M. In local equilibrium, i.e., slowly varying conditons from one equilibrium state to another, $S_B = S_G$. Otherwise $S_B \geq S_G$. In other words, one may argue that microscopic time evolution is reversible, but the coarse-graining procedure is not. The precise implementation of a quantum analog for the S_B for a generic out-of-equilibrium situation (not assuming local equilibrium) is still a matter of debate [122]. The definitons of computationally useful concepts like entropy or statistical ensemble lead to deep discussions in the philosophy of physics. It is worth pointing out their relevance in achieving full consistency between unitary QM and the second law of thermodynamics, but we shall not discuss them further.

2.7 Black Hole Thermodynamics

We finish this chapter by reviewing a topic that beautifully intertwines gravity, QM and thermodynamics: the laws of black hole thermodynamics [14, 123]. It illustrates the importance of the confluence of these three disciplines and suggests the existence of a microscopic description of macroscopical gravitational systems in terms of a yet unknown theory of quantum gravity.

Roughly speaking, a black hole is a physical object whose gravitational pull is so strong that even light (or any other massless particle) can become trapped inside it [48]. This trapping region is enclosed in the *event horizon* of the black hole, which characterizes its size[7]. According to the no-hair theorem [124–126], a stationary black hole in GR can be

[7]The definition of the event horizon requires knowledge about the full future history of light-like geodesics, which may not be known unless the black hole is stationary. Sometimes it is convenient to use the notion of apparent horizon instead, which can be defined with information about the light-like geodescics at a given space-like hypersurface.

described by its mass M, its angular momentum J and its electric charge Q[8]. It is unlikely that a black hole would keep a non-negligible electric charge for a long time, as it would attract more matter with charge of the opposite sign, so we will focus here on black holes with $Q = 0$, i.e., Kerr black holes [128].

Still, we will first discuss briefly the case $Q = J = 0$, as it is of great relevance as well. Such an object is called a Schwarzschild black hole. Its metric, discovered by Karl Schwarzschild in 1916 [129], is actually the first solution to Einstein's field equations ever found. It describes generically a static and spherically symmetric space-time, and so many relevant physical problems such as celestial orbits or light deflection are studied with this metric. Furthermore, it predicts the existence of an event horizon at the so called Schwarzschild radius

$$r_S = \frac{2GM}{c^2}\,, \tag{2.32}$$

unless the metric is generated by a mass of larger size. Even if the Schwarzschild black hole is a limiting case, it is a fair description when angular momentum is sufficiently small. Furthermore, PBH, already discussed in sec. 1.7, are predicted to have negligible angular momentum and are correctly described by the Schwarzschild metric.

Coming back to Kerr black holes, it is useful to parametrize their deviation from a Schwarzschild black holes by introducing the parameter $a = J/Mc$. The event horizon of a Kerr black hole is then located at

$$r_{EH} = \frac{r_S + \sqrt{r_S^2 - 4a^2}}{2}\,. \tag{2.33}$$

Even if the Kerr solution is stationary, it is legitimate to ask oneself how do the parameters M and J change, for instance if the black hole grows by matter accretion. This time evolution from one member of the Kerr-family to another is governed by the laws of black hole thermodynamics [14, 48, 123]:

- Zeroth law. For every Kerr black hole, the surface gravity κ is constant and a function of M and J only. Its precise form is

$$\kappa = \frac{\sqrt{M^2 - a^2}}{2M\left(M + \sqrt{M^2 - a^2}\right)}\,. \tag{2.34}$$

- First law. The variation of the black hole mass after any physical process is a function of the variation of its event horizon area and its angular momentum.

$$dM = \frac{\kappa}{8\pi} dA + \Omega_H dJ\,, \tag{2.35}$$

[8]Electric charges are defined in GR in a way analogous to flat space-time. Mass and angular momentum are trickier. For an asymptotic space-time, however, one can make sense of a global mass and angular momentum associated with the space-time metric in terms of Komar integrals [127]. One speaks of this Komar mass and angular momentum as belonging to the black hole itself.

where $A = \pi r_S^2$ and Ω_H is the angular velocity of the horizon[9].

- Second law. The variation of the black hole area after any physical process is always non-negative [130]
$$dA \geq 0\,. \tag{2.36}$$

- Third law. No finite amount of physical processes can result in $\kappa = 0$ [131].

These laws were first constructed as the laws of black holes mechanics, but its similarity with the well-known laws of thermodynamics was soon realized. Of course, this similarity was not enough to claim the thermodynamical nature of black holes. It was first argued by Jacob Bekenstein in a thought experiment that the entropy of a black hole should scale as its area [105]. Even if he did not showed what the proportionality coefficient should be, we now understand the Bekenstein-Hawking entropy of a black hole to be

$$S_{BH} = k_B \frac{Ac^3}{4G\hbar}\,. \tag{2.37}$$

Later, Stephen Hawking found that a quantum field in Schwarzschild space-time is put in a thermal state [100], with temperature proportional to the surface gravity

$$T_H = \frac{\hbar\kappa}{2\pi c k_B}\,, \tag{2.38}$$

so that a black hole emits black-body radiation, the so called Hawking radiation, decreasing its mass and potentially leading to its evaporation. Note that this does not contradict the second law, as the latter is proven for classical GR and a stress-energy tensor satisfying certain conditions, which are violated by a quantum field.

We kept all physical constants to illustrate the underlying quantum nature of black hole thermodynamics. Indeed, black holes are macroscopical objects and, as such, can be understood to a great extent with classical physics alone. This can be seen from the fact that the product $T_H S_{BH}$ does not depend on the Planck constant $\hbar$. On the contrary, both T_H and S_{BH} do depend individually on $\hbar$. Hawking radiation and the micro-structure from which Bekenstein entropy emerges are quantum phenomena. As mentioned in sec. 2.3, it is still a matter of debate whether the area dependency of S_{BH} can be linked to quantum entanglement.

In any case, the thermodynamical nature of black holes will play an important role when embedding them as one of the components of non-equilibrium cosmology in chapter 6. Furthermore, it will serve as inspiration for the treatment of other horizons in chapter 7, such as the cosmic horizon.

[9] Ω_H is obtained as the polar component of the Killing vector field normal to the event horizon surface.

We finish this section with the remark that the formation of a PBH by the gravitational collapse of the radiation contained inside the Hubble scale is accompanied by an enormous increase in classical entropy, as one would expect from an out-of-equilibrium process that follows the laws of thermodynamics [1]. Indeed, the entropy of the gas of relativistic particles within the Hubble scale can be written as [13, 132]

$$S_{\text{gas}} = \frac{2\pi^2}{45} g_{*S}(T) T^3 V_H \,, \tag{2.39}$$

where V_H is the Hubble volume, $g_*(T)$ is the number of relativistic degrees of freedom and natural units including $k_B = 1$ were used, so that the entropy is a dimensionless quantity. On the other hand, the resulting PBH carries the Bekenstein-Hawking entropy, which is proportional to its event horizon area

$$S_{\text{PBH}} = \frac{A_H}{4A_P} = 4\pi\gamma^2 \frac{t^2}{t_P^2} \,, \tag{2.40}$$

where $A_P = 4\pi L_P^2$ is the Planck area, L_P is the Planck length and t_P is the Planck time. Since the Hubble scale is time-dependent, so are the mass and the entropy of the PBH. Time and temperature are related in a radiation-dominated universe [13, 132]

$$\frac{t}{t_P} = \left(\frac{45}{16\pi^3 g_*(T)}\right)^{1/2} \left(\frac{T_P}{T}\right)^2 . \tag{2.41}$$

This way we can express both the entropy of the relativistic gas and the entropy of the Primordial Black Hole as a function of temperature

$$\begin{aligned} S_{\text{gas}} &= \frac{4}{3} \frac{T_P^3}{T^3} \left(\frac{45}{16\pi^3 g_*}\right)^{1/2} \\ S_{\text{PBH}} &= 4\pi\gamma^2 \left(\frac{45}{16\pi^3 g_*}\right) \left(\frac{T_P^4}{T^4}\right. \end{aligned} \tag{2.42}$$

and so the ratio of both quantities is a function of temperature as well

$$\frac{S_{\text{PBH}}}{S_{\text{gas}}} = \left(\frac{405}{16\pi}\right)^{1/2} \gamma^2 g_*^{-1/2} \frac{T_P}{T} \,. \tag{2.43}$$

Let us apply this equation to the QCD phase transition temperature. Then $T \simeq 200\,\text{MeV}$ and $g_* \simeq 10$. Taking into account that $T_P = 1.22 \times 10^{19}$ GeV one gets

$$\frac{S_{\text{PBH}}}{S_{\text{gas}}} \simeq \gamma^2 \cdot 5 \times 10^{19} \,. \tag{2.44}$$

This large number suggests that gravitational collapse via PBH formation is an extremely efficient way of generating a burst of entropy production which could fill the universe with entropy. Even if PBH do not exist, black holes are known to give the largest contribution to the entropy of the universe [133].

Part II

The quantum universe

Chapter 3

A first approach

> If you wish to make an apple pie from scratch, you must first invent the universe.
>
> Carl Sagan, *Cosmos* (1980).

3.1 Motivation

The common thread of part II is the study of correlations in cosmological perturbations arising from inflation. Regardless of their origin, these perturbations are a crucial ingredient of the standard cosmological model, ΛCDM. They are responsible for cosmological observables such as CMB anisotropies or structure formation. According to the standard framework reviewed in chapter 1, they arise as amplification or stretching of quantum fluctuations during inflation, which reenter the horizon at later times.

More concretely, the starting question of this thesis was: can primordial black holes (PBH) be entangled quantum-mechanically? We recall from sec. 1.7 that PBH are black holes formed by gravitational collapse induced by large curvature perturbations. If they have a quantum-mechanical origin in the sense described in sec. 1.5, we find our question to be a natural and relevant one. The fact that genuinely quantum features cannot be found easily in standard cosmological observables [117, 134, 135] already shows that this is a non-trivial issue.

Entangled black holes are involved in one of the most fascinating conjectures proposed in fundamental physics in the last years, namely the ER = EPR proposal [76]. Introduced by Maldacena and Susskind in 2012, it states that wormholes and quantum entanglement are analogous phenomena[1]. Since PBH may be formed copiously in the early universe, their quantum entanglement would lead one to postulate the existence of a wormhole network filling up spacetime.

The present chapter will be, however, less ambitious. We will illustrate how long-range correlations can be present in the early universe and how this is related to entanglement entropy, a quantity introduced in sec. 2.3. As we already discussed, quantum entanglement is present even in the Minkowski vacuum state in the form of the area law of entanglement entropy. It is known that the vacuum state of de Sitter spacetime is entangled in a way that goes beyond the area law found in Minkowski spacetime, as it was found by Maldacena and Pimentel [136]. Its corresponding entanglement entropy includes both UV-divergent and UV-finite terms. The former arise from local physics, while the latter are expected to be related to true long-range or non-local correlations. If this entanglement arises in de Sitter spacetime, it must be at least partially created during inflation as well. Entanglement may occur between different momentum modes as well as between localized modes, and it may change during time evolution, since it may not be unitary when restricted to individual modes due to interactions among them. However, the whole quantum state of the field must remain pure as dictated by unitary evolution. In this chapter we explore how some terms can be related to the entanglement of isotropic modes across a spherical entangling surface.

Even though quantum entanglement is easier understood when dealing with single particles in quantum mechanics, it is in fact an inevitable and natural feature of any quantum field theory. If we take the whole field to be the quantum system of interest, then it can be split into subsystems whose correlations are measured by their entanglement entropy. This entanglement entropy is dependent on the quantum state of the field and the choice of subsystems. For instance, if we consider the vacuum state of a scalar field theory in Minkowski spacetime, it can be expressed as a product state of single momentum mode vacua and therefore there is no entanglement between them

$$|0\rangle = \otimes_k |0\rangle_k \ . \tag{3.1}$$

However, if we choose the subsystems to be the localized modes inside and outside of a sphere of radius R, then one finds quantum entanglement between the inner and the outer modes with a UV-divergent entanglement entropy that scales with the area of the sphere [103, 104]

$$S \sim \frac{R^2}{\epsilon^2} \,, \tag{3.2}$$

[1]This is motivated by a previous proposal in holography, according to which a maximally extended AdS-Schwarzschild BH is dual to the thermofield double state in a conformal field theory. Similar ideas were already exposed by Israel in [92], without yet a reference to holography or the AdS/CFT correspondence. Intuitively, it can be understood from the fact that a mixed state can be purified by embedding it in a larger Hilbert space.

where ϵ acts as a UV regulator. This is the celebrated area law and describes the dominant contribution to the entanglement entropy of the vacuum state in Minkowski spacetime. It is interpreted as the entanglement degrees of freedom close to the surface of the sphere and is therefore related to local physics [136].

When the quantum field is coupled to gravity, particle creation can take place, as explained in sec. 1.5. In momentum space, this can lead to quantum entanglement between different momentum modes, as it is the case of cosmological perturbations. This phenomenon can also affect entanglement in real space and add both UV-divergent and UV-finite contributions beyond the area law. For a massless free minimally coupled scalar field in de Sitter spacetime these are given by [136]

$$\begin{aligned} S_{\text{dS, UV-divergent}} &= c_1 \frac{R^2}{\epsilon^2} + \log\left(\epsilon H\right)\left(c_2 + c_3 R^2 H^2\right) \\ S_{\text{dS, UV-finite}} &= c_4 R^2 H^2 + c_5 \log\left(-\eta\right) + \text{constant}\,. \end{aligned} \tag{3.3}$$

The term $\sim \log(-\eta)$ signals the presence of long-range quantum correlations. They arise from short-range physics due to the streching out of length-scales with the expansion. Since during inflation the background metric can be regarded as approximate de Sitter spacetime, we argue that such long-range quantum correlations may also be created during inflation and survive during the subsequent radiation-dominated era.

In this chapter we inspect this question, reviewing ref. [1]. The remainder of it is organized as follows. In section 3.2 we construct the spherical modes for the quantum state after inflation. In section 3.3 we perform a restriction of these modes over a sphere in order to compute its entanglement entropy. In section 3.4 we discuss the connection with the result in de Sitter, as well as phenomenological consequences, such as PBH entanglement.

3.2 Spherical modes

3.2.1 The quantum state after inflation

Consider a massless field Φ, which can be used for instance to describe primordial curvature perturbations. As such, it is related with the Mukhanov-Sasaki variable introduced in section 1.5 as $v = a\Phi$. Since primordial gravitational waves are described by the same dynamics, our results will also be valid for them. Following the usual prescription, we place it in the Bunch-Davies vacuum state in the distant past. This is particularly safe in applications to inflation, since only a piece of de Sitter is actually needed to describe a short period of accelerated expansion and those modes with wavelength larger than the event horizon at the beginning of inflation are phenomenologically irrelevant. On the other hand, some phenomenologically relevant scales were smaller than the Planck scale at the beginning of inflation. As the laws of physics at such small scales are not probed, deviations from the usual predictions of inflation may take place, which is known as the Transplanckian problem [137]. We assume that these deviations, if exist, are negligible.

In the Schrödinger picture, the Bunch-Davies vacuum evolves into a squeezed state due to the action of the time-evolution operator (S-matrix)

$$\hat{U}(\eta, \eta_0) = e^{-i(\eta-\eta_0)\hat{H}(\eta)} \tag{3.4}$$

where η_0 is the conformal time at the beginning of inflation. The Hamiltonian operator contains a squeezing term, which is proportional to a'/a

$$\hat{H}(\eta) = \frac{1}{2}\int d^3k \left[k\left(\hat{a}_{\vec{k}}(\eta)\hat{a}^{\dagger}_{\vec{k}}(\eta) + \hat{a}^{\dagger}_{\vec{k}}(\eta)\hat{a}_{\vec{k}}(\eta)\right) + i\frac{a'}{a}\left(\hat{a}^{\dagger}_{\vec{k}}(\eta)\hat{a}^{\dagger}_{-\vec{k}}(\eta) - \hat{a}_{\vec{k}}(\eta)\hat{a}_{-\vec{k}}(\eta)\right)\right] \tag{3.5}$$

It can be shown that the time-evolution operator can be rewritten in the following way [138]

$$\log \hat{U}(\eta, \eta_0) = \int d^3k \frac{\tau_k(\eta)}{2}\left[\hat{a}_{\vec{k}}(\eta_0)\hat{a}_{-\vec{k}}(\eta_0)e^{-i\phi(\vec{k},\eta)} - \hat{a}^{\dagger}_{\vec{k}}(\eta_0)\hat{a}^{\dagger}_{-\vec{k}}(\eta_0)e^{i\phi(\vec{k},\eta)}\right] \tag{3.6}$$

and it acts on the vacuum creating a two-mode squeezed state, which entangles the $\vec{k}$ and $-\vec{k}$ modes as

$$|0,\eta\rangle = \hat{U}(\eta,\eta_0)\,|0,\eta_0\rangle = \otimes_k \frac{1}{\cosh\tau_k}\sum_{n=0}^{\infty}\left(e^{-i\phi(\vec{k},\eta)}\tanh\tau_k\right)^n |n\rangle_{\vec{k}}\,|n\rangle_{-\vec{k}}\ , \tag{3.7}$$

where τ and ϕ are respectively the squeezing parameter and phase, which depend only on the conformal time η and the norm of the momentum k. We refer the reader to [56] for a review of the physics and mathematics of squeezed states as well as to the original references on two-mode squeezed states [57, 58]. In the problem at hand one finds that $\tau \sim N$ where N is the number of e-folds between horizon exit and the end of inflation, i.e., $N \sim \log(\eta/\eta_0)$.

This state shows entanglement between $\vec{k}$ and $-\vec{k}$ modes, measured by an entanglement entropy given by [139]

$$S(\vec{k}) = 2\left[\log(\cosh\tau_k) - \log(\tanh\tau_k)\sinh^2\tau_k\right], \tag{3.8}$$

which reduces to $S(\vec{k}) \simeq 2\tau_k$ in the limit $\tau_k \gg 1$ as it is usually the case. Indeed, due to inflation the squeezing parameter can take values much larger than those attainable in the laboratory [140]. This entanglement entropy is related to the coarsed-grained entropy of primordial perturbations computed by Brandenberger, Mukhanov and Prokopec [59]. Indeed they found the entropy density to be

$$s = \int d^3k \log\sinh^2\tau_k \simeq \int d^3k\, 2\tau_k\,. \tag{3.9}$$

Intuitively, this coarse-grained entropy seems to be equivalent to tracing over one of the two subsystems of the 2-mode squeezed state. It must be noted, however, that the procedure used in its computation is different.

It is true that apparently we are comparing entropy density with total entropy, but it is not the case since after integrating the entanglement entropy over all possible momentum modes we get a quantity in units of entropy density. The scaling can be properly regularized via discretization

$$\int d^3k \to \sum_k = \left(\frac{k_{max}}{k_{min}}\right) \sim k_{max}^3 L^3\,, \tag{3.10}$$

which indeed grows as the volume.

The squeezing formalism readily allows us to understand the presence of quantum entanglement in cosmological perturbations in momentum space. Here we are interested in going beyond this statement and checking other ways in which quantum entanglement may be present in this state. Therefore, we will try to elucidate the entanglement in real or position space and, more precisely, between modes restricted to the interior and the exterior of a sphere of radius R.

3.2.2 Canonical quantization in spherical coordinates

In order to achieve the restriction mentioned above, we perform a canonical quantization in spherical coordinates. Introducing the auxiliary field $\chi = a\Phi$ [2] the equation of motion of the scalar field takes a simple form [53]:

$$\chi'' - \nabla^2\chi - \frac{a''}{a}\chi = 0\,. \tag{3.11}$$

Using the fact that during the radiation-dominated era $a \sim \eta$ the equation of motion reduces to that on Minkowski spacetime and therefore its solutions are the well-known plane waves. In spherical coordinates this is equivalent to

$$\frac{\partial^2\chi}{\partial\eta^2} - \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\chi) - \frac{1}{r^2}\Delta_{S_2}\chi = 0\,, \tag{3.12}$$

where the Laplacian on the 2-sphere is given by

$$\Delta_{S_2} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\,. \tag{3.13}$$

[2] The field χ is roughly equivalent to the Mukhanov-Sasaki variable v. Its dynamics, however, is simplified. For instance we take $z = a$. For this reason, we keep the notation χ in order to avoid confusion.

The solutions to this equation are known to be (up to an overall constant N_k that we will fix later)

$$\chi_{k,l,m}(\eta, r, \theta, \varphi) = \frac{N_k}{\sqrt{2\omega}} e^{-i\omega\eta} j_l(kr) Y_{lm}(\theta, \varphi)\,, \tag{3.14}$$

where $j_l(z) = \sqrt{\frac{\pi}{2z}} J_{l+1/2}(z)$ are the spherical Bessel functions and $Y_{lm}(\theta, \varphi)$ are the spherical harmonics. Notice that for a massless field, as it is our case, the dispersion relation reads $\omega = k$.

These mode functions need to be normalized with respect to the Klein-Gordon inner product as

$$(\chi_{klm}, \chi_{k'l'm'}) = i \int_0^\infty r^2 dr \int d\Omega \left(\chi^*_{klm} \overleftrightarrow{\partial}_\eta \chi_{k'l'm'} \right) = \frac{\pi}{2k^2} \delta(k - k') \delta_{ll'} \delta_{mm'}\,. \tag{3.15}$$

The choice of functions makes therefore perfect sense from the point of view of the Klein-Gordon inner product, since they are orthogonal. We reabsorb the factor $1/k^2$ into the definition of the mode functions since we anticipate it to be important for the operator field expansion. We also reabsorb the constant factor $\pi/2$ and finally get

$$\chi_{klm}(\eta, r, \theta, \varphi) = \frac{1}{\sqrt{2\omega}} e^{-i\omega\eta} \sqrt{\frac{2}{\pi}}\, k j_l(kr) Y_{lm}(\theta, \varphi)\,. \tag{3.16}$$

The field operator χ can be expanded in terms of these functions:

$$\hat{\chi}(\eta, r, \theta, \varphi) = \int_0^\infty dk \sum_{l=0}^\infty \sum_{m=-l}^{l} \frac{k}{\sqrt{2\omega}} j_l(kr) \left(Y^*_{lm}(\theta, \varphi) e^{i\omega\eta} \hat{a}_{klm} + Y_{lm}(\theta, \varphi) e^{-i\omega\eta} \hat{a}^\dagger_{klm} \right)\,. \tag{3.17}$$

The field operator must of course satisfy the Canonical Commutation Relation

$$[\hat{\chi}(\eta, r, \theta, \varphi), \hat{\Pi}(\eta, r', \theta', \varphi')] = i\delta^{(3)}(\vec{r} - \vec{r}') \tag{3.18}$$

which is achieved by imposing

$$\begin{aligned} [\hat{a}_{klm}, \hat{a}_{k'l'm'}] = 0 = \left[\hat{a}^\dagger_{klm}, \hat{a}^\dagger_{k'l'm'}\right] \\ \left[\hat{a}_{klm}, \hat{a}^\dagger_{k'l'm'}\right] = \delta(k - k')\delta_{ll'}\delta mm'\,. \end{aligned} \tag{3.19}$$

As one would expect, this canonical quantization in spherical coordinates is completely equivalent to the usual canonical quantization in cartesian coordinates. The destruction and creation operators in both descriptions are related by the following expression

$$\hat{a}_{\vec{k}} = \sum_{l=0}^\infty \sum_{m=-l}^{l} \frac{i^l}{k} Y_{lm}(\hat{k}) \hat{a}_{klm} \tag{3.20}$$

and its inverse

$$\hat{a}_{klm} = (-i)^l k \int d\Omega Y^*_{lm}(\hat{k})\hat{a}_{\vec{k}}\,, \tag{3.21}$$

where $\hat{k} = \vec{k}/k$ and is simply parametrized by two angular variables. In terms of this creation and annihilation operators in spherical coordinates the time-evolution operator becomes

$$\begin{aligned}\log \hat{U}(\eta) = \int d^3k \frac{\tau_k(\eta)}{2} \sum_{l,l',m,m'} \Bigg[&\frac{i^{l+l'}}{k^2} Y_{lm}(\hat{k})Y_{l'm'}(-\hat{k})\hat{a}_{klm}\hat{a}_{kl'm'}e^{-i\phi(\vec{k},\eta)} \\ &- \frac{(-i)^{l+l'}}{k^2} Y^*_{lm}(\hat{k})Y^*_{l'm'}(-\hat{k})\hat{a}^\dagger_{klm}\hat{a}^\dagger_{kl'm'}e^{i\phi(\vec{k},\eta)}\Bigg]\end{aligned} \tag{3.22}$$

After applying some properties of the spherical harmonics and integrating over the angular variables one gets a simpler expression for the operator:

$$\log \hat{U}(\eta) = \int dk \frac{\tau_k(\eta)}{2} \sum_{l,m} (-1)^m \left[\hat{a}_{klm}\hat{a}_{kl,-m}e^{-i\phi} - \hat{a}^\dagger_{klm}\hat{a}^\dagger_{kl,-m}e^{i\phi}\right]. \tag{3.23}$$

This operator has a slightly different effect for $l = 0$ and $l \neq 0$. Indeed by expressing

$$\hat{U}(\eta) = \prod_{l,m} \hat{U}_{lm}(\eta) \tag{3.24}$$

we see that

$$\log \hat{U}_{00}(\eta) = \int dk \frac{\tau_k(\eta)}{2} \left[\hat{a}_{k00}\hat{a}_{k00}e^{-i\phi(\vec{k},\eta)} - \hat{a}^\dagger_{k00}\hat{a}^\dagger_{k00}e^{i\phi(\vec{k},\eta)}\right]. \tag{3.25}$$

The operator U_{00} creates nothing but a one-mode squeezed operator out of the vacuum. By factoring the state as well

$$|0,\eta\rangle = \otimes_{lm} |0,\eta\rangle_{lm} \tag{3.26}$$

we find that

$$\begin{aligned}|0,\eta\rangle_{00} &= \hat{U}_{00}(\eta)\,|0\rangle \\ &= \otimes_{k^2} \frac{1}{\sqrt{\cosh \tau_k(\eta)}} \sum_{n=0}^{\infty} \frac{\sqrt{(2n!)}}{n!} \left(-\frac{1}{2}e^{2i\phi(\vec{k},\eta)} \tanh \tau_k(\eta)\right) |2n\rangle_{k00}\,.\end{aligned} \tag{3.27}$$

On the other hand, for the other modes U_{lm} is a two-mode squeezing operator

$$\log \hat{U}_{lm}(\eta) = \int dk \frac{\tau_k(\eta)}{2} (-1)^m \left[\hat{a}_{klm}\hat{a}_{kl,-m}e^{-i\phi(\vec{k},\eta)} - \hat{a}^\dagger_{klm}\hat{a}^\dagger_{kl,-m}e^{i\phi(\vec{k},\eta)}\right], \tag{3.28}$$

which creates a two-mode squeezed state. This kind of state carries entanglement between the m and $-m$ modes, as can be seen from the form of the state

$$|0,\eta\rangle_{lm} = \otimes_{k^2} \sum_{n=0}^{\infty} \frac{\left(e^{2i\phi(\vec{k},\eta)}(-1)^{m+1}\tanh\tau_k(\eta)\right)^n}{\cosh\tau_k(\eta)} |n\rangle_{klm} |n\rangle_{kl,-m} . \tag{3.29}$$

To sum up, in spherical coordinates the quantum state after inflation has the following properties. First, the isotropic mode $l = 0$ is found in a one-mode squeezed state. Second, the anisotropic modes $l \neq 0$ are found in a two-mode squeezed state, which entangles m and $-m$ modes. This is one source of entanglement, but there is still another one due to the in and out bipartition by a spherical entangling surface of radius R.

3.3 Entanglement across a sphere

3.3.1 Isotropic entanglement entropy

As stated in the previous section, the anisotropic modes (i.e. those with $l \neq 0$) are found in two-mode squeezed states and show therefore entanglement between m and $-m$ modes. This entanglement is related directly to the entanglement between $\vec{k}$ and $-\vec{k}$ modes that is found in Cartesian coordinates. The computation of its entanglement entropy follows analogously and delivers the same result $S_k \simeq 2\tau_k$ for large τ_k.

The second simplest form of entanglement is the one across a spherical entangling surface of radius R for isotropic modes, i.e., those with $l = 0$. This entanglement is most interesting when R is taken to be the Hubble radius, but we will keep it as a free parameter for now. We will proceed with the Ansatz that the creation and annihilation operators can be split into an inner and an outer component as follows

$$\hat{a}_{k00} \equiv \hat{a}_k = \alpha\hat{a}_{k,\text{in}} + \beta\hat{a}_{k,\text{out}} , \tag{3.30}$$

with $|\alpha|^2 + |\beta|^2 = 1$. With this choice, the inner and outer operators commute

$$\begin{aligned} \left[\hat{a}_{k,\text{in}}, \hat{a}_{k',\text{in}}\right] &= \left[\hat{a}_{k,\text{out}}, \hat{a}_{k',\text{out}}\right] = 0 \\ \left[\hat{a}^\dagger_{k,\text{in}}, \hat{a}^\dagger_{k',\text{in}}\right] &= \left[\hat{a}^\dagger_{k,\text{out}}, \hat{a}^\dagger_{k',\text{out}}\right] = 0 \\ \left[\hat{a}_{k,\text{in}}, \hat{a}_{k',\text{out}}\right] &= \left[\hat{a}^\dagger_{k,\text{in}}, \hat{a}^\dagger_{k',\text{out}}\right] = \left[\hat{a}_{k,\text{in}}, \hat{a}^\dagger_{k',\text{out}}\right] = 0 . \end{aligned} \tag{3.31}$$

as expected from the CCR. Later we will deal with the fact that, in general, the following commutators do not satisfy the canonical relations

$$\left[\hat{a}_{k,\text{in}}, \hat{a}^\dagger_{k',\text{in}}\right] \neq \delta(k-k') \neq \left[\hat{a}_{k,\text{out}}, \hat{a}^\dagger_{k',\text{out}}\right] . \tag{3.32}$$

Note that the splitting performed in eq. (3.30) has the particularity of leaving the vacuum state invariant when interpreted as a Bogolyubov transformation. We shall elaborate later on this non-trivial statement. In a nutshell, this should be valid since i) isotropic modes could at most be linked with logarithmic contributions to the entanglement entropy and ii) we asume long- and short-range entanglement to be essentially independent phenomena, the former being due to the structure of vacuum and the latter due to particle production.

Taking this partition, any quantum state can be expressed in terms of n-particle states created by these inner and outer operators, which take the following form

$$\begin{aligned} |n\rangle &= \frac{1}{\sqrt{n!}}\left(\hat{a}^{\dagger}\right)^{n}|0\rangle = \left(\alpha^{*}\hat{a}^{\dagger}_{in} + \beta^{*}\hat{a}^{\dagger}_{\text{out}}\right)^{n}|0\rangle \\ &= \sum_{m=0}^{n}\binom{n}{m}^{1/2}\alpha^{m}\beta^{n-m}\,|m\rangle_{\text{in}}\otimes|n-m\rangle_{\text{out}}\ , \end{aligned} \tag{3.33}$$

where we dropped the subscript k for simplicity. Now, the $l = 0$ sector of the vacuum state is a one-mode squeezed state, which can be written in its standard particle basis decomposition and then split into inner and outer components

$$\begin{aligned} |0,\eta\rangle_{00} &= \frac{1}{\sqrt{\cosh\tau}}\sum_{n=0}^{\infty}\frac{\sqrt{(2n)!}}{n!}\left(-\frac{1}{2}e^{2i\phi}\tanh\tau\right)^{n}\times \\ &\times\sum_{m=0}^{2n}\binom{2n}{m}^{1/2}\alpha^{m}\beta^{n-m}\,|m\rangle_{\text{in}}\otimes|2n-m\rangle_{\text{out}} \end{aligned} \tag{3.34}$$

and we can build the corresponding density matrix

$$\begin{aligned} \hat{\rho}_{00} &= |0,\eta\rangle_{00}\,\langle 0,\eta|_{00} \\ &= \frac{1}{\cosh\tau}\sum_{n,n'=0}^{\infty}(-2)^{-(n+n')}\frac{\sqrt{(2n)!(2n')!}}{n!n'!}\times \\ &\times e^{2i\phi(n-n')}\tanh^{n+n'}(\tau)\cdot\sum_{m,m'=0}^{2n,2n'}\binom{2n}{m}^{1/2}\binom{2n'}{m'}^{1/2}\times \\ &\times\alpha^{m+m'}\beta^{(n-m)+(n'-m')}\,|m\rangle_{\text{in}}\,\langle m'|_{\text{in}}\otimes|2n-m\rangle_{\text{out}}\,\langle 2n'-m'|_{\text{out}}\ . \end{aligned} \tag{3.35}$$

Now we trace out the inner degrees of freedom in order to obtain the reduced density matrix of the outer degrees of freedom

$$\begin{aligned}\hat{\rho}_{\text{out}} &= \text{Tr}_{\text{in}}\hat{\rho} = \sum_{q=0}^{\infty} \langle q|_{\text{in}}\, \hat{\rho}\, |q\rangle_{\text{in}} \\ &= \frac{1}{\cosh\tau}\sum_{n,n'=0}^{\infty}\sum_{l=0}^{\min(2n,2n')}(-2)^{-(n+n')}\frac{\sqrt{(2n)!(2n')!}}{n!n'!}e^{2i\phi(n-n')}\times \\ &\times \tanh^{n+n'}(\tau)\alpha^{2l}\beta^{n+n'-2l}\binom{2n}{l}^{1/2}\binom{2n'}{l}^{1/2}|2n-l\rangle_{\text{out}}\,\langle 2n'-l|_{\text{out}}\,.\end{aligned} \tag{3.36}$$

In order to compute the von Neumann entropy of this density matrix we would in principle need to compute its logarithm and, therefore, diagonalize it. Its complicated structure and infinite size make it seem an impossible task. Hence, we will compute it using a different method, namely exploiting the available knowledge of the von Neumann entropy of generic two-mode Gaussian states. Even though it may not seem obvious that $\hat{\rho}_{00}$ is a Gaussian state, it has been proven that any quantum state created by a time evolution driven by a bilinear two-mode Hamiltonian is a two-mode Gaussian state [56]. This means that, even though the state itself is characterized by an infinite set of coefficients, it only contains a much more reduced amount of information codified in its first and second statistical moments, that is, in its expected values and covariance matrix. In other words: the density matrix of a single mode is created from the vacuum by acting with a squeezing operator, which depends on a few parameters, two per momentum mode. Therefore, its entanglement entropy should also depend on these parameters only. This means that, even though one needs in principle all the matrix elements to compute the logarithm of the matrix, it cannot have any non-trivial dependence that is not encoded in the dependence on the parameters. We use in the following the formalism described in [141] to compute the entanglement entropy.

We introduce the following auxiliary field and conjugated momentum operators

$$\begin{aligned}\hat{\chi}_{\text{in/out}} &= \frac{1}{\sqrt{2}}\left(\hat{a}_{\text{in/out}} + \hat{a}^{\dagger}_{\text{in/out}}\right) \\ \hat{\pi}_{\text{in/out}} &= \frac{-i}{\sqrt{2}}\left(\hat{a}_{\text{in/out}} - \hat{a}^{\dagger}_{\text{in/out}}\right).\end{aligned} \tag{3.37}$$

Then we construct the covariance matrix σ of a quantum state as follows:

$$\sigma_{ij} = \frac{1}{2}\langle \hat{x}_i\hat{x}_j + \hat{x}_j\hat{x}_i\rangle - \langle \hat{x}_i\rangle\langle \hat{x}_j\rangle\,, \tag{3.38}$$

where $i = 1, 2$ and the vector x is defined as $x = (\chi_{\text{in}}, \pi_{\text{in}})^T$.

The expected values $\langle \hat{x}_i \rangle$ can be set to zero without loss of generality. As a matter of fact, they are zero in our case. Let us use the short notation

$$\hat{\rho}_{\text{out}} = \sum_{n,n'=0}^{\infty} \sum_{l=0}^{\min(2n,2n')} c_{nn'l} \, |2n-l\rangle_{\text{out}} \langle 2n'-l|_{\text{out}} \, . \tag{3.39}$$

Then it follows

$$\left\langle \hat{a}^{\dagger}_{\text{out}} \right\rangle = \text{Tr}\left(\hat{\rho}_{\text{out}} \hat{a}^{\dagger}_{\text{out}} \right) = \sum_{n,n'=0}^{\infty} \sum_{l=0}^{max(2n,2n')} c_{nn'l} \sqrt{2n'-l} \cdot \delta_{2n-l,2n'-l-1} = 0 \, . \tag{3.40}$$

This is 0 because the condition of the Kronecker delta can never be fulfilled since n and n' are integers. Similarly one obtains $\langle \hat{a}_{\text{out}} \rangle = 0$. Hence, we focus on the second statistical moments

$$\begin{aligned}
\left\langle \hat{a}^{\dagger} \hat{a} \right\rangle &= \text{Tr}\left(\hat{\rho} \hat{a}^{\dagger} \hat{a} \right) = \text{Tr}\left(\hat{a} \hat{\rho} \hat{a}^{\dagger} \right) \\
&= \text{Tr}\left(\sum_{n,n'=0}^{\infty} \sum_{l=0}^{\min(2n,2n')} c_{nn'l} \sqrt{(2n-l)(2n'-l)} \, |2n-l-1\rangle \langle 2n'-l-1| \right) \\
&= \sum_{n,n'=0}^{\infty} \sum_{l=0}^{\min(2n-1,2n'-1)} c_{nn'l} \sqrt{(2n-l)(2n'-l)} \, \delta_{2n-l-1,2n'-l-1} \\
&= \frac{1}{\cosh \tau} \sum_{n=0}^{\infty} (-2)^{-2n} \frac{(2n)!}{(n!)^2} \tanh^{2n} \tau \cdot 2n \sum_{l=0}^{2n-1} \frac{(2n-1)!}{l!(2n-l-1)!} \alpha^{2l} \beta^{2(n-l)} \\
&= \frac{1}{\cosh \tau} \sum_{n=0}^{\infty} 2^{-2n} \frac{(2n)!}{(n!)^2} \tanh^{2n} \tau \cdot 2n \beta^2 = \beta^2 \sinh^2 \tau \, .
\end{aligned} \tag{3.41}$$

Similarly for the other moment

$$
\begin{aligned}
\langle \hat{a}\hat{a} \rangle &= \mathrm{Tr}\,(\hat{\rho}\hat{a}\hat{a}) = \mathrm{Tr}\,(\hat{a}\hat{\rho}\hat{a}) \\
&= \mathrm{Tr}\left(\sum_{n,n'=0}^{\infty} \sum_{l=0}^{\min(2n-1,2n')} \left(c_{nn'l} \cdot \sqrt{(2n'-l+1)(2n-l)} \cdot |2n-l-1\rangle \langle 2n'-l+1| \right) \right) \\
&= \sum_{n,n'=0}^{\infty} \sum_{l=0}^{\min(2n-1,2n')} \left(c_{nn'l} \cdot \sqrt{(2n'-l+1)(2n-l)} \cdot \delta_{2n-l-1,2n'-l+1} \right) \\
&= \frac{1}{\cosh\tau} \sum_{n=1}^{\infty} \sum_{l=0}^{2n-2} \sqrt{(2n-l-1)(2n-l)}\,(-2)^{-2n+1} \frac{\sqrt{(2n)!(2n-2)!}}{n!(n-1)!} \cdot \\
&\cdot e^{2i\phi} \tanh^{2n-1}\tau \binom{2n}{l}^{1/2} \binom{2n-2}{l}^{1/2} \alpha^{2l}\beta^{4n-2l-2} \\
&= \frac{1}{\cosh\tau} \sum_{n=1}^{\infty} 2^{-2n+1} \frac{(2n)!}{n!(n-1)!} e^{2i\phi} \tanh^{2n-1}\tau \sum_{l=0}^{2n-2} \binom{2n-2}{l} \alpha^{2l}\beta^{4n-2l-2} \\
&= \frac{1}{\cosh\tau} \sum_{n=1}^{\infty} 2^{-2n+1} \frac{(2n)!}{n!(n-1)!} e^{2i\phi}\beta^2 \tanh^{2n-1}\tau = e^{2i\phi}\beta^2 \sinh\tau\cosh\tau\,.
\end{aligned}
\tag{3.42}
$$

We will neglect in the following the contribution of the phase, since we can always reabsorb it by means of the transformation $\hat{a} \to e^{-i\phi}\hat{a}$ which does not affect the physics of the problem.

Now we are ready to compute the elements of the covariance matrix

$$\sigma_{\chi\chi} = \langle \hat{\chi}\hat{\chi} \rangle = \beta^2 e^{\tau} \sinh\tau + \frac{1}{2}\,. \tag{3.43}$$

$$\sigma_{\pi\pi} = \langle \hat{\pi}\hat{\pi} \rangle = \frac{1}{2} - \beta^2 e^{-\tau} \sinh\tau\,. \tag{3.44}$$

$$\sigma_{\chi\pi} = 0\,. \tag{3.45}$$

The entanglement entropy of the quantum state is related to the determinant of the covariance matrix as follows

$$S = \frac{1-\mu}{2\mu} \ln\left(\frac{1+\mu}{1-\mu}\right) - \ln\left(\frac{2\mu}{1+\mu}\right), \tag{3.46}$$

with

$$\mu = \frac{1}{2^n \sqrt{\det\sigma}}\,, \tag{3.47}$$

where n is the number of quantum modes. In our present case, $n = 1$. The determinant is given here by

$$\det\sigma = \sigma_{\chi\chi}\sigma_{\pi\pi} - \sigma_{\pi\chi}^2 = \frac{1}{4} + \beta^2(1-\beta^2)\sinh^2\tau\,. \tag{3.48}$$

Notice that this result is symmetric under the exchange of β^2 and $\alpha^2 = 1-\beta^2$, as it should. We then get the expression

$$\mu = \frac{1}{2\sqrt{\det\sigma}} = \frac{1}{\sqrt{1+4\beta^2\alpha^2\sinh^2\tau}} \tag{3.49}$$

and the following result for the entanglement entropy

$$\begin{aligned} S = &\log\left[\frac{1}{2}\left(1+\sqrt{1+4\beta^2\alpha^2\sinh^2\tau}\right)\right] \\ &+\frac{1}{2}\left(-1+\sqrt{1+4\beta^2\alpha^2\sinh^2\tau}\right)\log\left(\frac{1+\sqrt{1+4\beta^2\alpha^2\sinh^2\tau}}{-1+\sqrt{1+4\beta^2\alpha^2\sinh^2\tau}}\right). \end{aligned} \tag{3.50}$$

Now, let us consider a completely equal bipartiton, i.e. $\alpha = \beta = 1/\sqrt{2}$, so that

$$\mu = \frac{1}{\sqrt{1+\sinh^2\tau}} = \text{sech}\tau\,. \tag{3.51}$$

For $\tau \gg 1$, as it is usually the case in cosmological applications, this in turn leads to

$$S \sim 2\tau\,, \tag{3.52}$$

which means that the entanglement between inner and outer modes grows linearly with τ and vanishes for $\tau = 0$. This turns out to be the case as well for any other value of β. The main difference is that the linear behaviour is preceded by a slow exponential growth before becoming linear, and the more β departs from its equipartion value $\beta = 1/\sqrt{2}$, the longer this linear behavior appears.

On the other hand, for fixed τ the following dependence for $\alpha < \frac{1}{\sqrt{2}}$ is observed

$$S \sim \log\alpha\,. \tag{3.53}$$

We will discuss this in a later section but we advance the following Ansatz for the scaling of the coefficients α and β

$$\alpha = \sqrt{\frac{R}{L}} \quad \text{and} \quad \beta = \sqrt{1-\frac{R}{L}}\,, \tag{3.54}$$

so that

$$S \sim \log\frac{R}{L}\,, \tag{3.55}$$

where L is an IR regulator. Therefore, an IR divergence arises due to the term $\log L$. But actually for *really small* α we have that $S \to 0$. This can be checked taking the complete formula or, more easily, performing a Taylor expansion around $\alpha = 0$

$$S \simeq \alpha^2 \left[1 - \log\left(\alpha^2 \sinh^2 \tau\right)\right] \sinh^2 \tau \,. \tag{3.56}$$

This result should be interpreted carefully. Indeed, if we take the limit $L \to \infty$ this is in a sense equivalent to taking the limit $R \to 0$. This would mean that all degrees of freedom have been traced out and so the entanglement entropy must vanish. The actual quantity should be regularized. We think a reasonable regularization scheme would be taking the Hubble scale during inflation as initial size of the universe and then expand it exponentially during the N e-folds that inflation lasts

$$L = H^{-1} e^{N} \,. \tag{3.57}$$

This prescription is borrowed from regularization schemes in quantum cosmology and stochastic inflation [142–144]. It is also consistent with the Bunch-Davies prescription for the vacuum state, since it cannot be applied to modes whose wavelength was larger than the Hubble scale at the beginning of inflation.

The key statement is the scaling of the entropy as $S \sim \log R$. This is a sub-dominant correction to the area law, which seems to be unrelated to the isotropic modes. This form of entanglement arises solely due to the squeezing and vanishes the moment the limit $\tau \to 0$ is taken. The usual short-range UV-divergent and area-scaling contribution to the entanglement entropy must still be present when the total entanglement entropy is computed but is not related to the isotropic modes. From our expression it can be inferred that the entanglement entropy given by the long-range correlations between isotropic modes is in any case subdominant. However, to make a proper judgement it should still be integrated for all the available modes.

3.3.2 Scaling of the bipartition

The expression we used to split the creation and annihilation operators of the scalar field theory defined on the whole spacetime manifold seems a bit obscure. In this section we will argue why the coefficients α and β should scale as indicated before.

In order to do this, let us place the theory in a spherically symmetric lattice, so that the radial coordinate is discretized while keeping the angular coordinates continuous. Then the field itself is discretized into a set of fields $\chi_r(\theta, \varphi)$ living at each point of the lattice and can be expanded in terms of its associated annihilation and creation operators a_r and $a_r^\dagger$. They satisfy the canonical commutation relations

$$\left[\hat{a}_r, \hat{a}_{r'}^\dagger\right] \sim \delta_{rr'} \tag{3.58}$$

or, in the continuum limit,

$$\left[\hat{a}_r, \hat{a}^\dagger_{r'}\right] = \frac{1}{4\pi r^2}\delta(r - r')\,. \tag{3.59}$$

The usual momentum-defined creation and annihilation operators are recovered through a Bessel transform in the continuum limit

$$\hat{a}_k = \int d^3r \sqrt{\frac{2}{\pi}}\, j_0(kr)\hat{a}_r\,. \tag{3.60}$$

We can split this integral into two regions and so define the inner and outer components of the operator

$$\hat{a}_k = 4\pi \int_0^R drr^2k\sqrt{\frac{2}{\pi}}\, j_0(kr)\hat{a}_r + 4\pi \int_R^\infty drr^2k\sqrt{\frac{2}{\pi}}\, j_0(kr)\hat{a}_r \tag{3.61}$$

and we can approximately identify

$$\begin{aligned} \hat{a}_{k,\text{in}} &\sim 4\pi \int_0^R drr^2k\sqrt{\frac{2}{\pi}}\, j_0(kr)\hat{a}_r \\ \hat{a}_{k,\text{out}} &\sim 4\pi \int_R^\infty drr^2k\sqrt{\frac{2}{\pi}}\, j_0(kr)\hat{a}_r\,. \end{aligned} \tag{3.62}$$

The integrals are defined in three dimensions and the delta function is defined to be the spherically symmetric three dimensional one. This is done so in order to show that this formalism can be generalized to include anistropic modes, even though we will not need them here.

From this point of view it is clear that it is legitimate to perform a bipartition of the local degrees of freedom of the scalar field into inner and outer components with respect to some spherical surface of radius R. For cosmological applications it is of particular interest to pick R to be the Hubble radius. Formally, our results can be applied to any arbitrary R but, as we will discuss in more detail in sec. 3.4, they can be physically trusted for R of the order or larger than the Hubble scale.

Then there is an alternative field operator expansion in terms of inner and outer mode functions. We restrict ourselves in the present analysis to the isotropic modes $l = 0$ but it could be extended to the anisotropic modes as well. The expansion is then

$$\hat{\chi}_0 = \int_0^\infty dk\frac{k}{\sqrt{2\omega}}\left(f_{k,in}\hat{a}_{k,in} + f_{k,out}\hat{a}_{k,out} + \text{h.c.}\right)\,, \tag{3.63}$$

where h.c. stands for hermitian conjugate. The mode functions need to be normalized with respect to the Klein-Gordon inner product

$$\begin{aligned} \int_0^R drr^2 j_0(kr)j_0(kr) &\sim R \\ \int_R^L drr^2 j_0(kr)j_0(kr) &\sim L - R\,, \end{aligned} \tag{3.64}$$

where an IR regulartor L has once more been introduced. We find it reasonable to suggest the following scaling for the coefficients of the mode splitting

$$\alpha = \sqrt{\frac{R}{L}} \quad \& \quad \beta = \sqrt{1 - \frac{R}{L}} \tag{3.65}$$

as it was used in the previous section. Notice once more that $\alpha^2 + \beta^2 = 1$.

The creation and annihilation operators so constructed must be treated carefully, since they do not exactly satisfy the canonical commutation relations

$$\left[\hat{a}_{k,\mathrm{in}}, \hat{a}^{\dagger}_{k',\mathrm{out}}\right] \propto \int_0^R dr dr' r r' j_0(kr) j_0(k'r') \left[\hat{a}_r, \hat{a}^{\dagger}_{r'}\right] \propto \int_0^R dr r^2 j_0(kr) j_0(k'r) \tag{3.66}$$

This integral does not give anything proportional to $\delta_{kk'}$ even though it is clearly peaked at $k = k'$. Of course, this means that the scalar product $\langle k \mid k' \rangle$ will also be proportional to this integral and, therefore, the set of states $\hat{a}^n_{k,\mathrm{in}} |0\rangle$ can be used to span the whole inner Hilbert space but it does not form an orthonormal basis. However, once the Hilbert space is restricted to one momentum mode, the set of vectors does form an orthonormal basis on that Hilbert subspace thanks to the $\delta_{nn'}$ factor appearing in the computation of the scalar product. The same applies of course to the outer Hilbert space.

These considerations do not change the form of the quantum state after inflation as we treated it in sec. 3.2. The reason is that, even though a single inner or outer operator may affect several momentum modes, the combination $\hat{a}_{k,\mathrm{in}} + \hat{a}_{k,\mathrm{out}} = \hat{a}_k$ does not.

One may wonder as well about the validity of the computation of the entanglement entropy, since it involves the computation of two partial traces and no orthonormal basis is available. We argue that, even though the partial traces indeed cannot be computed exactly, our approximation is good enough. Let us assume that we have at our disposal an orthonormal basis $|j\rangle$ where j stands as a multi-index that labels momentum and particle number. This basis is related to our non-orthonormal basis $|\tilde{j}\rangle$ via a linear transformation

$$|\tilde{j}\rangle = \hat{C} |j\rangle \, . \tag{3.67}$$

We actually have meaningful information regarding the linear operator C. Its matrix elements are given by

$$C_{pqnm} \equiv C_{jh} \equiv \langle \tilde{j} | \hat{C} |h\rangle = \left\langle \tilde{j} \middle| \tilde{h} \right\rangle \propto \int_0^R dr r^2 j_0(pr) j_0(qr) \delta_{nm} \, . \tag{3.68}$$

The mode functions are normalized and therefore we have that $C_{jj} = 1$ and so the linear operator can be splitted into the identity plus corrections $C = 1 + \epsilon$. Since the integral is peaked at $p = q$ we assume ϵ to be small. In particular, the inverse of the operator can be written as $C^{-1} \simeq 1 - \epsilon$. Furthermore, it is traceless and so it does not affect at first order the computation of the relevant traces for our problem. Let us see how this works out for the trace of some linear operator A

$$\begin{aligned} \mathrm{Tr} A &= \sum_j = \langle j | \hat{A} | j \rangle = \sum_{j'} \langle \tilde{j} | \hat{C}^{-1} \hat{A} \hat{C}^{-1} | \tilde{j} \rangle \\ &= \sum_{j'} \left[\langle \tilde{j} | \hat{A} | \tilde{j} \rangle - \mathrm{Re} \left(\langle \tilde{j} | \hat{A} \epsilon | \tilde{j} \rangle \right) + \mathcal{O}\left(\epsilon^2\right) \right] . \end{aligned} \tag{3.69}$$

Now let use this expression for the density matrix $\hat{\rho}$ of a separable state with respect to the momentum modes such as the one created after inflation. This operator is diagonal, whereas all diagonal elements in ϵ vanish. Hence, the expected value of the product of both operators is 0. This leaves the approximate result

$$\mathrm{Tr} A \simeq \sum_{\tilde{j}} \langle \tilde{j}' | A | \tilde{j} \rangle . \tag{3.70}$$

This finishes the argument that the computation of the entanglement entropy above is a good approximation.

3.4 Discussion

3.4.1 Mode counting and the area law

The computation presented in sec. 3.3 is far from accounting for the whole entanglement entropy of the region inside a sphere of radius R. In fact, it is limited for two reasons: it accounts only for isotropic modes ($l = 0$) and only those with a given momentum k. Hence, it is a measure of the entanglement per isotropic mode. It is characterized by its squeezing parameter τ, which is in turn a function of the momentum k and in particular the number of e-folds N_k between horizon exit and the end of inflation. Roughly one gets $\tau \sim N$ [138].

Then one simply needs to integrate

$$S \sim \int dk \; \tau_k \log R \tag{3.71}$$

This integral could be in principle model-dependent, although roughly $\tau_k \simeq N(k)$. Notice that there is no dependence on R^2 as opposed to the standard area law for entanglement in QFT on 3+1 dimensions. We can understand this from the point of view that, effectively, the restriction to isotropic modes delivers a (1+1)-dimensional theory. Such theories are known to have a logarithmic scaling of the entanglement entropy.

In the computation of the entanglement entropy done by Maldacena and Pimentel they also found a term proportional to the number of e-folds or, more explicitly, to $\log(-\eta)$. This computation is performed in the limit of very late time and therefore we can consider that every mode has crossed the inflationary event horizon long time ago. In that case

$$S = \int_0^\infty dk N(k) \log \frac{R}{L} = \int_0^\Lambda dk \log(-\eta k) \log \frac{R}{L} = \Lambda \log \frac{R}{L} \left[\log(-\eta) + \log \Lambda - 1\right] , \tag{3.72}$$

where Λ is a UV cut-off. In the limit $L \to \infty$ the logarithm must be replaced by a term that goes as $\sim \frac{R}{L}$ and so tends to 0. At the same time we take the limits $\Lambda \to \infty$ and keeping the product $\Lambda \frac{R}{L}$ constant. Then we get the following contributions to the entropy

$$S = c \log(-\eta) + c' \log \Lambda \, , \tag{3.73}$$

with some coefficients c and c' to be determined. Both kind of terms exist in dS and therefore also in a radiation-dominated universe if we assume it is preceded by an extremely long inflationary epoch.

In order to recover the usual UV-divergent area-law scaling entanglement entropy, as well as additional UV-finite terms proportional to the area, the whole tower of l and m modes must be taken into account. Restricting ourselves now to the true vacuum state $|0\rangle$, it carries no angular momentum, i.e. $l = 0$ and $m = 0$. Angular momentum can be shown to be a good quantum number of the particle states in spherical coordinates introduced in sec. 3.2. This means that $\hat{L}^2 |l, m\rangle = l(l+1) |l, m\rangle$ and $\hat{L}_z |l, m\rangle = m |l, m\rangle$. Therefore, if the vacuum is to be splitted, it must be done in a way that preserves the total angular momentum. This can be done with the formalism of the Clebsch-Gordan coefficients, widely used in Quantum Mechanics. One should therefore find an analogous of the singlet state of two-particle systems with spin. However, the issue is not trivial, as in QFT the total number of particles is not fixed *a priori* and there can be many contributions to the vacuum state.

3.4.2 Phenomenological implications.

Formally, the computation showed here can be applied to any entangling sphere of radius R, let it be smaller or larger than the Hubble scale R_H. However, from a more physical point of view, it is only justified for $R > R_H$. In this regime, arguably dominated by super-Hubble physics, perturbation modes are frozen and do not interact. On the contrary, when modes re-enter the horizon, this interaction begins and can scramble the interior quantum state, thus erasing long-range correlations inside the Hubble sphere, although not the correlation of the observable universe with other causal domains. In addition, non-linear interactions are likely to play a role in this process. Depending on the scales giving a stronger contribution to the entanglement entropy, this may have a non-negligible impact on the entanglement entropy.

Following our earlier motivation in sec. 3.1, this scenario may change should a PBH be formed during the radiation era. As mentioned in sec. 1.7, PBH are formed by gravitational collapse, triggered by enhanced primordial perturbations [64, 65]. The relevant scale for the formation of a PBH in a radiation-dominated universe is the Hubble scale, as we will briefly argue later and is supported by simple model estimates [69, 70] and numerical relativity simulations [66, 75]. This means that the PBH captures most of the long-range entanglement of the Hubble sphere and keeps therefore long-range correlations with the rest of the universe, including other causal domains that collapse to form a PBH as well.

It is in this precise context that we view gravitational collapse as an *entanglement trap* that prevents the long-range correlation between different PBH to be destroyed by scrambling. As time passes, the Hubble sphere grows and PBH formed in different causal domains come into causal contact. This creates a network of entangled PBH inside the observable universe. Note that the entanglement of super-Hubble modes arise during inflation as those modes are stretched beyond the horizon and keep this entanglement on non-causal patches. As these modes re-enter the Hubble scale after inflation and induce black hole collapse, the entanglement created during inflation is trapped inside these regions without allowing for scrambling to take place.

In other words, a PBH keeps a long-range entanglement with other PBH. This is because they trap entanglement before scrambling can take place, as scrambling is a sub-Hubble process and PBH form with a size of the order of the Hubble scale at the time of collapse. This entanglement exists regardless of whether they came into casual contact already or not. A PBH keeps a long-range entanglement as well with non-collapsed regions of the non-observable universe, as they didn't undergo scrambling yet.

Perhaps it should be clarified that our use of entanglement entropy is not linked in principle to the gravitational entropy associated to the event horizon of any black hole. Instead, it is a description of how the degrees of freedom inside a spherical region are entangled with the degrees of freedom existing outside. This concept is applicable to any surface enclosing a volume. When a black hole is formed, the exterior degrees of freedom cannot interact with the interior ones and therefore this entanglement is preserved. It may be that the interior degrees of freedom interact with other degrees of freedom inside the black hole. We do not make any claim regarding the nature of the degrees of freedom inside the black hole, but rather than the entanglement entropy across the surface is preserved by unitarity. As an analogy, we could think of a pair of entangled photons, one of them being captured by a black hole and another one kept outside. It is unknown how the swallowed photon will interact with the interior degrees of freedom of the black hole, but due to unitarity the entanglement entropy of the system formed by the black hole and the swallowed spin will be preserved.

If this gravitational collapse is assumed to be unitary, then the entanglement entropy will be conserved during the process. Nothing forbids, for instance, the formation of a black hole by the collapse of a large number of particles which are entangled with distant objects. Such a black hole would keep this quantum entanglement. Such a process is described for instance in [76] in the context of building a pair of maximally entangled black holes by the gravitational collapse of the Hawking radiation of an initially isolated black hole.

Entangled black holes have been considered before in the literature [76,92], being usually maximally entangled. We have presented here a viable mechanism to produce entangled PBH. It must be noted, however, that they would not be maximally entangled, as their long-range entanglement entropy does not saturate the Bekenstein bound [145]. Since two causally disconnected regions that collapse to form PBH far away from eachother are individually entangled with the rest of the universe, they must necessarily be themselves entangled with each other.

The *entanglement trap* is not, nevertheless, the only feasible behavior of long-range correlations due to entanglement when PBH are involved. Alternatively, it is possible that entanglement is not trapped, but rather is allowed to *leak*, so that the event horizon of a PBH forms sort of a *leaky barrier* and is, in fact, no special surface. In other words, the picture of discrete entangled particles, which may not escape the black hole, it is possible that a dynamical continuous field leads to correlations between the PBH that change with cosmic evolution. We will come back to this possibility in chapter 4 and discuss how it could induce non-trivial interactions between distant PBH.

3.4.3 Remarks

The results of this chapter suggest the existence of long-range entanglement in the universe due to the inflationary origin of cosmic structures. Indeed, due to inflation, the quantum state of a scalar field describing cosmological perturbations is highly squeezed. This squeezing leads to subdominant terms in the entanglement entropy that go beyond the (UV-divergent) area-law. This kind of term is also found in the entanglement entropy of a field living in dS and signals the survival during the radiation era of the entanglement created during inflation.

These terms arise due to the entanglement of super-Hubble modes that are stretched beyond the horizon during inflation and maintain entanglement on non-causal patches. In the case of modes that re-enter the Hubble scale after inflation and induce black hole collapse, the entanglement is trapped inside these regions without allowing for scrambling to take place.

It may seem puzzling that quantum entanglement of the state created during inflation should be conserved after its end. Indeed, if inflation is capable of creating entanglement, the next cosmological era may very likely destroy it. The creation or destruction of entanglement between quantum modes is possible since the time evolution of an individual mode can be non-unitary in presence of interactions, for instance thanks to a gravitational background. The time evolution of the total quantum state is of course unitary and remains pure. In order to gain some intuition about the survival of the entanglement, let us put in simpler, qualitative terms, the evolution that the quantum state undergoes during inflation.

Any quantum field coupled to a gravitational background, even if minimally, is sourced by it, which leads to particle creation in the form of entangled pairs in inflation. During the radiation era, the dynamics of the field is equivalent to that of a field in Minkowski spacetime and so there is no source that can affect the nature of the quantum state created during inflation.

Furthermore, the locality of QM imposes entanglement to be created or destroyed by local interactions only. Therefore, causally disconnected patches keep their correlations (both classical and quantum) with time evolution. We can also understand this as a consequence of the freezing of perturbations.

We have assumed throughout a standard single-field inflation because of the simplicity of its treatment from a quantum field-theoretic point of view. However, more sophisticated models of (multi-field) inflation might enhance the entanglement. In particular, it would be fascinating if those models leading to PBH formation were also related to enhanced long-range entanglement. Such long-range correlations may give rise to the growth of isocurvature perturbations on cosmological scales, which could have important consequences for large scale structure formation and evolution.

We will encounter this issue throughout this thesis. Gaussian states can be well described with a density matrix or a Wigner function, but non-gaussianities are usually described either by higher-point correlation functions or by a probability distribution for the field [67], which is a sufficient description for many relevant phenomena, but not a complete one from the quantum-mechanical point of view.

Finally, it is worth pointing out that inspecting the entanglement entropy gives only a hint towards the existence of long-range correlations and, possibly, quantum entanglement. Strictly speaking, it solely quantifies the entanglement between complementary patches. The scale of the correlation is then identified with the scale of the momentum mode involved. UV-divergent contributions to the entropy are expected to be dominated by short-range phenomena. Conversely, UV-finite contributions should be dominated by long-range phenomena. However, a finer analysis is in order. As following next logical step, the next chapter will be devoted to the computation of the *mutual information* between two separate (i.e., non-complementary) spatial regions.

Chapter 4

Mutual information from inflation

> Whatever the rhythm was, luck rewarded us, because, wanting connections, we found connections — always, everywhere, and between everything. The world exploded in a whirling network of kinships, where everything pointed to everything else, everything explained everything else...
>
> Casaubon in *Foucault's pendulum* (1988) by Umberto Eco.

4.1 Motivation

Entropy and information play a key role in our understanding of physics. They are important properties of quantum states and are useful in describing correlations between physical subsystems. Furthermore, they are thought to be a bridge between classical gravity and an underlying quantum theory of gravity. In fact, the study of entropy and information applied to black hole physics is a fruitful field of research. The introduction of bekenstein-hawking entropy [105], discussed in sec. 2.7 was followed by the discovery of the area law of entanglement entropy [103, 104], discussed in sec. 2.4. The link between these two concepts added quantum information to the already successful crossover between gravity and quantum field theory.

Cosmology also profits from this interplay between gravity and quantum physics. The idea of inflation introduced a quantum origin of primordial perturbations [45]. This was needed in order to explain the power spectra of the CMB and some features of the LSS of the universe. Less known alternatives to inflation also explain power spectra by means of quantum fluctuations [63]. Even though quantum fluctuations classicalize in the sense that their observable features appear classical [138, 139, 146], their quantum origin is still relevant. For instance, the study of the entropy of cosmological perturbations in momentum space has long been considered [59] and has recently been extended to include non-linear interactions [147]. In a more general sense, it has also been a matter of recent work the study of the universe as a storage of quantum information in gravitational d.o.f., which could in turn leave an imprint on primordial perturbations [148].

However, quantum information properties of primordial perturbations in real space have been less studied. Following the path started in chapter 3, we turn now to the study of mutual information in a cosmological set-up. As mentioned in sec. 2.3, mutual information quantifies the total (classical and quantum) correlations between two quantum subsystems. It is, therefore, a relevant quantity to understand the information content of the cosmological perturbations of quantum origin.

For complementary subsystems, mutual information is simply equal to twice the entanglement entropy, as it can be readily seen from eq. (2.15), and is a quantity of no particular interest. For two non-complementary subsystems, however, it provides additional insight. This is the case, for instance, of a quantum field restricted to two separated regions. For a scalar field in the Minkowski vacuum, the mutual information is a rapidly decaying function of the distance r between the involved regions. This was shown by Noburo Shiba in [111, 112], using a perturbative formalism that we will adapt to cosmological perturbations. The particular expression for two spheres of radius R_1 and R_2 and $R_1, R_2 \ll r$ is

$$I(A,B) \simeq \frac{1}{4}\frac{R_1^2 R_2^2}{r^4}\,, \tag{4.1}$$

which becomes quickly irrelevant with distance. We will see in the course of this chapter how this quantity is enhanced thanks to particle production (or, equivalently, stretching of quantum fluctuations) during inflation. Indeed, this same quantity for a scalar field in the squeezed state resulting from the stretching of quantum fluctuations during inflation at conformal time η is

$$I(A,B) \simeq \frac{1}{16}\frac{R_1^2 R_2^2}{\eta^4}\left[1 - \gamma + \log\left(\frac{-\eta_0}{r}\right)\right]^2\,, \tag{4.2}$$

where $\gamma \simeq 0.577216...$ is the Euler-Mascheroni constant. This much slower decay signals long-range correlations between these disjoint regions and is due to the dependency of the mutual information with the power spectrum. It is also a natural result: due to inflation distant regions were causally connected in the past. Enhanced mutual information is intuitively connected with the main dynamical prediction of inflation: an homogeneous and isotropic universe with a nearly scale-invariant spectrum of curvature perturbations.

This chapter is a review of the results presented in ref. [2] and is organized as folows. In sec. 4.2 we compute the relevant correlation functions of primordial perturbations during the inflationary and radiation eras. In sec. 4.3 we extend an existing formalism to perturbatively compute the mutual information of a Gaussian state and apply it to cosmological perturbations in sec. 4.4. We finish with a discussion of our results in sec. 4.5, in comparison with other work and for its relevance to our understanding of primordial perturbations and the possible emergence of entropic forces.

4.2 Correlation functions

4.2.1 The quantum state of scalar perturbations

In this chapter we will describe scalar perturbations by means of a sigle scalar d.o.f., the Mukhanov-Sasaki variable v, which was introduced in sec. 1.4. As we saw in sec. 1.5, at linear order the time evolution of v is characterized by a bilinear Hamiltonian, so that a Gaussian state remains Gaussian with time evolution. Hence, we describe the quantum state during inflation by means of its 1- and 2-point correlation functions.

We briefly recall that the dynamics of of the Mukhanov-Sasaki variable is derived from a perturbation of the action

$$\delta\mathcal{S} = \frac{1}{2}\int d^4x\left((v')^2 - c_s^2\delta^{ij}\partial_i v\partial_j v + \frac{z''}{z}v^2\right)\,, \tag{4.3}$$

where c_s is the speed of sound, which takes values $c_s = 1$ during inflation and $c_s = 1/\sqrt{3}$ during the radiation era. The corresponding equation of motion for the Fourier modes $v_k(\eta) = \int d^3x e^{i\vec{k}\cdot\vec{x}}v(\eta,\vec{x})$ is:

$$v'' + \left(c_s^2k^2 - \frac{z''}{z}\right)v = 0\,, \tag{4.4}$$

which is the equation of motion of a harmonic oscillator with time-dependent mass. Thus, whenever $c_s^2k^2 < z''/z$, particle creation can occur.

At the beginning of inflation, the perturbation field is assumed to be in the Bunch-Davies vacuum, i.e., mode functions behave as plane waves in the distant past [53]. Then these modes evolve and are put in a squeezed state after they become super-horizon. For each momentum mode k, the state is described by a squeezing parameter τ_k and angle δ_k. This time-evolution is due to the z''/z term in the equation of motion (4.4).

Similarly to what we argued in chapter 3, in this chapter we will refer mostly to curvature perturbations, but our conclusions can be extended to primordial gravitational waves as well, at least qualitatively, since they have effectively the same dynamics.

The time-evolution of the quantum state for general inflationary models is more practically obtained after performing a canonical transformation of the Hamiltonian obtained from the action (4.3). As discussed in sec. 1.5, this is equivalent to the addition of a total derivative to the action in order to get

$$\delta\mathcal{S} = \frac{1}{2}\int d^4x \quad (v')^2 - c_s^2\delta^{ij}\partial_i v\partial_j v - 2\frac{z'}{z}vv' + \left(\frac{z'}{z}\right)^2 v^2 \,. \tag{4.5}$$

Of course, from this action one gets the same equation of motion (4.4). The canonical momentum and the Hamiltonian are given by

$$\begin{aligned} p &= v' - \frac{a'}{a}v\,, \\ H &= \frac{1}{2}\int d^3x \left(p^2 + c_s^2\delta^{ij}\partial_i v\partial_j v + 2\frac{z'}{z}vp\right). \end{aligned} \tag{4.6}$$

We will use this Hamiltonian for the rest of the chapter. For a detailed discussion of the two Hamiltonians that can equivalently describe the time-evolution of primordial perturbations and the canonical transformation that relates them, we refer the reader to refs. [49, 54].

Inflation is succeeded by the radiation era. Recall that $\eta \in (-\infty, 0)$ for eternal inflation or dS and $\eta \in (0, \infty)$ for an eternal radiation era. Instead, we will consider that inflation starts at $\eta_0 < 0$ and finishes at $\eta_* < 0$ and then the radiation era starts at $-\eta_*$. The details of the matching between η_* and $-\eta_*$ depend on the reheating scenario, but have little effect on curvature perturbations. Nevertheless, the mode functions of the radiation era depend of course on the boundary conditions imposed at $-\eta_*$. First, we will obtain the correlation functions in quasi de-Sitter inflation by obtaining the time evolution of the mode functions and then generalize them by applying known results in the squeezing formalism.

4.2.2 Correlation functions in quasi de-Sitter

During quasi de-Sitter inflation $c_s^2 = 1$, $a = -1/(H\eta)$ and therefore $z''/z = 2/\eta^2$. In this scenario, the mode functions of the Bunch-Davies vacuum have a simple form

$$v_k^i = \frac{(k|\eta| + i)}{\sqrt{2}\,k^{3/2}|\eta|}e^{ik|\eta|}\,. \tag{4.7}$$

From them one computes the mode functions for the canonical momentum

$$p_k^i(\eta) = v_k^{i\prime}(\eta) - \frac{a'}{a}v_k^i(\eta) = \frac{i\sqrt{k}}{\sqrt{2}}e^{ik|\eta|}\,. \tag{4.8}$$

Mode functions allow us to build the mode expansions of the quantum field and its canonical momentum

$$\begin{aligned} v^i(\eta,\vec{x}) &= \int \frac{d^3k}{(2\pi)^{3/2}}\left(e^{i\vec{k}\vec{x}}v_k^{i*}(\eta)\hat{a}_k + e^{-i\vec{k}\vec{x}}v_k^i(\eta)\hat{a}_k^\dagger\right)\,, \\ p^i(\eta,\vec{x}) &= \int \frac{d^3k}{(2\pi)^{3/2}}\left(e^{i\vec{k}\vec{x}}\pi_k^{i*}(\eta)\hat{a}_k + e^{-i\vec{k}\vec{x}}\pi_k^i(\eta)\hat{a}_k^\dagger\right)\,. \end{aligned} \tag{4.9}$$

Now we can compute the correlation functions that characterize the Bunch-Davies vacuum during quasi de-Sitter inflation:

- 1-point correlation functions

$$v^i(x,\eta) \;=\; p^i(x,\eta) \;=0\,. \tag{4.10}$$

- 2-point correlation functions

$$\begin{aligned} v^i(\eta,\vec{x})v^i(\eta,\vec{y}) &= \int \frac{d^3k}{(2\pi)^3}\frac{1}{2k}\left(1+\frac{1}{k^2\eta^2}\right) e^{-i\vec{k}(\vec{x}-\vec{y})}\,, \\ p^i(\eta,\vec{x})p^i(\eta,\vec{y}) &= \int \frac{d^3k}{(2\pi)^3}\frac{k}{2} e^{-i\vec{k}(\vec{x}-\vec{y})}\,, \\ v^i(\eta,\vec{x})p^i(\eta,\vec{y})+p^i(\eta,\vec{y})v^i(\eta,\vec{x}) &= \int \frac{d^3k}{(2\pi)^3}\frac{1}{k|\eta|} e^{-i\vec{k}(\vec{x}-\vec{y})}\,. \end{aligned} \tag{4.11}$$

These integrals are taken over momenta that are affected by inflation, i.e. those that are sub-horizon when inflation starts and become super-horizon before it ends. These are momentum modes that satisfy

$$-\eta_0 > k^{-1} > -\eta_*\,. \tag{4.12}$$

When inflation ends at $\eta = \eta_*$, mode functions are matched at the beginning of the radiation era at $\eta = -\eta_*$. The radiation era satisfies $z''/z = 0$ and so solutions to the equation of motion (4.4) are plane waves. Once the boundary conditions are imposed and taking into account that $c_S^2 = 1/3$ during the radiation era we get the solution

$$\begin{aligned} v_k^r(\eta) =& \frac{e^{ik\eta_*}}{\sqrt{2}} \times \\ &\times \left[\frac{(-\sqrt{3}+(1+\sqrt{3})\eta_* k(\eta_* k+i))}{2\eta_*^2 k^{5/2}} e^{\frac{i}{\sqrt{3}}k(\eta+\eta_*)} \right. \\ &\left. + \frac{(\sqrt{3}+(1-\sqrt{3})\eta_* k(\eta_* k+i))}{2\eta_*^2 k^{5/2}} e^{-\frac{i}{\sqrt{3}}k(\eta+\eta_*)} \right] \end{aligned} \tag{4.13}$$

Note that this mode function is a linear combination of oscillating functions, unlike in the Minkowski vacuum, in which the oscillation affects only a global phase of the mode function. Modes significantly affected by inflation satisfy $k\eta_* \ll 1$ so it is enough to keep leading terms in inverse powers of $(k\eta_*)$, i.e.

$$v_k^r(\eta) \simeq \frac{e^{ik\eta_*}}{i\sqrt{2}\,\eta_*^2 k^{5/2}} \sin\left(\frac{k(\eta+\eta_*)}{\sqrt{3}}\right). \tag{4.14}$$

The dependence on the sin function of the mode function is a general result for modes significantly affected by inflation [45]. From (4.13) one can also get the explicit form of the canonical momentum mode function $\pi^r_k(\eta)$ by using the definition (4.6).

We will consider only super-horizon modes, i.e. those that satisfy $k\eta \ll 1$ at a given time during the radiation era. For those the correlation functions are:

- 1-point correlation functions

$$\langle v^r(x,\eta)\rangle = \langle \pi^r(x,\eta)\rangle = 0\,. \tag{4.15}$$

- 2-point correlation functions

$$\begin{aligned}
\langle v^r(\eta,\vec{x})v^r(\eta,\vec{y})\rangle &\simeq \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\times \\
&\times \left(\frac{1}{2k} + \frac{1}{2k^3\eta_*^2} + \frac{1}{2}\left(\frac{\eta+\eta_*}{|\eta_*|}\right)^2 \frac{1}{k^3\eta_*^2} + \ldots\right) \\
\langle v^r(\eta,\vec{x})p^r(\eta,\vec{y}) + p^r(\eta,\vec{y})v^r(\eta,\vec{x})\rangle &\simeq \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\times \\
&\times \left(\frac{1}{k\eta_*} - \frac{1}{3}\left(\frac{\eta+\eta_*}{|\eta_*|}\right)\frac{1}{k^3\eta_*^3} + \ldots\right) \\
\langle v^r(\eta,\vec{x})p^r(\eta,\vec{y}) + p^r(\eta,\vec{y})v^r(\eta,\vec{x})\rangle &\simeq \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\times \\
&\times \left(\frac{1}{k\eta_*} - \frac{1}{3}\left(\frac{\eta+\eta_*}{|\eta_*|}\right)\frac{1}{k^3\eta_*^3} + \ldots\right)
\end{aligned} \tag{4.16}$$

The quadratic term in the field-field correlator is clearly dominant, while the expansion in the others is a bit more involved and only the first term is shown for illustrative purposes. Hence, after inflation ends and the radiation era starts, 2-point correlation functions continue growing with conformal time η. This is a general result that can be understood as well in the squeezing formalism.

4.2.3 The squeezing formalism

For general inflationary models, one can treat the time-evolution of the Bunch-Davies vacuum using the squeezing formalism, which of course can be applied to the quasi de-Sitter case as well. Such a state was introduced in sec. 1.5 and widely used in chapter 3 in the operator formalism. As a Gaussian state, it is characterized by the following correlation functions involving the field v and its canonical conjugate p [59]

- 1-point correlation functions

$$\langle v(\eta,\vec{x})\rangle = \langle p(\eta,\vec{x})\rangle = 0\,. \tag{4.17}$$

- 2-point correlation functions

$$\begin{aligned}
\langle v(\eta,\vec{x})v(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\left(\frac{1}{2k}\left(1+2\sinh^2\tau_k - \sinh 2\tau_k \cos 2\delta_k\right)\right)\\
\langle p(\eta,\vec{x})p(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\left(\frac{k}{2}\left(1+2\sinh^2\tau_k + \sinh 2\tau_k \cos 2\delta_k\right)\right)\\
\langle v(\eta,\vec{x})p(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\left(\frac{i}{2}\left(1+ i\sinh 2\tau_k \sin 2\delta_k\right)\right)\\
\langle p(\eta,\vec{y})v(\eta,\vec{x})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\left(\frac{-i}{2}\left(1- i\sinh 2\tau_k \sin 2\delta_k\right)\right)
\end{aligned} \tag{4.18}$$

The squeezeng parameter τ_k and phase δ_k can be derived from the inflationary dynamics and the subsequent evolution in the radiation era and have a momentum-dependent expression. However, we will perform the following approximation: we will assume a random character of the phases δ_k so that integrals over $\sin 2\delta_k$ or $\cos 2\delta_k$ vanish. This is a standard procedure in the study of primordial perturbations and is justified by the effect of small self-interactions or interactions with other fields [59, 147]. It can be seen as a coarse-graining or decoherence procedure, where the off-diagonal elements of the density matix in momentum space $\rho(\vec{k},-\vec{k},\vec{p},-\vec{p})$ decay. Strictly speaking, this is a rather rough model for decoherence and there exist finer ways to account for it [149, 150]. Nevertheless, our results would not change significantly if the random phase approximation was not performed. Therefore, this approximation will serve mostly as a computational simplification. We leave this discussion to appendix A.1.

After averaging over the phases the correlators become

$$\begin{aligned}
\langle v(\eta,\vec{x})v(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\frac{1}{2\omega_k}\left(1+2\sinh^2\tau_k\right)\,,\\
\langle p(\eta,\vec{x})p(\eta,\vec{y})\rangle &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}(\vec{x}-\vec{y})}\frac{\omega_k}{2}\left(1+2\sinh^2\tau_k\right)\,,\\
\langle v(\eta,\vec{x})p(\eta,\vec{y}) + p(\eta,\vec{y})v(\eta,\vec{x})\rangle &= 0\,.
\end{aligned} \tag{4.19}$$

Because of the term $\left(1+2\sinh^2\tau_k\right)$ we get an effective enhancement of the field and conjugate correlations for those momentum modes that are affected by inflation, i.e. those that satisfy

$$-\eta_0 > k^{-1} > -\eta_*\,, \tag{4.20}$$

The affected modes are thus those with wavelength smaller than the horizon when inflation starts and larger than the horizon when it ends.

One could ask what should be the correlators for modes that are not squeezed. It is clear that, for modes with small wavelength $k^{-1} < -\eta_*$, we can take them to be equal to those of the Minkowski vacuum due to the Bunch-Davies prescription. However, there is little if anything we can say about those modes with large wavelength $k^{-1} > -\eta_0$ as they were already super-horizon when inflation started. Those modes should have physical effects only at extremely large scales, much larger than the observable universe. We expect them to give an irrelevant contribution to the correlator and thus we will treat them as if they were in the Minkowski vacuum as well.

In our discussion we will not pay too much attention to the particular inflationary dynamics. Instead, we will take the following quite general result for the squeezing parameter during inflation [138]

$$\tau_k^i = \log\left(\frac{1}{-\eta k}\right) \quad \text{for} \quad -\eta_0 > k^{-1} > -\eta\,, \tag{4.21}$$

and $\tau_k = 0$ otherwise. Notice that once inflation ends, this squeezing parameter will have a dependence on the conformal time at the end of inflation, but not at its beginning. The enhancement of the correlation functions for modes affected by inflation during inflation is then

$$1 + \sinh^2 \tau_k^i = \frac{1}{2}\left(\frac{1}{k^2\eta^2} + k^2\eta^2\right) \tag{4.22}$$

and the correlation functions themselves become become

$$\begin{aligned} v^i(\eta,\vec{x})v^i(\eta,\vec{y}) &= \int_k \frac{d^3k}{(2\pi)^3}\frac{1}{4k}\frac{1}{k^2\eta^2}e^{i\vec{k}\cdot(\vec{x}-\vec{y})}\,, \\ p^i(\eta,\vec{x})p^i(\eta,\vec{y}) &= \int_k \frac{d^3k}{(2\pi)^3}\frac{k}{4}\frac{1}{k^2\eta^2}e^{i\vec{k}\cdot(\vec{x}-\vec{y})}\,. \end{aligned} \tag{4.23}$$

Furthermore, during the radiation era the quantum state undergoes additional squeezing, so that its parameter is given by [138]

$$\tau_k^r = \log\left(\frac{1}{|\eta_*|k}\right) + \log\left(\frac{\eta}{|\eta_*|}\right) \quad \text{for} \quad k^{-1} > \eta\,. \tag{4.24}$$

This additional term stops growing once the mode re-enters the horizon at $\eta = k^{-1}$ and reaches $\tau_k^r = 2\log(|\eta_*|k)$. We will restrict ourselves to modes that remain super-horizon in order to avoid encountering non-linearities. It is important to notice that modes that are sub-horizon when inflation ends are not squeezed during the radiation era.

The enhancement of the correlation functions during the radiation era for modes affected by inflation is then

$$1 + 2\sinh^2 \tau_k^r = \frac{1}{2} \left(\frac{1}{k^2\eta_*^2} \left(\frac{\eta}{\eta_{\text{end}}}\right)^2 + k^2\eta_*^2 \left(\frac{\eta_{\text{end}}}{\eta}\right)^2 \right) . \tag{4.25}$$

The second term can be neglected because of the condition $k\eta_{\text{end}} \ll 1$ and the fact that $\eta > |\eta_{\text{end}}|$. The correlators in the random phase approximation for modes that are affect by inflation and stay super-horizon at conformal time η in the radiation era are then given by

$$\begin{aligned} \langle v^r(\eta,\vec{x}) v^r(\eta,\vec{y})\rangle &= \int_k \frac{d^3k}{(2\pi)^3} \frac{1}{4k} \frac{1}{k^2\eta_*^2} \left(\frac{\eta}{\eta_{\text{end}}}\right)^2 e^{i\vec{k}\cdot(\vec{x}-\vec{y})} , \\ \langle p^r(\eta,\vec{x}) p^r(\eta,\vec{y})\rangle &= \int_k \frac{d^3k}{(2\pi)^3} \frac{k}{4} \frac{1}{k^2\eta_*^2} \left(\frac{\eta}{\eta_{\text{end}}}\right)^2 e^{i\vec{k}\cdot(\vec{x}-\vec{y})} . \end{aligned} \tag{4.26}$$

The enhancement of the 2-point correlation functions is translated into a slower decay. The long range behavior of the Minkowski correlation functions is known to be [103, 111]

$$\int \frac{d^3k}{(2\pi)^3} \frac{1}{k} e^{i\vec{k}\cdot\vec{r}} \sim r^{-2} \quad \text{and} \quad \int \frac{d^3k}{(2\pi)^3} k e^{i\vec{k}\cdot\vec{r}} \sim r^{-4} , \tag{4.27}$$

where $r = |\vec{x}-\vec{y}|$. The result is similar when considering other powers of k in the integrand

$$\int \frac{d^3k}{(2\pi)^3} k^\alpha e^{i\vec{k}\cdot\vec{r}} = r^{-(3+\alpha)} \quad \text{for} \quad \alpha > -3 , \tag{4.28}$$

and thus correlations decay fast with distance. This is also true for several of the enhanced terms, as they satisfy this form with $\alpha > -3$. However, there is one term in the field-field correlation function that has $\alpha = -3$. We write this term schematically as[1]

$$\langle v(\eta,\vec{x}), v(\eta,\vec{y})\rangle \supset \mathcal{E}(\eta) I(r) , \tag{4.29}$$

with a function $\mathcal{E}(\eta)$ that carries the time-dependency as

$$\mathcal{E}(\eta) = \begin{cases} \dfrac{1}{4\eta^2} & \text{for} \quad \eta < \eta_* \quad \text{i.e., inflation} \\[2ex] \dfrac{1}{4\eta_*^2} \left(\dfrac{\eta}{\eta_*}\right)^2 & \text{for} \quad \eta > |\eta_*| \quad \text{i.e., radiation era} \end{cases} \tag{4.30}$$

and a function $I(r)$ that keeps track of the spatial dependency, i.e., the decay with distance

$$I(r) = \int_{k\in\text{inf}} \frac{d^3k}{(2\pi)^3} \frac{1}{k^3} e^{i\vec{k}\cdot\vec{r}} . \tag{4.31}$$

[1] Notice the change of notation with respect to ref. [2].

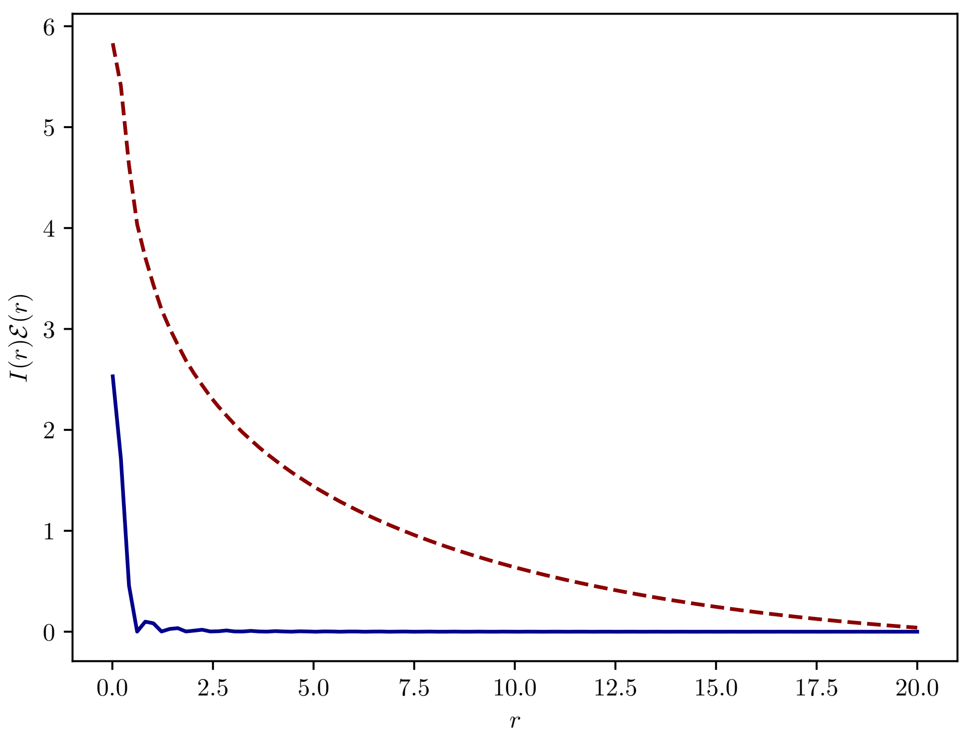

Figure 4.1: An example of the difference between the enhanced correlator (red dashed line) and the Minkowski one (restricted to inflationary modes, blue line) for $-\eta_0 = 10$, $-\eta_* = 0.1$, $\eta = \eta_*$. The Minkowski correlator decays very fast for distances larger than the scale of the largest momentum, while the enhanced correlator has a much slower decay. Adapted from ref. [2].

Strictly speaking, during inflation the upper limit of this integral is given by the comoving scale leaving the horizon at a given time, i.e., $k = |\eta|^{-1}$. Hence, the splitting into a a time-dependent and a spatial-dependent part is rough. In practice, we will also set a time-dependent upper limit during the radiation era, as squeezing stops when modes reenter the horizon and the spatial dependency of the correlation function changes.

In the long-range regime, this integral has an analytic expression

$$I(r) = \frac{1}{2\pi^2}\left[-\,\mathrm{Ci}\left(\frac{r}{-\eta_0}\right) + \mathrm{Ci}\left(\frac{r}{\eta}\right) + \frac{-\eta_0}{r}\sin\left(\frac{r}{-\eta_0}\right) - \frac{\eta}{r}\sin\left(\frac{r}{\eta}\right)\right] \tag{4.32}$$

where Ci is the cosine integral defined as

$$\mathrm{Ci}(x) = -\int_x^\infty \frac{\cos t\,dt}{t} = \gamma + \log x + \int_0^x \frac{\cos t - 1}{t}dt\,. \tag{4.33}$$

And $\gamma = 0.577216...$ is the Euler-Mascheroni constant. Because of the logarithmic behavior of the cosine integral, this term of the field-field correlator decays logarithmically with distance until $r \simeq -\eta_0$, i.e. the enhancement happens only up to length-scales comparable to the wavelength of the longest momentum modes affected by inflation.

If inflation lasts for a finite number of e-folds the correlation vanishes at infinity

$$\lim_{r\to\infty} I(r) = 0\,. \tag{4.34}$$

The expression above is not very intuitive, but we can approximate it by assuming that $r \ll -\eta_0$ which is a reasonable approximation until distances reach the scale of the horizon at the beginning of inflation. Then we have

$$\mathrm{Ci}\left(\frac{r}{-\eta_0}\right) \simeq \gamma + \log\left(\frac{r}{-\eta_0}\right)\,, \quad \sin\left(\frac{r}{-\eta_0}\right) \simeq \frac{r}{-\eta_0}\,. \tag{4.35}$$

Then

$$I(r) \simeq \frac{1}{2\pi^2}\left[\mathrm{Ci}\left(\frac{r}{\eta}\right) - \gamma + \log\left(\frac{-\eta_0}{r}\right) - \left(\frac{\eta}{r}\right)\sin\left(\frac{r}{-\eta_*}\right) + 1\right]. \tag{4.36}$$

Since we are limiting ourselves to super-horizon scales, we can also assume $r \gg \eta$ and perform further approximations

$$\mathrm{Ci}\left(\frac{r}{\eta}\right) \simeq 0\,, \quad \left(\frac{\eta}{r}\right)\sin\left(\frac{r}{\eta}\right) \simeq 0\,. \tag{4.37}$$

And we get the expression

$$I(r) \simeq \frac{1}{2\pi^2}\left[\log\left(\frac{-\eta_0}{r}\right) + 1 - \gamma\right]. \tag{4.38}$$

Even if this is an approximated expression, it will be the one we will make most use of. First, it shows intuitively that correlations are kept at large distances due to the logarithmic dependency. Second, it removes the additional dependency on η as it focuses on super-horizon distances. This makes the high momentum cut-off at $k = |\eta|^{-1}$ less of an issue. Even though it is clearly justified during inflation, it is not much so during the radiation era. In practice, we choose not to deal in detail with modes that re-enter the horizon, which may have a non-trivial time evolution.

The overall physical picture here is that field correlations are enhanced in those momentum modes affected by inflation. This can be understood as modes being stretched out from small scales and then occupied due to particle creation. Distant regions of the universe where in causal contact with the past and keep the resulting correlations as there are no long-range (acausal) interactions able to break these correlations. The next step will be to review the connection between correlation and entropy or information, with the goal of computing the mutual information in real space during inflation and the radiation era.

4.3 Perturbative mutual information

4.3.1 Entropy of the scalar field

Let us now revisit the problem of computing the entropy of a spatial region for a scalar field in a gaussian state. Gaussian states are simple enough for a systematic method to be developed but already include important states such as the Minkowski vacuum or the squeezed state from inflation. In order to do so, we will take advantage of the fact that Gaussian states can be fully characterized by its equal-time 1-point and 2-point correlation functions. We refer the reader to [97–99] for additional details.

The computation of the entropy becomes particularly simple in the case of vanishing expected values

$$\langle v(\vec{x})\rangle = 0 \quad \langle p(\vec{x})\rangle = 0 \tag{4.39}$$

and vanishing symmetrized 2-point cross-correlation function

$$\langle v(\vec{x})p(\vec{y}) + p(\vec{y})v(\vec{x})\rangle = 0\,. \tag{4.40}$$

This is the case for the squeezed state of the curvature perturbation field once the averaging over phases is performed. The other 2-point correlation functions are given by the operator kernels

$$X(\vec{x},\vec{y}) = \langle v(\vec{x})v(\vec{y})\rangle \quad P(\vec{x},\vec{y}) = \langle p(\vec{x})p(\vec{y})\rangle\ . \tag{4.41}$$

Then one defines the operator

$$\Lambda_\Omega = X \cdot P\,, \tag{4.42}$$

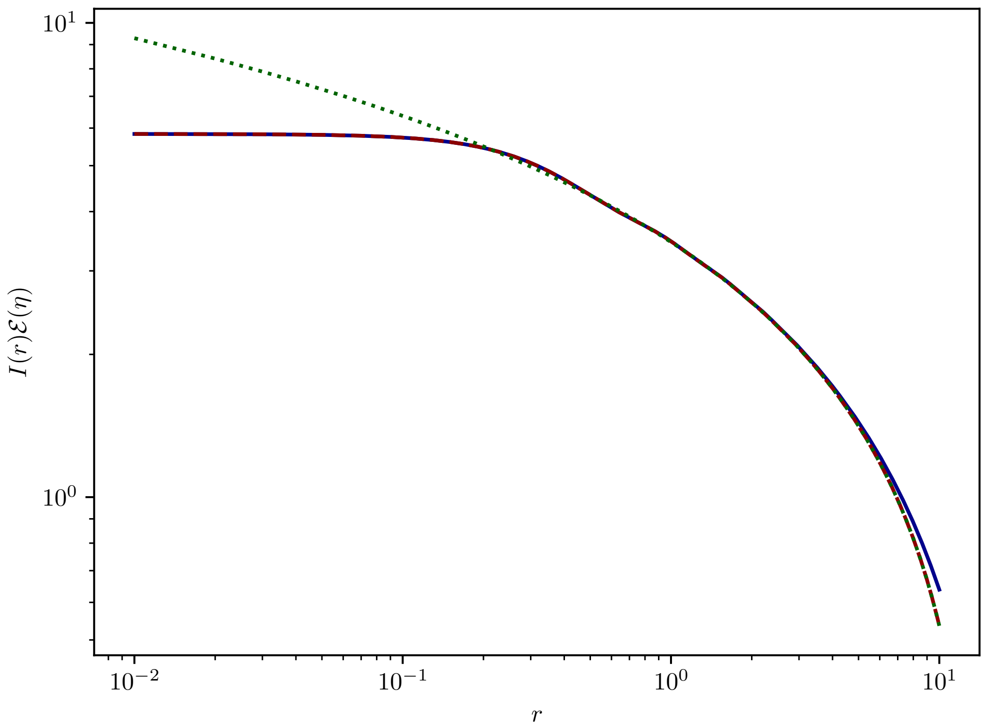

Figure 4.2: Comparison between the exact expression for the enhanced correlator $I(r)$ eq. (4.32) (blue line), its approximation eq. (4.36) (red dashed line), and the further logarithmic approximation eq. (4.38) (green dotted line), for $-\eta_0 = 10, -\eta_* = 0.1$, $\eta = \eta_*$. The agreement is excellent until distances of the order of $r/(-\eta_0) \sim 1$, where both approximations start to slowly diverge. Adapted from ref. [2].

where the operator product is equivalent to a convolution of the kernels

$$\Lambda_\Omega(\vec{x},\vec{y}) = \int_{\Omega^C} d^3z X(\vec{x},\vec{z})P(\vec{z},\vec{y})\,, \tag{4.43}$$

where the region Ω^C comprises the local d.o.f. that we wish to trace out, thereby being left with an operator kernel defined on Ω only. Then the entropy of the complementary region Ω can be computed as

$$S_\Omega = \mathrm{Tr}\Big[\Big(\sqrt{\Lambda_\Omega}+1/2\Big)\log\Big(\sqrt{\Lambda_\Omega}+1/2\Big) - \Big(\sqrt{\Lambda_\Omega}-1/2\Big)\log\Big(\sqrt{\Lambda_\Omega}-1/2\Big)\Big] \tag{4.44}$$

Note that the kernel of the square root is not the square root of the kernel and so we cannot give a closed expression for the kernel $\sqrt{\Lambda_\Omega}(\vec{x},\vec{y})$. However, in order to compute numerically this complicated expression, we do not need to know it. Instead, one needs to solve the eigenvalue problem for Λ_Ω, i.e. find those λ_i for which

$$\int_{\Omega} d^3y \Lambda_\Omega(\vec{x},\vec{y})f_i(\vec{x}) = \lambda_i f_i(\vec{y})\,, \tag{4.45}$$

where f_i is the eigenfunction of Λ_Ω with eigenvalue λ_i. Then one has

$$\begin{aligned} S_\Omega &= \sum_i h(\lambda_i) = \\ &= \sum_i \Big[\Big(\sqrt{\lambda_i}+1/2\Big)\log\Big(\sqrt{\lambda_i}+1/2\Big) - \Big(\sqrt{\lambda_i}-1/2\Big)\log\Big(\sqrt{\lambda_i}-1/2\Big)\Big] \end{aligned} \tag{4.46}$$

Nevertheless, we will compute the mutual information perturbatively, without needing to obtain exact results for S_Ω. That is, if we take $\Omega = A \cup B$, where A and B are, then we have that

$$S_{A\cup B}(r) = S_A + S_B - I(A,B)(r)\,. \tag{4.47}$$

As mentioned before, this method was introduced by Noburo Shiba in ref. [111], although it was applicable only to the vacuum state. We will adapt it to the case of cosmological perturbations by using a more general formalism. The key is that the operator Λ_Ω introduced here can be defined without any reference to the Lagrangian of the theory. Therefore, its validity can be extended to arbitrary Gaussian states, and so we will apply it to the quantum state following inflation. One expects that the mutual information should vanish at infinite distance

$$\lim_{r\to\infty} I(A,B)(r) = 0\,. \tag{4.48}$$

Conversely,

$$\lim_{r\to\infty} S_{A\cup B}(r) = S_A + S_B\,. \tag{4.49}$$

The idea then is to expand perturbatively the joint entropy $S_{A\cup B}$ as the individual entropies S_A and S_B and a term involving functions of the distance that vanish at infinity. This can be already done at the operator level by identifying what terms in $\Lambda_{A\cup B}$ depend on the distance r and expanding them.

For the case at hand, Λ will carry both contributions from the Minkowski vacuum as well as the squeezed modes. The former will be responsible for a mutual information that scales as r^{-4} and thus is of no interest to us. The latter, however, will be responsible for an enhanced mutual information that decays logarithmically.

4.3.2 The perturbative computation

We are interested in perturbative solutions to the eigenvalue problem

$$\int_{\Omega} d^3y \Lambda_{\Omega}(\vec{x},\vec{y}) f_i(\vec{x}) = \lambda_i f_i(\vec{y})\,, \tag{4.50}$$

with the choice

$$\Omega = A \cup B\,, \tag{4.51}$$

where A and B are two disjoint regions of size R_A and R_B separated by a large distance r such that $r \gg R_A, R_B$. Both regions need not be spherical, although this is the simplest and perhaps most interesting application.

We will find these perturbative solutions by following the next steps

- We identify the perturbative and non-perturbative contributions.
- We identify the leading perturbative contribution. In our case this will mean keeping only the enhancement of the correlation functions.

The behavior of Λ_{Ω} depends on whether x and y belong to the regions A or B. We represent this in matrix form

$$\Lambda_{\Omega}(x,y) = \begin{pmatrix} \Lambda_{\Omega}(\vec{x}_a,\vec{y}_a) & \Lambda_{\Omega}(\vec{x}_a,\vec{y}_b) \\ \Lambda_{\Omega}(\vec{x}_b,\vec{y}_a) & \Lambda_{\Omega}(\vec{x}_b,\vec{y}_b) \end{pmatrix}, \tag{4.52}$$

where it is understood that $\vec{x}_a, \vec{y}_a \in A$ and $\vec{x}_b, \vec{y}_b \in B$.

4.3.3 Perturbative part

We take first a look at the off-diagonal terms, as they clearly involve points belonging to different regions. First, we rewrite the off-diagonal terms using the relation

$$\Lambda_{\emptyset}(\vec{x}_{a/b},\vec{y}_{b/a}) = \delta^{(3)}(\vec{x}_{a/b},\vec{y}_{b/a}) = 0\,, \tag{4.53}$$

where $\emptyset = \{\mathbb{R}^3\}^C$ is the empty set. We will use the notation a/b to mean "a or b" and the order will matter if it appears several times in an equation. Then the Dirac delta equals 0 because $\vec{x}_{a/b} \neq \vec{y}_{b/a}$ when one point belongs to A and the other belongs to B. We can then rewrite

$$\Lambda_\Omega(\vec{x}_{a/b}, \vec{y}_{b/a}) = -\Lambda_{\Omega^C}(\vec{x}_{a/b}, \vec{y}_{b/a}), \tag{4.54}$$

with

$$\Lambda_{\Omega^C}(\vec{x}_{a/b}, \vec{y}_{b/a}) = \int_A d^3z_a X(\vec{x}_{a/b}, \vec{z}_a) P(\vec{z}_a, \vec{y}_{b/a}) + \int_B d^3z_b X(\vec{x}_{a/b}, \vec{z}_b) P(\vec{z}_b, \vec{y}_{b/a}). \tag{4.55}$$

Strictly speaking, $\Lambda_\emptyset \simeq \delta$ but the equality is not exact. The difference is small from the operator point of view and we will neglect it. It is also an artifact of assuming random phases.

Notice that for each of the integrals, either the kernel $X(\vec{x}, \vec{y})$ or $P(\vec{x}, \vec{y})$ has a long-distance behavior, i.e. it is evaluated at points belonging to different regions. Both kernels have the form of a Fourier transform, regardless of whether we consider the Minkowksi or the squeezed correlators

$$\begin{aligned} X(\vec{x}, \vec{y}) &= \int \frac{d^3k}{(2\pi)^3} X(k) e^{i\vec{k}(\vec{x}-\vec{y})}, \\ P(\vec{x}, \vec{y}) &= \int \frac{d^3k}{(2\pi)^3} P(k) e^{-i\vec{k}(\vec{x}-\vec{y})}, \end{aligned} \tag{4.56}$$

where the only dependence on the direction of $\vec{k}$ is encoded in the exponential. In the long-distance regime we can approximate

$$\int d\theta \sin\theta e^{ik|\vec{x}-\vec{z}|\cos\theta} \simeq \int d\theta \sin\theta e^{ikr\cos\theta} = \frac{2\sin(kr)}{kr} \tag{4.57}$$

and the integral over z will be irrelevant for this kernel since

$$|\vec{a} - \vec{b}| \simeq r \quad \text{for} \quad \forall \vec{a} \in A, \vec{b} \in B. \tag{4.58}$$

Hence, we will approximate from now on

$$X(\vec{x}_{a/b}, \vec{y}_{b/a}) \simeq \mathcal{E}(\eta) I(r) \tag{4.59}$$

and we will keep only terms involving $I(r)$ in the off-diagonal components of Λ_Ω, since they are the leading perturbative contribution. This leaves us with

$$\delta\Lambda_\Omega(r) = -\mathcal{E}(\eta) I(r) \begin{pmatrix} 0 & \int_B d^3z_b P(\vec{z}_b, \vec{y}_b) \\ \int_A d^3z_a P(\vec{z}_a, \vec{y}_a) & 0 \end{pmatrix}. \tag{4.60}$$

4.3.4 Non-perturbative part

The non-perturbative part of Λ_Ω needs some refinement. One would think first to simply choose its block-diagonal components

$$\Lambda_\Omega^D = \Lambda_\Omega(\vec{x}_{a/b}, \vec{y}_{a/b})\,, \tag{4.61}$$

but this still depends on r, as it integrates over $z \in \Omega^C = (A \cup B)^C$. Instead, we define the non-perturbative part as the limit

$$\Lambda_\Omega^0 = \lim_{r\to\infty} \Lambda_\Omega^D = \begin{pmatrix} \int_{A^C} d^3z X(\vec{x}_a, \vec{z}) P(\vec{z}, \vec{y}_a) & 0 \\ 0 & \int_{B^C} d^3z X(\vec{x}_b, \vec{z}) P(\vec{z}, \vec{y}_b) \end{pmatrix}.$$

The difference is given by a perturbative contribution that decays faster than $I(r)$, as it decays at most as slow as $I(r)$ times an additional perturbative term

$$\Lambda_\Omega^0 - \Lambda_\Omega^D = \begin{pmatrix} \int_B d^3z_b X(\vec{x}_a, \vec{z}_b) P(\vec{z}_b, \vec{y}_a) & 0 \\ 0 & \int_A d^3z X(\vec{x}_b, \vec{z}_a) P(\vec{z}_a, \vec{y}_b) \end{pmatrix}.$$

Since X will decay at most as slow as $I(r)$ and P will decay as some inverse power of r, it is clear that $\Lambda_\Omega^0 - \Lambda_\Omega^D$ is a negligible perturbative term.

We have now a well-posed perturbative approach for the eigenvalue problem.

4.3.5 Non-hermitian perturbation theory

The first thing we should notice when taking the perturbative approach is that neither Λ_Ω^0 nor $\delta\Lambda_\Omega$ are symmetric operators. This means that, in principle, it is not guaranteed that Λ_Ω is diagonalizable or that the computation of its eigenvalues admits the usual perturbative treatment. In practice, one can argue that Λ_Ω is diagonalizable [97], nevertheless the issue of applying perturbation theory remains. For a detailed treatment of non-hermitian perturbation theory we refer the reader to ref. [151]. We will need to work with symmetrized forms of both operators, which we will achieve by introducing the following operator

$$P_0 = \lim_{r\to\infty} P = \begin{pmatrix} P(\vec{x}_a, \vec{y}_a) & 0 \\ 0 & P(\vec{x}_b, \vec{y}_b) \end{pmatrix}, \tag{4.62}$$

so that the operator $P_0\Lambda_\Omega$ is indeed symmetric. Let us see why. For the perturbative part it is pretty straightforward to check that

$$\begin{aligned} &P_0\delta\Lambda_\Omega(\vec{x}_a, \vec{y}_b) = \\ &\quad = -\int_A d^3z_a \int_B d^3z_b P(\vec{x}_a, \vec{z}_a) X(\vec{z}_a, \vec{z}_b) P(\vec{z}_b, \vec{y}_b) \\ &\quad \simeq -\mathcal{E}(\eta) I(r) \int_A d^3z_a \int_B d^3z_b P(\vec{x}_a, \vec{z}_a) P(\vec{z}_b, \vec{y}_b)\,. \end{aligned} \tag{4.63}$$

and

$$
\begin{aligned}
&P_0 \delta\Lambda_\Omega(\vec{x}_b, \vec{y}_a) \\
&\quad = -\int_A d^3 z_a \int_B d^3 z_b P(\vec{x}_b, \vec{z}_b) X(\vec{z}_b, \vec{z}_a) P(\vec{z}_a, \vec{y}_a) \\
&\quad \simeq -\mathcal{E}(\eta) I(r) \int_A d^3 z_a \int_B d^3 z_b P(\vec{x}_b, \vec{z}_b) P(\vec{z}_a, \vec{y}_a)\,,
\end{aligned}
\tag{4.64}
$$

which is is clearly symmetric since P is symmetric. The non-perturbative part is perhaps less obvious

$$
P_0 \Lambda^0_\Omega(\vec{x}_a, \vec{y}_a) = \int_A d^3 z_a \int_{A^C} d^3 z P(\vec{x}_a, \vec{z}_a) X(\vec{z}_a, \vec{z}) P(\vec{z}, \vec{y}_a) \tag{4.65}
$$

and

$$
P_0 \Lambda^0_\Omega(\vec{x}_b, \vec{y}_b) = \int_B d^3 z_b \int_{B^C} d^3 z P(\vec{x}_b, \vec{z}_b) X(\vec{z}_b, \vec{z}) P(\vec{z}, \vec{y}_b)\,. \tag{4.66}
$$

Nevertheless, we can now make use of the relation that was argued previously

$$
\int_{\mathbb{R}^3} d^3 z X(\vec{x}, \vec{z}) P(\vec{z}, \vec{y}) = \delta^{(3)}(\vec{x} - \vec{y}) \tag{4.67}
$$

and rewrite the non-perturbative part as

$$
P_0 \Lambda^0_\Omega(\vec{x}_a, \vec{y}_a) = -\int_A d^3 z_1 \int_A d^3 z_2 P(\vec{x}_a, \vec{z}_1) X(\vec{z}_1, \vec{z}_2) P(\vec{z}_2, \vec{y}_a) + P(\vec{x}_a, \vec{y}_a)\,. \tag{4.68}
$$

One can proceed analogously for $P(\vec{x}_b, \vec{y}_b)$ and check that the result is symmetric.

Next, let us discuss the eigenvalue problem for Λ^0_Ω first. We know that it is diagonalizable and has real eigenvalues [97], but it is still a non-symmetric operator. Therefore, its right and left eigenvectors do not need to coincide. Let us consider a right eigenvector f_i

$$
\Lambda^0_\Omega f^0_i = \lambda_i f^0_i\,. \tag{4.69}
$$

We can apply P_0 on the left and define a new set of vectors $\tilde{f}^0_i := P_0 f^0_i$. Notice what happens if we compute

$$
P_0 \Lambda^0_\Omega f^0_i = \lambda^0_i P_0 f^0_i \equiv \lambda^0_i \tilde{f}^0_i\,. \tag{4.70}
$$

It turns out that $\tilde{f}^0_i$ are left eigenvectors of Λ^0_Ω

$$
\lambda^0_i \tilde{f}^0_i = P_0 \Lambda^0_\Omega f^0_i = \Lambda^{0\dagger}_\Omega P_0 f^0_i = \Lambda^{0\dagger}_\Omega \tilde{f}^0_i\,. \tag{4.71}
$$

For the perturbation theory to work, we would like this set of left and right eigenvectors to form a complete biorthonormal set, i.e. that the following identity is satisfied

$$
\tilde{f}^{0\dagger}_i f^0_j = f^{0\dagger}_i P_0 f^0_j = \delta_{ij}\,. \tag{4.72}
$$

Let us see when this is true, starting from the fact that $P_0\Lambda$ is a symmetric operator

$$0 = f_i^{0\dagger} P_0 \Lambda_\Omega^0 f_j - f_i^{0\dagger} \Lambda_\Omega^{0\dagger} P_0 f_j = (\lambda_j - \lambda_i) \tilde{f}_i^{0\dagger} f_j^0 \,, \tag{4.73}$$

which means that, if the eigenvalues are non-degenerate, then the set of left and right eigenvalues is guaranteed to be biorthonormal. If they are degenerate, one has to look into it more carefully.

We have the intuitive notion from QM that degeneracy arises when a symmetry is present. The corresponding transformation allows us to add additional labels to the degenerate eigenstates and also transform between them. Under which transformations is Λ_Ω^0 invariant? Let us think of the space-time symmetries, which are actually restricted to spatial symmetries, i.e. 3-dimensional rotations and translations, since we are working with equal time correlators.

Translational symmetry is clearly broken by the choice of the regions A and B. It may be only partially broken if these regions are infinite in some direction, but this is not of interest for the case at hand. Then we are left with rotational symmetry only, which is a symmetry only of Λ_Ω^0 restricted to either A or B when these are in turn spherically symmetric regions. In addition to this restricted rotational symmetry, the permutation $A \leftrightarrow B$ is also a symmetry if A and B have the same size and shape and this adds an additional degeneracy.

How can we know that this degeneracy brought by symmetry transformations T is not harmful? The key is that restricted rotations and permutations commute with P_0, which is the operator that maps between left and right eigenvectors

$$[T, P_0] = 0 \,. \tag{4.74}$$

Recall the discussion on complete sets of commuting observables in Quantum Mechanics. Here, because we are dealing with a non-hermitian operator that plays the role of a hamiltonian, not only do we need symmetry (i.e., $[\Lambda, T] = 0$) but also the commuting relation above in order to guarantee the existence of a complete biorthonormal set of eigenstates. It is clear that P_0 is both invariant under restricted rotations and permutations and this is why it commutes with T. Permutations are really not an issue, because it is clear that eigenfunctions defined on different regions A and B are orthogonal. Due to rotational symmetry, we can label the right eigenvectors with degenerated eigenvalue according to its angular momentum

$$f_{ilm} = f_i Y_{lm} \,, \tag{4.75}$$

where Y_{lm} are the spherical harmonics. Furthermore, the left eigenvectors are

$$\tilde{f}_{ilm} = P_0 f_{ilm} = P_0 f_i Y_{lm} = \tilde{f}_i Y_{lm} \,, \tag{4.76}$$

since P_0 commutes with rotations. This guarantees now the biorthonormality relation

$$\tilde{f}_{ilm}^{0\dagger} f_{jl'm'}^0 = \tilde{f}_i^{0\dagger} f_j^0 Y_{lm}^* Y_{l'm'} = \delta_{ij} \delta_{ll'} \delta_{mm'} \tag{4.77}$$

and, therefore, it is guaranteed that Λ^0_Ω is diagonalizable and has a complete biorthogonal set of eigenvectors. We will need this later and in particular we will need the resolution of identity

$$\sum_{ilm} \tilde{f}^0_{ilm} f^{0\dagger}_{ilm} = 1 \,. \tag{4.78}$$

4.3.6 Computation

Let us now deal with the perturbation theory itself. We will keep first- and second-order perturbations to the eigenvalues

$$\lambda_i = \lambda_i^0 + \delta\lambda_i^1 + \delta\lambda_i^2 \,, \tag{4.79}$$

so that the entropy can be computed in perturbation theory

$$S_{AB} = \sum_i h(\lambda_i) = S_A + S_B + \sum_i \left[\delta\lambda_i \frac{dh}{d\lambda_i}\bigg|_{\lambda_i=\lambda_i^0} + \frac{1}{2}(\delta\lambda_i)^2 \frac{d^2h}{d\lambda_i^2}\bigg|_{\lambda_i=\lambda_i^0} \right] , \tag{4.80}$$

where $\delta\lambda_i = \delta\lambda_i^1 + \delta\lambda_i^2$ is the combined first- and second-order perturbation and we simply denote by h the function of the eigenvalues that delivers the entropy. We can clearly identify the mutual information as the third term in the RHS. We will see that the first order perturbation to the entropy vanishes and so the second-order perturbation becomes the most relevant one. The following lines are to great extent a reproduction of the results from ref. [111].

We will try to keep $R_1 \neq R_2$ during the whole computation in order to keep it as general as possible. In fact, we will keep the regions A and B of arbitrary shape. Recall that the non-perturbative operator Λ^0_Ω is divided in two blocks, affecting either region A or B. Each of these blocks may have some common and some different eigenvalues. Then, let us introduce extra indices to take this into account, as well as other possible degeneracies. We label the eigenvalues in increasing order, i.e., $\lambda^0_m > \lambda^0_n$ when $m > n$ and the right eigenvectors with eigenvalue λ^0_m as

$$f^0_{m1\alpha} = \begin{pmatrix} f^0_{m1\alpha}(\vec{x}_a) \\ 0 \end{pmatrix} , \quad f^0_{m2\beta} = \begin{pmatrix} 0 \\ f^0_{m2\beta}(\vec{x}_b) \end{pmatrix} , \tag{4.81}$$

being α and β some possible degeneracies. With this notation, the orthogonality property is written as

$$\tilde{f}^{0\dagger}_{mi\alpha} f^0_{nj\beta} = \delta_{mn}\delta_{ij}\delta_{\alpha\beta} \,. \tag{4.82}$$

The right eigenvector $f_{m\gamma}$ of the full operator Λ_Ω is a linear combination of the eigenvectors of the blocks plus perturbations

$$f_{m\gamma} = \sum_\alpha a_{\gamma\alpha} f^0_{m1\alpha} + \sum_\beta b_{\gamma\beta} f^0_{m2\beta} + f^1_{m\gamma} + f^2_{m\gamma} \equiv \xi^0_{m\gamma} + f^1_{m\gamma} + f^2_{m\gamma} \,. \tag{4.83}$$

Note that if λ_m^0 is not a common eigenvalue of both blocks, then either the $a_{\gamma\alpha}$ or the $b_{\gamma\beta}$ coefficients vanish. We can now plug the perturbative expansion of the right eigenvector $f_{m\gamma}$ in the eigenvalue equation to find

$$\left(\Lambda_\Omega^0 + \delta\Lambda_\Omega\right) f_{m\gamma} = \left(\lambda_m^0 + \delta\lambda_{m\gamma}^1 + \delta\lambda_{m\gamma}^2\right) f_{m\gamma} \,. \tag{4.84}$$

The first order perturbation equation is obtained by neglecting second order perturbations and pluging in the solution to the unperturbed eigenvalue equation

$$\Lambda_\Omega^0 f_{m\gamma}^1 + \delta\Lambda_\Omega \xi_{m\gamma}^0 = \lambda_m^0 f_{m\gamma}^1 + \delta\lambda_{m\gamma}^1 \xi_{m\gamma}^0 \,. \tag{4.85}$$

Similarly, we obtain the second order perturbation equation

$$\Lambda_\Omega^0 f_{m\gamma}^2 + \delta\Lambda_\Omega f_{m\gamma}^1 = \lambda_m^0 f_{m\gamma}^2 + \delta\lambda_{m\gamma}^1 f_{m\gamma}^1 + \delta\lambda_{m\gamma}^2 \xi_{m\gamma}^0 \,. \tag{4.86}$$

We take now the first order perturbation equation and multiply it by $\tilde{f}^{0\dagger}$ on the left

$$\tilde{f}_{mj\gamma'}^{0\dagger} \Lambda_\Omega^0 f_{m\gamma}^1 + \tilde{f}_{mj\gamma'}^{0\dagger} \delta\Lambda_\Omega \xi_{m\gamma}^0 = \lambda_m^0 \tilde{f}_{mj\gamma'}^{0\dagger} f_{m\gamma}^1 + \delta\lambda_{m\gamma}^1 \tilde{f}_{mj\gamma'}^{0\dagger} \xi_{m\gamma}^0 \,. \tag{4.87}$$

Since $\tilde{f}_{mj\gamma'}^{0\dagger}$ is a left eigenvector of Λ_Ω^0, the first terms in the LHS and RHS cancel out, so that we are left with

$$\tilde{f}_{mj\gamma'}^{0\dagger} \delta\Lambda_\Omega \xi_{m\gamma}^0 = \delta\lambda_{m\gamma}^1 \tilde{f}_{mj\gamma'}^{0\dagger} \xi_{m\gamma}^0 \,. \tag{4.88}$$

If we decompose back $\xi_{m\gamma}^0 = \sum_\alpha a_{\gamma\alpha} f_{m1\alpha}^0 + \sum_\beta b_{\gamma\beta} f_{m2\beta}^0$ we can rewrite this equation as

$$\sum_\alpha a_{\gamma\alpha} V_{m\gamma' m\alpha}^{j1} + \sum_\beta b_{\gamma\beta} V_{m\gamma' m\beta}^{j2} = \delta\lambda_{m\gamma}^1 \left(a_{\gamma\gamma'}\delta^{j1} + b_{\gamma\gamma'}\delta^{j2}\right) \,, \tag{4.89}$$

where we have used the orthonormality relation $\tilde{f}_i^{0\dagger} f_j^0 = \delta_{ij}$ and we have introduced the operator

$$V_{m\alpha n\beta}^{ij} = \tilde{f}_{mi\alpha}^{0\dagger} \delta\Lambda_\Omega f_{nj\beta}^0 \,. \tag{4.90}$$

Because of the block structure of $P_0\delta\Lambda_\Omega$, it is clear that $V_{m\alpha n\beta}^{11} = V_{m\alpha n\beta}^{22} = 0$, while the other components take the following form

$$\begin{aligned} V_{m\alpha n\beta}^{12} &= \\ &= -\mathcal{E}(\eta) I(r) \iint_{A^2\times B^2} d^3x_a d^3z_a d^3z_b d^3y_b P(\vec{x}_a, \vec{z}_a) f_{m1\alpha}^0(\vec{x}_a) P(\vec{z}_b, \vec{y}_b) f_{n2\beta}^0(\vec{y}_b) \\ &\equiv -\mathcal{E}(\eta) I(r) C_{m\alpha n\beta} \,. \end{aligned} \tag{4.91}$$

Note the symmetry

$$V_{m\alpha n\beta}^{12} = V_{n\beta m\alpha}^{21} \,, \tag{4.92}$$

which makes the definition of $C_{m\alpha n\beta}$ meaningful. We further define the set of matrices

$$(C_{mn})_{\alpha\beta} \equiv C_{m\alpha n\beta}\,, \tag{4.93}$$

so that the equation for the first order perturbation $\delta\lambda^1_{m\gamma}$ can be rewritten as a block matrix equation

$$-\mathcal{E}(\eta)I(r)\begin{pmatrix}0 & C_{mm}\\ C^T_{mm} & 0\end{pmatrix}\begin{pmatrix}a_\gamma\\ b_\gamma\end{pmatrix} = \delta\lambda^1_{m\gamma}\begin{pmatrix}a_\gamma\\ b_\gamma\end{pmatrix}. \tag{4.94}$$

In the case that λ^0_m is not a common eigenvalue of Λ^0 in both regions A and B, then either the coefficients a_γ or b_γ (notice that they are vectors) vanish and so does the perturbation $\delta\lambda^1_m$. On the contrary, if λ^0_m is indeed a common eigenvalue, then this equation becomes an eigenvalue equation that is solved by means of a characteristic polynomial

$$\begin{aligned}\det\begin{pmatrix}x1_{M_m\times M_m} & -C_{mm}\\ -C^T_{mm} & x_{N_m\times N_m}\end{pmatrix}\\ &= \det(x1_{M_m\times M_m})\det\left(x1_{N_m\times N_m} - x^{-1}C^T_{mm}C_{mm}\right)\\ &= x^{M_m-N_n}\det\left(x^2 1_{N_m\times N_m} - C^T_{mm}C_{mm}\right)\,,\end{aligned} \tag{4.95}$$

where M_m and N_m are the degeneracies of the eigenvalues λ^0_m in each region with the convention $M_m \geq N_m$. In other words, the perturbation is linked to the eigenvalue problem for the matrix $C^T_{mm}C_{mm}$ which is a symmetric positive semi-definite matrix, since C_{mm} is real and symmetric. This means that for all its eigenvalues $c_{m\alpha} \geq 0$ and then the perturbation $\delta\lambda^1_m$ either vanishes or comes in pairs of opposite sign

$$\delta\lambda^1_{m\gamma} = \pm\mathcal{E}(\eta)I(r)\sqrt{c_{m\gamma}}\,, \tag{4.96}$$

and thus the first order perturbation to the entropy vanishes because the following combination also vanishes

$$\sum_\gamma \delta\lambda^1_{m\gamma}\left.\frac{dh}{d\lambda_m}\right|_{\lambda_m=\lambda^0_m} = 0\,. \tag{4.97}$$

Next, we need to deal with the second order perturbation. Recall the relevant equation

$$\Lambda^0_\Omega f^2_{m\gamma} + \delta\Lambda_\Omega f^1_{m\gamma} = \lambda^0_m f^2_{m\gamma} + \delta\lambda^1_{m\gamma}f^1_{m\gamma} + \delta\lambda^2_{m\gamma}\xi^0_{m\gamma}\,. \tag{4.98}$$

We can multiply this time my $\tilde{\xi}^{0\dagger}_{mi\gamma'}$ on the left in order to get rid of the first terms of the left- and right-hand side

$$\tilde{\xi}^{0\dagger}_{m\gamma'}\delta\Lambda_\Omega f^1_{m\gamma} = \tilde{\xi}^{0\dagger}_{m\gamma'}\delta\lambda^1_{m\gamma}f^1_{m\gamma} + \tilde{\xi}^{0\dagger}_{m\gamma'}\delta\lambda^2_{m\gamma}\xi^0_{m\gamma}\,. \tag{4.99}$$

We need an explicit expression for $f^1_{m\gamma}$. Let us look again at the first order perturbation

$$\Lambda^0_\Omega f^1_{m\gamma} + \delta\Lambda_\Omega\xi^0_{m\gamma} = \lambda^0_m f^1_{m\gamma} + \delta\lambda^1_{m\gamma}\xi^0_{m\gamma}\,. \tag{4.100}$$

This means that

$$f^1_{m\gamma} = \left(\Lambda^0_\Omega - \lambda^0_m\right)^{-1} \left(\delta\lambda^1_{m\gamma} - \delta\Lambda_\Omega\right) \xi^0_{m\gamma} \, . \tag{4.101}$$

We now insert the identity operator

$$\begin{aligned} f^1_{m\gamma} &= \left(\Lambda^0_\Omega - \lambda^0_m\right)^{-1} \left(\sum_{n,j,\alpha} f^0_{nj\alpha} \tilde{f}^{0\dagger}_{nj\alpha}\right) \left(\delta\lambda^1_{m\gamma} - \delta\Lambda_\Omega\right) \xi^0_{m\gamma} \\ &= \sum_{n\neq m,j,\alpha} \left(\lambda^0_m - \lambda^0_n\right)^{-1} f^0_{nj\alpha} \tilde{f}^{0\dagger}_{nj\alpha} \delta\Lambda_\Omega \xi^0_{m\gamma} \, . \end{aligned} \tag{4.102}$$

Note that the addend would vanish if $m = n$ due to the equation for the first-order perturbation. Now we can plug this in the equation for $\delta\lambda^2_{m\gamma}$

$$\begin{aligned} &\tilde{\xi}^{0\dagger}_{m\gamma'} \delta\lambda^2_{m\gamma} \xi^0_{m\gamma} \\ &\quad = \tilde{\xi}^{0\dagger}_{m\gamma'} \left(\delta\Lambda_\Omega - \delta\lambda^1_{m\gamma}\right) f^1_{m\gamma} \\ &\quad = \tilde{\xi}^{0\dagger}_{m\gamma'} \left(\delta\Lambda_\Omega - \delta\lambda^1_{m\gamma}\right) \sum_{n\neq m,j,\alpha} \left(\lambda^0_m - \lambda^0_n\right)^{-1} f^0_{nj\alpha} \tilde{f}^{0\dagger}_{nj\alpha} \delta\Lambda_\Omega \xi^0_{m\gamma} \\ &\quad = \sum_{n\neq m,j,\alpha} \left(\lambda^0_m - \lambda^0_n\right)^{-1} \tilde{\xi}^{0\dagger}_{m\gamma'} \delta\Lambda_\Omega f^0_{nj\alpha} \tilde{f}^{0\dagger}_{nj\alpha} \delta\Lambda_\Omega \xi^0_{m\gamma} \, . \end{aligned} \tag{4.103}$$

In the last line we used $\delta\lambda^1_{m\gamma} \tilde{\xi}^{0\dagger}_{m\gamma'} f^0_{nj\alpha} = 0$ for $n \neq m$. Finally, since $\tilde{\xi}^{0\dagger}_{m\gamma'} \xi^0_{m\gamma} = \delta_{\gamma\gamma'}$

$$\begin{aligned} \delta\lambda^2_{m\gamma} &= \sum_{n\neq m,j,\alpha} \left(\lambda^0_m - \lambda^0_n\right)^{-1} \tilde{\xi}^{0\dagger}_{m\gamma} \delta\Lambda_\Omega f^0_{nj\alpha} \tilde{f}^{0\dagger}_{nj\alpha} \delta\Lambda_\Omega \xi^0_{m\gamma} \\ &\equiv \sum_{n\neq m} \left(\lambda^0_m - \lambda^0_n\right)^{-1} \tilde{\xi}^{0\dagger}_{m\gamma} \delta\Lambda_\Omega \hat{\phi}_n \delta\Lambda_\Omega \xi^0_{m\gamma} \, , \end{aligned} \tag{4.104}$$

where we have introduced the projector onto the subspace spanned by the eigenvectors with eigenvalue λ_n

$$\hat{\phi}_n = \sum_{j,\alpha} f^0_{nj\alpha} \tilde{f}^{0\dagger}_{nj\alpha} \, . \tag{4.105}$$

Now we compute the perturbation to the entropy due to the second order perturbation

$$\begin{aligned}
&\sum_{m,\gamma} \delta\lambda^2_{m\gamma} \frac{dh}{d\lambda_m}\Big|_{\lambda_m=\lambda^0_m} \\
&\quad = \sum_{m,\gamma}\sum_{n\neq m} \left(\lambda^0_m - \lambda^0_n\right)^{-1} \tilde{\xi}^{0\dagger}_{m\gamma} \delta\Lambda_\Omega \hat{\phi}_n \delta\Lambda_\Omega \xi^0_{m\gamma} \frac{dh}{d\lambda_m}\Big|_{\lambda_m=\lambda^0_m} \\
&\quad = \sum_{m}\sum_{n\neq m} \left(\lambda^0_m - \lambda^0_n\right)^{-1} \mathrm{Tr}\left(\hat{\phi}_m \delta\Lambda_\Omega \hat{\phi}_n \delta\Lambda_\Omega\right) \frac{dh}{d\lambda_m}\Big|_{\lambda_m=\lambda^0_m} \\
&\quad = \sum_{n}\sum_{m>n} \left(\lambda^0_m - \lambda^0_n\right)^{-1} \mathrm{Tr}\left(\hat{\phi}_m \delta\Lambda_\Omega \hat{\phi}_n \delta\Lambda_\Omega\right) \cdot \left(\frac{dh}{d\lambda_m}\Big|_{\lambda_m=\lambda^0_m} - \frac{dh}{d\lambda_n}\Big|_{\lambda_n=\lambda^0_n}\right) .
\end{aligned} \tag{4.106}$$

In the last line we simply relabelled the indices so that $m > n$. Furthermore, the alternative expression for the projector was used

$$\sum_{\gamma} \xi^0_{m\gamma} \tilde{\xi}^{0\dagger}_{m\gamma} = \hat{\phi}_m \,. \tag{4.107}$$

What is the sign of this expression? Let us take a look at the trace

$$\begin{aligned}
&\mathrm{Tr}\left(\hat{\phi}_m \delta\Lambda_\Omega \hat{\phi}_n \delta\Lambda_\Omega\right) = \\
&\quad = \sum_{i,\alpha,j,\beta} \left(\tilde{f}^{0\dagger}_{ni\alpha} \delta\Lambda_\Omega f^0_{mj\beta}\right)\left(\tilde{f}^{0\dagger}_{mj\beta} \delta\Lambda_\Omega f^0_{ni\alpha}\right) = \sum_{i,\alpha,j,\beta} V^{ij}_{n\alpha m\beta} V^{ji}_{m\beta n\alpha} = \sum_{i,\alpha,j,\beta} \left(V^{ij}_{n\alpha m\beta}\right)^2 \\
&\quad = \sum_{\alpha\beta} \mathcal{E}(\eta)^2 I(r)^2 \left(C_{n\alpha m\beta}\right)^2 \geq 0 \,.
\end{aligned} \tag{4.108}$$

We compute now the derivatives of h

- Function

$$h(\lambda) = \left(\sqrt{\lambda} + 1/2\right) \log\left(\sqrt{\lambda} + 1/2\right) - \left(\sqrt{\lambda} - 1/2\right) \log\left(\sqrt{\lambda} - 1/2\right) . \tag{4.109}$$

- First derivative

$$\frac{dh}{d\lambda}(\lambda) = \frac{1}{2\sqrt{\lambda}} \left[\log\left(\sqrt{\lambda} + 1/2\right) - \log\left(\sqrt{\lambda} - 1/2\right)\right] > 0 \quad \text{for} \quad \lambda > 1/4 \,. \tag{4.110}$$

- Second derivative

$$\frac{d^2h}{d\lambda^2}(\lambda) = \frac{\frac{4\sqrt{\lambda}}{1-4\lambda} + \log\left(\sqrt{\lambda} - \frac{1}{2}\right) - \log\left(\sqrt{\lambda} + \frac{1}{2}\right)}{4\lambda^{3/2}} < 0 \quad \text{for} \quad \lambda > 1/2 \,. \tag{4.111}$$

Furthermore, the first derivative is positive but monotonically decreasing, while the second derivative is negative but monotonically increasing. Both tend to 0 for large λ and blow up for $\lambda \to 1/4$.

In particular, if $m > n$ then $\lambda_m > \lambda_n$ and so

$$\left(\left.\frac{dh}{d\lambda_m}\right|_{\lambda_m=\lambda_m^0} - \left.\frac{dh}{d\lambda_n}\right|_{\lambda_n=\lambda_n^0} \right) < 0 \tag{4.112}$$

and the sign of the perturbation is non-positive.

There is also a second order perturbation coming from the term

$$\sum_{m\gamma} \left(\delta\lambda_m^1\right)^2 \left.\frac{d^2h}{d\lambda_m^2}\right|_{\lambda_m=\lambda_m^0} \leq 0\,, \tag{4.113}$$

and thus the sign of this perturbation is non-positive as well.

The last step is to plug everything into the formula for the mutual information between the two regions

$$\begin{aligned} I(A,B) &= S_A + S_B - S_{AB} \\ &= -\sum_i \left[\delta\lambda_i \left.\frac{dh}{d\lambda_i}\right|_{\lambda_i=\lambda_i^0} + \frac{1}{2}(\delta\lambda_i)^2 \left.\frac{d^2h}{d\lambda_i^2}\right|_{\lambda_i=\lambda_i^0} \right] = -\mathcal{E}(\eta)^2 I(r)^2 G\,(A,B) \geq 0\,. \end{aligned} \tag{4.114}$$

Therefore, there is a non-negative mutual information between disjoin regions that is enhanced due to inflation. Here $G(A,B)$ is a function of the size and possibly the shape of the regions A and B, e.g., for two spherical regions of radii R_1 and R_2 we would have $G(A,B) = G(R_1,R_2)$, but its precise form is not that easy to compute.

Nevertheless, $G(R_1,R_2)$ is a function of the short-range behavior of the operator P and as such its leading term is expected to agree with the Minkowski computation. In that case, one has the following result for the mutual information [111]

$$I_M(A,B) = -\frac{1}{16\pi^4\, r^4} G(A,B)\,. \tag{4.115}$$

Notice that we use the convention of factoring out of $G(A,B)$ not only the long-range dependence on r but also numerical coefficients coming from $X(\vec{x},\vec{y})$. The function $G(A,B)$ was computed numerically by Shiba in ref. [112] and found

$$G(R_1,R_2) \simeq -\frac{1}{4} R_1^2 R_2^2 \times 16\pi^4\,. \tag{4.116}$$

We take this computation to be valid in leading order for our case, because the kernel $X(\vec{x},\vec{y})$ is equal to the Minkowski kernel for most momenta. Dimensions agree but notice that R_i are comoving, not physical, radii.

Having this expression for the perturbative mutual information, we are ready to apply it to cosmological perturbations during the inflationary and radiation eras by simply plugging in the relevant functions $\mathcal{E}(\eta)$ and $I(r)$.

4.4 Application to cosmological perturbations

In the previous section we obtained a perturbative expression for the mutual information in real space as a function of the correlation function $\mathcal{E}(\eta)I(r)$. Using the expressions obtained in sec. 4.2 we can obtain right away the expressions for the mutual information.

Let us first focus on inflation. Recall that during this era particle creation takes place on super-horizon scales. As a consequence, correlations are enhanced and the field-field 2-point correlation function takes the form given by eq. (4.23), i.e.,

$$\begin{aligned} \mathcal{E}(\eta) &= \frac{1}{4\eta^2} \\ I(r) &= \frac{1}{2\pi^2}\left[-\operatorname{Ci}\left(\frac{r}{-\eta_0}\right) + \operatorname{Ci}\left(\frac{r}{\eta}\right) + \frac{-\eta_0}{r}\sin\left(\frac{r}{-\eta_0}\right) - \frac{\eta}{r}\sin\left(\frac{r}{\eta}\right)\right], \end{aligned} \tag{4.117}$$

where the function $I(r)$ admits several approximations. Then the perturbative mutual information in inflation becomes

$$\begin{aligned} I^i(A,B) &\simeq \frac{1}{4}\mathcal{E}(\eta)^2 I(r)^2 R_1^2 R_2^2 \times 16\pi^4 \\ &\simeq \frac{1}{16}\frac{R_1^2R_2^2}{\eta^4}\left[1 - \gamma + \log\left(\frac{-\eta_0}{r}\right) + \operatorname{Ci}\left(\frac{r}{\eta}\right) - \left(\frac{\eta}{r}\right)\sin\left(\frac{r}{\eta}\right)\right]^2, \end{aligned} \tag{4.118}$$

where we already implemented the approximation from eq. (4.36), which is valid for $r < -\eta_0$. More compactly, we arrive at

$$I^i(A,B) \simeq \frac{1}{16}\frac{R_1^2R_2^2}{\eta^4}\left[1 - \gamma + \log\left(\frac{-\eta_0}{r}\right)\right]^2, \tag{4.119}$$

using the approximation from eq. (4.38), which is valid for $-\eta_0 > r > \eta$. We see that the long-range behavior of the correlation function is inherited by the mutual information and thus an enhancement is obtained due to particle creation during inflation. On the one hand, the decay with distance is logarithmic and, therefore, slower than inverse powers of r. On the other hand, the ratio $R_1^2R_2^2/\eta_*^4$ can be potentially very large and does not depend on the distance, as opposed to the mutual information for the Minkowski vacuum, which behaves as $R_1^2R_2^2/r^4$, which is necessarily small for the perturbative approach to work.

Let us now turn to the radiation era. Since solutions to the equation of motion are plane waves, it would seem that there is no additional particle creation during the radiation era.

However, squeezing of a given mode continues as long as it remains super-Hubble. This happens because initial conditions for plane waves fix the mode functions to grow for some time. This leaves an imprint in the function $\mathcal{E}(\eta)$, which takes the following form during the radiation era

$$\mathcal{E}(\eta) = \frac{1}{4\eta_{\rm end}^2}\left(\frac{\eta}{\eta_*}\right)^2 , \tag{4.120}$$

while $I(r)$ stays the same. As a consequence, the perturbative mutual information during the radiation era becomes

$$I^r(A,B) \simeq \frac{1}{16}\frac{R_1^2R_2^2}{\eta_*^4}\left(\frac{\eta}{\eta_*}\right)^4\left[1 - \gamma + \log\left(\frac{-\eta_0}{r}\right)\right]^2 , \tag{4.121}$$

where we already implemented the approximations for the regime $\eta_0 > r > \eta$ on $I(r)$. This result shows a continued growth of the perturbative mutual information with time as η^4/η_*^4 during the radiation era.

4.5 Discussion

4.5.1 Comparison with other work

Some time after the publication in ref. [2] of the results presented in this chapter, Jérôme Martin and Vincent Vennin developed a non-perturbative method to compute entanglement entropy, mutual information and quantum discord [152, 153]. Their formalism is based on coarse-groaning the quantum field on the regions of interest, which allows one the reduce an infinite-dimensional eigenvalue problem, only tractable with approximations, to a finite dimensional one. The similarities and discrepancies between our and their results are useful to delimitate the validity of the perturbative approach to computing mutual information.

Qualitatively, they also find an enhancement of the mutual information, in the sense that the decay is not a power law, as it would be the case in the Minkowski vacuum, but rather a logarithmic or log-logarithmic one. In this sense, the non-perturbative analysis confirms the translation of the long-range behavior of correlation functions into truly long-range mutual information.

Quantitatively, the perturbative and non-perturbative computations agree when the physical radius of the spheres involved is smaller than the Hubble radius during inflation. In our notation, this is equivalent to $R < \eta$, for $\eta < \eta_*$. For $R > \eta_*$, both results depart, having the non-perturbative one essentially a logarithmic dependency, on top of the also logarithmic dependency on the distance. This suggests that the enhancement we found, which goes as R^4/η^4 is actually the first term of a series that does not converge for large values of R/η. This can be understood right away from the Taylor expansion of the

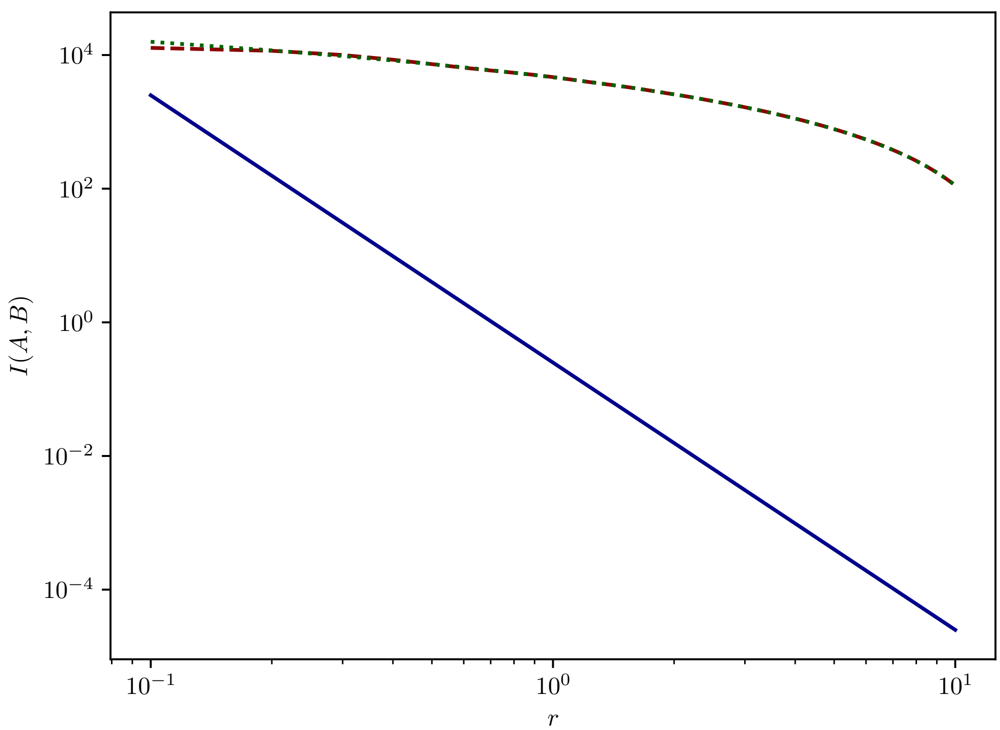

Figure 4.3: Comparison between the mutual information of the Minkowski vacuum eq. (4.115) (blue line) and the enhanced mutual information eqs. (4.118) and (4.119) (red dashed and green dotted lines, as in fig. 4.2), for $\eta_* = -0.1$, $\eta_0 = -10$, $\eta = \eta_*$ and $R_1 = R_2 = 1$ (gray vertical line). Adapted from ref. [2].

logarithm function

$$\log(1+x) = \sum_{k=0}^{\infty} \frac{x^k}{k}\,, \tag{4.122}$$

whose radius of convergence is 1, i.e., it converges only for $|x| < 1$.

Alternatively, it is also possible that the random phase approximation does have a non-negligible effect even at the perturbative level, despite the arguments presented in the appendix A.1.

Nevertheless, we emphasize the validity of the main physical picture: particle creation during inflation does lead to an enhancement of the mutual information between distant regions, which can even be causally disconnected at later times. This is a key feature of inflation that is consistent with our current understanding of some of the fundamental features of the universe. Namely, the Copernican principle can be satisfied thanks to the enhanced mutual information that is shared by causally disconnected patches. We will elaborate on this in the next subsection.

Martin and Vennin also present a way to compute quantum discord for fields non-perturbatively in [152, 153]. They found it to be non-vanishing for both the Minkowski vacuum and the quantum state of primordial perturbation during the inflationary and radiation eras. In chapter 5 we will study whether a non-vanishing quantum discord in field theory can be translated into genuine quantum observations, namely Bell inequality violations.

4.5.2 Long-range correlations

The enhanced mutual information seems intuitively to be connected to some of the main predictions of inflation, such as the leading homogeneous and isotropic nature of the universe and the common causal past of the observable universe. For instance, the CMB temperature anisotropies are characterized with the 2-point correlation function of curvature perturbations. The enhanced mutual information offers a new perspective on a well-known fact, namely that fluctuations in distant points in the sky are tightly correlated. Quantum correlations in the CMB have been explored by computing the quantum discord of primordial perturbations in momentum space [60]. The enhanced mutual information is a first step towards a similar study of quantum correlations in position space in the CMB and possibly other cosmological observables.

Following the ideas presented in [1] we state that, should certain regions collapse to form PBH during the radiation era, the PBH will inherit the enhanced mutual information by the collapsing regions. Furthermore, since the quantum discord is also non-vanishing, some of this mutual information is due to quantum entanglement. Whether this can lead to genuine quantum correlations will be discussed in chapter 5 in the context of Bell inequalities.

Similarly to chapter 3, in our computation we considered a toy model for inflation that delivers an exactly flat power spectrum. Under such circumstances the formation of a PBH is an extremely unlikely event. Hence, in order to compute the mutual information between two PBH, we would need to consider the power spectrum of the particular inflationary model leading to sufficiently abundant PBH formation [64]. It deviates from flatness at scales comparable to the comoving size of the PBH at formation time (or, equivalently, the size of the Hubble scale at formation time), but not for scales well-probed such as the CMB scales. However, this should make no difference for the mutual information shared by PBH separated by distances so large that the power spectrum at the corresponding scale is flat or nearly flat.

Entangled Black Holes have been considered previously in the literature, for instance in the context of the celebrated ER = EPR correspondence [76]. In this framework, one could picture the network of entangled PBH as a network of black holes connected by wormholes that fill the entire Universe. In that case, the mutual information shared by the PBH would most likely be relevant in order to characterize the wormholes that connect them, as long as genuinely quantum correlations are enhanced as well. For instance, two black holes connected by an Einstein-Rosen bridge would be maximally entangled in the ER = EPR correspondence, and so their mutual information would be maximal and equal to the Bekenstein-Hawking entropy of a single black hole.

We wonder whether the entropy of the PBH network can be interpreted as thermodynamical entropy and, in that case, lead to some kind of entropic forces that would affect the dynamics of the network. Entropic forces will be the main topic of part III, where a variational and covariant formulation of non-equilibrium thermodynamics in GR will be presented and some of its phenomenological consequences will be explored. For now, we discuss in the next subsection how entropic forces between PBH may work, although in a pair-wise and non-relativistic set-up.

4.5.3 Entropic forces

Physical forces are usually of two kinds: either fundamental or residual. Entropic forces belong to a third kind: they are due to collective behaviour and its tendency to increase the entropy of a physical system. Conversely, they can be seen as the tendency to decrease the Helmholtz free energy F

$$F = U - TS\,, \tag{4.123}$$

where U, T and S are defined as in sec. 2.6. Following Shiba (see ref. [111]), if the entropy of quantum fields admits a thermodynamic interpretation, then an entropic force X between two black holes arises and is given by

$$X = -\frac{\partial F}{\partial r} = -\frac{\partial U}{\partial r} + T\frac{\partial S}{\partial r}\,. \tag{4.124}$$

Here the physical system is the quantum field itself, not the black holes. Changes in the internal energy U are due to the Casimir effect, which decay quickly as $U \sim r^{-8}$ in the case of spheres. Changes in the entropy, however, decay much slower

$$\frac{\partial S}{\partial r} = -\frac{\partial \mathcal{I}}{\partial r} \sim \frac{1}{r}\,, \tag{4.125}$$

and lead to a repulsive interaction between black holes, which may eventually compete with the attractive gravitational interaction.

4.5.4 Remarks

The quantum origin of primordial curvature perturbations generated during inflation has provided a fascinating explanation for the origin of the matter distribution on large scales. However, it is often thought to offer no distinctive signature or observational feature compared to simply postulating the existence of a classical Gaussian (free) stochastic field of density perturbations. This is due to the suppression of the decaying mode thanks to squeezing, a phenomenon called *decoherence without decoherence* [146], which is actually necessary in order to reproduce the apparently classical features of the primordial power spectrum of matter fluctuations seen in the CMB and LSS.

Nevertheless, there has been recent interest on the quantum nature of the matter distribution and how to properly distinguish quantum from classical perturbations. Although the decaying mode is hopelessly suppressed in both slow-roll and ultra-slow-roll inflation [154], there are actually features of the primordial bi-spectrum (the 3-point correlation function) that would be distinctively quantum and may be probed in the future [102]. On the other hand, the quantum nature of inflationary fluctuations can be explored with rare but highly non-linear phenomena like primordial black hole collapse during the radiation era, that arises precisely because of large non-Gaussian tails due to quantum diffusion during inflation [67]. These events could provide the best clue as to the quantum nature of matter fluctuations generated during inflation, affecting structure formation and constituting a significant component of dark matter [155]. We believe the importance of the quantum origin of cosmological perturbations should not be understated.

In this chapter we have studied the perturbative mutual information between two disjoint regions during the inflationary and radiation eras, which shows an enhancement with respect to the mutual information in the Minkowski vacuum. However, the perturbative approach as presented here seems to overestimate the mutual information, as compared to later non-perturbative results [152, 153]. Even so, these studies found a similar long-distance logarithmic behaviour and pre-factors of $\mathcal{O}(1)$ or larger, which are clearly enhanced with respect to the Minkowski vacuum.

This phenomenon has a quantum origin, in the sense that is linked to squeezing and particle creation. However, this does not mean *per se* that enhanced correlations are genuinely quantum in the sense of chapter 2. It was also found in ref. [152, 153] that quantum discord in real space is non-vanishing for both the Minkowski vacuum and cosmological perturbations, but is enhanced for the latter. This finding is both exciting and striking. On the one hand, it suggests that particle creation during inflation leads to genuine quantum correlations. On the other hand, these correlations seem to be present in the Minkowski vacuum as well, albeit in smaller magnitude. In order to settle this issue, we explore in chapter 5 whether Bell inequalities are satisfied in these contexts.

Finally, it is worth pointing out that even if the enhanced mutual information is dominated by classical correlations, our results offer a new approach to the predictions of inflation. Enhanced mutual information is a fundamental prediction of inflation and is related to a scale-invariant power spectrum of primordial perturbations. Furthermore, future research in the topic of entropic forces, which has precedence in cosmology, could provide relevant observational features. We will deal with entropic forces in part III, although not in the context of PBH.

Chapter 5

Bell inequalities in de Sitter

All that is gold does not glitter,
Not all those who wander are lost;
The old that is strong does not wither,
Deep roots are not reached by the frost.

J.R.R. Tolkien, *The Lord of the Rings (1954)*.

5.1 Motivation

The quantum origin of primordial perturbations is a backbone of the inflationary paradigm, as it was reviewed in chapter 1. Thus, quantum mechanics offers an explanation to the origin of several cosmological observables, such as the CMB anisotropies and the emergence of LSS of the universe. The transition of quantum to classical perturbations is understood to take place either simply by the large squeezing of momentum modes, what John Archibald Wheeler called *decoherence without decoherence* [146], or due to a regular decoherence process [134]. Even though the question whether this explanation suffices is a matter of debate [156], we will assume it to do so and not dive into possible fundamental quantum issues, as observational predictions are unquestioned.

It may seem puzzling that a highly squeezed quantum state is regarded as a *quasi classical* state of some sort, as they have distinctive quantum properties, such as a large quantum discord [60] or violation of Bell inequalities [117], both features introduced in chapter 2. It must be noted, however, that these studies have been mostly carried out in Fourier space, whereas measurements are done in real space. Furthermore, the physical significance of Bell inequalities in Fourier space is unclear. Indeed, their violation is regarded as a genuine quantum feature, in the sense that it implies giving up either locality or realism. However, the requirement of locality only makes sense in real space and it does not seem to be much inconvenient to have non-locality in Fourier space. It may as well be that this is simply what the Bell inequality is signalling.

The study of quantum properties in QFT is in general cumbersome due to the infinite dimension of the Hilbert space. This is not much of an issue in Fourier space, as long as the theory is linear and the quantum state is Gaussian, for the state factorizes into Fourier modes. In real space, on the contrary, the quantum state, even if Gaussian, has a complicated entangled structure. Indeed, this is why only a particular kind of modes was considered in chapter 3 and a perturbative approach was taken in chapter 4. Nevertheless, the dimension of the Hilbert state can be drastically reduced by performing a coarse-graining of the quantum field over regions of interest, as first developed in ref. [152]. This allows several problems to be tackled analytically and non-perturbatively, such as the computation of entanglement entropy, mutual information and quantum discord.

Previous works have found that the quantum discord of a quantum field coarse-grained over two spheres is non-vanishing, both in Minkowski and de Sitter space-time [153], the latter surely being of particular interest for cosmological applications. Still, it is unclear why this happens, given that, contrary to de Sitter, there is no particle creation in Minkowski space-time.

The goal of this chapter is to extend these previous studies to the problem of Bell inequalities in real space. As such, it collects the results obtained in ref. [6]. By inspecting these Bell inequalities, we will attempt to settle whether genuine quantum correlations exist in real space in Minkowski and Sitter space-time. This is a natural continuation of some of the questions raised in chapters 3 and 4 and closes our discussion on the quantum universe that is developed in part II.

This chapter is organized as follows. In sec. 5.2 we present the formalism to build Bell inequalities for quantum fields by means of a particular set of pseudo-spin operators. We apply this to Minkowski and de Sitter space-times in secs. 5.3 and 5.4. We extend this to additional pseudo-spin operators in sec. 5.5 and finish with our discussion of the results in sec. 5.6.

5.2 Bell inequalities for quantum fields

Recall the introduction to Bell inequalities in sec. 2.2. They are usually set up in the context of bipartite systems over which dichotomic measurements can be performed. A paradigmatic example of such systems is two particles with spin, which are separated a large distance.

Quantum fields are quite distinct from discrete particle systems in many respects. First, they take values over all space and one can hardly speak of the position of a quantum field. Second, its phase space described by continuous variables, in particular the value of the field or the conjugate momentum.

In order to be able to construct a Bell inequality for quantum fields, a two-step procedure must be followed. First, one needs to perform a coarse-graining of the field, as mentioned in sec. 5.1, over two spherical regions around given spatial points $\vec{x}_1$ and $\vec{x}_2$. Second, one needs to introduce dichotomic observables as functions of the continuous variables that describe the phase space of quantum fields.

5.2.1 Coarse-grained bipartite systems

First, let us review how to cast two-point measurements of a quantum field in terms of a quantum bipartite system, following the proposal made in ref. [153], where further details can be found. Let $\phi(\vec{x})$ be a real scalar quantum field (since all measurements are performed at the same time, the time argument is omitted for notation convenience) and $\pi(\vec{x})$ its conjugated momentum. We define the field coarse-grained at a location $\vec{x}$ over a radius R as

$$\phi_R(\vec{x}) \equiv \left(\frac{a}{R}\right)^3 \int \mathrm{d}^3\vec{y}\,\phi(\vec{y})\,W\left(\frac{a\,|\vec{y}-\vec{x}|}{R}\right), \tag{5.1}$$

with a similar expression for $\pi_R(\vec{x})$. In this formula, a is the scale factor of the universe, such that space is labelled by comoving coordinates[1], and W is a window function that asymptotes a constant at small arguments and decays at large arguments. It is normalised such that

$$\int_0^\infty z^2 W(z)\mathrm{d}z = 1/(4\pi)\,, \tag{5.2}$$

i.e, such that a uniform field is left invariant by the coarse-graining procedure. Moreover, in order for the coarse-grained configurations of the field to commute when evaluated at two distant spatial locations, the support of W must be taken as compact. In practice, we denote this supporte to be of size $1+\delta$, i.e., $W(z)=0$ for $z\geq 1+\delta$.

Let us then consider two spatial points $\vec{x}_1$ and $\vec{x}_2$ distant by $d \equiv a|\vec{x}_1-\vec{x}_2| > 2R(1+\delta)$. Because of the compactness of W, one has

$$[\phi_R(\vec{x}_1), \phi_R(\vec{x}_2)] = [\pi_R(\vec{x}_1), \pi_R(\vec{x}_2)] = 0\,, \tag{5.3}$$

while the canonical commutation relation $[\phi(\vec{x}), \pi(\vec{y})] = i\delta(\vec{x}-\vec{y})$ gives rise to

$$[\phi_R(\vec{x}_i), \pi_R(\vec{x}_j)] = i4\pi\left(\frac{a}{R}\right)^3 \int_0^{1+\delta} \mathrm{d}z W^2(z)\,\delta_{ij} \equiv i\frac{3}{4\pi}\left(\frac{a}{R}\right)^3 G\,\delta_{ij}\,, \tag{5.4}$$

[1] This is to make the formalism directly applicable to cosmology in sec. 5.4. Otherwise, in flat space-time, one may simply set $a=1$ and use physical coordinates, as in sec. 5.3.

which defines the parameter G, and where the prefactor is arranged such that $G = 1$ for a constant window function with $\delta = 0$. As a consequence, canonical commutation relations for the coarse-grained fields are recovered only after rescaling the fields according to

$$\tilde{\phi}_R(\vec{x}) = \left(\frac{R}{a}\right)\sqrt{\frac{4\pi}{3G(\delta)}}\,\phi_R(\vec{x}) \qquad \text{and} \qquad \tilde{\pi}_R(\vec{x}) = \left(\frac{R}{a}\right)^2\sqrt{\frac{4\pi}{3G(\delta)}}\,\phi_R(\vec{x}). \tag{5.5}$$

The coarse-grained rescaled fields thus describe a bipartite system with canonical commutation relations.

5.2.2 Pseudo-spin operators

Second, we require observables suitable to build a Bell inequality. In a nutshell, this amounts to build a set of *pseudo-spin* operators $\{\hat{\mathcal{S}}_x, \hat{\mathcal{S}}_y, \hat{\mathcal{S}}_z\}$, which satisfy two conditions:

1. $\hat{\mathcal{S}}_x^2 = \hat{\mathcal{S}}_y^2 = \hat{\mathcal{S}}_z^2 = 1$, so that their eigenvalues are ± 1.
2. The $SU(2)$ commutation relations $\left[\hat{\mathcal{S}}_i, \hat{\mathcal{S}}_j\right] = 2i\epsilon_{ijk}\hat{\mathcal{S}}_k$, where ϵ_{ijk} is totally antisymmetric and $\epsilon_{xyz} = 1$.

Several sets fulfilling this criteria can be defined, see ref. [117]. We will focus for the main argument of the chapter on the Gour-Khanna-Mann-Revzen (GKMR) pseudo-spin operators, although another set will also be considered alter.

GKMR operators are built from the eigenstates $\left|\tilde{\phi}_R(\vec{x})\right\rangle$ of the coarse-grained field configuration. Let us first introduce the auxiliary states

$$\begin{aligned} |\mathcal{E}(\vec{x})\rangle &= \frac{1}{2}\left[\left|\tilde{\phi}_R(\vec{x})\right\rangle + \left|-\tilde{\phi}_R(\vec{x})\right\rangle\right] \\ |\mathcal{O}(\vec{x})\rangle &= \frac{1}{2}\left[\left|\tilde{\phi}_R(\vec{x})\right\rangle - \left|-\tilde{\phi}_R(\vec{x})\right\rangle\right] \end{aligned} \tag{5.6}$$

in terms of which the GKMR operators are defined as

$$\begin{aligned} \hat{\mathcal{S}}_x(\vec{x}) &= \int_0^\infty \mathrm{d}\tilde{\phi}_R(\vec{x}) \left[|\mathcal{E}(\vec{x})\rangle\langle\mathcal{O}(\vec{x})| + |\mathcal{O}(\vec{x})\rangle\langle\mathcal{E}(\vec{x})|\right] \\ \hat{\mathcal{S}}_y(\vec{x}) &= i\int_0^\infty \mathrm{d}\tilde{\phi}_R(\vec{x}) \left[|\mathcal{O}(\vec{x})\rangle\langle\mathcal{E}(\vec{x})| - |\mathcal{E}(\vec{x})\rangle\langle\mathcal{O}(\vec{x})|\right] \\ \hat{\mathcal{S}}_z(\vec{x}) &= -\int_0^\infty \mathrm{d}\tilde{\phi}_R(\vec{x}) \left[|\mathcal{E}(\vec{x})\rangle\langle\mathcal{E}(\vec{x})| - |\mathcal{O}(\vec{x})\rangle\langle\mathcal{O}(\vec{x})|\right]. \end{aligned} \tag{5.7}$$

5.2.3 Gaussian states

Now that we have a way to define bipartite states from a quantum field and pseudo-spin operators, we need to characterize the quantum states to be studied within this formalism. We will work with Gaussian states, because they are of particular relevance to cosmology, as they are obtained at linear order in perturbation theory[2]. Furthermore, they are easily dealt with within the phase space formalism of QM, which was reviewed in sec. 2.5. The Wigner function of a Gaussian state is then

$$W_{\hat{\rho}}(\boldsymbol{q}) = \frac{e^{-\frac{1}{2}\boldsymbol{q}^{\mathrm{T}}\boldsymbol{\gamma}^{-1}\boldsymbol{q}}}{(2\pi)^2\sqrt{\det\boldsymbol{\gamma}}}\,, \tag{5.8}$$

where we have arranged the bipartite phase-space variables into the vector $\boldsymbol{q} = (\tilde{\phi}_R(\vec{x}_1), \tilde{\pi}_R(\vec{x}_1), \tilde{\phi}_R(\vec{x}_2), \tilde{\pi}_R(\vec{x}_2))^{\mathrm{T}}$. This Wigner function is fully described by its covariance matrix γ, which can be written in terms of the anticommutator $\{\hat{A}, \hat{B}\} \equiv (\hat{A}\hat{B} + \hat{B}\hat{A})/2$ as [152][3]

$$\begin{aligned}\gamma_{ab} \equiv& \langle\{\hat{q}_a, \hat{q}_b\}\rangle \\ =&\frac{4\pi}{3G}\left(\frac{R}{a}\right)^3\int \mathrm{d}\ln k\,\widetilde{W}^2\left(\frac{R}{a}k\right) \\ &\times\begin{pmatrix} \frac{a}{R}\mathcal{P}_{\phi\phi}(k) & \mathcal{P}_{\phi\pi}(k) & \frac{a}{R}\mathcal{P}_{\phi\phi}(k)\,\mathrm{sinc}\left(\frac{kd}{a}\right) & \mathcal{P}_{\phi\pi}(k)\,\mathrm{sinc}\left(\frac{kd}{a}\right) \\ - & \frac{R}{a}\mathcal{P}_{\pi\pi}(k) & \frac{a}{R}\mathcal{P}_{\phi\phi}(k)\,\mathrm{sinc}\left(\frac{kd}{a}\right) & \frac{R}{a}\mathcal{P}_{\pi\pi}(k)\,\mathrm{sinc}\left(\frac{kd}{a}\right) \\ - & - & \frac{a}{R}\mathcal{P}_{\phi\phi}(k) & \mathcal{P}_{\phi\pi}(k) \\ - & - & - & \frac{R}{a}\mathcal{P}_{\pi\pi}(k)\end{pmatrix}.\end{aligned} \tag{5.9}$$

Note that this expression casts the result in terms of the Fourier transform of the window function

$$\widetilde{W}(z) \equiv 4z^{-3}\int_0^\infty W(u/z)u\sin u\,\mathrm{d}u \tag{5.10}$$

and the reduced power spectra of the field and its momentum, defined as

$$\langle\{\hat{\phi}^\dagger_{\vec{k}}, \hat{\phi}_{\vec{k}'}\}\rangle = 2\pi^2 k^{-3}\mathcal{P}_{\phi\phi}(k)\delta(\vec{k} - \vec{k}') \tag{5.11}$$

with similar expressions for $\mathcal{P}_{\phi\pi}$ and $\mathcal{P}_{\pi\pi}$.

[2] We neglect here unavoidable non-Gaussianities coming from quantum difusion, which lead to non-Gaussian tails in the probability distribution [67].

[3] Note that there is a factor 2 difference in the definition of the covariance matrix with respect to ref. [152].

Here, the Fourier transform is defined as $\hat{\phi}(\vec{x}) = (2\pi)^{-3/2} \int \mathrm{d}\vec{k} e^{-i\vec{k}\cdot\vec{x}} \hat{\phi}(\vec{k})$ with a similar expression for $\hat{\pi}(x)$, and the above definition of the power spectrum assumes isotropy and homogeneity, i.e., the Copernican Principle.

Note that the covariance matrix is symmetric by definition, so that only the upper triangular part has been written explicitly. Furthermore, in our setup subsystems 1 and 2 are taken to be equal, so that the covariance matrix is also symmetric under their exchange. As a consequence, there are only 6 independent entries, namely γ_{11}, γ_{12}, γ_{22}, γ_{13}, γ_{14} and γ_{24}.

It is important to stress that even if the quantum state of the field is pure, the state of the bipartite system we consider is, in general, mixed. This can be understood as a consequence of the quantum state not being a product state in real space, as opposed to Fourier space, and can be seen by computing the purity parameter

$$\mathfrak{p} \equiv \mathrm{Tr}(\hat{\rho}^2) = \frac{1}{4\sqrt{\det \boldsymbol{\gamma}}}, \tag{5.12}$$

which equals one for a pure state but is smaller than one otherwise, and where the second expression is valid for Gaussian state.

This transition from a pure to a mixed state due to tracing over every spatial point that does not lie within the spheres around $\vec{x}_1$ and $\vec{x}_2$ can be understood as an *effective decoherence* mechanism [152, 153], a consequence of the correlations that exist everywhere in real space. This can potentially blur the presence of a genuine quantum signal. Indeed, classical and quantum correlations become harder to tell apart the more mixed the state is. In ref. [152, 153], its effect of quantum discord was investigated. While discord was found to be non-vanishing, its magnitude is still smaller than that of Fourier space [60]. In the following sections we will show how it affects Bell-inequality violations.

Note that tracing-out in Hilbert space is equivalent to phase-space marginalisation (see Appendix D of ref. [157]). This is implemented in the phase-space formulation by integrating the Wigner function over the appropriate phase-space coordinates. The resulting Wigner function is still Gaussian.

5.2.4 Spin correlators

Recall from sec. 2.5 that in the phase-space formulation of QM, a Hilbert space operator $\hat{\mathcal{O}}$ os mapped to a phase-space function $W_{\mathcal{O}}$. Its expectation value is then given by the integral

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}(\hat{\rho}\,\hat{O}) = (2\pi)^2 \int \mathrm{d}\boldsymbol{q} W_{\hat{\rho}}(\boldsymbol{q}) W_{\hat{O}}(\boldsymbol{q}). \tag{5.13}$$

This formula can be used to compute the spin correlators that appear in the definition of the Bell operator. First, we need the Wigner-Weyl transform of the GKMR operators, which are given by

$$
\begin{aligned}
W_{\hat{\mathcal{S}}_x(\vec{x})}\left[\tilde{\phi}_R(\vec{x}), \tilde{\pi}_R(\vec{x})\right] &= \frac{1}{(2\pi)}\text{sign}\left[\tilde{\phi}_R(\vec{x})\right] \\
W_{\hat{\mathcal{S}}_y(\vec{x})}\left[\tilde{\phi}_R(\vec{x}), \tilde{\pi}_R(\vec{x})\right] &= -\frac{1}{(2\pi)}\delta\left[\tilde{\phi}_R(\vec{x})\right]\mathcal{P}\left[1/\tilde{\pi}_R(\vec{x})\right] \\
W_{\hat{\mathcal{S}}_z(\vec{x})}\left[\tilde{\phi}_R(\vec{x}), \tilde{\pi}_R(\vec{x})\right] &= -\frac{1}{2}\delta\left[\tilde{\phi}_R(\vec{x})\right]\delta\left[\tilde{\pi}_R(\vec{x})\right],
\end{aligned}
\tag{5.14}
$$

where $\mathcal{P}$ denotes the principal part. Since $\hat{\mathcal{S}}_i(\vec{x}_1)$ and $\hat{\mathcal{S}}_j(\vec{x}_2)$ act on two separate sectors of the full Hilbert space, where $i,\ j = x,\ y$ or z, the Wigner-Weyl transform of their product is simply given by the product of their Wigner-Weyl transforms, i.e.

$$
W_{\hat{\mathcal{S}}_i(\vec{x}_1)\otimes\hat{\mathcal{S}}_j(\vec{x}_2)}(\boldsymbol{q}) = W_{\hat{\mathcal{S}}_i(\vec{x}_1)}(q_1, q_2)W_{\hat{\mathcal{S}}_j(\vec{x}_2)}(q_3, q_4). \tag{5.15}
$$

From the above expressions, one can thus readily compute the spin correlators in the state eq. (5.8).

In general, one is free to set the directions of the spin measurements in an arbitrary way. It is however common practice to consider the case where $\hat{\mathcal{S}}_a = \hat{\mathcal{S}}_z$, $\hat{\mathcal{S}}_{a'} = \hat{\mathcal{S}}_x$, and $\hat{\mathcal{S}}_b$ and $\hat{\mathcal{S}}_{b'}$ are set in the (xz) plane, i.e. $\hat{\mathcal{S}}_b = \sin\theta\hat{\mathcal{S}}_x + \cos\theta\hat{\mathcal{S}}_z$ and $\hat{\mathcal{S}}_{b'} = \sin\theta'\hat{\mathcal{S}}_x + \cos\theta'\hat{\mathcal{S}}_z$. Since $\left\langle\hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle = 0$ (see below), upon optimising the polar angles θ and θ' such as to get a maximal value for B, one obtains

$$
B = 2\sqrt{\left\langle\hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle^2 + \left\langle\hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle^2}. \tag{5.16}
$$

Therefore, it is enough to compute the correlation functions of two pseudo-spin operators. We will first show the result and afterwords how to obtain them. First we have

$$
\left\langle\hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle = \frac{1}{4\sqrt{\det\boldsymbol{\gamma}}} = \mathfrak{p}, \tag{5.17}
$$

where one recovers the purity parameter introduced in eq. (5.12). This already indicates that the *effective decoherence* mechanism mentioned above leads to a suppression of the expectation value of the Bell operator, since

$$
B = 2\sqrt{\mathfrak{p}^2 + \left\langle\hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle^2}, \tag{5.18}
$$

which can be understood as quantum correlations being reduced. One also has

$$
\left\langle\hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle = -\frac{2}{\pi}\arctan\left[a_{12}(a_{11}a_{22} - a_{12}^2)^{-1/2}\right] \tag{5.19}
$$

where a_{11}, a_{12} and a_{22} are the entries of the symmetric two-by-two matrix

$$\boldsymbol{a} = (\boldsymbol{\gamma}^{-1})^{\phi\phi} - (\boldsymbol{\gamma}^{-1})^{\phi\pi}[(\boldsymbol{\gamma}^{-1})^{\pi\pi}]^{-1}(\boldsymbol{\gamma}^{-1})^{\pi\phi}. \tag{5.20}$$

In this expression, the two overscripts indicate a restriction of the $\boldsymbol{\gamma}^{-1}$ matrix to the lines labelled by the first index, and to the columns labelled by the second index.

Now, let us see how the integrals leading to these correlators are actually performed. Plugging eq. (5.8) and eq. (5.14) into eq. (5.13), one first has

$$\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle = \frac{1}{(2\pi)^2\sqrt{\det\boldsymbol{\gamma}}}\int \mathrm{d}\boldsymbol{q}\ \mathrm{sign}(q_1)\mathrm{sign}(q_3)e^{-\frac{1}{2}\boldsymbol{q}^{\mathrm{T}}\boldsymbol{\gamma}^{-1}\boldsymbol{q}}\,. \tag{5.21}$$

Since the field and momentum coordinates play different roles in this integral, let us first re-arrange the entries of the $\boldsymbol{q}$ vector such that the field coordinates appear first, and then the momentum coordinates

$$\bar{\boldsymbol{q}} = \begin{pmatrix} \tilde{\phi}_R(\vec{x}_1) \\ \tilde{\phi}_R(\vec{x}_2) \\ \tilde{\pi}_R(\vec{x}_1) \\ \tilde{\pi}_R(\vec{x}_2) \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{\boldsymbol{P}} \boldsymbol{q}\,, \tag{5.22}$$

which defines the permutation matrix $\boldsymbol{P}$. In this new basis, the matrix $\boldsymbol{\gamma}^{-1}$ reads

$$\overline{\boldsymbol{\gamma}^{-1}} = \boldsymbol{P}^{\mathrm{T}}\boldsymbol{\gamma}^{-1}\boldsymbol{P} = \begin{pmatrix} (\boldsymbol{\gamma}^{-1})^{\phi\phi} & (\boldsymbol{\gamma}^{-1})^{\phi\pi} \\ (\boldsymbol{\gamma}^{-1})^{\pi\phi} & (\boldsymbol{\gamma}^{-1})^{\pi\pi} \end{pmatrix}, \tag{5.23}$$

the sub-blocks of which are given by

$$\begin{aligned} (\boldsymbol{\gamma}^{-1})^{\phi\phi} &= \begin{pmatrix} (\gamma^{-1})_{11} & (\gamma^{-1})_{13} \\ (\gamma^{-1})_{31} & (\gamma^{-1})_{33} \end{pmatrix}, \qquad & (\boldsymbol{\gamma}^{-1})^{\phi\pi} &= \begin{pmatrix} (\gamma^{-1})_{12} & (\gamma^{-1})_{14} \\ (\gamma^{-1})_{32} & (\gamma^{-1})_{34} \end{pmatrix}, \\ (\boldsymbol{\gamma}^{-1})^{\pi\phi} &= \begin{pmatrix} (\gamma^{-1})_{21} & (\gamma^{-1})_{23} \\ (\gamma^{-1})_{41} & (\gamma^{-1})_{43} \end{pmatrix}, \qquad & (\boldsymbol{\gamma}^{-1})^{\pi\pi} &= \begin{pmatrix} (\gamma^{-1})_{22} & (\gamma^{-1})_{24} \\ (\gamma^{-1})_{42} & (\gamma^{-1})_{44} \end{pmatrix}. \end{aligned} \tag{5.24}$$

We now want to diagonalise the quadratic form $\boldsymbol{q}^{\mathrm{T}}\boldsymbol{\gamma}^{-1}\boldsymbol{q} = \overline{\boldsymbol{q}}^{\mathrm{T}}\overline{\boldsymbol{\gamma}^{-1}}\overline{\boldsymbol{q}}$, in a way that does not modify its two first entries (such that the argument of the sign functions in eq. (5.21) remains unaffected). This can be done by introducing the new variable $\boldsymbol{Q}$ defined as

$$\overline{\boldsymbol{q}} = \begin{pmatrix} \boldsymbol{1} & 0 \\ -\left[(\boldsymbol{\gamma}^{-1})^{\pi\pi}\right]^{-1}(\boldsymbol{\gamma}^{-1})^{\pi\phi} & \boldsymbol{1} \end{pmatrix}\boldsymbol{Q}\,. \tag{5.25}$$

One has

$$\boldsymbol{q}^{\mathrm{T}}\boldsymbol{\gamma}^{-1}\boldsymbol{q} = \boldsymbol{Q}_\phi^{\mathrm{T}}\boldsymbol{a}\boldsymbol{Q}_\phi + \boldsymbol{Q}_\pi^{\mathrm{T}}(\boldsymbol{\gamma}^{-1})^{\pi\pi}\boldsymbol{Q}_\pi\,, \tag{5.26}$$

where we have introduced

$$\boldsymbol{a} = (\boldsymbol{\gamma}^{-1})^{\phi\phi} - (\boldsymbol{\gamma}^{-1})^{\phi\pi}[(\boldsymbol{\gamma}^{-1})^{\pi\pi}]^{-1}(\boldsymbol{\gamma}^{-1})^{\pi\phi} \tag{5.27}$$

and where $\boldsymbol{Q}_\phi$ and $\boldsymbol{Q}_\pi$ are the two-dimensional vectors that compose $\boldsymbol{Q}$, i.e. $\boldsymbol{Q} = \begin{pmatrix}\boldsymbol{Q}_\phi \\ \boldsymbol{Q}_\pi\end{pmatrix}$. Since the Jacobian of the transformation that goes from $\boldsymbol{q}$ to $\boldsymbol{Q}$ is unity, eq. (5.21) gives rise to

$$\begin{aligned}\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle = \frac{1}{(2\pi)^2\sqrt{\det\boldsymbol{\gamma}}} \int \mathrm{d}Q_1\mathrm{d}Q_2\ \mathrm{sign}(Q_1)\mathrm{sign}(Q_2)e^{-\frac{1}{2}\boldsymbol{Q}_\phi^{\mathrm{T}}\boldsymbol{a}\boldsymbol{Q}_\phi} \\ \times \int \mathrm{d}Q_3\mathrm{d}Q_4 e^{-\frac{1}{2}\boldsymbol{Q}_\pi^{\mathrm{T}}(\boldsymbol{\gamma}^{-1})^{\pi\pi}\boldsymbol{Q}_\pi}\,.\end{aligned} \tag{5.28}$$

The integral over $\boldsymbol{Q}_\pi$ is a simple Gaussian integral and can be readily performed. Upon splitting the integral over Q_1 and Q_2 according to their sign, one then finds

$$\begin{aligned}\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle = \frac{1}{2\pi\sqrt{\det\boldsymbol{\gamma}\det(\boldsymbol{\gamma}^{-1})^{\pi\pi}}}\left[\int \mathrm{d}Q_1\mathrm{d}Q_2 e^{-\frac{1}{2}\boldsymbol{Q}_\phi^{\mathrm{T}}\boldsymbol{a}\boldsymbol{Q}_\phi}\right. \\ \left. -2\int_0^\infty \mathrm{d}Q_1\int_{-\infty}^0 \mathrm{d}Q_2 e^{-\frac{1}{2}\boldsymbol{Q}_\phi^{\mathrm{T}}\boldsymbol{a}\boldsymbol{Q}_\phi} - 2\int_{-\infty}^0 \mathrm{d}Q_1\int_0^\infty \mathrm{d}Q_2 e^{-\frac{1}{2}\boldsymbol{Q}_\phi^{\mathrm{T}}\boldsymbol{a}\boldsymbol{Q}_\phi}\right].\end{aligned} \tag{5.29}$$

The first integral is again a simple Gaussian integral, while the second and third integrals are equal because of the invariance of the problem under exchanging $\vec{x}_1$ and $\vec{x}_2$. It can be computed by first integrating over Q_2 and then over Q_1

$$\begin{aligned}&\int_0^\infty \mathrm{d}Q_1\int_{-\infty}^0 \mathrm{d}Q_2 e^{-\frac{1}{2}\boldsymbol{Q}_\phi^{\mathrm{T}}\boldsymbol{a}\boldsymbol{Q}_\phi} = \\ &= \int_0^\infty \mathrm{d}Q_1\int_{-\infty}^0 \mathrm{d}Q_2 e^{-\frac{1}{2}(a_{11}Q_1^2+a_{22}Q_2^2+2a_{12}Q_1Q_2)} \\ &= \int_0^\infty \mathrm{d}Q_1 e^{\left(-\frac{a_{11}}{2}+\frac{a_{12}^2}{2a_{22}}\right)Q_1^2}\int_{-\infty}^0 \mathrm{d}Q_2 e^{-\frac{a_{22}}{2}\left(Q_2+\frac{a_{12}}{a_{22}}Q_1\right)^2} \\ &= \int_0^\infty \mathrm{d}Q_1 e^{\left(-\frac{a_{11}}{2}+\frac{a_{12}^2}{2a_{22}}\right)Q_1^2}\sqrt{\frac{\pi}{2a_{22}}}\left[1+\mathrm{erf}\left(\frac{a_{12}}{\sqrt{2a_{22}}}Q_1\right)\right] \\ &= \frac{\frac{\pi}{2}+\arctan\left(\frac{a_{12}}{a_{11}a_{22}-a_{12}^2}\right)}{\sqrt{a_{11}a_{22}-a_{12}^2}}.\end{aligned} \tag{5.30}$$

Combining the above results, one obtains

$$\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle = -\frac{2}{\pi}\sqrt{\frac{\det\boldsymbol{\gamma}^{-1}}{\det(\boldsymbol{\gamma}^{-1})^{\pi\pi}\det\boldsymbol{a}}}\arctan\left(\frac{a_{12}}{a_{11}a_{22}-a_{12}^2}\right)\,. \tag{5.31}$$

This expression can be further simplified as follows. Using the formula for determinants of block matrices in eq. (5.23), one has

$$\begin{aligned}\det \boldsymbol{\gamma}^{-1} &= \det \overline{\boldsymbol{\gamma}^{-1}} \\ &= \det\left(\boldsymbol{\gamma}^{-1}\right)^{\pi\pi} \det \left\{(\boldsymbol{\gamma}^{-1})^{\phi\phi} - (\boldsymbol{\gamma}^{-1})^{\phi\pi}[(\boldsymbol{\gamma}^{-1})^{\pi\pi}]^{-1}(\boldsymbol{\gamma}^{-1})^{\pi\phi}\right\} \\ &= \det\left(\boldsymbol{\gamma}^{-1}\right)^{\pi\pi} \det \boldsymbol{a}\,,\end{aligned} \tag{5.32}$$

where we have recognised the matrix $\boldsymbol{a}$ defined in eq. (5.27). Upon replacing $\det \boldsymbol{a} = a_{11}a_{22} - a_{12}^2$ in eq. (5.31) by $\det \boldsymbol{\gamma}^{-1}/\det\left(\boldsymbol{\gamma}^{-1}\right)^{\pi\pi}$, one finally obtains

$$\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle = -\frac{2}{\pi}\arctan\left[a_{12}(a_{11}a_{22} - a_{12}^2)^{-1/2}\right], \tag{5.33}$$

which is the equation used in the main text.

The other spin correlators are more straightforward to evaluate. One has

$$\begin{aligned}&\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle = \\ &= \frac{1}{(2\pi)^2\sqrt{\det\boldsymbol{\gamma}}}\int \mathrm{d}\boldsymbol{q}\left[-\pi\delta(q_1)\right]\delta(q_2)\mathrm{sign}(q_3)) e^{-\frac{1}{2}\boldsymbol{q}^{\mathrm{T}}\boldsymbol{\gamma}^{-1}\boldsymbol{q}} \\ &= \frac{-1}{4\pi\sqrt{\det\boldsymbol{\gamma}}}\int \mathrm{d}q_3\mathrm{d}q_4\mathrm{sign}(q_3)e^{-\frac{1}{2}q_3(\gamma^{-1})_{33}q_3-\frac{1}{2}q_4(\gamma^{-1})_{44}q_4-q_4(\gamma^{-1})_{43}q_3} \\ &= \frac{-1}{4\pi\sqrt{\det\boldsymbol{\gamma}}}\sqrt{\frac{2\pi}{(\gamma^{-1})_{44}}}\int \mathrm{d}q_3\mathrm{sign}(q_3)e^{-\frac{1}{2}q_3(\gamma^{-1})_{33}q_3+\frac{\left[(\gamma^{-1})_{43}q_3\right]^2}{2(\gamma^{-1})_{44}}} \\ &= 0\end{aligned} \tag{5.34}$$

since the last integrand is an odd function, to be integrated over the real line. One finally has

$$\begin{aligned}\left\langle \hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle &= \frac{1}{(2\pi)^2\sqrt{\det\boldsymbol{\gamma}}}\int \mathrm{d}\boldsymbol{q}\pi^2\delta(q_1)\delta(q_2)\delta(q_3)\delta(q_4)e^{-\frac{1}{2}\boldsymbol{q}^{\mathrm{T}}\boldsymbol{\gamma}^{-1}\boldsymbol{q}} \\ &= \frac{1}{4\sqrt{\det\boldsymbol{\gamma}}}\,.\end{aligned} \tag{5.35}$$

Before proceeding, let us comment on the window function. As mentioned above, it needs to be compact for the phase-space operators at two different locations to commute. The simplest choice would then be the Heaviside function. Nevertheless, such a function can lead to divergences ref. [152,153] in intermediate, non-observable quantities. Therefore, it is more convenient to consider a continuous window function that is made of a constant piece and of a linear piece:

$$W(x) = \frac{3}{4\pi\mathcal{F}(\delta)}\begin{cases}1 & \text{for} \quad x \leq 1\,, \\ -\frac{1}{\delta}(x-1)+1 & \text{for} \quad 1 < x \leq 1+\delta\,, \\ 0 & \text{for} \quad x > 1+\delta\,,\end{cases} \tag{5.36}$$

where $\mathcal{F}(\delta) = (\delta + 2)(\delta^2 + 2\delta + 2)/4$ is such that the normalisation condition mentioned above is satisfied.

With that expression, the Fourier transform of the window function is given by

$$\widetilde{W}(z) = \frac{3\{z\sin(z) - (1+\delta)z\sin[(1+\delta)z] + 2\cos(z) - 2\cos[(1+\delta)z]\}}{\delta\mathcal{F}(\delta)z^4} \tag{5.37}$$

and one has

$$G(\delta) = \frac{8(\delta^3 + 5\delta^2 + 10\delta + 10)}{5(\delta+2)^2(\delta^2 + 2\delta + 2)^2} . \tag{5.38}$$

Now we have all the ingredients required to compute the expected value of the Bell operator for any Gaussian state. As a test, we will first apply it to the Minkowski vacuum and then go on with the quantum state relevant to cosmological perturbations: the Bunch-Davies vacuum of de Sitter space-time.

5.3 Flat space-time

Now that we have set up the tools required to study Bell inequalities in real space, we consider as first application a massless scalar field placed in the vacuum state of Minkowski space-time. This is the simplest setup and will allow us to test our formalism with a small number of parameters, thus facilitating the discussion on whether violations occur or not. Even though it may seem a trivial case, the fact that quantum discord is non-vanishing [152] leaves the door open for Bell inequalities to be violated. The exception to this is the limit $\delta \to 0$, for which discord does vanish. The aim of this section is to clarify the presence or absence of genuine quantum correlations in the sense of Bell inequalities, regardless of the fact that the Minkowski vacuum contains no particles.

5.3.1 Covariance matrix

After expanding the field into independent Fourier modes, the mode functions in the vacuum state are given by $\phi_{\vec{k}} = e^{-ikt}/\sqrt{2k}$ and $\pi_{\vec{k}} = \dot{\phi}_{\vec{k}} = -i\sqrt{k/2}\,e^{-ikt}$, which give rise to the reduced power spectra

$$\mathcal{P}_{\phi\phi} = k^2/(4\pi^2) , \quad \mathcal{P}_{\pi\pi} = k^4/(4\pi^2) \quad \text{and} \quad \mathcal{P}_{\phi\pi} = 0 \tag{5.39}$$

Plugging those expressions into eq. (5.9), the entries of the covariance matrix can be computed and are given by

$$\begin{aligned} \gamma_{11} &= \frac{\mathcal{K}_1(\delta)}{3\pi G(\delta)} , \qquad \gamma_{12} = 0 , \qquad \gamma_{22} = \frac{\mathcal{K}_3(\delta)}{3\pi G(\delta)} \\ \gamma_{13} &= \frac{\mathcal{L}_1(\alpha,\delta)}{3\pi G(\delta)} , \qquad \gamma_{14} = 0 , \qquad \gamma_{24} = \frac{\mathcal{L}_3(\alpha,\delta)}{3\pi G(\delta)} , \end{aligned} \tag{5.40}$$

where we have introduced the integrals

$$\begin{aligned}\mathcal{K}_\mu(\delta) &= \int_0^\infty z^\mu \widetilde{W}^2(z)\mathrm{d}z \\ \mathcal{L}_\mu(\alpha,\delta) &= \int_0^\infty z^\mu \widetilde{W}^2(z)\,\mathrm{sinc}(\alpha z)\mathrm{d}z\,,\end{aligned} \tag{5.41}$$

which depend on the parameter

$$\alpha \equiv \frac{d}{R}\,, \tag{5.42}$$

which measures the distance between the two patches in units of the patch radius. Note that $\alpha > 2(1+\delta)$ is required in order for the two patches not to overlap. By plugging the expression for $\widetilde{W}$ given below eq. (5.36) into eq. (5.41), those integrals can be performed analytically, and the corresponding expressions can be found in ref. [152].

Let us now evaluate the GKMR spin correlators following the method outlined in subsec. 5.2.4. Since the field-momentum correlators vanish, namely $\gamma_{12} = \gamma_{14} = 0$, one can show that it is also true for the inverse covariance matrix, i.e., $(\boldsymbol{\gamma}^{-1})^{\phi\pi} = \mathbf{0}$. As a consequence, eq. (5.20) leads to

$$\boldsymbol{a} = (\boldsymbol{\gamma}^{-1})^{\phi\phi} = \frac{1}{\gamma_{11}^2 - \gamma_{13}^2}\begin{pmatrix}\gamma_{11} & -\gamma_{13} \\ -\gamma_{13} & \gamma_{11}\end{pmatrix}, \tag{5.43}$$

so eq. (5.19) and eq. (5.17) give rise to

$$\begin{aligned}&\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle \\ &\quad= \frac{2}{\pi}\arctan\left(\frac{\gamma_{13}}{\sqrt{\gamma_{11}^2-\gamma_{13}^2}}\right) = \frac{2}{\pi}\arctan\left[\frac{\mathcal{L}_1(\alpha,\delta)}{\sqrt{\mathcal{K}_1^2(\delta)-\mathcal{L}_1^2(\alpha,\delta)}}\right] \\ &\left\langle \hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle \\ &\quad= \frac{1}{4\sqrt{\left(\gamma_{11}^2-\gamma_{13}^2\right)\left(\gamma_{22}^2-\gamma_{24}^2\right)}} = \frac{9\pi^2 G^2(\delta)}{4\sqrt{\left[\mathcal{K}_1^2(\delta)-\mathcal{L}_1^2(\alpha,\delta)\right]\left[\mathcal{K}_3^2(\delta)-\mathcal{L}_3^2(\alpha,\delta)\right]}}\end{aligned} \tag{5.44}$$

where the result is also given in terms of the integrals introduced in eq. (5.41).

By plugging those expressions into eq. (5.16), one obtains an explicit formula for the expectation value of the Bell operator in terms of the two parameter α and β. The result is displayed in the left panel of fig. 5.1 for $\delta = 0.01$ and as a function of α. One can see that $B(\vec{x}_1, \vec{x}_2)$ decreases with α and reaches an asymptotic value at large distances between the two patches. This can be understood by expanding the above formulas in the limit where

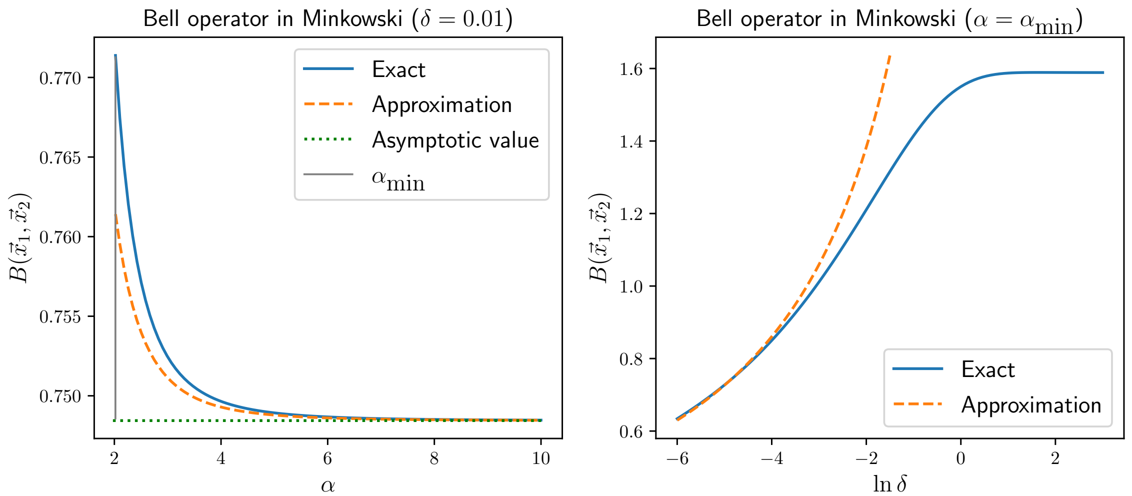

Figure 5.1: Expectation value of the GKMR Bell operator in the Minkowski vacuum. Left panel: $\delta = 0.01$ and α is varied from its minimum allowed value, $\alpha_{\rm min} = 2(1+\delta)$, to larger values. The blue solid line stands for the full result, the orange dashed line is obtained from the small-δ, large-α approximation eq. (5.46), and the green dotted line corresponds to the asymptotic value at large α. Right panel: $\alpha = \alpha_{\rm min}$ (which maximises the expectation value of the Bell operator, see left panel) and δ is varied. The approximation eq. (5.46), displayed in orange, still provides a good fit to the full result at small δ, even though $\alpha_{\rm min}$ is not so much larger than one. From these figures one concludes that Bell inequalities are never violated in this setup. From ref. [6]

δ is small but α is large, which gives rise to

$$\begin{aligned}\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle &\simeq \frac{8}{9\pi\alpha^2}(1+\delta) + \mathcal{O}\left(\frac{\delta^2}{\alpha^2}, \frac{1}{\alpha^4}\right), \\ \left\langle \hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle &\simeq \frac{4\pi^2}{9\left(1-2\ln\frac{\delta}{2}\right)}\left[1 + \frac{8}{81\alpha^4} + \mathcal{O}\left(\delta, \frac{1}{\alpha^6}\right)\right]\end{aligned} \tag{5.45}$$

Together with eq. (5.16), this leads to

$$B \simeq \frac{8\pi^2}{9\left(1-2\ln\frac{\delta}{2}\right)}\left\{1 + \frac{2}{\alpha^4}\left[\frac{4}{81} + \left(\frac{1-2\ln\frac{\delta}{2}}{\pi^3}\right)^2\right]\right\}, \tag{5.46}$$

which is displayed as the orange dashed line in fig. 5.1. One can check that, when $\alpha \gg 1$, it provides a good fit to the full result indeed. At large α, B reaches a constant that is given by the first term of eq. (5.46) and which is controlled by the purity of the state. It is displayed with the green dotted line. Note that the case $\delta = 0$ is singular, and leads to $B \simeq 16/(9\pi\alpha^2)$ at large α (so the asymptotic value vanishes).

Since B is maximal when α is minimal, in the right panel of fig. 5.1 we set α to its minimal value and let δ vary, so as to optimise the expectation value of the Bell operator. One can see that B increases with δ,[4] and reaches an asymptotic value at large δ of order 1.6. This is therefore the largest value one can obtain in this setup, and since it is smaller than 2, we conclude that GKMR Bell inequalities are never violated in flat space time.

5.3.2 Discussion

We thus conclude this section by reporting no real-space Bell-inequality violation with the GKMR pseudo-spin operators in the Minkowski vacuum state. This settles the question raised earlier and establishes that, even though quantum discord in real space is non-vanishing for this state, there is still no Bell inequality violation. This can be understood from the fact that the interpretation of quantum discord for mixed states is less clear than when dealing with pure states. One could argue that this result is actually a consequence of the choice of pseudo-spin operators. Therefore, we will generalize our discussion to a larger class of spin operators in sec. 5.5.

One may argue that this result was to be expected from the fact that the Minkowski vacuum contains no particles. In the next section we take a next step and perform the same computation for the Bunch-Davies vacuum in de Sitter space-time, in order to find out whether the situation changes when particle creation takes place.

It is worth point out that it was found in ref. [152] that quantum discord decays as α^{-4} at large distances. The behaviour of quantum discord as a function of α is therefore the same as for the Bell expectation value, and in that sense, it may be seen as a useful tracer for identifying the configurations that are most likely to yield quantum effects. However, as we shall now see, this is not always true, since this behaviour similarity is lost in de-Sitter space times.

5.4 De-Sitter space-time

Let us now turn our attention to de-Sitter space times, in order to address the case of primordial cosmological perturbations. Since particle creation takes place in this setup, it is worth exploring how the situation changes with respect to Minkowski space-time.

[4] When $\delta \to 0$, $\alpha_{\rm min} \to 2$ and one has $\mathcal{L}_1 = 3(13 - 16\ln 2)/20$, $\mathcal{L}_3 = 3(\ln 2 - 1)/2$, $\mathcal{K}_1 = 9/4$ and $\mathcal{K}_3$ diverges logarithmically with δ. This leads to $B \simeq 0.16$, which corresponds to the lower asymptotic value in the right panel of fig. 5.1 that would be reached if the horizontal axis extended to large enough negative values.

Recall that we describe scalar primordial perturbations by means of the Mukhanov-Sasaki variable, as discussed in chapter 1. It is placed in the Bunch-Davies state [55], which is in excellent agreement with observations of the cosmic microwave background [38]. The Fourier mode functions of the field v and its conjugated momentum p are thus given by

$$v_{\vec{k}} = \frac{e^{-ik\eta}}{\sqrt{2k}}\left(1 - \frac{i}{k\eta}\right) \quad \text{and} \quad p_{\vec{k}} = v'_{\vec{k}} - \frac{a'}{a}v_{\vec{k}} = -i\sqrt{\frac{k}{2}}\, e^{-ik\eta}\,, \tag{5.47}$$

and allow us to compute the reduced power spectra.

5.4.1 Covariance matrix

The reduced power spectra associated to the mode functions in eq. (5.47) read

$$\mathcal{P}_{vv}(k) = \frac{1+k^2\eta^2}{4\pi^2\eta^2}\,, \qquad \mathcal{P}_{pp}(k) = \frac{k^4}{4\pi^2}\,, \qquad \mathcal{P}_{vp}(k) = \frac{k^2}{4\pi^2\eta}\,. \tag{5.48}$$

The covariance matrix is then obtained by plugging these expressions into eq. (5.9), and this leads to

$$\begin{aligned}
\gamma_{11} &= \frac{(HR)^2}{3\pi G(\delta)}\left[\mathcal{K}_{-1}(\beta,\delta) + \frac{1}{(HR)^2}\mathcal{K}_1(\beta,\delta)\right],\\
\gamma_{12} &= -\frac{HR}{3\pi G(\delta)}\mathcal{K}_1(\beta,\delta)\,, \qquad \gamma_{22} = \frac{\mathcal{K}_3(\beta,\delta)}{3\pi G(\delta)}\,,\\
\gamma_{13} &= \frac{(HR)^2}{3\pi G(\delta)}\left[\mathcal{L}_{-1}(\alpha,\beta,\delta) + \frac{1}{(HR)^2}\mathcal{L}_1(\alpha,\beta,\delta)\right],\\
\gamma_{14} &= -\frac{HR}{3\pi G(\delta)}\mathcal{L}_1(\alpha,\beta,\delta)\,, \qquad \gamma_{24} = \frac{\mathcal{L}_3(\alpha,\beta,\delta)}{3\pi G(\delta)}\,.
\end{aligned} \tag{5.49}$$

Therefore, it depends on four parameters, namely HR, α, β and δ. The parameters α and δ are defined identically to those introduced in sec. 5.3. We recall that they respectively correspond to the distance between the two patches in units of their radius, see eq. (5.42), and to the smoothing parameter of the window function, see eq. (5.36). In addition, there are the parameters HR and β, which include the effects of space-time dynamics. The parameter HR corresponds to the ratio between the size of the patches and the Hubble radius, which is the typical distance that characterises the curvature of space-time. The parameter β is defined as the ratio between the size of the observed patches and the size of the entire observable universe, i.e., the size of the region over which observations are performed,

$$\beta \equiv \frac{R}{R_{\text{obs}}} < 1\,. \tag{5.50}$$

The reason to do that is that, in practice, cosmological perturbations are measured as fluctuations away from an average configuration. This average is computed as a mean value over a finite part of the universe, the size of which is denoted R_{obs}. This implies that, in eq. (5.9), the window function needs to be replaced according to

$$\widetilde{W}(kR/a) \to \widetilde{W}(kR/a) - \widetilde{W}(kR_{\mathrm{obs}}/a)\,. \tag{5.51}$$

This can be simply modelled by imposing an infra-red cutoff $k > \beta a/R$ in the integral of eq. (5.9), see ref. [153] for further details. The integrals $\mathcal{K}$ and $\mathcal{L}$ are thus defined in a similar way as in eq. (5.41) but with β as a lower bound, namely

$$\begin{aligned} \mathcal{K}_\mu(\beta,\delta) &= \int_\beta^\infty z^\mu \widetilde{W}^2(z)\mathrm{d}z\,, \\ \mathcal{L}_\mu(\alpha,\beta,\delta) &= \int_\beta^\infty z^\mu \widetilde{W}^2(z)\,(z)\,\mathrm{sinc}(\alpha z)\mathrm{d}z\,. \end{aligned} \tag{5.52}$$

These integrals can be computed analytically in terms of the cosine integral function. The relevant formulas can be found in appendix A of ref. [153], where a systematic expansion in the regime $\beta \ll 1$, $\delta \ll 1$ and $\alpha \gg 1$ is also performed. Let us finally note that, in the limit where $H = 0$ (i.e., static space time), eq. (5.49) becomes the Minkowski formula in eq. (5.40), which serves as a consistency check.

5.4.2 Spin and Bell correlators

We now compute the expectation value of the Bell operator by plugging the covariance matrix eq. (5.49) into the formulas of subsec. 5.2.4. The result is displayed in fig. 5.2. Since there is at most a logarithmic dependence of the result on these parameters, they do not play a crucial role. Hence, we choose to show in 5.2 how the result depends on HR and α instead. The dependence on δ and β is shown for completeness in appendix B.1.

One can see that two regimes need clearly to be distinguished, depending on whether $HR \ll 1$ (i.e. the size of the patches is smaller than the Hubble radius) or $HR \gg 1$ (i.e. the patches are larger than the Hubble radius).

When $HR \ll 1$, the result seems to carry little dependence on α, and coincides with the values obtained in the left panel of fig. 5.1 in the Minkowski vacuum. This is because, when $HR \ll 1/\alpha$, all distances involved in the problem (namely R and d) are smaller than the Hubble radius, hence the setup is equivalent to a local Minkowski background. This is why the results of sec. 5.3 are recovered in this regime, which can be formally verified by expanding the above formulas in HR and then in α^{-1}, leading to

$$
\begin{aligned}
\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle &\simeq \\
&\simeq \frac{8}{9\pi\alpha^2} + (HR)^2\left\{\frac{8}{9\pi}\left[\gamma_{\mathrm{E}} + \ln(\alpha\beta) - 1\right] + \frac{32\left[5\gamma_{\mathrm{E}} - 11 + 5\ln(2\beta)\right]}{405\alpha^2\pi}\right\}, \\
\left\langle \hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle &\simeq \frac{4\pi^2}{9|1-2\ln\frac{\delta}{2}|} + \frac{8\pi^2}{81}(HR)^2 \\
&\times \frac{1}{(1-2\ln\frac{\delta}{2})|(1-2\ln\frac{\delta}{2})|}\Big(1 + 2\gamma_E(1+2\ln 2) - 5\ln 2 + 4\ln^2 2 + \\
&+ \ln\beta(2-4\ln\frac{\delta}{2}) + (7-4\gamma_{\mathrm{E}} - 4\ln 2)\ln\delta\Big)
\end{aligned}
\tag{5.53}
$$

where γ_{E} is Euler's constant and the result is further expanded in δ and β. One thus recovers eq. (5.45), with corrections suppressed by $(HR)^2$.

An in-between regime is give if $1/\alpha \ll HR \ll 1$, R is smaller than the Hubble radius but not d, hence the flat space-time result may be modified a priori. That is, the two spheres are smaller than the Hubble sphere and exist in different Hubble patches. However, this regime cannot be seen in fig. 5.2 since it does not display large-enough values of α. This is why, in fig. 5.3, the expectation value of the Bell operator is shown as a function of α, where β and δ are fixed to the same value as in fig. 5.2, and where we have set $HR = 10^{-2}$. For comparison, the flat space-time result is also displayed. No strong deviation from the de-Sitter result can be observed, even when d is larger than the Hubble radius. In any case, one can see that B decreases with α. Therefore, when $HR \ll 1$, B is maximal in the Minkowski limit, where we have already shown that there is no Bell-inequality violation.

When $HR \gg 1$, one can see in fig. 5.2 that an asymptotic value is also reached, which decreases with α. This can be understood analytically by performing a large HR, large α

expansion of the above formulas, which leads to

$$
\begin{aligned}
\left\langle \hat{\mathcal{S}}_x(\vec{x}_1)\hat{\mathcal{S}}_x(\vec{x}_2)\right\rangle \simeq \\
&\simeq \frac{2}{\pi}\arctan\left\{\frac{4\left[1-\gamma_{\mathrm{E}}-\ln(\alpha\beta)\right]}{\sqrt{\left(\beta+4\ln\frac{\alpha}{2}\right)\left[11-8\gamma_{\mathrm{E}}-4\ln(2\alpha\beta^2)\right]}}\right\}, \\
\left\langle \hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle \simeq \\
&\simeq \frac{2\pi^2}{(HR)^2}\left\{\left[4\gamma_{\mathrm{E}}(1+2\ln 2)-1-9\ln 2+4\ln^2 2+2\ln\left(\alpha\beta^2\right)\left(1-2\ln\frac{\delta}{2}\right)\right.\right. \\
&\left.+\ln\delta\left(11-8\gamma_{\mathrm{E}}-4\ln 2\right)\right]\times \\
&\left.\times\left[3-\ln 2+4\ln^2 2-\ln\alpha\left(2-4\ln\frac{\delta}{2}\right)+(3-4\ln 2)\ln\delta\right]\right\}^{-1/2}.
\end{aligned}
\tag{5.54}
$$

In addition to the clear distinction between the two regimes, the main conclusion of our analysis is that maximum expectation value for the Bell operator is obtained for large HR and α close to its minimum value. This happens when the coarse-graining scale R is large compared to the Hubble radius, and the two patches are almost adjacent. In appendix B.1, we further show that decreasing δ and β make B larger, but not to the extent of leading to a Bell inequality violation. In fact, we can derive an upper bound on B as follows. Formally, when $\beta \to 0$, the integrals $\mathcal{K}_{-1}$ and $\mathcal{L}_{-1}$ logarithmically diverge, and in the limit $\delta \to 0$, $\mathcal{K}_3$ logarithmically diverges too. This behaviour is such that $\mathfrak{p} = \left\langle \hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle \propto 1/\ln(\beta\delta) \to 0$ in this limit, and such that the argument of the arctan function in eq. (5.19) goes to a finite constant (that only depends on α if one further lets $HR \to \infty$). This proves that $\left\langle \hat{\mathcal{S}}_z(\vec{x}_1)\hat{\mathcal{S}}_z(\vec{x}_2)\right\rangle < 1$ in this limit, hence $B < 2$, see eq. (5.16), which therefore applies to the whole parameter space.

5.4.3 Discussion

The fact that no Bell-inequality violation is found in de Sitter is non trivial. One would expect that, since entangled pairs of particles with opposite Fourier momenta are produced on super-Hubble scales, this would lead to genuine quantum correlations. Indeed, the quantum state in Fourier space in highly squeezed, which means that its quantum discord is large as well [60,150] and Bell inequalities are violated (both with the GKMR operators and with other pseudo-spin operators, see ref. [117,158]). The reason why this is no longer the case in real space is subtle. Because the quantum state is correlated everywhere and large spatial regions are traced over, one deals with mixed states. This impacts quantum discord as well, so that it becomes smaller in real space than it is in Fourier space [153], although it is still non zero. This suggests that quantum discord may not always provide a direct probe of genuine quantum correlations in the context of mixed states.

The relationship between quantum discord and Bell inequalities gives a rich scale dependency. In fig. 5.4 we show these quantities and other relevant ones, such as mutual information and purity, as a function of HR. The parameters α, β and δ are kept fixed. One finds that B reaches a plateau in both the $HR \ll 1$ (Minkowski) and $HR \gg 1$ limits, being the latter higher than the former, with a transition from one to the other around $HR \sim \mathcal{O}(1)$. In contrast, quantum discord vanishes in these two limits, and is maximal when HR is of order one. Therefore, contrary to the flat space-time case discussed in sec. 5.3, discord cannot be used to identify the setup configuration that maximises our ability to detect quantum features.

For comparison, the state purity introduced in eq.(5.12) is also shown in fig 5.4. In the limit $HR \ll 1$, it shares the same behaviour as $B/2$, as already explained in sec. 5.3. In this regime, the more mixed the quantum state is, the smaller the value of B is, which is intuitive. However, in the large HR limit, the behaviour of the state purity and of the Bell expectation value are opposite: $\mathfrak{p}$ decreases with HR while B increases. This can be understood as follows. Since more entangled particle are created at large scales, the field becomes more correlated in real space as R increases, as can be seen at the level of the mutual information $\mathcal{I}$, which only increases with HR. It explains why the state purity decreases (one traces over regions of space to which the system is more and more entangled).

Both quantum discord and the Bell operator are driven by a compromise between the amount of quantum entanglement (measured by mutual information $\mathcal{I}$) and the state purity $\mathfrak{p}$. But since these two quantities evolve in opposite ways, how the trade-off is settled is a priori not trivial, and it happens to be settled in different ways for $\mathcal{D}$ and $\mathcal{B}$.

5.5 Other pseudo-spin operators

In the previous sections we have studied GKMR pseudo-spin operators in field theory, and use the general formalism to show that real-space Bell inequalities built with them are not violated neither in Minkowski nor in de Sitter space-time. Since GKMR are built from the fields and, in principle, one of possibly many pseudo-spin operators, one may argue that our result is a mere consequence of the choice of pseudo-spin operator. Therefore, one may hope to achieve Bell inequality violations by considering other operators. Unfortunately, it is not possible to verify (at least with the present approach) all possible pseudo-spin operators, given that there may exist an infinite number of them and that only a few explicit constructions are known [117, 159]. However, in this section we will still consider another set of pseudo-spin operators: the Larsson spin-operators [160], which is in fact an infinite, one-parameter family of spin operators.

5.5.1 Larsson pseudo-spin operators

The idea of the Larsson pseudo-spin operators is to split the real axis describing the scalar field value into intervals of size ℓ, where ℓ can be freely chosen by the observer. One then introduces [160]

$$
\begin{aligned}
\hat{S}_x^\ell(\vec{x}) &= \sum_{n=-\infty}^{\infty} \int_{2n\ell}^{(2n+1)\ell} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left[\left|\tilde{\phi}_R(\vec{x})+\ell\right\rangle\left\langle\tilde{\phi}_R(\vec{x})\right| + \left|\tilde{\phi}_R(\vec{x})\right\rangle\left\langle\tilde{\phi}_R(\vec{x})+\ell\right| \right], \\
\hat{S}_y^\ell(\vec{x}) &= -i \sum_{n=-\infty}^{\infty} \int_{2n\ell}^{(2n+1)\ell} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left[\left|\tilde{\phi}_R(\vec{x})+\ell\right\rangle\left\langle\tilde{\phi}_R(\vec{x})\right| - \left|\tilde{\phi}_R(\vec{x})\right\rangle\left\langle\tilde{\phi}_R(\vec{x})+\ell\right| \right], \\
\hat{S}_z^\ell(\vec{x}) &= \sum_{n=-\infty}^{\infty} (-1)^n \int_{n\ell}^{(n+1)\ell} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left|\tilde{\phi}_R(\vec{x})\right\rangle\left\langle\tilde{\phi}_R(\vec{x})\right| .
\end{aligned}
\tag{5.55}
$$

One can check that these operators are indeed pseudo-spin operators, as they satisfy the relations given below eq. (5.7). Their Wigner-Weyl transforms are given by [117]

$$
\begin{aligned}
W_{\hat{S}_x^\ell(\vec{x})} &= \sum_{n=-\infty}^{\infty} 2\cos\left[\tilde{\pi}_R(\vec{x})\ell\right] \left\{ \theta\left[\tilde{\phi}_R(\vec{x}) - \frac{\ell}{2} - 2n\ell\right] - \theta\left[\tilde{\phi}_R(\vec{x}) - \frac{\ell}{2} - (2n+1)\ell\right] \right\}, \\
W_{\hat{S}_y^\ell(\vec{x})} &= \sum_{n=-\infty}^{\infty} 2\sin\left[\tilde{\pi}_R(\vec{x})\ell\right] \left\{ \theta\left[\tilde{\phi}_R(\vec{x}) - \frac{\ell}{2} - 2n\ell\right] - \theta\left[\tilde{\phi}_R(\vec{x}) - \frac{\ell}{2} - (2n+1)\ell\right] \right\}, \\
W_{\hat{S}_z^\ell(\vec{x})} &= \sum_{n=-\infty}^{\infty} (-1)^n \left\{ \theta\left[\tilde{\phi}_R(\vec{x}) - n\ell\right] - \theta\left[\tilde{\phi}_R(\vec{x}) - (n+1)\ell\right] \right\}
\end{aligned}
\tag{5.56}
$$

where θ is here the Heaviside function. By plugging these expressions into eq. (5.13), one obtains explicit expressions for the spin correlators in terms of double infinite sums of integrals involving the error function, which we provide later in this section.

These expressions do not admit general analytic expressions, but can be evaluated numerically. Before displaying the result, it is worth mentioning that further analytical insight can be gained by expanding those formulas in the limits $\ell \ll 1$ and $\ell \gg 1$. Those expansions are carried out later in this section. We give first the final result.

When $\ell \ll 1$, one obtains

$$
\begin{aligned}
\left\langle \hat{S}_x^\ell(\vec{x}_1)\hat{S}_x^\ell(\vec{x}_2)\right\rangle &\simeq \frac{1}{4}\sum_{\boldsymbol{\epsilon}=(\pm 1,\pm 1)^{\mathrm{T}}} e^{\frac{\ell^2}{2}\left\{\frac{a_{11}\tilde{a}_2^2+a_{22}\tilde{a}_1^2-2a_{12}\tilde{a}_1\tilde{a}_2}{a_{11}a_{22}-a_{12}^2}+\boldsymbol{\epsilon}^T\cdot[(\gamma^{-1})^{\pi\pi}]\cdot\boldsymbol{\epsilon}\right\}} \underset{\ell\to 0}{\longrightarrow} 1\,, \\
\left\langle \hat{S}_z^\ell(\vec{x_1})\hat{S}_z^\ell(\vec{x}_2)\right\rangle &\simeq e^{-\frac{\pi^2(a_{11}+a_{22}-2a_{12})}{2\ell^2(a_{11}a_{22}-a_{12}^2)}} \underset{\ell\to 0}{\longrightarrow} 0\,,
\end{aligned}
\tag{5.57}
$$

where $\tilde{a}_1$ and $\tilde{a}_2$ are functions of the entries of the covariance matrix defined later in this section.

Let us inspect this limit. The approximations above show that $B^\ell \to 2$ as $\ell \to 0$, hence there is no Bell-inequality violation in this regime. Let us note that, when ℓ decreases, the size of the ℓ-intervals in eq. (5.55) decreases, hence numerically one has to include more terms before truncating the sum. This is why the small-ℓ regime is numerically challenging, and there is always a minimum value of ℓ below which the computation cannot be performed, given finite numerical capacities. For this reason, having an analytical control on the small-ℓ regime is convenient and even necessary in order for the analysis to be complete.

When $\ell \gg 1$, one finds that

$$
\left\langle \hat{S}_x^\ell(\vec{x}_1)\hat{S}_x^\ell(\vec{x}_2)\right\rangle \underset{\ell\to\infty}{\longrightarrow} 0\,,
\tag{5.58}
$$

while $\hat{S}_z^\ell(\vec{x})$ approaches the $\hat{\mathcal{S}}_x$ component of the GKMR operator,

$$
\hat{S}_z^\ell(\vec{x}) \underset{\ell\to\infty}{\longrightarrow} \hat{\mathcal{S}}_x^\ell(\vec{x}).
\tag{5.59}
$$

Its two-point function is thus given by eq. (5.19) in this limit. Considering eq. (5.16), this allows us to establish the bound

$$
\lim_{\ell\to\infty} B^\ell < B^{GKMR}\,,
\tag{5.60}
$$

that is, B^ℓ is smaller than the GKMR result in the limit $\ell \to \infty$. Hence, no Bell-inequality violation can be obtained in this regime either.

In between those two regimes, as mentioned above, one has to resort to numerical computations, which we present in the next subsection.

Intermediate analytical expressions

By plugging eq. (5.8) and eq. (5.56) into eq. (5.13), one obtains explicit expressions for the two-point correlation functions of the Larsson spin operators, involving a double sum of double integrals. One of these integrals [say the one over $\tilde{\phi}_R(\vec{x}_2)$] can be performed in terms of the error function, and one obtains

$$\begin{aligned}
\left\langle \hat{S}_z^\ell(\vec{x}_1)\hat{S}_z^\ell(\vec{x}_2)\right\rangle &= \frac{1}{2\pi\sqrt{\det\boldsymbol{\gamma}\det(\boldsymbol{\gamma}^{-1})^{\pi\pi}}}\sum_{n,m=-\infty}^{\infty}(-1)^{n+m}\mathcal{Z}_{n,m}(\vec{x}_1,\vec{x}_2),\\
\left\langle \hat{S}_x^\ell(\vec{x}_1)\hat{S}_x^\ell(\vec{x}_2)\right\rangle &= \frac{1}{2\pi\sqrt{\det\boldsymbol{\gamma}\det(\boldsymbol{\gamma}^{-1})^{\pi\pi}}}\sum_{n,m=-\infty}^{\infty}\mathcal{X}_{n,m}(\vec{x}_1,\vec{x}_2),\\
\left\langle \hat{S}_x^\ell(\vec{x}_1)\hat{S}_z^\ell(\vec{x}_2)\right\rangle &= 0\,.
\end{aligned}\tag{5.61}$$

The functions $\mathcal{Z}_{n,m}$ and $\mathcal{X}_{n,m}$ are defined as

$$\begin{aligned}
&\mathcal{Z}_{n,m}(\vec{x}_1,\vec{x}_2)=\\
&\quad\sqrt{\frac{\pi}{2a_{22}}}\int_{n\ell}^{(n+1)\ell}\mathrm{d}\phi e^{-\frac{1}{2}\phi^2\left(a_{11}-\frac{a_{12}^2}{a_{22}}\right)}\left\{\mathrm{erf}\left[\frac{a_{12}\phi+a_{22}(m+1)\ell}{\sqrt{2a_{22}}}\right]-\mathrm{erf}\left[\frac{a_{12}\phi+a_{22}m\ell}{\sqrt{2a_{22}}}\right]\right\}\\
&\mathcal{X}_{n,m}(\vec{x}_1,\vec{x}_2)=\\
&\quad\int_{\frac{\ell}{2}+2nl}^{\frac{\ell}{2}+(2n+1)\ell}\mathrm{d}\phi\sum_{\epsilon_1,\epsilon_2=-1,1}\sqrt{\frac{\pi}{2a_{22}}}e^{-\frac{\phi^2}{2}\left(a_{11}-\frac{a_{12}^2}{a_{22}}\right)+\frac{i\ell\phi}{a_{22}}(a_{12}\tilde{a}_y-a_{22}\tilde{a}_1)-\frac{\ell^2\tilde{a}_y^2}{2a_{22}}-\frac{\ell^2}{2}\boldsymbol{\epsilon}^{\mathrm{T}}\cdot(\boldsymbol{\gamma}^{-1})^{\pi\pi}\cdot\boldsymbol{\epsilon}}\\
&\quad\times\left\{\mathrm{erf}\left[\frac{a_{12}\phi+i\ell\tilde{a}_2+a_{22}\left(2m+\frac{3}{2}\right)\ell}{\sqrt{2a_{22}}}\right]-\mathrm{erf}\left[\frac{a_{12}\phi+i\ell\tilde{a}_2+a_{22}\left(2m+\frac{1}{2}\right)\ell}{\sqrt{2a_{22}}}\right]\right\},
\end{aligned}\tag{5.62}$$

where we recall that the matrix $\boldsymbol{a}$ was introduced in eq. (5.27), and where the integration variable ϕ physically correspond to $\tilde{\phi}_R(\vec{x})$. We have also introduced the vector $\boldsymbol{\epsilon}=(\epsilon_1,\epsilon_2)^{\mathrm{T}}$, and the quantities $\tilde{a}_1$ and $\tilde{a}_2$ defined as

$$\begin{aligned}
\tilde{a}_1 =&\frac{1}{2}\Big\{(\gamma^{-1})_{12}[(\gamma^{-1})^{\pi\pi}]^{-1}_{11}\epsilon_x+(\gamma^{-1})_{12}[(\gamma^{-1})^{\pi\pi}]^{-1}_{12}\epsilon_y\\
&+(\gamma^{-1})_{14}[(\gamma^{-1})^{\pi\pi}]^{-1}_{21}\epsilon_x+(\gamma^{-1})_{14}[(\gamma^{-1})^{\pi\pi}]^{-1}_{22}\epsilon_y\Big\},\\
\tilde{a}_2 =&\frac{1}{2}\Big\{(\gamma^{-1})_{32}[(\gamma^{-1})^{\pi\pi}]^{-1}_{11}\epsilon_x+(\gamma^{-1})_{32}[(\gamma^{-1})^{\pi\pi}]^{-1}_{12}\epsilon_y+\\
&+(\gamma^{-1})_{34}[(\gamma^{-1})^{\pi\pi}]^{-1}_{21}\epsilon_x+(\gamma^{-1})_{34}[(\gamma^{-1})^{\pi\pi}]^{-1}_{22}\epsilon_y\Big\}.
\end{aligned}\tag{5.63}$$

In general, the remaining integral and double sum need to be carried out numerically. However, more analytical insight can be gained in the small-ℓ and the large-ℓ limits.

Small-ℓ limit

When $\ell \ll 1$, the functions $\mathcal{Z}_{n,m}$ and $\mathcal{X}_{n,m}$ involve differences of error functions evaluated at nearby points. They can therefore be Taylor expanded as follows

$$\mathrm{erf}\left[b_1 + b_2(m+1)\ell\right] - \mathrm{erf}(b_1 + b_2 m\ell) \simeq b_2\ell \frac{\mathrm{d}}{\mathrm{d}(b_2 m\ell)} \mathrm{erf}(b_1 + b_2 m\ell) = \frac{2b_2\ell}{\sqrt{\pi}} e^{-(b_1+b_2 m\ell)^2} , \tag{5.64}$$

and

$$\begin{aligned} \mathrm{erf}\left[b_1 + b_2\left(\left(2m+\frac{3}{2}\right)\ell\right] - \mathrm{erf}\left[b_1 + b_2\left(\left(2m+\frac{1}{2}\right)\ell\right]\right. \right. \simeq \\ \simeq \ell b_2 \frac{\mathrm{d}}{\mathrm{d}(2mb_2\ell)} \mathrm{erf}\left[b_1 + b_2\ell(2m+1/2)\right] = \frac{2b_2\ell}{\sqrt{\pi}} e^{-\left[b_1+b_2\ell\left(2m+\frac{1}{2}\right)\right]^2} . \end{aligned} \tag{5.65}$$

The remaining integrals in $\mathcal{Z}_{n,m}$ and $\mathcal{X}_{n,m}$ become Gaussian integrals and can thus be performed analytically. Similarly, the sums over n and m can be approximated by Riemann integrals upon introducing $x = n\ell$ and $y = m\ell$ and by noticing that

$$\sum_{n,m=-\infty}^{\infty} \ell^2 g(n\ell, m\ell) \underset{\ell\ll 1}{\simeq} \int_{-\infty}^{\infty} \mathrm{d}x\mathrm{d}y g\left(x,y\right) , \tag{5.66}$$

if g is a sufficiently smooth function.

In the particular case of interest to us, since $g(n,m)$ is Gaussian, one can compute its Riemann integral right away. This finally gives rise to

$$\left\langle \hat{S}_z^\ell(\vec{x}_1)\hat{S}_z^\ell(\vec{x}_2)\right\rangle \simeq e^{-\frac{\pi^2(a_{11}+a_{22}-2a_{12})}{2\ell^2(a_{11}a_{22}-a_{12}^2)}} \underset{\ell\to 0}{\longrightarrow} 0 \tag{5.67}$$

and

$$\left\langle \hat{S}_x^\ell(\vec{x}_1)\hat{S}_x^\ell(\vec{x}_2)\right\rangle \simeq \frac{1}{4}\sum_{\boldsymbol{\epsilon}} e^{\frac{\ell^2}{2}\left\{\frac{a_{11}\tilde{a}_2^2+a_{22}\tilde{a}_1^2-2a_{12}\tilde{a}_1\tilde{a}_2}{a_{11}a_{22}-a_{12}^2}+\boldsymbol{\epsilon}^T\cdot[(\gamma^{-1})^{\pi\pi}]\cdot\boldsymbol{\epsilon}\right\}} \underset{\ell\to 0}{\longrightarrow} 1 . \tag{5.68}$$

Large-ℓ limit

When $\ell \to \infty$, in the expression for $\hat{S}_x^\ell(\vec{x})$ given in eq. (5.55), one can see that only the term with $n = 0$ has a non-empty integration domain. However, this term involves the field eigenstate $|\infty\rangle$, which necessarily vanishes when evaluated on a normalised state. This implies that

$$\left\langle \hat{S}_x^\ell(\vec{x}_1)\hat{S}_x^\ell(\vec{x}_2)\right\rangle \underset{\ell\to\infty}{\longrightarrow} 0 , \tag{5.69}$$

which can be further checked by noticing that for all m, the two error functions appearing in the expression of $\mathcal{X}_{n,m}$ given in eq. (5.62) are evaluated at the same point (i.e. either $+\infty$ or $-\infty$), hence the difference always vanishes.

For $\hat{S}_z^\ell(\vec{x})$, when evaluating the expression given in eq. (5.55) in the limit $\ell \to \infty$, only the terms $n = -1$ and $n = 0$ remain, which leads to

$$
\begin{aligned}
\hat{S}_z^\ell(\vec{x}) \underset{\ell\to\infty}{\longrightarrow} & \int_{-\infty}^{0} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left| \tilde{\phi}_R(\vec{x}) \right\rangle \left\langle \tilde{\phi}_R(\vec{x}) \right| + \int_{0}^{\infty} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left| \tilde{\phi}_R(\vec{x}) \right\rangle \left\langle \tilde{\phi}_R(\vec{x}) \right| \\
& = \int_{-\infty}^{\infty} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left| \tilde{\phi}_R(\vec{x}) \right\rangle \left\langle \tilde{\phi}_R(\vec{x}) \right| .
\end{aligned}
\tag{5.70}
$$

This formula coincides with the one for the $\hat{\mathcal{S}}_x$ component of the GKMR operator. Indeed, by plugging eq. (5.6) into eq. (5.7), one obtains

$$
\begin{aligned}
\hat{\mathcal{S}}_x(\vec{x}) = & \frac{1}{2} \int_{0}^{\infty} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left[\left| \tilde{\phi}_R(\vec{x}) \right\rangle \left\langle \tilde{\phi}_R(\vec{x}) \right| - \left| -\tilde{\phi}_R(\vec{x}) \right\rangle \left\langle -\tilde{\phi}_R(\vec{x}) \right| \right] \\
& = \int_{-\infty}^{\infty} \mathrm{d}\tilde{\phi}_R(\vec{x}) \left| \tilde{\phi}_R(\vec{x}) \right\rangle \left\langle \tilde{\phi}_R(\vec{x}) \right| ,
\end{aligned}
\tag{5.71}
$$

where the change of integration variable $\tilde{\phi}_R(\vec{x}) \to -\tilde{\phi}_R(\vec{x})$ has been performed in the second term. One thus has

$$
\hat{S}_z^\ell(\vec{x}) \underset{\ell\to\infty}{\longrightarrow} \hat{\mathcal{S}}_x(\vec{x}), \tag{5.72}
$$

hence the two-point function of the $\hat{S}_x^\ell(\vec{x})$ operator is given by eq. (5.19) in the limit $\ell \to \infty$.

5.5.2 Flat space-time

In fig. 5.5, we display the expectation value of the Larsson Bell operator in the Minkowski vacuum, as a function of ℓ, for $\alpha = 3$ and $\delta = 0.1$. One can check that the small-ℓ and the large-ℓ approximations derived above provide good fits to the full result in their respective domains of validity. In between, we find that B^ℓ is a decreasing function of ℓ, and this behaviour is observed for any value of δ and α. As a consequence, one has $B^\ell < B^{\ell\to 0} = 2$, hence there is no Bell-inequality violation in flat space time.

5.5.3 De-Sitter space-time

Similarly, the expectation value for the Larsson Bell operator is displayed as a function of ℓ in the de-Sitter Bunch-Davies vacuum state in fig. 5.6, for $\delta = 0.1$, $\beta = 10^{-4}$, $\alpha = 3$ and for a few values of HR. One can check that the small-ℓ and the large-ℓ approximations derived above still provide good fits to the full result. In between, B^ℓ goes through a local minimum at intermediate values of ℓ, hence it is always smaller than 2. This same behaviour is observed with other values for the parameters δ, β and α, which allows us to conclude that no Bell-inequality violation can be obtained with the Larsson operators.

5.6 Discussion

In this chapter we have discussed how to build real-space Bell operators in QFT and obtained its expectation value when the field is placed in a Gaussian state. This allowed us to continue our discussion on the existence of quantum correlations between distant regions of the universe. We have found that there is no Bell inequality violation in both the Minkowski vacuum and the Bunch-Davies vacuum of de Sitter space-time, the latter being relevant to characterize primordial perturbations, in particular by means of the Mukhanov-Sasaki variable.

This is to some extent a natural continuation of the discussion in chapters 3 and 4 and closes part II. In addition, it follows a serious of works dealing with this fascinating topic, which we can trace back to refs. [60, 161], where quantum discord in Fourier space was computed for two-mode squeezed state, revealing that the creation of pairs of particles with opposite Fourier momenta in de-Sitter geometries is associated with the production of a large quantum discord, i.e.m with the presence of genuine quantum correlations. Fourier-space Bell operators were then constructed in refs. [117, 158], confirming that Bell inequalities between opposite Fourier modes can indeed be violated, and hinting towards the presence of quantum features in primordial fluctuations. However, as it was discussed in sec. 2.2, Bell inequalities are build on the assumption of locality, whose violation has not a clear significance in Fourier space.

Therefore, entanglement entropy, mutual information and quantum discord have been studied in real space, in particular in refs. [1, 2], on which chapters 3 and 4 are based, as well as in refs. [152, 153]. It was found that, although they remain non vanishing, their typical values are greatly reduced compared to the Fourier-space setup, casting some doubt on the ability of cosmological structures to display quantum correlations. We can understand this phenomenon in real space due to the existence of local correlations, so that when regions of space are traced over, the rest are left in a mixed state. This effect, called *effective decoherence*, does not take place in Fourier space, for the two-mode squeezed state is a product state of each Fourier mode.

The formalism of ref. [152] was employed in this chapter to be build Bell operators in real-space QFT and to compute its expected value for Gaussian states. We have found that no Bell inequality violation takes place in both Minkowski and de Sitter space-time, despite the fact that quantum discord is non-vanishing in both cases [152, 153]. In addition, the notable difference between both states in Fourier space, the former being a Fock space vacuum the latter being a two-mode squeezed state with large quantum discord, does not seem to play a role in our results.

This illustrates that the interpretation of quantum discord for mixed states is subtle. *Effective decoherence* seems to act as a quantumness censor, at least in this setup. Moreover, the configuration where it is maximal (namely when the two patches have size comparable to the Hubble radius and are almost adjacent [153]) does not coincide with the one where the expectation value of the Bell operator is maximal (namely when the patches are large compared to the Hubble radius and are almost adjacent). This illustrates again the subtleties of quantum discord for mixed states.

It is worth mentioning a few possible directions along which this research program could be carried on. First, even though we have generalised our finding to another family of spin operators in sec. 5.5, we have not tested *all* possible Bell operators (only a few explicit constructions are known). Therefore, strictly speaking, we cannot claim that real-space Bell inequalities can never be violated in de Sitter, and it would be interesting to derive a generic mathematical argument (or expose a counter-example).

Second, there are other classes of Bell inequalities, which rely on measuring the system at different times. Those are the temporal Bell inequalities [162–164], the Legget-Garg inequalities [165], and the bipartite temporal Bell inequality [166]. The last two were shown to be violated by cosmological perturbations in Fourier space in refs. [167] and [168] respectively, and their investigation in real space remains to be carried out.

Third, it would be interesting to investigate correlations and entanglement between more than two spheres. This may effectively reduce the size of the traced-out regions, hence the importance of the *effective decoherence* effect. This may also require to account for non-Gaussianities, which have been shown to be relevant for the search of primordial quantum signals [102, 169]. Indeed, non-Gaussian tails are known to be present in cosmological perturbations [67] and may give rise to genuine quantum correlations. The study of classical and quantum correlations between more than two spheres is also relevant in trying to understand how many-body entropic forces may exist between black holes, following the arguments developed in chapter 4.

On top of the *effective decoherence* effect, a *physical decoherence* mechanism may take place in the context of cosmology, arising from the fact that the scalar field describing cosmological adiabatic perturbations usually couples to other, unobserved degrees of freedom (additional fields, unobserved scales, etc.). This may come as an additional quantumness censor and would have to be studied, if one of the previously-mentioned directions turns out successful. Recently, in ref. [150], it was found that there exists a wide region in parameter space where the Fourier-space quantum discord is unaffected by environmental effects even where they make the state of the system fully decohere. Generalising this calculation to real-space setups would further test the relationship between quantum discord, Bell-inequalities violation, and the detectability of quantum features in cosmological fields.

This chapter closes part II, which dealt on the study of classical and quantum correlations in cosmological perturbations. We conclude that finding genuine quantum correlations is inherently hard, if possible at all, due to the unavoidable *effective decoherence* present in any local QFT.

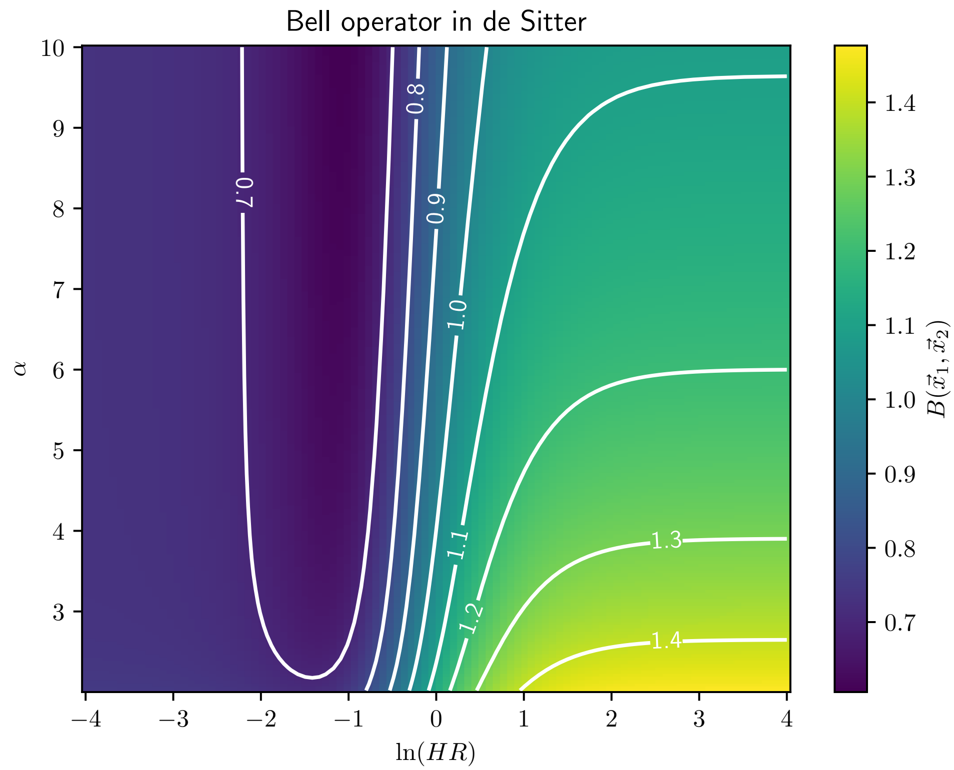

Figure 5.2: Expectation value of the GKMR Bell operator in the Bunch-Davies vacuum of the de-Sitter space-time, as a function of the parameters $\alpha = d/R$ and HR. Here α varies from its minimal value $\alpha_{\text{min}} = 2(1 + \delta)$. The colour encodes the value of B, and a few contour lines are displayed in white. The UV and IR regulators (on which there is at most a logarithmic dependence) have been respectively set to $\delta = 0.01$ and $\beta = 10^{-4}$ (see appendix B.1 for other slices in parameter space). Different behaviours are obtained depending on whether $HR < 1$ or $HR > 1$, i.e. depending on the size of the measured patches with respect to the Hubble radius (see main text for further details). From ref. [6].

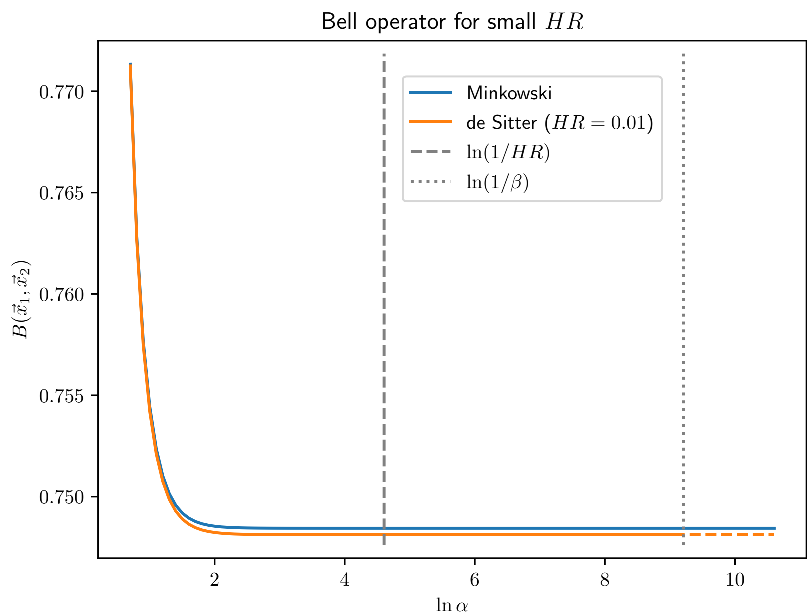

Figure 5.3: Expectation value of the GKMR Bell operator in the Bunch-Davies vacuum of the de-Sitter space time for $\beta = 10^{-4}$, $HR = 10^{-2}$, $\delta = 10^{-2}$, and as a function of the parameter $\alpha = d/R$. For $\alpha \ll 1/(HR)$, all distances involved in the problem are smaller than the Hubble radius hence the de-Sitter and Minkowski results coincide. Note that values of $\alpha > 1/\beta$ are not displayed since they would correspond to $d > R_{\rm obs}$. From ref. [6].

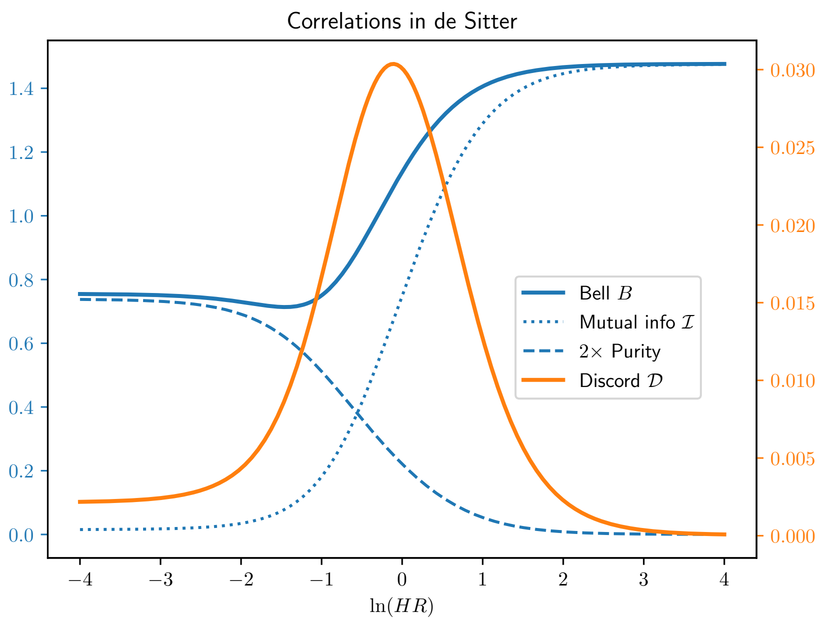

Figure 5.4: Expectation value of the GKMR Bell operator B in the de-Sitter space time, as a function of HR and for $\alpha = \alpha_{\text{min}} = 2(1+\delta)$, $\beta = 10^{-4}$ and $\delta = 10^{-2}$. For comparison, we also display (two times) the state purity $\mathfrak{p}$, to which B asymptotes in the small-HR limit, as well as mutual information $\mathcal{I}$ and quantum discord $\mathcal{D}$, the latter being labelled with the rightmost vertical axis. From ref. [6].

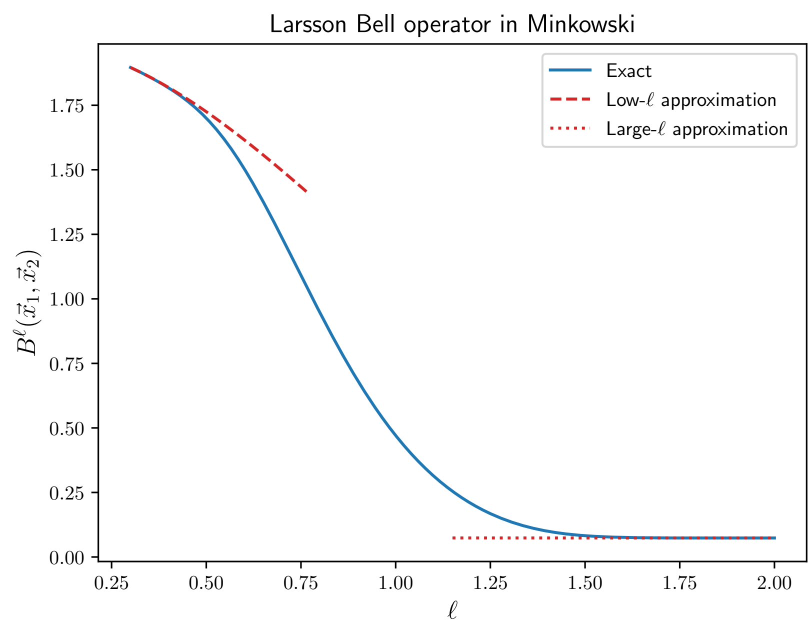

Figure 5.5: Expectation value of the Larsson Bell operator in the Minkowski vacuum, as a function of ℓ, for $\alpha = 3$ and $\delta = 0.1$. The blue solid line corresponds to the full result, the red dashed line to the low-ℓ approximation eq. (5.57), and the red dotted line to the large-ℓ limit eq. (5.58) and eq. (5.59). From ref. [6].

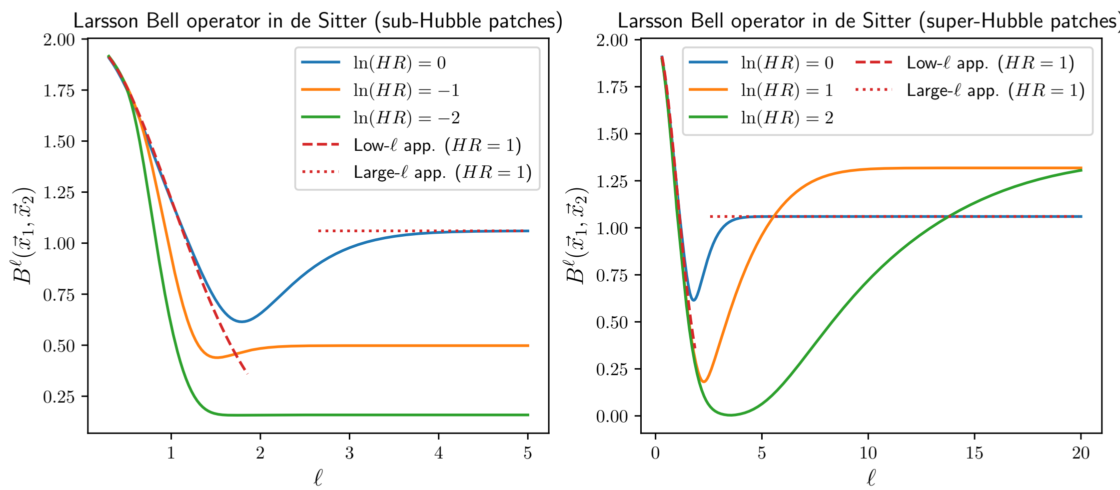

Figure 5.6: Expectation value of the Larsson Bell operator in the de-Sitter space-time, as a function of ℓ, for $\alpha = 3$ and $\delta = 0.1$ and $\beta = 10^{-4}$. A few sub-Hubble values of HR are shown in the left panel, and a few super-Hubble values in the right panel. The red dashed line corresponds to the low-ℓ approximation eq. (5.57), and the red dotted line to the large-ℓ limit eq. (5.58) and eq. (5.59), both in the case $HR = 1$. From ref. [6].

Part III

The non-equilibrium universe

Chapter 6

Irreversible gravity

> Someone once told me that time was a predator that stalked us all our lives. But I rather believe that time is a companion who goes with us on the journey and reminds us to cherish every moment because they'll never come again. What we leave behind is not as important as how we've lived. After all, Number One, we're only mortal.
>
> Jean-Luc Picard in *Star Trek: Generations* (1994).

6.1 Motivation

Forces are key elements of the classical description of a physical system. They dictate the equation of motion of a physical object in compliance with Newton's second law, $\vec{F} = m\vec{a}$. Forces can be generalized to relativistic physics (both SR and GR), taking the form of tensors. They can be classified in three types depending on their microscopic origin:

- Fundamental forces. They are due to the fundamental interactions between the elements of a physical systems and are functions of the charges of each element and their phase space coordinates. The four fundamental interactions are the strong, weak, electromagnetic and gravitational interaction.
- Residual forces. They are due to the microstructure of the elements of a physical system. These elements are composite, so that their total total charge with respect to a fundamental interaction vanishes, but the charge of the constituents does not. The fundamental interaction between constituents of different elements leads to a

residual force between them. Examples of residual forces include the nuclear and van der Waals forces.

- Entropic forces. They are due to the tendency of collective macroscopic systems to increase their entropy. An example is diffusion due to Brownian motion.

In theoretical physics we are mostly used to characterizing and working with fundamental forces and, to a lesser extent, residual forces. Nevertheless, entropic forces also play a role in theoretical physics and couple microscopic and macroscopic dynamics. Furthermore, since they are linked to the increase of entropy, they break the symmetry under time inversion and cause irreversible phenomena.

As we saw in sec. 4.5, repulsive entropic forces may arise between PBH due to their tendency to increase the entropy of quantum field of cosmological perturbations. Such proposal is derived from classical thermodynamics and non-relativistic forces. We would like to understand how to generally formulate entropic forces in a fully general-relativistic setup.

The goal of this chapter is to provide a variational and covariant formulation of non-equilibrium thermodynamics. This first principles approach includes existing descriptions of non-equilibrium phenomena, such as real fluids, but allows for other sources of entropy and reconciles the irreversible nature of the laws of thermodynamics with the symmetries of the Einstein-Hilbert action. Entropic forces between PBH will serve as motivation, but we will not develop here the variational treatment of the thermodynamic variables associated to the quantum field.

The link between gravity and thermodynamics is deep and provides insight into the need of a UV-complete theory of quantum gravity. The work of Hawking [100] and Bekenstein [105] introduced the notion of temperature and entropy of a black hole, leading to the formulation of black hole thermodynamics [123]. This points towards the existence of unknown microphysical quantum degrees of freedom (d.o.f.), being the geometric description of gravity an emergent macrophysical phenomenon. The link between gravity and thermodynamics has only grown ever since. It has been argued that it constitutes the first piece of the connection between classical and quantum gravity [106]. The discovery of the area law of entanglement entropy [103, 104] particularly supports this idea.

Motivated by the relevance of thermodynamics in gravity, we argue for the need of a proper understanding of the interplay between GR and non-equilibrium thermodynamics. GR, like other physical theories that can be deduced from the stationary action principle, is a time-reversible theory. It is true that the dynamics of horizons has irreversible features, as dictated for instance by the already mentioned black hole thermodynamics, in particular the second law [130]. Still, irreversible phenomena are not included into GR in a complete and systematic way. It is the purpose of the work presented in this paper to provide such an inclusion, i.e. a covariant formulation of non-equilibrium thermodynamics in GR. Our results show that non-equilibrium phenomena, either in the matter content or space-time itself, lead to a back-reaction on the gravitational field equations with potential observational consequences.

This chapter is organized as follows. In sec. 6.2 we review existing work on the variational formulation of non-equilibrium thermodynamics. In sec. 6.3 we apply this concept to gravity and show how it fits with both the Lagrangian and Hamiltonian formulation of GR. In sec. 6.4 we argue that temperature and entropy are naturally included in the matter or gravitational Lagrangian. In sec. 6.5 we look for applications of our results and obtain the non-equilibrium Friedmann and Raychaudury equations. In sec. 6.6 we include real fluids into the formalism. We finish with a discussion of our results in sec. 6.7.

6.2 Variational formulation

In this section we review the variational formulation for non-equilibrium thermodynamical systems, which was developed by Gay-Balmaz and Yoshimura in refs. [170, 171]. Such formulation is the synthesis of two physical frameworks. On the one hand, one has the laws of thermodynamics in the axiomatic formulation of Stückelberg (see also sec. 2.6):

- *First law* or energy conservation. For every thermodynamic system there is an extensive scalar quantity E called *energy*, which can only change due to interactions with the environment
$$\frac{dE}{dt} = P^{ext}(t)\,. \tag{6.1}$$
- *Second law* or positive entropy production. For every thermodynamic system there is an extensive scalar quantity S called *entropy*, which is a monotonically increasing function of time
$$\frac{dS}{dt} = I(t) \geq 0\,, \tag{6.2}$$
where the equality holds only once the system is in equilibrium.

On the other hand, the dynamics of a mechanical system is dictated by the stationary action principle:

- *Stationary action principle*. For a dynamical system with configuration manifold Q and Lagrangian function $L(q, \dot{q}) : TQ \to \mathbb{R}$, the physical curve defined on an interval $t \in [t_1, t_2]$, satisfies the variational condition
$$\delta \int_{t_1}^{t_2} dt L(q, \dot{q}) = 0\,, \tag{6.3}$$

which delivers the well-known Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0\,. \tag{6.4}$$

In order to merge these principles, let us now consider a mechanical system whose Lagrangian function depends on the entropy S as well. The stationary action principle dictates that the physical curve $(q(t), S(t))$ on $Q \times \mathbb{R}$, defined on an interval $t \in [t_1, t_2]$, satisfies the variational condition

$$\delta \int_{t_1}^{t_2} dt L(q, \dot{q}, S) = 0\,. \tag{6.5}$$

Since the thermodynamical system is out of equilibrium, it must be supplemented with the laws of thermodynamics. Energy conservation is related to the symmetry of the Lagrangian under time translations and so is already encoded in the variational formulation. On the other hand, the second law requires the introduction of a friction or entropic force $F : TQ \times \mathbb{R} \to T^*Q$ and is implemented by a variational constraint

$$\frac{\partial L}{\partial S}(q, \dot{q}, S)\delta S = \langle F(q, \dot{q}, S), \delta q\rangle\ , \tag{6.6}$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product. This variational constraint comes also with a *phenomenological* constraint

$$\frac{\partial L}{\partial S}(q, \dot{q}, S)\dot{S} = \langle F(q, \dot{q}, S), \dot{q}\rangle\ . \tag{6.7}$$

The curve $(q(t), S(t))$ that satisfies all three conditions is given by:

$$\begin{aligned} &\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = F(q, \dot{q}, S) \\ &\frac{\partial L}{\partial S}\dot{S} = \langle F(q, \dot{q}, S), \dot{q}\rangle\ . \end{aligned} \tag{6.8}$$

Hence, once the effect of non-equilibrium thermodynamics is enforced by the second law, one obtains the Euler-Lagrangian equation with an additional force of entropic origin. This variational formulation of non-equilibrium thermodynamics applies as it is to isolated systems, i.e. thermodynamic systems that do not exchange energy (heat and work) nor matter with its environment. In order to consider a closed thermodynamic system, i.e. one that exchanges energy but not matter with its environment, one must include the effect of external work in eq. (6.5) and external heat supply in eq. (6.7). The generalization to open systems, i.e. that allow both energy and matter exchange, is developed in [172]. As we will see later, one often finds that the *temperature* of the thermodynamic system can be introduced as

$$\frac{\partial L}{\partial S} = -T\,, \tag{6.9}$$

although it is not necessary to do so in the general case.

The thermodynamical nature of the system implies the explicit or implicit coarse-grain of some d.o.f. Its detailed microphysics may be unknown, but its macrophysics has an effect on the dynamics of other physical variables whose microphysics is known. This effect is encoded by the second law of thermodynamics, which restricts the configuration space and delivers a modified equation of motion, and it allows us to study the coupling between these d.o.f.

The full variational implementation of the continuum case is a bit more involved, should the entropy be allowed to have a spatial dependence [171]. The reason is that friction causes internal entropy production, but entropy can also increase or decrease locally due to entropy fluxes. For the sake of clarity and when required, we will instead follow a short-cut and introduce the required additional equations from physical considerations.

6.3 Non-equilibrium dynamics in GR

After reviewing the variational formulation of non-equilibrium thermodynamics we are ready to apply this same formalism to General Relativity. The coupling of the gravitational field to coarse-grained physical d.o.f. delivers an effective modification of Einstein field equations. We will first show this by supplementing the Einstein-Hilbert action with the constraints given by the second law of thermodynamics. Then, we will check that it is also consistent with the Hamiltonian formulation of General Relativity. We will also provide a physical insight onto the effects of this effective modification of the gravitational dynamics by inspecting the Raychauduri equation.

6.3.1 Lagrangian formulation

The variational formalism can be applied directly to the Einstein-Hilbert action without any particular assumption on the metric. However, it requires the introduction of a foliation of the space-time manifold. This cannot be avoided: the second law of thermodynamics is linked to the existence of the arrow of time. Nevertheless, the Einstein field equations keep its general covariance, as we will check shortly.

Let us build our action as the sum of the Einstein-Hilbert action of General Relativity plus a matter term

$$\frac{1}{2\kappa}\int d^4x\sqrt{-g}\,R + \int d^4x\mathcal{L}_m(g_{\mu\nu}, S)\,, \tag{6.10}$$

where the coupling is $\kappa = 8\pi G$ and we allow the matter Lagrangian $\mathcal{L}_m$, which is a tensor density, to have a dependency on the entropy S. It may as well depend on additional fields that describe the matter content. In this setup, the stationary action principle takes the form $\delta(6.10) = 0$. That is

$$\int d^4x \left(\frac{1}{2\kappa} \frac{\delta(\sqrt{-g}\,R)}{\delta g^{\mu\nu}} + \frac{\delta \mathcal{L}_m}{\delta g^{\mu\nu}} \right) \delta g^{\mu\nu} + \int d^4x \frac{\partial \mathcal{L}_m}{\partial S} \delta S = 0\,, \tag{6.11}$$

which is now supplemented with the variational constraint given by the second law of thermodynamics

$$\frac{\partial L_m}{\partial S} \delta S = \frac{1}{2} F_{\mu\nu} \delta g^{\mu\nu}\,, \tag{6.12}$$

where $F_{\mu\nu}$ is the tensorial friction or entropic force. Analogously to the Lagrangian density one can define the friction density as

$$F_{\mu\nu} = \int d^3x \sqrt{-g}\, f_{\mu\nu}\,. \tag{6.13}$$

The constrained stationary action principle gives the non-equilibrium Einstein field equations

$$R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} = \kappa \left(T_{\mu\nu} - f_{\mu\nu} \right)\,, \tag{6.14}$$

which includes the usual geometric and matter terms plus an entropic one. This equation is one of the main results of our work and shows how non-equilibrium thermodynamics is very relevant in gravitation.

Note that the Bianchi identities, a reflection of the general covariance of the theory, allow the covariant non-conservation of the energy-momentum tensor

$$D^{\mu} T_{\mu\nu} = D^{\mu} f_{\mu\nu}\,. \tag{6.15}$$

One can include a dependence of the entropy on the spatial position by introducing the entropy density $s(\vec{x}, t)$ and rewriting the variational constraint as

$$\frac{\partial \mathcal{L}_m}{\partial s} \delta s = \frac{1}{2} \sqrt{-g}\, f_{\mu\nu} \delta g^{\mu\nu}\,, \tag{6.16}$$

provided that there is no dependence of the Lagrangian on the partial derivatives $\partial_\mu s$.

For now, we have shown that the variational constraint is enough to obtain the non-equilibrium Einstein field equations. We will deal with the phenomenological constraint in the next subsection, once a foliation of space-time is explicitly introduced in the context of the ADM formalism. The phenomenological constraint will allow us to obtain an implicit expression for the force $f_{\mu\nu}$.

The fully rigorous implementation of the variational constraint becomes a bit more subtle once this spatial dependence is introduced. In practice, the function s is not the entropy itself, but rather a function that plays a role in the entropy balance equation. In particular δs is the entropy density variation due to internal processes and not to entropy fluxes. We leave the discussion of this equation to the next section, as it also requires the introduction of a foliation.

6.3.2 Hamiltonian formulation

The variational formalism delivers a modification of Einstein field equations due to the appearence of a force of entropic origin. We will make the effect of this entropic force more concrete by employing the Hamiltonian formulation of General Relativity or Arnowitt-Deser-Misner (ADM) formalism. That is, we perform a (3+1)-splitting of space-time, a foliation that parametrizes the 4-dimensional metric $g_{\mu\nu}$ by means of a 3-dimensional metric h_{ij} and the lapse and shift functions N and N^i. Space-time dynamics is treated as the evolution of space-like hypersurfaces Σ_t, parametrized by some parameter t, which is usually taken to be the time coordinate. We already reviewed this formalism in sec. 1.4 in the context of Cosmological Perturbation Theory. Here, it will allow us to include non-equilibrium phenomena in a general way. For more details, see e.g. [48]. In the ADM formalism, an arbitrary metric takes the form

$$ds^2 = -(Ndt)^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt)\,. \tag{6.17}$$

We will denote as Σ the 3-dimensional hypersurface and n its normal vector:

$$n_\alpha = (-N, 0, 0, 0)\,, \tag{6.18}$$

which is a unit vector, i.e. $n_\alpha n^\alpha = -1$. Space-time indices are lowered and raised as usual by $g_{\mu\nu}$. Spatial indices, however, are lowered and raised by h_{ij}, which furthermore satisfies $h_{ij}h^{jk} = \delta_i^k$.

Equivalently, one can write the splitting of the metric as:

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu\,, \tag{6.19}$$

so that it is clear that $h_{\mu\nu}$ is purely tangential to the hypersurface. Then its spatial part h_{ij} is equal to the pull-back of the 4-dimensional metric $g_{\mu\nu}$ onto Σ and is a legitimate 3-dimensional metric.

The Einstein-Hilbert action for this parametrization of the metric is given by the following gravitational Lagrangian

$$\mathcal{L}_G = \sqrt{-g}\,R = N\sqrt{h}\left({}^{(3)}R + K_{ij}K^{ij} - K^2\right)\,, \tag{6.20}$$

where K_{ij} is the extrinsic curvature of the 3-hypersurface Σ and is given by the Lie derivative along the normal vector n

$$K_{ij} = \frac{1}{2}\pounds_n h_{ij} = \frac{1}{2N}\left(\partial_0 h_{ij} - \nabla_i N_j - \nabla_j N_i\right)\,. \tag{6.21}$$

where ∇ denotes the covariant derivative on Σ with respect to the 3-metric h_{ij}. Its trace and traceless part are

$$\begin{aligned} K &= h^{ij}K_{ij} = \frac{1}{N}\left(\partial_0 \ln\sqrt{h} - \nabla_i N^i\right) \\ \bar{K}_{ij} &= K_{ij} - \frac{1}{3}K h_{ij}\,. \end{aligned} \tag{6.22}$$

Unlike the intrinsic curvature, described by the Riemann tensor $R^{\rho}_{\mu\nu\lambda}$ and its contractions, the extrinsic curvature is a quantity that depends on the embedding of a surface in a larger manifold.

The extrinsic curvature can be a complicated function of the parameters. Therefore, it is convenient to shift to the Hamiltonian formulation of the stationary-action principle. Note that the only quantity whose time derivative appears in the gravitational Lagrangian is the 3-spatial metric h_{ij} and, thus, it is the only dynamical or propagating d.o.f. Correspondingly, one defines its conjugate momentum as

$$\Pi^{ij} = \frac{\partial \mathcal{L}_G}{\partial \dot{h}_{ij}} = \sqrt{h}\left(K^{ij} - K h^{ij}\right)\,. \tag{6.23}$$

With this, the gravitational Lagrangian can be rewritten as

$$\begin{aligned} \mathcal{L}_G &= N\sqrt{h}\,{}^{(3)}R - \frac{N}{\sqrt{h}}\left(\Pi_{ij}\Pi^{ij} - \frac{1}{2}\Pi^2\right) - 2\Pi^{ij}\nabla_i N_j \\ &= \Pi^{ij}\dot{h}_{ij} - N\mathcal{H} - N_i\mathcal{H}^i - 2\nabla_i\left(\Pi^{ij}N_j\right), \end{aligned} \tag{6.24}$$

where $\Pi = h_{ij}\Pi^{ij}$ and we introduced the functions

$$\begin{aligned} \mathcal{H} &= -\sqrt{h}\,{}^{(3)}R + \frac{1}{\sqrt{h}}\left(\Pi_{ij}\Pi^{ij} - \frac{1}{2}\Pi^2\right) \\ \mathcal{H}^i &= -2\nabla_j\left(h^{-1/2}\Pi^{ij}\right). \end{aligned} \tag{6.25}$$

Since N and N_i are not dynamical variables, they merely enter the gravitational Lagrangian as Lagrange multipliers. One defines the gravitational Hamiltonian as

$$\mathcal{H}_G = \Pi^{ij}\dot{h}_{ij} - \mathcal{L}_G = N\mathcal{H} + N_i\mathcal{H}^i + \nabla_i\left(\Pi^{ij}N_j\right), \tag{6.26}$$

with the Hamiltonian and momentum constraints

$$\frac{\delta\mathcal{H}_G}{\delta N} = \mathcal{H} = 0 \qquad \frac{\delta\mathcal{H}_G}{\delta N_i} = \mathcal{H}^i = 0\,. \tag{6.27}$$

The evolution equations are obtained upon taking variations of the Hamiltonian, but these need to be modified once the second law of thermodynamics is enforced and entropic forces come into play. The first Hamilton equation is

$$\frac{\delta\mathcal{H}_G}{\delta\Pi^{ij}} = \dot{h}_{ij} - \frac{\partial\dot{h}_{kl}}{\partial\Pi^{ij}}\Pi^{kl} - \frac{\partial\mathcal{L}_G}{\partial\dot{h}_{kl}}\frac{\partial\dot{h}_{kl}}{\partial\Pi^{ij}} = \dot{h}_{ij}\,. \tag{6.28}$$

This equation is true regardless of the constraint imposed by the second law of thermodynamics. The second Hamilton equation will carry the effect of non-equilibrium thermodynamics. Let us compute it starting from the derivative

$$\frac{\partial \mathcal{H}_G}{\partial h_{ij}} = \Pi^{kl}\frac{\partial \dot{h}_{kl}}{\partial h_{ij}} - \frac{\partial \mathcal{L}_G}{\partial \dot{h}_{kl}}\frac{\partial \dot{h}_{kl}}{\partial h_{ij}} - \frac{\partial \mathcal{L}_G}{\partial h_{ij}} = -\frac{\partial \mathcal{L}_G}{\partial h_{ij}} = -\frac{\partial \mathcal{L}_G}{\partial h^{kl}}\frac{\partial h^{kl}}{\partial h_{ij}}\,. \tag{6.29}$$

One usually applies the field equation in order to obtain the second Hamilton equation (see e.g. [173]). Here, we will do the same but taking into account the constraints imposed by the second law of thermodynamcs. The 3+1 splitting of the space-time manifold allows us to identify the 3-metric h_{ij} as the dynamical d.o.f. Then we argue that the phenomenological constraint should involve only those and, therefore, relates their dynamical evolution to changes in the entropy density

$$\frac{\partial \mathcal{L}}{\partial s}\pounds_n s = \frac{1}{2}N\sqrt{h}\,\tilde{f}_{ij}\pounds_n h^{ij}\,. \tag{6.30}$$

The Lie derivative $\pounds_n$ along the normal vector n serves here as a generalization of the time derivative. Note that the same equation for the phenomenological constraint is obtained if one characterizes the evolution of the hypersurfaces by the flow along the vector $m = Nn$, which may be preferred as it satisfies $g(\partial_t, m) = 1$. The variational constraint should only involve dynamical d.o.f. as well

$$\frac{\partial \mathcal{L}}{\partial s}\delta s = \frac{1}{2}N\sqrt{h}\,\tilde{f}_{ij}\delta h^{ij}\,. \tag{6.31}$$

The tensor $\tilde{f}_{ij}$ should now be understood as the pull-back of the projection of $f_{\mu\nu}$ on Σ, i.e.

$$\tilde{f}_{ij} = h^{\mu}_{i}h^{\nu}_{j}f_{\mu\nu} \tag{6.32}$$

We argue that this is the only non-vanishing part of $f_{\mu\nu}$. Our claim is supported by the fact that

$$\pounds_n(n^\mu n^\nu) = 0 \tag{6.33}$$

The tensor $\tilde{f}_{ij}$ will have contributions from its trace and trace-less component according to the tensor decomposition

$$\tilde{f}_{ij} = \frac{1}{3}\tilde{f}h_{ij} + \nabla_{(i}\tilde{f}_{j)} + \nabla_i\nabla_j\bar{f} + f^{TT}_{ij}\,, \tag{6.34}$$

where

$$\tilde{f} = \tilde{f}_{ij}h^{ij} \quad \nabla^i\tilde{f}_i = 0 \quad \nabla^i\nabla_i\bar{f} = 0 \quad \nabla^i f^{TT}_{ij} = h^{ij}f^{TT}_{ij} = 0\,. \tag{6.35}$$

We point out now that the interpretation of $s(t,\vec{x})$ as the entropy density is subtle. Instead, it is a function that satisfies the following entropy balance equation

$$\pounds_n s = \pounds_n s^{tot} - \nabla_i j^i_s\,, \tag{6.36}$$

where $\pounds_n s^{tot}$ is the total entropy production and j_s is the entropy flux in the hypersurface. Hence, $\pounds_n s$ is interpreted as the internal entropy production. It is important to bear this balance in mind when applying the phenomenological constraint to actual physical scenarios. We refer the interested reader to the appendix and to the original work on the variational formulation of non-equilibrium thermodynamics in the continuum [171] for the description of a fully variational formulation and its consistency with the shortcut version presented here.

Once we have properly taken into account the constraints given by the second law of thermodynamics, we are ready to obtain the field equation for the 3-metric as

$$\frac{\delta \mathcal{L}_G}{\delta h^{ij}} = \frac{\partial \mathcal{L}_G}{\partial h^{ij}} - \partial_\mu \frac{\partial \mathcal{L}_G}{\partial \partial_\mu h^{ij}} = -\frac{1}{2} N \sqrt{h}\, \tilde{f}_{ij} \,. \tag{6.37}$$

One can then recast it as

$$\frac{\partial \mathcal{L}_G}{\partial h^{kl}} \frac{\partial h^{kl}}{\partial h_{ij}} = \left(\partial_\mu \frac{\partial \mathcal{L}_G}{\partial \partial_\mu h^{kl}} - \frac{1}{2} N \sqrt{h}\, \tilde{f}_{kl} \right) \frac{\partial h^{kl}}{\partial h_{ij}} \tag{6.38}$$

and rewrite the derivative

$$\frac{\partial \mathcal{H}_G}{\partial h_{ij}} = -\left(\partial_\mu \frac{\partial \mathcal{L}_G}{\partial \partial_\mu h^{kl}} - \frac{1}{2} N \sqrt{h}\, \tilde{f}_{kl} \right) \frac{\partial h^{kl}}{\partial h_{ij}} \,. \tag{6.39}$$

Now, by using the relations

$$\begin{aligned} \frac{\partial h_{ij}}{\partial h^{kl}} &= -\frac{1}{2} \left(h_{ik} h_{jl} + h_{il} h_{jk} \right) \\ \frac{\partial \partial_\mu h_{ij}}{\partial \partial_\nu h^{kl}} &= -\frac{1}{2} \delta^\nu_\mu \left(h_{ik} h_{jl} + h_{il} h_{jk} \right) \end{aligned} \tag{6.40}$$

we get

$$\frac{\partial \mathcal{H}_G}{\partial h_{ij}} = -\dot{\Pi}^{ij} + \partial_k \frac{\partial \mathcal{H}_G}{\partial \partial_k h_{ij}} - \frac{1}{2} N \sqrt{h}\, \tilde{f}^{ij} \tag{6.41}$$

and introducing the functional derivative

$$\frac{\delta \mathcal{H}_G}{\delta h_{ij}} = \frac{\partial \mathcal{H}_G}{\partial h_{ij}} - \partial_\mu \frac{\partial \mathcal{H}_G}{\partial \partial_\mu h_{ij}} \tag{6.42}$$

we obtain the second Hamilton equation

$$\frac{\delta \mathcal{H}_G}{\delta h_{ij}} = -\dot{\Pi}^{ij} - \frac{1}{2} N \sqrt{h}\, \tilde{f}^{ij} \,. \tag{6.43}$$

This equation is modified by the existence of an entropic force in consistency with the thermodynamical constraint. Physically, it is this equation that describes the dynamical evolution, for it implicitly contains a second time derivative of the field.

Matter can be included in the Lagrangian density as

$$\mathcal{L} = \mathcal{L}_G(h_{ij}, \dot{h}_{ij}) + 2\kappa\, \mathcal{L}_m(h_{ij}, S)\,, \tag{6.44}$$

where we introduced the gravitational coupling in the matter Lagrangian for convenience. Then the Hamilton equations become

$$\begin{aligned} \frac{\delta \mathcal{H}_G}{\delta \Pi^{ij}} &= \dot{h}_{ij} \\ \frac{\delta \mathcal{H}_G}{\delta h_{ij}} &= -\dot{\Pi}^{ij} - 2\kappa\, \frac{\delta \mathcal{L}_m}{\delta h_{ij}} - \kappa\, N\sqrt{h}\,\tilde{f}^{ij}\,, \end{aligned} \tag{6.45}$$

where the entropic term carries the coupling κ as well if it comes from the matter Lagrangian. The Hamiltonian and momentum constraints are likewise modified by the introduction of matter

$$\frac{\delta \mathcal{H}_G}{\delta N} = \mathcal{H} = 2\kappa \frac{\partial \mathcal{L}_m}{\partial N}\,, \quad \frac{\delta \mathcal{H}_G}{\delta N_i} = \mathcal{H}^i = 2\kappa \frac{\partial \mathcal{L}_m}{\partial N_i}\,. \tag{6.46}$$

The variational formalism for non-equilibrium thermodynamics developed in refs. [170,171] fits nicely in both the Lagrangian and Hamiltonian formulation of General Relativity. This means that one can naturally consider effects of non-equilibrium thermodynamics in General Relativity and obtain analytical or numerical solutions to the equations of motion.

6.3.3 The Raychauduri equations

The appearance of an entropic term in Einstein's field equations can have dynamical effects that may look as a violation of the energy conditions. We wil look now into this possibility by studying a congruence of worldlines in an arbitrary space-time. These need not be geodesics and have tangent vector n. The congruence is then characterized by the tensor

$$\Theta_{\mu\nu} = D_\nu n_\mu = \frac{1}{3}\Theta h_{\mu\nu} + \sigma_{\mu\nu} + \omega_{\mu\nu} - a_\mu n_\nu \tag{6.47}$$

where θ is the expansion rate of the congruence, $\sigma_{\mu\nu}$ is its shear or symmetric trace-less part and $\omega_{\mu\nu}$ is its vorticity or antisymmetric part. If the worldline is not a geodesic, then the congruence suffers an acceleration given by

$$a_\mu = n^\nu D_\nu n_\mu \tag{6.48}$$

One can compute the Lie derivative of the expansion of the congruence along its tangent vector and find the Raychauduri equation [48]

$$\pounds_n \Theta = -\frac{1}{3}\Theta^2 - \sigma_{\mu\nu}\sigma^{\mu\nu} + \omega_{\mu\nu}\omega^{\mu\nu} - R_{\mu\nu}n^\mu n^\nu + D_\mu a^\mu\,. \tag{6.49}$$

Let us perform the standard analysis of the sign of this equation. It is clear that $\sigma_{\mu\nu}\sigma^{\mu\nu} > 0$ and $\Theta^2 > 0$. On the other hand, if the congruence is chosen to be orthogonal to the spatial hypersurfaces, as we have been considering, then the vorticity vanishes $\omega_{\mu\nu} = 0$. Lastly, it is left to consider the term $R_{\mu\nu}n^\nu n^\nu$, which we can rewrite with the help of the field equations

$$R_{\mu\nu}n^\mu n^\nu = 8\pi G\left(T_{\mu\nu}n^\mu n^\nu + \frac{1}{2}T - f_{\mu\nu}n^\mu n^\nu - \frac{1}{2}f\right) \tag{6.50}$$

If the strong energy condition is satisfied, then

$$T_{\mu\nu}n^\mu n^\nu \geq -\frac{1}{2}T \tag{6.51}$$

and, in the absence of intrinsic acceleration, $a_\mu = 0$, we can establish the bound

$$\pounds_n\Theta + \frac{1}{3}\Theta^2 \leq 8\pi G\left(f_{\mu\nu}n^\mu n^\nu + \frac{1}{2}f\right) \tag{6.52}$$

For a vanishing entropic force $f_{\mu\nu} = 0$, this means that an expanding congruence cannot indefinitely sustain its divergence and will eventually recollapse. On the contrary, a positive and sufficiently large entropic contribution can avoid such recollapse. This may become relevant for an expanding universe, but also to generic gravitational collapse and the singularity theorems [174–176].

The shear $\sigma_{\mu\nu}$ is also affected by the inclusion of an entropic force. Its evolution equation is given by

$$\pounds_n\sigma_{\mu\nu} = -\frac{2}{3}\theta\,\sigma_{\mu\nu} - \sigma_{\mu\lambda}\sigma^\lambda{}_\nu - \omega_{\mu\lambda}\omega^\lambda{}_\nu + C_{\lambda\mu\rho\nu}n^\lambda n^\rho + \frac{1}{3}h_{\mu\nu}(\sigma_{\lambda\rho}\sigma^{\lambda\rho} - \omega_{\lambda\rho}\omega^{\lambda\rho}) + \frac{1}{2}\hat{R}_{\mu\nu}\,, \tag{6.53}$$

where $C_{\lambda\mu\rho\nu}$ is the Weyl tensor and $\hat{R}_{\mu\nu}$ is the spatial, trace-free part of the Ricci tensor

$$\hat{R}_{\mu\nu} = h_{\mu\lambda}h_{\nu\rho}R^{\lambda\rho} - \frac{1}{3}h_{\mu\nu}h_{\lambda\rho}R^{\lambda\rho} \tag{6.54}$$

This explicit dependence on the Ricci tensor allows us to directly include the effect of the entropic force and establish a bound. Indeed, using the modified Einstein field equation we get

$$\hat{R}_{\mu\nu} = 8\pi G\left(\hat{T}_{\mu\nu} - \hat{f}_{\mu\nu}\right), \tag{6.55}$$

where $\hat{f}_{\mu\nu}$ and $\hat{T}_{\mu\nu}$ are the analogously defined spatial, trace-free part of the friction and stress-energy tensors. Then we can rewrite the evolution equation for the shear as:

$$\begin{aligned}\pounds_n\sigma_{\mu\nu} = &-\frac{2}{3}\theta\,\sigma_{\mu\nu} - \sigma_{\mu\lambda}\sigma^\lambda{}_\nu - \omega_{\mu\lambda}\omega^\lambda{}_\nu + C_{\lambda\mu\rho\nu}n^\lambda n^\rho \\ &+ \frac{1}{3}h_{\mu\nu}(\sigma_{\lambda\rho}\sigma^{\lambda\rho} - \omega_{\lambda\rho}\omega^{\lambda\rho}) + 4\pi G\left(\hat{T}_{\mu\nu} - \hat{f}_{\mu\nu}\right),\end{aligned} \tag{6.56}$$

which means that the entropic force directly sources the shear in a way similar to that of the stress-energy tensor.

These results also apply to a congruence of worldlines which are not normal to the hypersurfaces that define the foliation of the space-time. In that case, the vorticity is non-vanishing and has the evolution equation

$$\pounds_n \omega_{\mu\nu} = -\frac{2}{3}\theta\, \omega_{\mu\nu} - 2\sigma^{\lambda}_{[\nu}\omega_{\mu]\lambda}\,, \tag{6.57}$$

which is not directly sourced by the entropic term. Of course, it is still affected indirectly due to modifications in the metric, the expansion and the shear.

The decomposition of the 2-tensor describing the congruence of geodesics into global expansion, shear and vorticity, which are affected by the entropic forces via the corresponding Raychaudhuri equations, brings to mind the evolution of large scale structures in the cosmic web due to gravitational collapse of initial fluctuations. The growth of structure brings order into an otherwise homogeneous universe, so we expect a corresponding entropy production in the outskirts of large structures like galaxies and clusters of galaxies. According to our formulation, on supergalactic scales, such an entropy production should give rise to a local acceleration, leaving large voids between superclusters, enhancing the contrast induced by the usual gravitational collapse. Moreover, in the formation of the first spiral galaxies there is also an associated entropy production which could give rise to a tiny acceleration, that may explain part of the rotation curves of galaxies, beyond that produced by the dark matter in the halos of galaxies.

6.4 Temperature and entropy

So far we have imposed the second law of thermodynamics by a constraint which contains the derivative $\partial L/\partial S$. The goal of this section is to understand how this term is often linked to the concept of temperature of a thermodynamical system, not only in a mechanical system but also in General Relativity. In doing so, we will consider two sources of entropy: hydrodynamical matter and gravity itself.

6.4.1 Bulk entropy: Hydrodynamical matter

Let us first consider a mechanical system with Lagrangian given by

$$L(q, \dot{q}, S) = E_K(q, \dot{q}) - U(q, S)\,, \tag{6.58}$$

where E_K and U are, respectively, the kinetic and internal energy. Notice that only the latter depends on the entropy S. One way of obtaining the temperature of this thermodynamic system is by definition:

$$T = \frac{\partial U}{\partial S} = -\frac{\partial L}{\partial S}\,. \tag{6.59}$$

Then the entropic constraint can also be written as

$$T\dot{S} = -F\dot{q} > 0\,. \tag{6.60}$$

We can generalize this to a fluid whose Lagrangian is pure internal energy, as it is the case for instance of the cosmic fluid [45]. The matter Lagrangian is then given by

$$L = \int d^3x\mathcal{L} = -\int d^3x\sqrt{-g}\,\rho(g_{\mu\nu}, s)\,, \tag{6.61}$$

where $\rho(g_{\mu\nu}, s)$ is the energy density of the fluid. Hence, hydrodynamic matter has a well defined notion of temperature

$$T = -\frac{1}{\sqrt{-g}}\frac{\partial \mathcal{L}_m}{\partial s} = -\frac{\partial \rho}{\partial s}\,. \tag{6.62}$$

If the fluid is homogeneous and isotropic this definition is equivalent to

$$T = -\frac{\partial L}{\partial S}\,. \tag{6.63}$$

The tensor entropic force for a space-time filled with hydrodynamic matter in the ADM formalism is then given implicitly by

$$F_{ij}\dot{h}^{ij} = -T\dot{S} \leq 0\,. \tag{6.64}$$

Since entropy is a monotonically increasing function of time, the second law of thermodynamics constraints the sign of the tensor entropic force.

6.4.2 Surface terms: Entropy in the boundary

One can also wonder about the effect of the entropy associated to space-time itself, in particular to horizons. It can be incorporated in a natural way by extending the Einstein-Hilbert action with a surface term, the Gibbons-Hawking-York (GHY) term of refs. [177, 178].

Let us consider a space-time manifold $\mathcal{M}$ with metric $g_{\mu\nu}$, which has a horizon hypersurface that we denote by $\mathcal{H}$. This is a submanifold of the whole space-time. By taking n^μ, the normal vector to the hypersurface $\mathcal{H}$, we can define an inherited metric on $\mathcal{H}$

$$g_{\mu\nu} = h_{\mu\nu} + n_\mu n_\nu\,. \tag{6.65}$$

With this, one can define the GHY term as

$$\mathcal{S}_{GHY} = \frac{1}{8\pi G} \oint_{\mathcal{H}} d^3y \sqrt{h} K \,, \tag{6.66}$$

where K is the trace of the extrinsic curvature of the surface. We already considered this quantity when discussing the ADM formalism. Notice, however, that here we are not foliating the entire space-time, but rather considering the properties of a particular hypersurface, the horizon. From the thermodynamic point of view, the GHY term contributes to the internal energy of the system. Hence, it can be related to the temperature and entropy of the horizon as

$$\mathcal{S}_{GHY} = -\int dt\, N(t)\, TS \,. \tag{6.67}$$

where we have kept the lapse function $N(t)$, to indicate that the variation of the total action with respect to it will generate a Hamiltonian constraint with an entropy term together with the ordinary matter/energy terms. In order to illustrate this, let us now compute the GHY for two horizons of interest: the event horizon of a Schwarzschild black hole and the horizon of black holes in FLRW universe.

Schwarzschild black hole

In order to illustrate this, let us now compute the GHY term for the event horizon of a Schwarzschild black hole of mass M. Its space-time is described by the metric

$$ds^2 = -\left(1 - \frac{2GM}{r}\right) dt^2 + \left(1 - \frac{2GM}{r}\right)^{-1} dr^2 + r^2 d\Omega_2^2 \,. \tag{6.68}$$

The normal vector to a 2-sphere of radius r around the origin of coordinates is

$$n = -\sqrt{1 - \frac{2GM}{r}}\, \partial_r \,. \tag{6.69}$$

With this, the trace of the extrinsic curvature for such a sphere scaled by the metric determinant is

$$\sqrt{h} K = (3GM - 2r) \sin\theta \,. \tag{6.70}$$

Integrating over the angular coordinates and setting the 2-sphere at the event horizon, i.e. $r = 2GM$, and restoring for a moment $\hbar$ and c, the GHY becomes

$$\mathcal{S}_{GHY} = -\frac{1}{2} \int dt M c^2 = -\int dt T_{BH} S_{BH} \,, \tag{6.71}$$

where T_{BH} is the Hawking temperature and S_{BH} is the Bekenstein entropy of the Schwarzschild black hole

$$k_{\mathrm{B}} T_{BH} = \frac{\hbar c^3}{8\pi G M} \,, \qquad S_{BH} = k_{\mathrm{B}} \frac{A c^3}{4 G \hbar} = k_{\mathrm{B}} \frac{4\pi G M^2}{\hbar c} \,. \tag{6.72}$$

This favors the interpretation of the GHY term of a horizon as a contribution to the internal energy in the thermodynamic sense.

Cosmological black holes

The natural inclusion of temperature and entropy from surface terms allows is also useful when embedding black holes into an expanding universe. This embedding is not unique [68], but one can keep the discussion rather generic by considering the generalized McVittie solution

$$ds^2 = -N(t)^2 \frac{B(t,\bar{r})^2}{A(t,\bar{r})^2} dt^2 + a(t)^2 A(t,\bar{r})^4 \left(d\bar{r}^2 + \bar{r}^2 d\Omega_2^2\right) \,, \tag{6.73}$$

where

$$\begin{aligned} A(t,\bar{r}) &= 1 + \frac{m(t)}{2\bar{r}} \\ B(t,\bar{r}) &= 1 - \frac{m(t)}{2\bar{r}} \,, \end{aligned} \tag{6.74}$$

being $m(t) > 0$ the comoving mass of the black hole, i.e. $m(t) = M(t)/a(t)$, and $N(t)$ the lapse function linked to the residual gauge freedom. Note the use of isotropic coordinates, which are obtained by introducing a new comoving radial coordinate $\bar{r}$, related to the usual areal radius r by

$$r = a(t)\bar{r}\left(1 + \frac{m(t)}{2\bar{r}}\right)^2 \,. \tag{6.75}$$

For a black hole much smaller than the Hubble scale, its apparent horizon is located at its Schwarzschild radius [68] and we can assign to it the usual Bekenstein entropy and Hawking temperature. Performing a computation similar to that of the Schwarzschild black hole, we arrive at the following result for the GHY term

$$\mathcal{S}_{GHY} = -\oint dt N(t) T_{BH} S_{BH} \,. \tag{6.76}$$

The growth of black holes comes with an increase in the entropy and an associated entropic force, which may have an impact on the dynamics of the scale factor. Furthermore, if the universe is populated by many black holes, one can compute their average contribution to the stress-energy tensor from these surface terms. Indeed, if one takes now the homogeneous and isotropic flat FLRW metric, which is valid at sufficiently large scales, then the GHY term can be approximated as

$$\mathcal{S}_{GHY} = -\sum_i \oint dt N(t) T_{BH} S_{BH} \simeq -\int d^4x \sqrt{-g}\, n_{BH} T_{BH} S_{BH} \,, \tag{6.77}$$

where n_{BH} is the number density of the black holes. This delivers the following contribution to the stress-energy tensor

$$T_{00} = N(t)^2 \rho_{BH} \,. \tag{6.78}$$

The other components of the stress-energy tensor depend on the accretion onto the black holes. If there is no accretion, as it is the case of the original McVittie metric [68], then the T_{ij} and T_{0i} components vanish and so does the pressure p and we recover the standard interpretation of a collection of black holes as dust. Other accretion conditions may lead to different equations of state.

Interpretation as a thermodynamic system

One may interpret the effects of the GHY term as the inclusion of a thermodynamic system. For a localized object like a black hole, its properties are characterised by the Lagrangian

$$L = -U\,, \tag{6.79}$$

where U is the internal energy of the system, which we find to be

$$U = -NTS\,. \tag{6.80}$$

If we ignore the lapse function, linked to the freedom in choosing the time coordinate, this expression is similarly found in usual thermodynamics.

Furthermore, if the thermodynamic system is extended, as in the case of the cosmological black holes, one may interpret this thermodynamic system not as an isolated object but rather as a fluid. In that case the internal thermodynamic energy can be written as a spatial integral of an energy density

$$U = \iiint d^3x\sqrt{-g}\,\rho \tag{6.81}$$

and deliver the Lagrangian of a perfect fluid. This fluid satisfies the second law of thermodynamics and may be considered as an effective real fluid after allowing an increase in entropy. In sec. 6.6 we discuss how the variational formalism includes the theory of real fluids and provides an extension thereof.

6.5 Non-equilibrium Cosmology

Let us now illustrate the potential of our covariant formulation of non-equilibrium thermodynamics in General Relativity by studying how it affects the trajectory of particles. We will consider a particularly relevant example of a space-time, an FLRW universe, and show how the Friedmann equations get modified in this context. These equations directly affect the geodesics followed by inertial observers.

The effect of non-equilibrium thermodynamics in an expanding FLRW universe requires the consideration of a homogeneous and isotropic space-time described by the metric

$$ds^2 = -N(t)^2 dt^2 + a^2(t)\left(\frac{dr^2}{1-kr^2} + r^2 d\Omega_2^2\right). \tag{6.82}$$

This fits naturally with the ADM formalism upon the choice for the shift functions

$$N^i = 0 \tag{6.83}$$

as well as the 3-dimensional metric h

$$\begin{aligned} h_{rr} &= \frac{a^2(t)}{1-kr^2} \\ h_{\theta\theta} &= a^2(t)\, r^2 \\ h_{\varphi\varphi} &= a^2(t)\, r^2 \sin^2\theta\,. \end{aligned} \tag{6.84}$$

These are imposed by the Copernican Principle, i.e. homogeneity and isotropy. On the contrary, the lapse function N is not determined a priori, so we will keep it free for now. It is related to the freedom in choosing the time coordinate. The square root of the 3-metric determinant is

$$\sqrt{h} = \frac{a^3(t)\, r^2 \sin\theta}{\sqrt{1-kr^2}}\,. \tag{6.85}$$

We can then compute the extrinsic curvature and find the conjugate momentum to the 3-metric

$$K^{ij} = \frac{1}{N}\frac{\dot a}{a} h^{ij} \qquad \Pi^{ij} = -\frac{2}{N}\frac{\dot a}{a}\sqrt{h}\, h^{ij} \tag{6.86}$$

and the corresponding traces

$$K = K^{ij} h_{ij} = \frac{3}{N}\frac{\dot a}{a} \qquad \Pi = \Pi^{ij} h_{ij} = -\frac{6}{N}\frac{\dot a}{a}\sqrt{h}\,, \tag{6.87}$$

as well as the 3-dimensional Ricci scalar

$${}^{(3)}R = \frac{6k}{a^2}\,. \tag{6.88}$$

The first Hamilton equation provides no additional information by itself, so the dynamics is obtained from the second Hamilton equation and the Hamiltonian constraint. Let us begin with the Hamiltonian constraint. We need the quantity

$$\Pi_{ij}\Pi^{ij} - \frac{1}{2}\Pi^2 = -\frac{6}{N^2}\left(\frac{\dot a}{a}\right)^2 h\,. \tag{6.89}$$

Then

$$\mathcal{H} = -\sqrt{h}\frac{6k}{a^2} - \frac{6}{N^2}\sqrt{h}\left(\frac{\dot a}{a}\right)^2 = 2\kappa\frac{\delta \mathcal{L}_m}{\delta N}\,. \tag{6.90}$$

The RHS is related with the stress-energy tensor in the following way

$$\frac{\delta \mathcal{L}_m}{\delta N} = -\frac{\delta \mathcal{L}_m}{\delta g_{00}} 2N = -T^{00} N^2 \sqrt{h}\,. \tag{6.91}$$

Note the slightly different definitions for the contravariant and covariant stress-energy tensor, due to the sign flip of the functional derivative

$$\begin{aligned} T_{\mu\nu} &= \frac{-2}{\sqrt{-g}} \frac{\delta \mathcal{L}_m}{\delta g^{\mu\nu}} \\ T^{\mu\nu} &= \frac{2}{\sqrt{-g}} \frac{\delta \mathcal{L}_m}{\delta g_{\mu\nu}}\,. \end{aligned} \tag{6.92}$$

An FLRW universe is filled with a cosmological perfect fluid, whose stress-energy tensor is given by

$$T^{\mu\nu} = (\rho + p) u^\mu u^\nu + p g^{\mu\nu}\,, \tag{6.93}$$

where the density ρ and pressure p are allowed to have a dependence on the entropy S as well as on the scale factor a. Since the fluid that we are considering is isotropic and homogeneous, its 4-velocity is

$$u^\mu = \left(\frac{1}{N}, 0, 0, 0\right) \Bigg(\quad g_{\mu\nu} u^\mu u^\nu = -1\,. \tag{6.94}$$

Then we can identify the time-time component of the stress-energy tensor with the energy density of the fluid

$$T^{00} = \rho N^{-2} \tag{6.95}$$

and the Hamiltonian constraint becomes

$$\mathcal{H} = -\sqrt{h}\frac{6k}{a^2} - \sqrt{h}\frac{6}{N^2}\left(\frac{\dot{a}}{a}\right)^2 = -2\kappa\rho\sqrt{h}\,. \tag{6.96}$$

This expression can be rearranged as

$$\frac{1}{N^2}\left(\frac{\dot{a}}{a}\right)^2 + \frac{k}{a^2} = \frac{8\pi G}{3}\rho \tag{6.97}$$

This is the first Friedmann equation, which is nothing but a constraint on the dynamics of the FLRW space-time. If we make the choice $N = 1$, which corresponds to the choice of cosmic time as time coordinate, we get the first Friedmann equation in its usual form

$$\left(\frac{\dot{a}}{a}\right)^2 + \frac{k}{a^2} = \frac{8\pi G}{3}\rho\,. \tag{6.98}$$

Of course, one can work with conformal time and choose $N = a$. Then the first Friedmann equation becomes

$$\left(\frac{a'}{a}\right)^2 + k = \frac{8\pi G}{3}\rho a^2\,, \tag{6.99}$$

which is consistent with a direct coordinate transformation.

Let us take a look now at the equation of motion involving the trace of the conjugate momentum

$$\begin{aligned}\dot{\Pi} =& \dot{\Pi}^{ij} h_{ij} + \Pi^{ij}\dot{h}_{ij} \\ =& -\frac{\delta \mathcal{H}_G}{\delta h_{ij}} h_{ij} + 2\kappa \frac{\delta \mathcal{L}_m}{\delta h_{ij}} h_{ij} - \kappa N\sqrt{h}\,\tilde{f}^{ij} h_{ij} + \Pi^{ij}\frac{\delta \mathcal{H}_G}{\delta \Pi^{ij}} \\ =& \frac{1}{2} N\sqrt{h}\,^{(3)}R + \frac{3}{2}N\sqrt{h}\left(K_{ij}K^{ij} - K^2\right) + 2\kappa\frac{\delta \mathcal{L}_m}{\delta h_{ij}} h_{ij} - \kappa N\sqrt{h}\,\tilde{f}^{ij} h_{ij}\,.\end{aligned} \tag{6.100}$$

The only term left to compute in this expression is

$$K_{ij}K^{ij} - K^2 = -\frac{6}{N^2}\left(\frac{\dot{a}}{a}\right)^2\,. \tag{6.101}$$

Then:

$$\dot{\Pi} = \frac{1}{2} N\sqrt{h}\frac{6k}{a^2} + \frac{3}{2}N\sqrt{h}\left(-\frac{6}{N^2}\left(\frac{\dot{a}}{a}\right)^2\right) + \kappa\sqrt{h}\,N T^{ij} h_{ij} - \kappa N\sqrt{h}\,\tilde{f}\,, \tag{6.102}$$

where we used the definition of the spatial components of the stress-energy tensor

$$N\sqrt{h}\,T^{ij} = 2\frac{\delta \mathcal{L}_m}{\delta h_{ij}} \tag{6.103}$$

On the other hand, we have the geometric relation

$$\dot{\Pi} = -2\sqrt{h}\,\dot{K} - 2N\sqrt{h}\,K^2 = -6\sqrt{h}\left[\frac{\ddot{a}}{aN} - \frac{\dot{a}\dot{N}}{aN^2} + 2\left(\frac{\dot{a}}{a}\right)^2\right], \tag{6.104}$$

where we used

$$\dot{K} = 3\left(\frac{\ddot{a}}{aN} - \frac{\dot{a}^2}{a^2 N} - \frac{\dot{a}\dot{N}}{aN^2}\right). \tag{6.105}$$

Using both expressions for $\dot{\Pi}$, the first Friedmann equation (i.e. the Hamiltonian constraint) and the spatial trace of the stress-energy tensor,

$$\frac{1}{6}\kappa T^{ij} h_{ij} = \frac{4\pi G}{3} 3p\,, \tag{6.106}$$

we get the equation of motion

$$\frac{\ddot{a}}{aN^2} - \frac{\dot{a}\dot{N}}{aN^3} = -\frac{4\pi G}{3}(\rho + 3p) + \frac{4\pi G}{3} N \tilde{f} \,. \tag{6.107}$$

Of course, for $N = 1$ this is nothing but the second Friedmann equation with an additional term of entropic origin. The effect of non-equilibrium thermodynamics is now encoded in the spatial trace

$$\tilde{f} = \tilde{f}^{ij} h_{ij} \,. \tag{6.108}$$

This trace is related to the rate of entropy production by the second law of thermodynamics, encoded in the phenomenological constraint. Let us check how

$$\frac{1}{2\kappa}\frac{\delta L}{\delta S}\dot{S} = \frac{1}{2} a^3 \tilde{f}_{ij} \dot{h}^{ij} = -\dot{a} a^2 \tilde{f} \,. \tag{6.109}$$

Introducing the temperature of the cosmological fluid,

$$\frac{1}{2\kappa}\frac{\partial L}{\partial S} = -T \,, \tag{6.110}$$

we get the expression for the trace of the entropic force

$$\tilde{f} = \frac{T\dot{S}}{\dot{a}a^2} \,. \tag{6.111}$$

With this, the equation of motion becomes

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3p) + \frac{4\pi G}{3} \quad \frac{T\dot{S}}{a^2\dot{a}} \Bigg)\Bigg(, \tag{6.112}$$

which is the second Friedmann equation modified by the enforcement of the second law of thermodynamics.

Most of the expansion history of the universe is adiabatic and thus remains unaffected by the inclusion of the effects of non-equilibrium thermodynamics in the Friedmann equations. Nevertheless, we can think of several phenomena in the expansion history during which entropy is copiously produced, such as the reheating of the universe, phase transitions and gravitational collapse to form black holes. We claim that these and other non-adiabatic phenomena in cosmology should be revisited, as their effect on the expansion rate may be non-negligible.

The assumption of homogeneity and isotropy implies that the tensor friction or entropic force $\tilde{f}_{ij}$ has only a trace component $\tilde{f}$. If we perturb around this solution, we expect the trace-less components to play a role as well, following the tensor decomposition in eq. (6.35). We leave the exploration of its consequences to a future publication where we will study the theory of cosmological perturbations in the presence of entropic forces arising from the trace, shear and vortical components of f.

Certain processes like gravitational collapse and structure formation are highly non-linear and cannot be understood within perturbation theory. It may be useful to treat this regime, highly non-linear and out of equilibrium, as an effective fluid. In this regard, we consider in the next section the similarities between generic entropic forces and the viscosity of a real fluid.

In principle, out of equilibrium phenomena could be incorporated into N-body simulations that study structure formation. This could be achieved by taking the non-relativistic limit of the non-equilibrium gravitational equations of motion in order to obtain a Newtonian plus entropic force.

6.6 Real fluids in the variational formalism

The results obtained in the previous sections are consistent with the relativistic dynamics of real fluids, i.e. fluids with viscosity and heat transfer. Such fluids are described by a stress-energy tensor that deviates from that of a perfect fluid [179, 180]

$$T_{\mu\nu} = (\rho + p)u_\mu u_\nu + p g_{\mu\nu} + \tau_{\mu\nu}\,. \tag{6.113}$$

This can be seen as a particular case of the variational formalism if the following equation is satisfied

$$\tau_{\mu\nu} = -f_{\mu\nu} \tag{6.114}$$

The additional term satisfies the orthogonality property

$$u^\mu \tau_{\mu\nu} = 0\,. \tag{6.115}$$

This is consistent with our description in the ADM formalism. In the comoving orthogonal gauge, $u^\mu = n^\mu$ and so the motion of the fluid is orthogonal to the constant time hypersurfaces.

For a vanishing chemical potential, the second law of thermodynamics of a real fluid takes the form

$$T D_\mu(\sigma u^\mu) = \tau^\nu_\mu D_\nu u^\mu \tag{6.116}$$

The LHS can be split into parallel and perpendicular components to the hypersurfaces, so that

$$D_\mu(\sigma u^\mu) = n_\mu n^\alpha D_\alpha(\sigma u^\mu) + \nabla_\mu(\sigma u^\mu) = n_\mu \pounds_n(\sigma u^\mu) + n_\mu \sigma u^\alpha D_\alpha n^\mu + \nabla_\mu(\sigma u^\mu)\,, \tag{6.117}$$

where σ is the local entropy density of the fluid. In the comoving orthogonal gauge this expression becomes

$$D_\mu(\sigma u^\mu) = \pounds_n \sigma + \nabla_\mu(\sigma n^\mu)\,. \tag{6.118}$$

On the other hand, in this gauge we have

$$D_\mu u_\nu = \frac{1}{2}\pounds_n h_{\mu\nu} \tag{6.119}$$

and the temperature of the fluid can be identified with

$$T = -\frac{1}{N\sqrt{h}}\frac{\partial \mathcal{L}}{\partial s} \tag{6.120}$$

We find then that the second law of thermodynamics of a real fluid can be rewritten in terms of the phenomenological constraint. This requires the following identifications

$$f_{\mu\nu} = -\tau_{\mu\nu} \quad s^{tot} = \sigma \quad j^i_s = -\sigma u^i\,. \tag{6.121}$$

We can still go one step further in the identification between the entropic force tensor and the viscosity tensor by inspecting its usual form

$$\tau_{\mu\nu} = -\,\eta\left(D_\nu u_\mu + D_\mu u_\nu - u_\nu u^\alpha D_\alpha u_\mu - u_\mu u^\alpha D_\alpha u_\nu\right) - \left(\zeta - \frac{2}{3}\eta\right)\Big(D_\alpha u^\alpha \left(g_{\mu\nu} + u_\mu u_\nu\right)\,, \tag{6.122}$$

where η and ζ are, respectively, the shear and bulk viscosity coefficients. Let us now focus on a homogeneous and isotropic fluid filling an FLRW universe. In this example, the covariant derivatives are given by

$$D_\mu u^\nu = \frac{\dot a}{a}\delta^\nu_\mu\,, \tag{6.123}$$

which means that the viscosity tensor is reduced to

$$\tau_{\mu\nu} = -3\zeta\frac{\dot a}{a}h_{\mu\nu}\,. \tag{6.124}$$

We can compare this with the expression of the trace of the entropic force obtained previously

$$\frac{T\dot S}{a^3 H} = \tilde f = \tilde f^{ij} h_{ij} = -\tau_{ij} h^{ij} \tag{6.125}$$

and obtain the following identity for the bulk viscosity coefficient

$$\zeta = \frac{T\dot S}{9H^2 a^3} > 0\,. \tag{6.126}$$

Let us elaborate a bit on the results of this section. First of all, the conventional formulation of general relativistic real fluids can be recovered by means of the variational formulation of non-equilibrium thermodynamics in General Relativity. In fact, one does not even need to impose additional terms on the energy momentum tensor. Instead, they are effectively generated by simply assuming the pressure and the energy density of the fluid to have a dependency on the entropy.

The variational description allows the inclusion of dissipative effects to any matter or gravity content, as long as it has time-dependent entropy. This means that we can interpret non-equilibrium phenomena in General Relativity as an effective viscosity term of a real (i.e. non ideal) fluid. In this sense, our results allow for a variational, first principles formulation of real fluids and the generalization of their dissipative effects to arbitrary matter and gravity contents.

We point out that the variational and phenomenological constraints are imposed before obtaining the equations of motion and must be satisfied at all times. This is a fundamental difference with the theory of real fluids.

Here we considered a vanishing chemical potential, which means that we did not impose particle number conservation. This excludes thermal conduction effects. Nevertheless, one could in principle impose also particle number conservation at the Lagrangian [171].

In the homogeneous and isotropic limit there is only bulk viscosity, parametrized by ζ. However, shear viscosity, parametrized by η, may play a role in characterizing entropic forces in gravitational collapse and structure formation.

6.7 Discussion

In this chapter we constructed a variational formulation of non-equilibrium thermodynamics in GR. This allows for a synthesis of two key physical principles: the extremal action and the laws of thermodynamics. More precisely, thermodynamics is included as a variational constraint, which modifies the variational problem posed by the extremal action principle. Consequently, the equations of motion are modified in compliance with the laws of thermodynamics, allowing for a departure of (global) equilibrium.

Applications to Cosmology are immediate. Non-equilibrium phenomena lead to a modification of the usual cosmic dynamics, with the inclusion of a repulsive (accelerating) term in the second Friedmann equation. We identify two possible contributions to the entropy of the universe: fluids (*bulk* entropy) and horizons (*boundary* entropy), such that dissipative phenomena in real fluids and horizon growth lead to entropy production. In contrast to the usual formulation of real fluids, we point out that ours is based on first principles and allows for the inclusion of other irreversible phenomena that do not admit, in principle, a fluid description.

It is key to explore possible contributions to the entropy of the universe and identify whether entropy-producing phenomena could dominate the dynamics of the universe, thus leading to an accelerated expansion. This will be the main goal of the following chapter.

Chapter 7

Entropic cosmic acceleration

> Andábamos sin buscarnos pero sabiendo que andábamos para encontrarnos.
>
> Julio Cortázar, *Rayuela* (1963).

7.1 Motivation

Gravity is usually regarded to be a purely attractive force. Indeed, Newton's law of Gravitation admits only positive charges (gravitational mass), as opposed to Coulomb's law of electrostatics, which admits both positive and negative (electric) charges. Even though this requirement was first imposed by hand, as in our daily experience no negative gravitational mass is ever observed, can be deeply justified within field theory. While the photon is a spin-1 field and admits both positive and negative charges, the graviton is a spin-2 field and admits only positive charges.

A similar observation can be done in the geometric language provided by GR and its description of the gravitational interaction. Indeed, geodesic congruences tend to converge due to Penrose-Hawking theorems [174–176], as we discussed in sec. 6.3. However, in order for these theorems to hold, certain conditions on the stress-energy tensor must be imposed. They are satisfied by ordinary matter, but not a first principles requirement of theory. Hence, GR allows gravity to act as a repulsive force.

We just mentioned that we do not observe negative gravitational mass (energy) in our daily experience. Indeed, negative energy is considered to be unphysical, since Hamiltonians that are unbounded from below lead to instabilities. However, pressure gravitates in GR and it is possible for gravity to become repulsive while keeping energy positive if there is a sufficiently strong negative pressure. Specifically, such matter should satisfy the weak energy condition, but violate the strong one. This is enough for the hyphotheses of the Penrose-Hawking theorem not to be satisfied.

We do not observe this negative pressure in our daily experience either, but it has at least two paramount contributions to the expansion history of the universe. One is inflation, a period in which an accelerated expansion of the universe is required in order to solve the horizon problem (see sec. 1.3). The other is the current accelerated expansion of the universe, confirmed by cosmological observations since the late 1990s. The former can be explained by the action of one or multiple scalar fields, although its dynamics is loosely constrained today. The latter is currently best modeled by the simple addition of a cosmological constant Λ (see sec. 1.2), which behaves as a fluid with equation of state $p = w\rho$, with $w = -1$, which violates the strong energy condition. Despite this, ΛCDM currently suffers from observational tensions that suggest the need to replace it by another model. Indeed, early- and late-time measurements of H_0, the current expansion rate of the universe, seem to be inconsistent [181]. There exists a plethora of alternative proposals to replace the cosmological constant by either modifying gravity (MG) or adding an extra fluid called dark energy (DE), but none of them seems to be able to solve the tension while providing a competitive fit to cosmological data [36, 182, 183].

In chapter 6 we presented the variational formulation of non-equilibrium thermodynamics in GR. As a consequence of the inclusion of thermodynamics as a constraint, the second Friedmann equation gets an accelerating term of entropic energy. Therefore, entropy production gravitates similarly to negative pressure

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\left(\rho + 3p - \frac{T\dot{S}}{a^2\dot{a}}\right). \tag{7.1}$$

This can be interpreted in two ways. One is to see irreversible phenomena as a way to produce an accelerated divergence of a geodesic congruence without violating the energy conditions, i.e., regarding the entropic force tensor as a separate entity. Alternatively, we can include the entropic force tensor as a contribution to the stress-energy tensor of a real fluid. Either way, an acceleration of the expansion of the universe can be achieved.

We note that the relations between entropy and cosmic evolution have been explored before, for instance in emergent gravity [108] or in the thermodynamic interpretation of the bare Friedmann equations [184, 185].

This chapter is devoted to explore whether the cosmological constant can be replaced by an acceleration of entropic origin. This can be achieved if the entropic force term is large enough to overcome the attractive terms coming from energy density and usual (positive) pressure. In section 7.2 we outline how entropic forces can arise in the universe and illustrate it with some examples, of which the horizon growth is the most promising one. In section 7.3 we present how this leads to General Relativistic Entropic Acceleration

(GREA) theory, which is compared against ΛCDM in section 7.4 using recent cosmological data. We finish with some discussion of our results in section 7.5.

7.2 Contributions to entropy

In this section we discuss several cosmic contributions to entropy and whether they can be considered serious candidates to give a positive and dominant contribution to the acceleration of the universe. We will distinguish two groups: the matter content of the universe, even if exotic, gives *bulk* entropy, while horizons give gravitational *boundary* entropy.

Bulk entropy

Bulk entropy is produced during cosmic expansion during certain out-of-equilibrium processes, such as (p)reheating, phase transitions or gravitational collapse. However, most of the expansion history of the universe is adiabatic and deviations from it are expected to be short-lived. This means that, although it may provide interesting phenomenology, it seems unable to explain the current accelerated expansion of the universe.

Furthermore, out-of-equilibrium ordinary particle matter is unlikely to provide even a short-lived acceleration of the universe. This matter is fully described microscopically by the phase space coordinates of all its particles. As dictated by statistical mechanics (see sec. 2.6), its associated macroscopic variables are phase space functions. A comoving observer with 4-velocity u^μ measures an effective pressure given by

$$p_{\text{eff}} = \frac{1}{3}\left(R_{ij} - \frac{1}{2}R g_{ij}\right) u^i u^j = \frac{1}{3}\left(T_{ij} - f_{ij}\right) u^i u^j = p - \frac{1}{3}\frac{T\dot{S}}{a^2\dot{a}}\,. \tag{7.2}$$

If the matter content of the universe admits a description in terms of usual statistical mechanics, then this pressure is a function of phase space as

$$p_{\text{eff}} = g\int \frac{d^3p}{(2\pi)^3}\frac{|\vec{p}|^2}{3\sqrt{|\vec{p}|^2+m^2}} f(\vec{p}) > 0\,, \tag{7.3}$$

where $f(\vec{p})$ is the probability distribution in phase space and m is the rest mass of the particle. Thus, a negative effective pressure does not seem to be consistent with usual statistical mechanics and somewhat exotic[1] matter should be advocated. However, such matter models have been proposed, for instance in refs. [186, 187] and can even lead to sustain entropy growth.

[1] Motivated by the breakdown of the usual statistical interpretation of pressure, in this chapter we will refer to matter with negative effective pressure as *exotic*. We will not consider matter with negative mass or energy density.

Alternatively, one could think of particle creation scenarios, where entropy is increased to a fast growth of occupation numbers. This is the situation, for instance, during (p)reheating. It must be noted, however, that entropy production comes with an increase in energy density

$$\frac{T}{a^2\dot{a}}\dot{S} = \frac{T}{a^2\dot{a}}\left(a^3\dot{s} + 3a^2\dot{a}s\right) = Ta\frac{ds}{da} + 3Ts\,. \tag{7.4}$$

A simpler way to achieve an acceleration with ordinary matter may come from particle creation. Here we outline a first approach to the issue. Let us first use the thermodynamic relation

$$Ts = (\rho + p) \rightarrow Ts - p = \rho \tag{7.5}$$

in order to rewrite the second Friedmann equation as

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\left(-2\rho - Ta\frac{ds}{da}\right). \tag{7.6}$$

If we consider the extreme case of the particle number density to be constant during a particle-creation process, then $ds/da = 0$ and an acceleration of the universe takes place. This may be achieved with slower particle creation rates too. However, it must be noted that particle creation needs to be sourced by some other (possibly exotic) matter component, either directly or indirectly via space-time geometry. Whether such an entropic force emerges and is relevant during particle-creation events such as (p)reheating is a relevant question, but out of the scope of this thesis.

Boundary entropy

Boundary entropy is given by the existence of horizons that determine the causal structure of the universe, limiting causal contact to finite patches. It can be incorporated in a natural way by extending the Einstein-Hilbert action with a surface term, the Gibbons-Hawking-York (GHY) term [3, 177, 178]. From the thermodynamic point of view, the GHY term also contributes to the internal energy of the system. Hence, it can be related to the temperature and entropy of the horizon as

$$\mathcal{S}_{GHY} = \frac{1}{8\pi G}\int_{\mathcal{H}} d^3y\,\sqrt{h}\,K = -\int dt\,N(t)\,TS\,, \tag{7.7}$$

where we used the notation of the ADM formalism. Note that we have kept the lapse function $N(t)$, to indicate that the variation of the total action with respect to it will generate a Hamiltonian constraint with an entropy term together with the ordinary matter/energy terms. Of course, this is a consequence of the symmetry under time reparametrization.

In sec. 6.4 we already computed the contribution to the action of the GHY term associated with black holes, let them be of astrophysical or primordial origin. Their temperature and entropy is given by the Hawking and Bekenstein formulas. Assuming their total comoving number is conserved, their contribution to the total energy and entropy density is given by ($\hbar = c = 1$)

$$\rho_{BH} = n_{BH}\, M\,, \qquad s_{BH} = n_{BH}\, 4\pi G M^2\,, \tag{7.8}$$

and therefore the contribution to the second Friedmann equation becomes

$$a^3 \frac{d}{dt}(\rho_{BH} a^3) = T_{BH} \frac{d}{dt}(s_{BH} a^3) = 0\,, \tag{7.9}$$

since the number density of black holes dilutes with the volume. Therefore, static black holes do not have an entropic contribution to the dynamics of the universe.

Next, it is natural to consider the entropy associated with cosmic horizons. These perhaps make the breaking of symmetry under time inversion most clear, as they keep growing with time. We will also describe them by means of a GHY term. There are two reasons for this, in addition to the motivation from black hole thermodynamics. First, since they also scale with the area, they can accommodate a Bekenstein-like formula in a thermodynamic contribution to the action. Second, it provides an effective fluid description (with effective density, pressure and entropic force), which is a requirement of the variational formalism in its present form.

A first natural choice of boundary hypersurface in FLRW metric is the apparent cosmological horizon [188]. The reason for this is that it can be defined locally in time, without reference to the past or future history of the universe. It is located at the physical radial coordinate

$$r_{AH} = \frac{1}{\sqrt{H^2 - k^2/a^2}}\,. \tag{7.10}$$

Let us now compute its GHY term. We can consider a comoving sphere around the origin of coordinates $r = 0$ with unit normal vector

$$n = g^{rr}\partial_r = a^{-1}\sqrt{1 - kr^2}\,\partial_r\,. \tag{7.11}$$

Then the trace of its extrinsic curvature is

$$\sqrt{h}\,K = 2N(t)\, r\, a\sqrt{1 - kr^2}\,\sin\theta \tag{7.12}$$

the GHY term (7.7) for the apparent horizon is

$$S_{GHY} = -\frac{1}{2G}\int dt\, N(t)\, H\, r_{AH}^2 = -\int dt\, N(t)\, T_{AH} S_{AH}\,,$$

where T_{AH} is the temperature and S_{AH} the entropy associated with the apparent horizon,

$$k_{\mathrm{B}} T_{AH} = \frac{\hbar c\, H}{2\pi}\,, \qquad S_{AH} = \frac{k_{\mathrm{B}} c^3}{\hbar}\frac{\pi\, r_{AH}^2}{G}\,. \tag{7.13}$$

This type of cosmological horizon does not contribute with a sufficient amount of entropy growth to affect the expansion of the universe. Therefore, we need to consider another kind of horizon. We suggest a contribution coming from the causal (particle) horizon, which does keep track of the history of the universe and the regions that came into causal contact.

We turn now to the causal cosmological horizon of a FLRW universe. Let us start by considering an arbitrary comoving 2-sphere around the origin of coordinates. Then the trace of its extrinsic curvature is given by eq. (7.12) and the GHY term (7.7) for the causal cosmological horizon, $d_H = a\,\eta$, with $r = \sinh\left(\eta\sqrt{-k}\right)/\sqrt{-k}$, where η is conformal time, can be written as

$$\mathcal{S}_{GHY} = -\frac{1}{2G}\int dt\, N(t)\,\frac{a}{\sqrt{-k}}\,\sinh\left(2\eta\sqrt{-k}\right) = -\int dt\, N(t)\, T_H S_H = -\int dt\, N\, a^3 \rho_H\,,$$

where T_H is the temperature and S_H the entropy associated with the causal cosmological horizon

$$k_\mathrm{B} T_H = \frac{\hbar c}{2\pi}\,\frac{\sinh\left(2\eta\sqrt{-k}\right)}{a\eta^2\sqrt{-k}}\,, \qquad S_H = k_\mathrm{B}\frac{\pi c^3}{\hbar}\frac{a^2\eta^2}{G}\,. \tag{7.14}$$

The fact that we can naturally assign a temperature and an entropy to a hypersurface is a signal of the existence of an underlying quantum description of gravity and thermodynamics. This is made explicit by the appearance of $\hbar$ in both quantities. Their product, however, does not depend on $\hbar$ and leads to a classical emergent phenomenon, the acceleration of the universe.

This kind of entropic term can actually lead to cosmic acceleration. Contrary to the apparent horizon, the causal horizon keeps growing with time and can be large enough to reach scales where curvature is non-negligible and the non-linearity of GHY in an open universe becomes relevant.

7.3 GREA theory

General Relativistic Entropic Acceleration (GREA) theory is a proposal to explain the current accelerated expansion of the universe. In its formulation based on horizon entropy, it relies on the existence of a large causal horizon in an open universe that underwent open inflation in the past.

Open inflation is a scenario that allows the universe to be non-flat. The universe is nucleated in de Sitter space, i.e., in eternal inflation [189] with curvature of order one. This nucleation takes place due to the tunneling of a quantum field from the false to the true vacuum. Inside the true vacuum bubble, local space-time as seen by a comoving observer is essentially flat if inflation lasts long enough, e.g. of order $N \sim 70$ e-folds. Nevertheless, there is still a given casual horizon with $\sqrt{-k} = a_0 H_0$. Inspired by this scenario we propose a GHY thermodynamic term that induces an entropic contribution satisfying [4]

$$\rho_H\, a^2 = \frac{T_H S_H}{a} = \frac{1}{2G}\,\frac{\sinh(2a_0 H_0 \eta)}{a_0 H_0}\,, \qquad \frac{\Omega_K}{1-\Omega_K} = e^{-2N}\left(\frac{T_{\rm rh}}{T_{\rm eq}}\right)^2 (1+z_{\rm eq})\,, \tag{7.15}$$

where η is the conformal time, Ω_K is the curvature parameter inside the inflated patch, $T_{\rm rh}$ is the reheating temperature, $T_{\rm eq}$ and $z_{\rm eq}$ are, respectively, the temperature and redshift at matter-radiation equality. We now introduce, for convenience, the time coordinate $\tau = a_0 H_0 \eta$ and denote with primes the derivatives w.r.t. to τ. Then the second Friedmann equation becomes

$$\left(\frac{a'}{a_0}\right)^2 = \Omega_M\,\frac{a}{a_0} + \Omega_K\,\frac{a^2}{a_0^2} + \frac{4\pi}{3}\,\Omega_K^{3/2}\,\frac{a^2}{a_0^2}\,\sinh(2\tau)\,, \tag{7.16}$$

where Ω_M is the matter density parameter.

Thus, the expansion of the universe is affected by the increase in entropy of the causal horizon. Since the causal horizon keeps growing, the entropic term eventually dominates and leads to a late-time cosmic acceleration. Contrary to a cosmological constant, however, the entropic term is diluted with the expansion, albeit at a slower rate than radiation and dust, and the universe ends in Minkowski space-time in the far future.

From the mathematical point of view, this modified second Friedmann equation is a differential equation in re-scaled conformal time τ. It is, however, an integro-differential equation in cosmic time t, unlike the usual second Friedmann equation. Physically, this is related to the nature of the entropic term associated to the causal horizon: it builds up as the expansion proceeds.

7.4 GREAT against ΛCDM

The GREA theory is successful in providing an explanation for the current accelerated expansion of the universe. As such, it joins the plethora of possible alternatives to the cosmological constant Λ. Therefore, it is paramount to test GREAT against Λ using current cosmological data and find which one is preferred statistically.

This analysis was performed in ref. [5] and provided promising results for GREAT. In this section we present a summary of the datasets, numerical methods and the obtained results. We will not, however, dive into the details, which are available in the paper for the interested reader.

First, we must note that, at the time at which the analysis was performed, no cosmological perturbation theory has been developed within the context of GREA. This is also true at the time of the writing of this thesis. The cosmological effects of entropic forces are only available at the background level, as presented in sec. 6.5. It is for this reason that the choice of datasets is limited to those that test the background evolution of the universe. We note, however, that we built variational non-equilibrium thermodynamics in the ADM formalism (see sec. 6.3), so that one can consistently build a cosmological perturbation theory as well.

7.4.1 Datasets

Taking this issue into account, the datasets included in the analysis are:

- $H(z)$ data. It is obtained from two sources: redshift drift of distant objects over long periods of time [190] and Baryon Acoustic Oscillations (BAO) in the radial direction [191]. It is assumed that the $H(z)$ data are uncorrelated with each other. The compilation is used as in ref. [192], which contains 36 points in the redshift range $0.07 \leq z \leq 2.34$ and which are in the form (z_i, H_i, σ_{H_i}).

- Supernovae type Ia data coming from the Pantheon compilation [193]. It containes 1048 Supernovae Ia points in the redshift range $0.01 < z < 2.26$, along with their covariance matrix.

- BAO data, including points from 6dFGS [194], WiggleZ [195], the MGS, ELG, LRG, quasars and DR12 galaxy samples BAO points from the completed SDSS-IV eBOSS survey [196], the year 3 DES [197] and the Lyman-α (Lyα) absorption and quasars, auto and cross correlation points from ref. [198]. It is assumed that the data are independent with each other. However, it must be noted that, since some of the points are derived by the same survey, inevitably there will be common overlapping galaxies between the datasets, which will result to strong covariances that are not included in the analysis. Even if some of them are, such as the covariance matrix of the WiggleZ data, full correlations are not publicly available. This is clearly a limitation in the analysis.

- CMB shift parameters [199, 200]. They encapsulate the geometric information in the CMB spectrum, via the location of the peaks and are in a sense a compressed form of the CMB likelihood. This allows us to use information from CMB surveys at the background level, without needing to include entropy in cosmological perturbation theory. As GREA requires a non-flat universe, the Planck 2018 chains base_omegak_plikHM_TTTEEE_lowl_lowE_lensing are used to estimate the data vectors.

- Riess et al H_0 prior. The measurement of H_0 from ref. [201] is included as well. It comes from a sample of 75 Milky Way Cepheids, which were used to recalibrate the extragalactic distance ladder. This approach gives a value

$$H_0^{(\mathrm{R})} = 73.2 \pm 1.3\,\mathrm{km\,s^{-1}\,Mpc^{-1}}. \tag{7.17}$$

- Freedman et al H_0 prior. Finally, the measurement of H_0 from ref. [202] is also included. It comes from the Tip of the Red Giant Branch (TRGB) method using stars in the Large Magellanic Cloud (LMC). This approach gives a value

$$H_0^{(\mathrm{TRGB})} = 69.6 \pm 0.8\,(\mathrm{stat}) \pm 1.7\,(\mathrm{syst})\ \mathrm{km\,s^{-1}\,Mpc^{-1}}. \tag{7.18}$$

These datasets provide complete information on the background evolution of the universe. They are used in ref. [5] to perform a Bayesian model comparison between GREAT and the cosmological constant using Markov Chain Monte Carlo (MCMC) techniques.

Given that the H_0 priors seem to be in tension with other data [203, 204], they must be taken with care. The H_0 tension is the observational discrepancy between the values of H_0 obtained by early- and late-time measurements. The tension seems to be statistically significant and it currently lacks a compelling enough solution. In order to factor out the effects of the tension, three different analysis are performed: 1) without including any of the H_0 priors, 2) including the Riess et al prior and 3) including the Freedman et al prior.

7.4.2 Bayesian inference and model comparison

Since statistics was not used before in the thesis, we will take now a small detour to introduce some key concepts. There are two main interpretations of the concept of probability: frequentist and Bayesian. In the former, probabilities describe the frequency or propensity of some phenomenon; while according to the latter probabilities are interpreted as a reasonable expectation or a quantification of belief. This philosophical distinction has direct consequences on parameter estimation, which is one of the main tasks of statistics. For instance, physical parameters Θ are treated as immutable values within classical (frequentist) statistics, while Bayesian statistics treats them as random variables. The latter is the standard approach in modern Cosmology. In Bayesian statistics, *prior probability* $p(\Theta)$ is updated according to Bayes' theorem by the likelihood $\mathcal{L}$ of data being observed given an outcome of the random variables describing the physical parameters

$$p(\Theta|data) = \frac{\mathcal{L}(data|\Theta)}{\int d\Theta \mathcal{L}(data|\Theta) p(\Theta)} p(\Theta)\,, \tag{7.19}$$

giving the *posterior probability* $p(\Theta|data)$. Estimates for Θ can be obtained from the posterior distribution, for instance by finding its maximum. Since it can be a complicated multivariate function, MCMC techniques are useful to sample it and find local maxima.

Following this approach, each dataset mentioned above carries a likelihood $\mathcal{L}$. Since they are assumed to be uncorrelated, the total likelihood can be written as the product

$$\mathcal{L}_{\rm tot} = \mathcal{L}_{\rm SnIa} \times \mathcal{L}_{\rm BAO} \times \mathcal{L}_{\rm H(z)} \times \mathcal{L}_{\rm cmb} \times \mathcal{L}_{\rm H_0}. \tag{7.20}$$

Furthermore, since the likelihoods are assumed to be Gaussian[2], they can also be easily described in terms of a χ^2 distribution. Total likelihood can be translated into the total χ^2 as a sum, taking into account that $\chi^2_{\rm tot} = -2\ln \mathcal{L}_{\rm tot}$, i.e.

$$\chi^2_{\rm tot} = \chi^2_{\rm SnIa} + \chi^2_{\rm BAO} + \chi^2_{\rm H(z)} + \chi^2_{\rm cmb} + \chi^2_{\rm H_0}. \tag{7.21}$$

Note that maximal likelihood is equivalent to minimal χ^2. For the included dataset, the total χ^2 is given by eq. (7.21) and the parameter vectors for both the ΛCDM and GREAT models are given by: $\Theta_{\rm Model} = \left(\Omega_{m0}, \Omega_b h^2, h, \Omega_k\right)$. Then, the best-fit parameters and their uncertainties are obtained via an MCMC code written by Savvas Nesseris[3]. Regarding the prior distribution $p(\Theta_{\rm Model})$ for each model, in the case of ΛCDM model they are given by $\Omega_{m0} \in [0.01, 0.5]$, $\Omega_b h^2 \in [0.015, 0.035]$, $\Omega_k \in [-0.1, 0.1]$, $h \in [0.5, 1]$, while for the GREAT model they are given by $\Omega_{m0} \in [0.01, 0.5]$, $\Omega_b h^2 \in [0.015, 0.035]$, $\Omega_k \in [0.00001, 0.1]$, $h \in [0.5, 1]$[4]. In the sampling approximately $\mathcal{O}(10^5)$ points are obtained for each of the models.

MCMC techniques allow to obtain the best parameter fit for each model. Now, in order to compare the quality of fit, an additional step must be taken. Bayesian model comparison is based on the Bayesian evidence B, which is calculated as the integral

$$E = \int d\Theta \mathcal{L}(data|\Theta) p(\Theta)\,, \tag{7.22}$$

which is computed using thermodynamic integration, a method based on MCMC techniques and described in the paper. Interestingly, the evidence is a likelihood function in which all parameters of the model have been marginalized. Hence, it quantifies the probability of the data giving a model regardless of the particular realization of the parameters understood as random variables. Qualitatively, it can be immediately understood that models with larger E are preferred. Quantitatively, this is expressed with the Bayes ratio between two models i and j as

$$B_{ij} = \frac{E_i}{E_j}\,. \tag{7.23}$$

The Bayes ratio is interpreted by means of the Jeffreys' scale [205] as follows:

- For $\ln B_{ij} < 1.1$ the preference of j over i is said to be *weak*.

[2] This is usually justified in application of the central limit theorem.

[3] https://github.com/snesseris/GREAT-project

[4] Note that for the GREAT model Ω_k has to be positive as otherwise the square of the Hubble parameter may become negative.

- For $1.1 < \ln B_{ij} < 3$ the preference of j over i is said to be *definite*.
- For $3 < \ln B_{ij} < 5$ the preference of j over i is said to be *strong*.
- For $\ln B_{ij} > 5$ the preference of j over i is said to be *very strong*.

In this way, we can obtain a quantitive comparison between two models that aim to explain a given dataset (i.e., physical observations).

7.4.3 Results

Let us collect here the results of the model comparison between GREAT and ΛCDM:

- Table 7.1 shows the results of the MCMC analysis when no H_0 prior is included. The logarithmic Bayes ratio $\ln B_{\Lambda,G} \simeq -9.006$ indicates a very strong preference of GREAT over ΛCDM.
- Table 7.2 shows the results of the MCMC analysis when the Riess et al H_0 is included. The logarithmic Bayes ratio $\ln B_{\Lambda,G} \simeq 0.386$ renders the test inconclusive, giving only weak evidence in favor of ΛCDM.
- Table 7.3 shows the results of the MCMC analysis when the Riess et al H_0 is included. The logarithmic Bayes ratio $\ln B_{\Lambda,G} \simeq -0.373$ renders the test inconclusive, giving only weak evidence in favor of GREAT.

These results have two immediate consequences. First, GREAT is a serious and viable alternative to ΛCDM. Indeed, excluding the H_0 priors in the analysis gives a very strong preference of GREAT over ΛCDM. Most of the difference in $\chi^2_{\rm min}$ comes from the CMB data, as can be seen in table 7.4. Second, the tension between the H_0 priors and the rest of the data dilutes this statistical preference, rending the model comparison inconclusive. We may interpret this result as steaming from the fact that the CMB data is driving most of this preference, so that the early-late universe tension is playing a key role.

7.5 Discussion

General Relativistic Entropic Acceleration is a proposal to explain the current accelerated expansion of the universe by means of an entropic force associated to the causal horizon. In particular, the size of the causal horizon is large enough and is controlled by the curvature parameter Ω_k thanks to open inflation.

No priors		
Parameter	ΛCDM	GREAT
$\Omega_{m,0}$	0.3057 ± 0.0056	0.3522 ± 0.0190
$\Omega_{b,0}h^2$	0.0224 ± 0.0002	0.0225 ± 0.0001
$\Omega_{k,0}$	0.0012 ± 0.0018	0.0010 ± 0.0002
H_0	68.08 ± 0.58	68.38 ± 0.48
$\chi^2_{\rm min}$	1075.63	1071.35
$\ln E$	-557.515	-548.509
$\ln B_{ij}$	0	-9.006

Table 7.1: Here we present the results of the MCMC analysis when not including any H_0 prior. In particular, we show the mean values, 1σ errors of the parameters for the GREAT and ΛCDM models respectively, along with the minimum χ^2 and the log-evidence $\ln E$, and the difference of the log-evidence with respect to the ΛCDM model $\ln B_{ij}$. The latter give a Bayes ratio of $B_{\Lambda,G} = \exp(-9.006) \sim 1/8150$, thus resulting in very strong evidence in favor of the GREAT model according to the Jeffreys' scale [205]. Note that H_0 is given in units of $\mathrm{km\,s^{-1}\,Mpc^{-1}}$.

Including Riess et al H_0 prior		
Parameter	ΛCDM	GREAT
$\Omega_{m,0}$	0.2995 ± 0.0051	0.3350 ± 0.0155
$\Omega_{b,0}h^2$	0.0224 ± 0.0002	0.0225 ± 0.0001
$\Omega_{k,0}$	0.0029 ± 0.0017	0.0008 ± 0.0002
H_0	68.85 ± 0.53	68.98 ± 0.44
$\chi^2_{\rm min}$	1088.79	1083.39
$\ln E$	-557.588	-557.974
$\ln B_{ij}$	0	0.386

Table 7.2: Here we present the results of the MCMC analysis when we include all the available data and the Riess et al H_0 prior. In particular, we show the mean values, 1σ errors of the parameters for the GREAT and ΛCDM models respectively, along with the minimum χ^2 and the log-evidence $\ln E$ and the difference of the log-evidence with respect to the ΛCDM model $\ln B_{ij}$. The latter give a Bayes ratio of $B_{\Lambda,G} = \exp(0.386) \sim 1.47$, thus resulting in the two models being considered statistically equivalent according to the Jeffreys' scale [205]. Note that H_0 is given in units of $\mathrm{km\,s^{-1}\,Mpc^{-1}}$.

Current cosmological data show that this proposal is a serious alternative to the cosmological constant. Indeed, if no prior on the current expansion rate of the universe H_0 is set, datasets involving the background expansion of the universe ($H(z)$, SnIa, BAO and CMB

Including Freedman et al H_0 prior		
Parameter	ΛCDM	GREAT
$\Omega_{m,0}$	0.3047 ± 0.0052	0.3502 ± 0.0157
$\Omega_{b,0}h^2$	0.0224 ± 0.0001	0.0225 ± 0.0001
$\Omega_{k,0}$	0.0015 ± 0.0017	0.0010 ± 0.0002
H_0	68.20 ± 0.54	68.46 ± 0.45
$\chi^2_{\rm min}$	1076.23	1071.74
$\ln E$	-550.484	-550.111
$\ln B_{ij}$	0	-0.373

Table 7.3: Here we present the results of the MCMC analysis when we include all the available data and the Freedman et al H_0 prior. In particular, we show the mean values, 1σ errors of the parameters for the GREAT and ΛCDM models respectively, along with the minimum χ^2 and the log-evidence $\ln E$ and the difference of the log-evidence with respect to the ΛCDM model $\ln B_{ij}$. The latter give a Bayes ratio of $B_{\Lambda,G} = \exp(-0.373) \sim 0.689$, thus resulting in the two models being considered statistically equivalent according to the Jeffreys' scale [205]. Note that H_0 is given in units of $\mathrm{km\,s^{-1}\,Mpc^{-1}}$.

No priors breakdown					
Model	CMB	BAO	SnIa	$H(z)$	$\chi^2_{\rm tot}$
ΛCDM	4.28	13.99	1034.84	22.52	1075.63
GREAT	0.07	14.39	1034.82	22.10	1071.35

Table 7.4: Here we present the breakdown of the χ^2 for both ΛCDM and GREAT for the different datasets used in our analysis, in the case of not including any H_0 prior. The best-fit parameters from the MCMC are given in Table 7.1. As can be seen, the main contribution in the difference of the χ^2s comes from the CMB and to a lesser extent from the $H(z)$ and BAO data, while the values for the SnIa are practically the same.

shift parameters) give a very strong preference of GREAT over ΛCDM, if one interpretes the Bayesian ratio with Jeffreys' scale. However, this preference disappears when the priors are included, so that the model comparison is inconclusive. This is probably due to the tension between early- and late-time measurements.

If the cosmological constant is unnecessary to explain cosmological observations, this would partly solve the cosmological constant problem, in the sense that a vanishing cosmological constant can be understood to be protected by a high-energy symmetry, which is yet to be discovered. On the contrary, a tiny cosmological constant, as the one considered in ΛCDM is hard to justify within QFT. Likewise, the issue of why vacuum energy does not seem to gravitate would still need to be solved.

Future surveys like CMB-S4, Euclid, DESI and LSST will provide tighter constraints and hopefully shed light as to which model is preferred by data. To see how this will happen, let us parametrize the equation of state GREAT by the redshift expansion

$$w(z) = w_0 + w_a \frac{z}{1+z}\,, \tag{7.24}$$

known as the Chevallier-Polarski-Linder (CPL) parametrization [206, 207]. For ΛCDM one simply has $w_0 = -1$ and $w_a = 0$, while GREAT and other dark energy models typically have different values. We show in fig. 7.1 the contour plots for (w_0, w_a) given the datasets $H(z)$, SnIa, BAO, CMB shift parameters and the Riess et al H_0 prior. As it can be seen in this plot, both GREAT and ΛCDM are compatible with the data, although the value of GREAT is closer to the maximum of the posterior distribution. Future surveys will hopefully shrink the contour plots and allow us to distinguish both models.

It is worth pointing out that a positive contribution to the Friedmann equation when non-equilibrium phenomena are present and, thus, it may well be that other sources of entropy need to be taken into account in addition to that of the causal horizon. An example of this relevant to late-time cosmology would be ordering and formation of LSS. This process is clearly irreversible, and may perhaps be characterized in terms of growing of the total entropy of the universe, even if ordering means a local decrease in entropy.

In our view GREAT is a powerful explanation to the current accelerated expansion of the universe, as it fits the data well and does not require additional parameters, which would be disfavored from the point of view of statistics. Furthermore, the thermodynamic bridge between the physics of yet unknown quantum gravitational degrees of freedom and large-scale cosmological physics makes it a compelling argument in light of the success of black hole thermodynamics. We look forward to further developments and both theory and observations that will clarify the role of these entropic forces in the cosmic expansion.

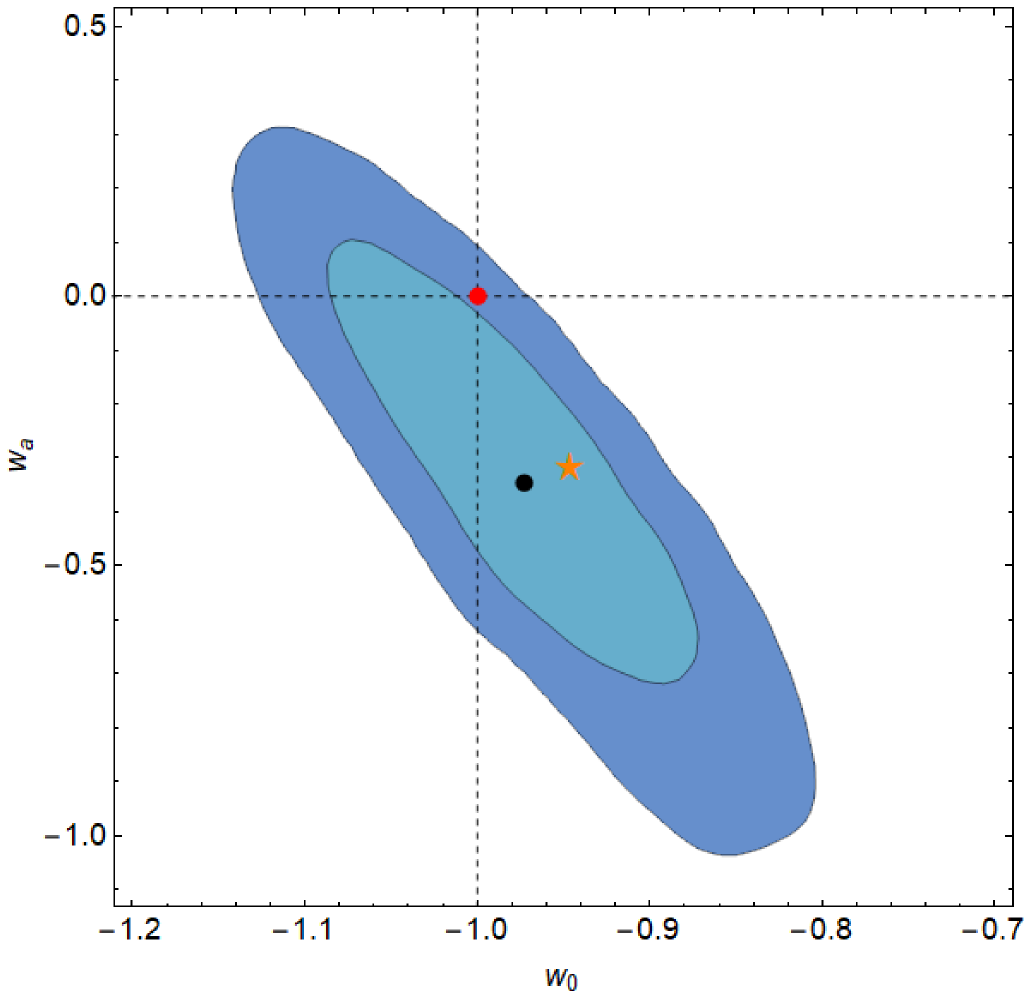

Figure 7.1: The 68.3% and 95.5% confidence contours for the CPL model for the w_0, w_a parameters, when including all data and the Riess prior. The black dot corresponds to the best-fit value, the red dot to the ΛCDM model and the orange star to the prediction of GREAT $(w_0, w_a) = (-0.946, -0.318)$ [4]. From ref. [5]

Part IV

Conclusions

Chapter 8

Conclusions

Theoretical cosmology sits at a fascinating crossroad between gravity, quantum mechanics, and thermodynamics. Indeed, general relativity is a theory of spacetime itself, quantum field theory explains the physics of the very early universe and the origin of perturbations, while thermodynamics and statistical mechanics constitute the indispensable bridge between the microscopic and macroscopic descriptions of physical reality.

In this thesis we have explored several topics related to the quantum and thermal nature of the universe. Motivated by an initial question: *can primordial black holes be entangled?*, we have taken a path to other questions like: *what else can we learn from cosmic correlations? Are they genuinely quantum?* Or also: *Can entanglement between black holes lead to an entropic force in the universe? How would we characterize entropic forces and generic non-equilibrium phenomena within the usual description of the universe? How do they impact the expansion of the universe?*

The quantum origin of primordial perturbations is an unavoidable consequence of the inflationary paradigm. These perturbations are responsible for the anisotropies in the cosmic microwave background, seeding the structure formation in the universe and possibly forming primordial black holes by inducing gravitational collapse during the radiation era. These have been mostly studied in Fourier space and many of its quantum-information properties were known. In part II we have investigated some of these quantities in real space, which is relevant in order to understand the quantum nature of the correlations between distant regions of the universe, not between distinct momentum modes.

In chapter 3 we have studied the entanglement entropy of a spherical region in the early universe, in particular for a quantum field placed in a squeezed state. We have found UV-finite contributions that are suspected to be due to long-range correlations and, thus, could lead to classically correlated or quantum entangled primordial black holes, as they are formed by collapse triggered by the quantum field of primordial perturbations. This is a realistic proposal of the existence of a network of entangled black holes in the universe. Should the ER = EPR correspondence hold, then these black holes could be connected via wormholes.

In chapter 4 we have computed the perturbative mutual information of primordial perturbations for inflation and the radiation era. We have found a two-fold enhancement. On the one hand, the decay is logarithmic with distance, thus much slower than the quartic decay found in the Minkowski vacuum. This shows the existence of long-range correlations due to inflation. On the other hand, mutual information seems to be larger the longer inflation lasts. Later non-perturbative studies cast doubt on the latter, which may be an artifact of the perturbative expansion, which may lead to a divergent series. Nevertheless, it confirms the logarithmic decay, which means that distant regions of the universe do share large amounts of information due to their common origin during inflation.

In chapter 5 we have attempted to show a distinctive signal of genuine quantum correlations by studying Bell inequalities in real space for both the Minkowski vacuum and the Bunch-Davies vacuum of de Sitter space-time. Despite the fact that quantum discord, a measure of such genuine correlations, is non-vanishing in both cases, we have found no violation of Bell inequalities. This shows the difficulty of finding these genuine quantum correlations in field theory, due to effective decoherence taking place. Furthermore, it casts doubt on the ability of quantum discord to quantify them when dealing with mixed states.

Even though we have not exhausted all possible constructions of Bell and similar inequalities, further attempts to probe the quantum nature of primordial perturbations may need go beyond Gaussian states. Primordial non-gaussianities are inevitable due to quantum diffusion during inflation [67] and may lead to interesting, observable quantum phenomena. In this sense, there exist proposals to probe this quantumness by means of the 3-point correlation function [102].

Entropic forces between PBH may still arise even if long-distance correlations are mostly classical, as they still have an impact on the overall entropy of the quantum field of primordial perturbations. We look forward to a more complete characterization of the primordial black hole network and the multi-partite information shared by them, as well as whether multi-partite Bell inequalities may provide distinctive quantum signals.

In our usual understanding of physical forces, we are used to both fundamental and residual forces. Entropic forces constitute a third kind and are due to the emergent phenomena in the collective motion of many particles. In part III we have taken a new perspective on out-of-equilibrium phenomena in gravity and cosmology, leading to potentially observable consequences.

In chapter 6 we have developed the variational and covariant formulation of non-equilibrium thermodynamics in general relativity. Built on an existing mathematical framework, this allows for the logical synthesis of the laws of thermodynamics and the extremal action principle in the context of General Relativity. As a consequence, the Einstein field equations get a contribution in the form an entropic force. When applied to cosmology, this delivers the non-equilibrium Friedmann equations, which also get an entropic force term.

In chapter 7 we have followed these ideas to understand the effect of entropy-producing processes in the universe, as the entropic force always tends to accelerated its expansion. We have found that the increase in entropy associated to the cosmic horizon from open inflation may be responsible for the current accelerated expansion in the universe. This proposal, called general relativistic entropic acceleration (GREA) is, thus, a viable alternative to the cosmological constant. According to latest cosmological data, not only is GREA a serious competitor, but is also favored when H_0 priors are not included.

We currently find ourselves at a fascinating, golden age in cosmology. Observations are not only able to confirm qualitatively our description of the universe, but also provide true precision tests. In years and decades to come, they will be able to powerfully constrain cosmological parameters and reach a conclusion as to whether GREA can statistically overpower the cosmological constant.

It is our firm opinion that the feedback between theoretical and observational Physics will continue to foster exciting developments at the fascinating crossover of physical realms and human motivations that is Cosmology.

Chapter 9

Conclusiones

La cosmología teórica se asienta en una encrucijada fascinante entre gravedad, mecánica cuántica y termodinámica. En efecto, la relatividad general es una teoría del propio espacio-tiempo, la teoría cuántica de campos explica la física del universo muy temprano y el origen de las perturbaciones, mientras que la termodinámica y la mecánica estadística constituyen el indispensable puente entre las descripciones microscópica y macroscópica de la realidad física.

En esta tesis hemos explorado varios temas relaciones con la naturaleza cuántica y térmica del universo. Motivados por la pregunta inicial: *¿es posible que los agujeros negros primordiales estén entrelazados?*, hemos explorado otras preguntas como: *¿qué queda por aprender de las correlaciones cósmicas? ¿Son genuinamente cuánticas?* O también: *¿es posible que el entrelazamiento entre agujeros negros conlleve una fuerza entrópica en el universo? ¿Cómo se caracterizan las fuerzas entrópicas y los fenómenos fuera del equilibrio en la descripción habitual del universo? ¿Qué impacto tienen en la expansión del universo?*.

El origen cuántico de las perturbaciones primordiales es una consecuencia inevitable del paradigma inflacionario. Estas perturbaciones son responsables de las anisotropías del fondo de radiación de microondas, del inicio de la formación de estructura en el universo y, posiblemente, de la formación de agujeros negros primordiales por colapso gravitacional inducido durante la era de radiación. Estas perturbaciones se han estudiado principalmente en espacio de Fourier, en el que se conocen muchas de sus propiedades de información cuántica. En la parte II hemos investigado algunas de estas cantidades en espacio real, lo que es relevante para entender la naturaleza cuántica de las correlaciones entre regiones distantes del universo, no entre diferentes modos de momento.

En el capítulo 3 hemos estudiado la entropía de entrelazamiento de una región esférica en el universo temprano, considerando en particular un campo cuántico en un estado comprimido[1]. Hemos encontrado contribuciones UV-finitas que, sospechamos, se deben a correlaciones de largo alcance y, por tanto, podrían conllevar la existencia de agujeros negros primordiales correlacionados clásicamente o entrelazados cuánticamente, debido a su formación por colapso estimulado por el campo cuántico de perturbaciones primordiales. Se trata de una postura realista para la existencia de una red de agujeros negros entrelazados en el universo. Si la conjetura ER = EPR es correcta, estos agujeros negros podrían estar conectados mediante agujeros de gusano.

En el capítulo 4 hemos calculado la información cuántica perturbativa de las perturbaciones primordiales durante inflación y la era de radiación. Hemos encontrado un incremento doble. Por un lado, la dependencia con la distancia es logarítmica y, por tanto, mucho más lenta que la dependencia cuártica típica del vacío de Minkowski. Esto muestra la existencia de correlaciones de largo alcance debido a inflación. Por otro lado, la información mutua parece ser mayor cuanto más tiempo dura inflación. Estudios no perturbativos posteriores ponen en duda la validez del segundo punto, que podría ser un artefacto de la expansión perturbativa, quizá ligada a una serie divergente. No obstante, confirma la dependencia logarítmica, lo que significa que, en efecto, regiones distantes del universo comparten grandes cantidades de inforamción debido a su origen común durante inflación.

En el capítulo 5 hemos intentado mostrar una señal característica de las correlaciones cuánticas genuinas, estudiando las desigualdades de Bell en espacio real, tanto para el vacío de Minkowski como para el vacío de Bunch-Davies del espacio de de Sitter. A pesar de que la discordancia cuántica[2], una medida de correlaciones cuántica genuinas, es distinta de cero para ambos casos, no hemos contrado violación alguna de las desigualdades de Bell. Esto muestra la dificultad de encontrar estas correlaciones cuánticas genuinas en teoría de campos, debido al mecanismo de decoherencia efectiva. Además, cuestiona la habilidad de la discordandia cuántica a la hora de cuantificarlas en el contexto de estados mixtos.

A pesar de que no hemos agotado todas las posibles construcciones de desigualdades de Bell y similares, es posible que los intentos ulteriores de explorar la naturaleza cuántica de las perturbaciones primordiales requiran ir más allá de los estados Gaussianos. Las no-Gaussianidades primordiales son inevitables debido a la difusión cuántica que ocurre durante inflación [67] y podrían conllevar fenónmenos cuánticos interesantes y observables. En este sentido, hay propuestas para su estudio mediante la función de correlación de 3 puntos [102].

Es posible que surjan fuerzas entrópicas entre agujeros negros primordiales, incluso si las correlaciones de largo alcance son principalmente clásicas, pues tendrían igualmente un impacto en la entropía del campo cuántico de perturbaciones primordiales. Esperamos el desarrollo futuro de una caracterización más completa de la red de agujeros negros

[1] *Squeezed state* en inglés.
[2] *Quantum discord* en inglés.

primordiales y la información mutua multipartita que comparten, así como el estudio de desigualdades de Bell multipartitas, que podrían desvelar señales cuánticas genuinas.

En nuestra concepción habitual de las fuerzas físicas, estamos acostumbrados a las fuerzas fundamentales y residuales. Las fuerzas entrópicas son un tercer tipo y se deben a fenómenos emergentes del movimiento colectivo de muchas partículas. En la parte III hemos tomado una nueva perspectiva sobre los fenómenos fuera del equilibrio en gravedad y cosmología, lo cual podría tener consecuencias observables.

En el capítulo 6 hemos desarrollado la formulación variacional y covariante de la termodinámica fuera del equilibrio en relatividad general. Basada en un formalismo matemático existente, permite la síntesis lógica de las leyes de la termodinámica y el prncipio de acción extrema en el contexto de la relatividad general. En consecuencia, las ecuaciones de campo de Einstein reciben una contribución en forma de fuerza entrópica. Al aplicar esta modificación a cosmología se obtienen las ecuaciones de Friedmann fuera del equilibrio, que también contienen un término de fuerza entrópica.

En el capítulo 7 hemos continuado estas ideas con el fin de entender el efecto de procesos productores de entropía en el universo, puesto que la fuerza entrópica siempre tiende a acelerar su expansión. Hemos encontrado que el incremento de entropía asociado con el horizonte cósmico en inflación abierta podría ser responsable de la actual expansión acelerada del universo. Esta propuesta, llamada aceleración entrópica relativista general (GREA[3]) es, por tanto, una alternativa viable a la costante cosmológica. De acuerdo con las observaciones cosmológicas recientes, GREA no es solo un competidor serio, sino que es preferido estadísticamente cuando no se incluyen las probabilidades *a priori* de H_0.

Nos encontramos en una fascinante era dorada de la cosmología. Las observaciones permiten confirmar cualitativamente nuestra descripción del universo y proporcionan auténticos tests de precisión. En las próximas décadas y años tendrán la capacidad suficiente para constreñir los parámetros cosmológicos y llegar a una conclusión sobre la preferencia o no de GREA sobre la constante cosmológica.

En nuestra opinión, la retroalimentación de la física teórica y observacional continuarán impulsando desarollos apasionantes en la fascinante encrucijada de campos físicos y motivaciones humanas que constituyen la cosmología.

[3] *General relativistic entropic acceleration* en inglés.

Part V

Appendices

Appendix A

Mathematical addenda

Some computational shortcuts were taken at different point of the thesis. For their relevance we can highlight the random phase approximation in chapter 4 and the treatment of variational non-equilibrium thermodynamics for continuum systems in chapter 6. The aim of this appendix is to provide these shortcuts with further support and motivation.

A.1 Non random phases

One may wonder whether assuming that the squeezing phases δ_k are random has a noticeable effect on the mutual information of primordial perturbations computed in chapter 4. In the following we argue why it is not the case.

In the case that $\langle vp + pv \rangle \neq 0$ then one cannot simply compute the entropy of the quantum state by finding the eigenvalues of the operator Λ, as described in sec. 4.3. Instead, one needs to consider an operator built from the larger field

$$\chi = \begin{pmatrix} v \\ \pi \end{pmatrix} . \tag{A.1}$$

Its 2-point correlation function contains all the 2-point correlation functions of the state

$$\Delta(\vec{x}, \vec{y}) = \frac{1}{2} \langle \chi(\vec{x}) \chi(\vec{y} \rangle = \begin{pmatrix} X(\vec{x}, \vec{y}) & \frac{1}{2} C(\vec{x}, \vec{y}) \\ \frac{1}{2} C(\vec{x}, \vec{y} & P(\vec{x}, \vec{y}) \end{pmatrix} , \tag{A.2}$$

where

$$C(\vec{x}, \vec{y}) = \langle v(\vec{x}) p(\vec{y}) + p(\vec{y}) v(\vec{x}) \rangle . \tag{A.3}$$

This correlation function transforms under symplectic transformations as

$$\Delta \to S \Delta S^{\dagger} . \tag{A.4}$$

Such transformations are not similarity transformation and, hence, do not leave the eigenvalues of Δ invariant. Still, Williamson's theorem guarantees that there exists a symplectic transformation that brings Δ to a diagonal form [97]. Note that any symplectic transformation S preserves the symplectic form

$$S\Omega S^\dagger = \Omega \quad \text{where} \quad \Omega = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \tag{A.5}$$

or, equivalently

$$S^\dagger = \Omega S^{-1}\Omega\,. \tag{A.6}$$

This means that the problem of finding symplectic eigenvalues of Δ is equivalent to finding conventional eigenvalues of $\Delta\Omega$

$$\Delta\Omega = \begin{pmatrix} -\frac{i}{2}C & iX \\ -iP & \frac{i}{2}C \end{pmatrix}. \tag{A.7}$$

If we assume random phases, then $C = 0$ and the eigenvalues of $\Delta\Omega$ are those of $\sqrt{\Lambda}$, so that both the formalism used in section IV and the one presented here are consistent. If $C \neq 0$, we need to study the eigenvalue problem of this operator. The determinant of a block matrix admits the following decomposition

$$\begin{aligned} M &= \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \\ \det(M) &= \det(M_{22})\det(M_{11} - M_{12}M_{22}^{-1}M_{21})\,. \end{aligned} \tag{A.8}$$

We are interested in the determinant of $\Delta\Omega - \lambda$ in order to find the eigenvalues of $\Delta\Omega$ and thus

$$\begin{aligned} &\det(\Delta\Omega - \lambda) = \\ &\det\left(\frac{i}{2}C - \lambda\right)\det\left(\frac{i}{2}C - \lambda - X\left(\frac{i}{2}C - \lambda\right)^{-1} P\right)\,. \end{aligned} \tag{A.9}$$

This expression admits two approximations. First, since we are interested in the perturbative regime, C will have a subdominant contribution in the first determinant and can be neglected. This argument is valid as well for the first term of the second determinant. Second, since C deals with only a subset of momentum modes, we can assume that it has a norm smaller than that of the identity and hence we can expand the inverse as

$$-\lambda^{-1}\left(1 - \lambda^{-1}\frac{i}{2}C\right)^{-1} \simeq -\lambda^{-1}\left(1 + \lambda^{-1}\frac{i}{2}C\right), \tag{A.10}$$

and thus

$$\det(\Delta\Omega - \lambda) \simeq \det\left[-\lambda + \lambda^{-1}X(1 + i\lambda^{-1}C/2)P\right]. \tag{A.11}$$

Recall that the dominant perturbative contribution is given by X being perturbative and P being non-perturbative. Then, C will be non-perturbative as well. Since it is only non-vanishing for momenta affeced by inflation, it does not affect the more relevant high-momentum modes of P. Hence, we can conclude than the effect of averaging over the squeezing phases has a negligible effect on the mutual information of primordial perturbations.

A.2 Non-equilibrium in the continuum

Here we connect the variational formulation for continuous systems described by Gay-Balmaz and Yoshimura [171] with the shortcut used in the Hamiltonian formulation of non-equilibrium thermodynamics in General Relativity, see sec. 6.3.

The original rigorous variational formulation of non-equilibrium thermodynamics requires the addition of a new term in the Lagrangian and the introduction of new variables

$$\delta \int d^4x\sqrt{-g}\left(\mathcal{L} + (S-\Sigma)\dot{\Gamma}\right) = 0\,. \tag{A.12}$$

Γ is the thermodynamic displacement, while S and Σ are functions whose time derivatives will be linked to internal and total entropy production. The variation of the action is equal to

$$\int d^4x\sqrt{-g}\left(\frac{\delta\mathcal{L}}{\delta\phi}\delta\phi + \frac{\partial\mathcal{L}}{\partial S}\delta S - (\dot{S}-\dot{\Sigma})\delta\Gamma + (\delta S - \delta\Sigma)\dot{\Gamma}\right). \tag{A.13}$$

The stationary-action principle is now supplemented with the phenomenological and variational constraints

$$\begin{aligned} \frac{\partial\mathcal{L}}{\partial S}\dot{\Sigma} &= -P^i\nabla_i\dot{\phi} + J^i\nabla_i\dot{\Gamma} \\ \frac{\partial\mathcal{L}}{\partial S}\delta\Sigma &= -P^i\nabla_i\delta\phi + J^i\nabla_i\delta\Gamma\,, \end{aligned} \tag{A.14}$$

which assume that there is no external power supply. We will restrict ourselves to the simple case where the field is scalar and so the tensor P is a vector, but it could have a higher order. In the original work the authors describe a fluid in its material representation. In that case ϕ is a position vector and P is a 2-tensor.

With this constraints, the variation of the action is equal to

$$\begin{aligned} \int d^4x\sqrt{-g}\Bigg[&\left(\frac{\delta\mathcal{L}}{\delta\phi} + \dot{\Gamma}\left(\frac{\partial\mathcal{L}}{\partial S}\right)^{-1} P^i\nabla_i\right)\delta\phi + \left(\dot{\Gamma} + \frac{\partial\mathcal{L}}{\partial S}\right)\delta S \\ &+ \left(\dot{\Sigma} - \dot{S} - \dot{\Gamma}\left(\frac{\partial\mathcal{L}}{\partial S}\right)^{-1} J^i\nabla_i\right)\delta\Gamma\Bigg] = 0\,. \end{aligned} \tag{A.15}$$

Integrating by parts we get

$$\int d^4x\sqrt{-g}\Bigg[\left(\frac{\delta\mathcal{L}}{\delta\phi} - \nabla_i\left(\dot{\Gamma}\left(\frac{\partial\mathcal{L}}{\partial S}\right)^{-1}P^i\right)\right)\delta\phi + \left(\dot{\Gamma} + \frac{\partial\mathcal{L}}{\partial S}\right)\delta S + \left(\dot{\Sigma} - \dot{S} + \nabla_i\left(\dot{\Gamma}\left(\frac{\partial\mathcal{L}}{\partial S}\right)^{-1}J^i\right)\right)\delta\Gamma\Bigg] = 0\,. \tag{A.16}$$

The equations of motion are obtained as usual by noticing that each variation is independent. From δS we get

$$\dot{\Gamma} = -\frac{\partial\mathcal{L}}{\partial S} \equiv T\,, \tag{A.17}$$

while $\delta\phi$ and $\delta\Gamma$ give

$$\begin{aligned}&\frac{\delta\mathcal{L}}{\delta\phi} + \nabla_i P^i = 0\\ &\dot{\Sigma} = \dot{S} + \nabla_i J^i\,.\end{aligned} \tag{A.18}$$

These equations of motion and the phenomenological constraint fully describe the time evolution of the system. The last one is the entropy balance equation. Even though we imposed it earlier, this shows that it can also be derived from the stationary-action principle.

We will now perform a variable transformation that will affect only the phenomenological constraint, in order for it to have the form used throughout the paper. Note that the variational condition is invariant under the following redefinitions

$$\begin{aligned}\frac{\partial\mathcal{L}}{\partial S}\delta\Sigma &\to \frac{\partial\mathcal{L}}{\partial\Sigma}\delta\Sigma + \nabla_i\left(J^i\delta\Gamma\right) - \nabla_i\left(P^i\dot{\phi}\right)\\ \frac{\partial\mathcal{L}}{\partial S}\delta S &\to \frac{\partial\mathcal{L}}{\partial S}\delta S + \nabla_i\left(J^i\delta\Gamma\right) - \nabla_i\left(P^i\dot{\phi}\right)\end{aligned} \tag{A.19}$$

and the equivalent changes in the derivatives

$$\begin{aligned}\frac{\partial\mathcal{L}}{\partial S}\dot{S} &\to \frac{\partial\mathcal{L}}{\partial S}\dot{S} + \nabla_i\left(J^i\dot{\Gamma}\right) - \nabla_i\left(P^i\dot{\phi}\right)\\ \frac{\partial\mathcal{L}}{\partial S}\dot{\Sigma} &\to \frac{\partial\mathcal{L}}{\partial S}\dot{\Sigma} + \nabla_i\left(J^i\dot{\Gamma}\right) - \nabla_i\left(P^i\dot{\phi}\right).\end{aligned} \tag{A.20}$$

These replacements add total derivatives to the varied Lagrangian and so have no physical effect. The equations of motion stay the same. In fact, these are the kind of terms added when integrating by parts before obtaining the equations of motion. The temperature also stays the same, since $\partial S/\partial S' = 1$, being S' the newly defined entropy.

As already mentioned, the only final equation that is transformed is the phenomenological constraint, which becomes

$$T\dot{\Sigma} = \nabla_i P^i\dot{\phi} + T\nabla_i J^i\,, \tag{A.21}$$

that is

$$T\dot{S} = \nabla_i P^i \dot{\phi}\,, \tag{A.22}$$

where $\nabla_i P^i$ is what we called the friction or entropic force tensor, only that it is a scalar here. In our formulation we replace the time derivative by a more covariant notion of time evolution, the Lie derivative along the normal vector n.

We conclude that both formulations are equivalent. Our choice is motivated by simplicity and physical intuition, as a homogeneous and isotropic entropy function becomes a particular case in a clearer way.

Appendix B

Suplementary material

In this appendix we provide supplementary material that supports the arguments presented in some chapters of the thesis. First, we provide additional results on the Bell inequalities studied in chapter 5, in particular by using Larsson operators. Second, we provide additional details on the analysis reviewed in chapter 7, more precisely in sec. 7.4.

B.1 Bell graphs

In this appendix, we provide additional figures, figs. B.1, B.2 and B.3, which are not directly relevant to the discussion presented in the main text in chapter 5, but which nonetheless complete the parameter-space exploration.

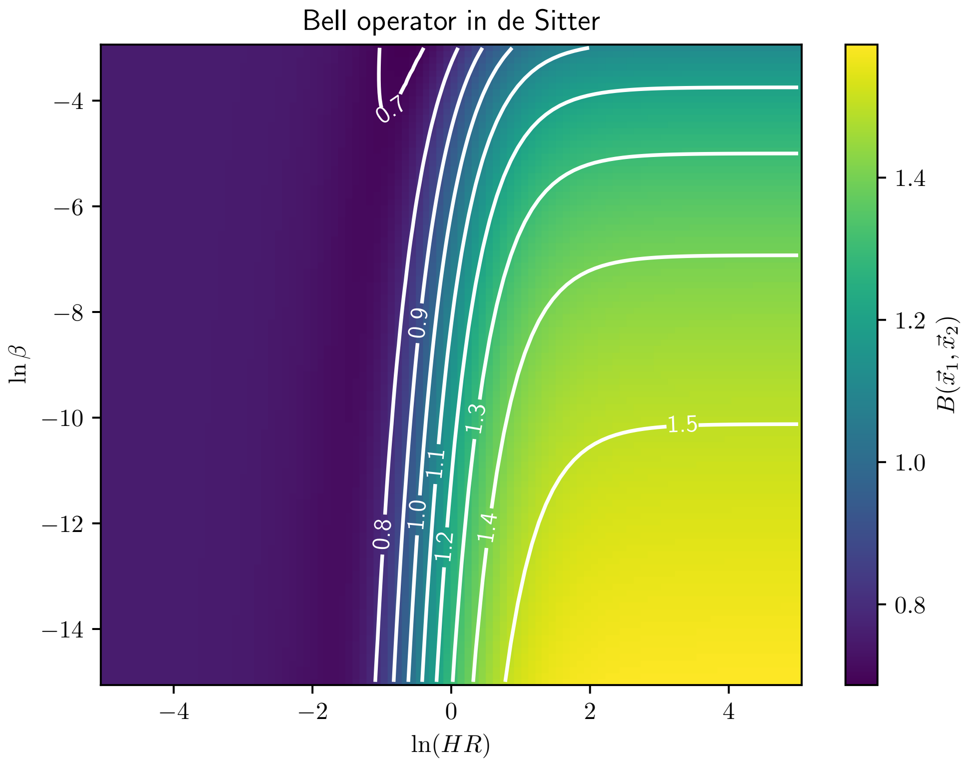

Figure B.1: Expectation value of the GKMR Bell operator in the Bunch-Davies vacuum of the de-Sitter space-time, as a function of the parameters β and HR. The colour encodes the value of B, and a few contour lines are displayed in white. The UV regulator is set to $\delta = 0.01$ and $\alpha = d/R$ is set to the minimum $\alpha = 2(\delta + 1)$.

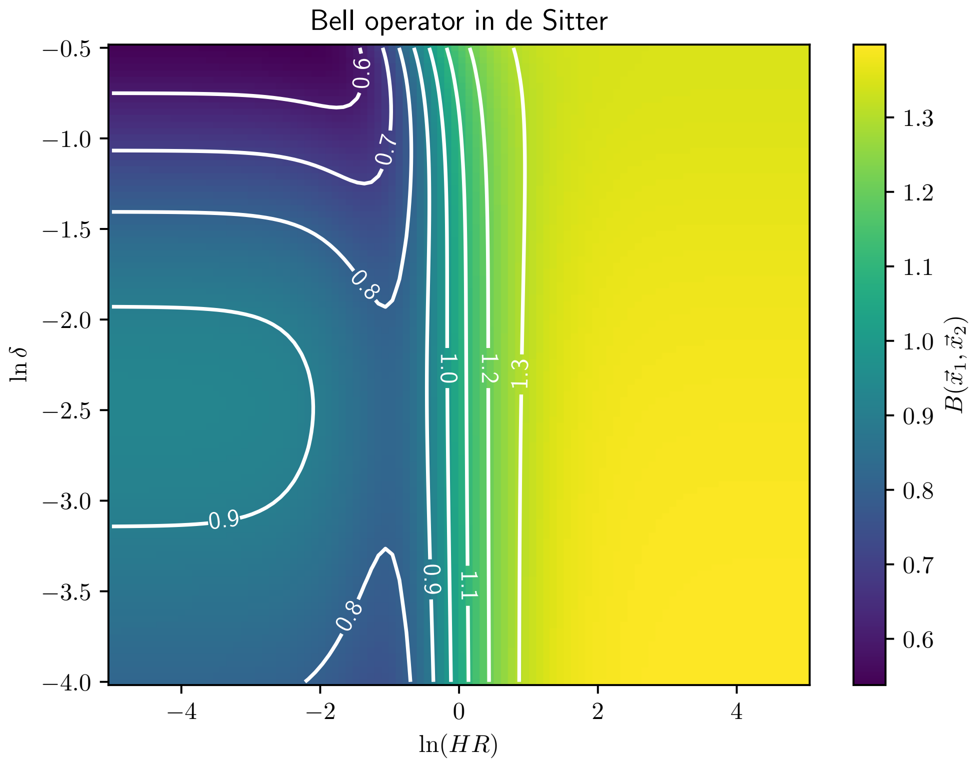

Figure B.2: Expectation value of the GKMR Bell operator in the Bunch-Davies vacuum of the de-Sitter space-time, as a function of the parameters β and HR. The colour encodes the value of B, and a few contour lines are displayed in white. The IR regulator is set to $\beta = 10^{-3}$ and $\alpha = d/R$ is set to the minimum $\alpha = 2(\delta + 1)$.

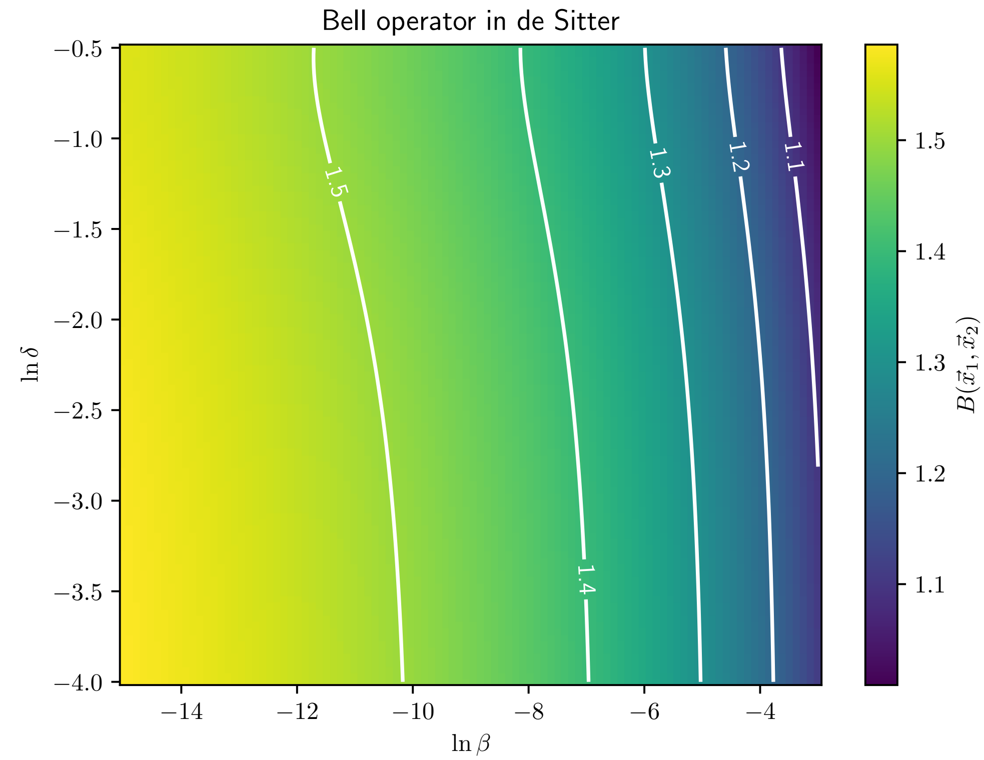

Figure B.3: Expectation value of the GKMR Bell operator in the Bunch-Davies vacuum of the de-Sitter space-time, as a function of the parameters β and HR. The colour encodes the value of B, and a few contour lines are displayed in white. The size of the patch is set to $HR = 10^3$ and $\alpha = d/R$ is set to the minimum $\alpha = 2(\delta + 1)$.

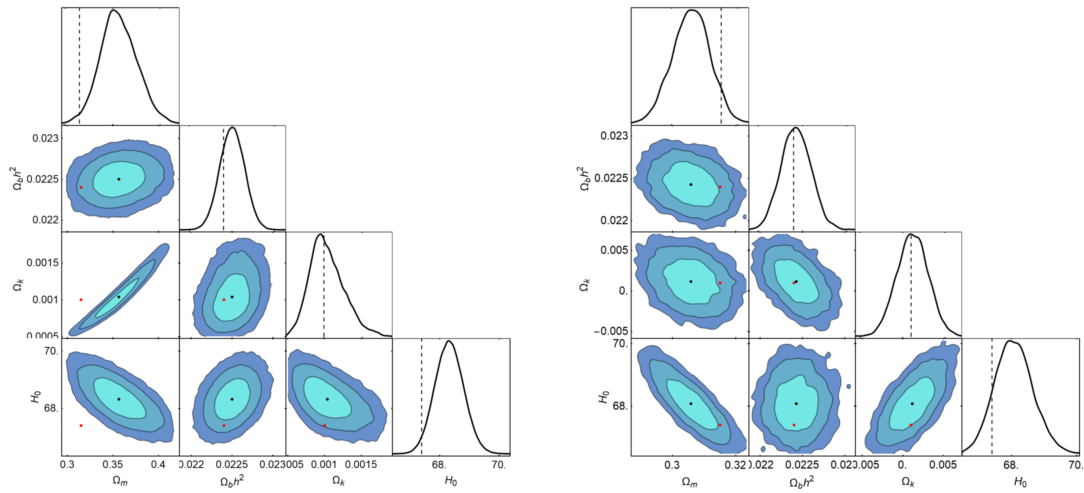

Figure B.4: The 68% and 95% confidence contours for the GREAT (left panel) and ΛCDM(right panel) models respectively, including all the data, but no prior on H_0. The red points/dashed lines correspond to the Planck best-fit $(\Omega_{m,0}, \Omega_{b,0}h^2, \Omega_{k,0}, H_0) = (0.315, 0.0224, 0.001, 67.4)$, where H_0 is given in units of $\mathrm{km\,s^{-1}\,Mpc^{-1}}$.

B.2 GREAT vs ΛCDM

For completeness, we show here the contour plots of confrontation of GREAT and ΛCDM against cosmological data. These are figs. B.4, B.5 and B.6. This complements the best fit parameters provided in section 7.4.

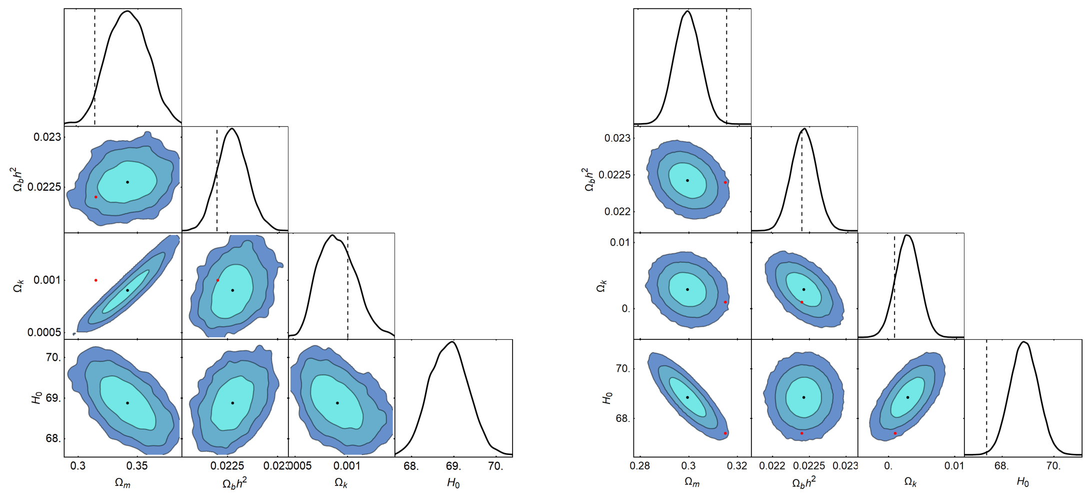

Figure B.5: The 68.3%, 95.5% and 99.7% confidence contours for the GREAT (left panel) and ΛCDM(right panel) models respectively, including all data and the Riess H_0 prior. The red points/dashed lines correspond to the Planck best-fit $(\Omega_{m,0}, \Omega_{b,0}h^2, \Omega_{k,0}, H_0) = (0.315, 0.0224, 0.001, 67.4)$, where H_0 is given in units of $\mathrm{km\,s^{-1}\,Mpc^{-1}}$.

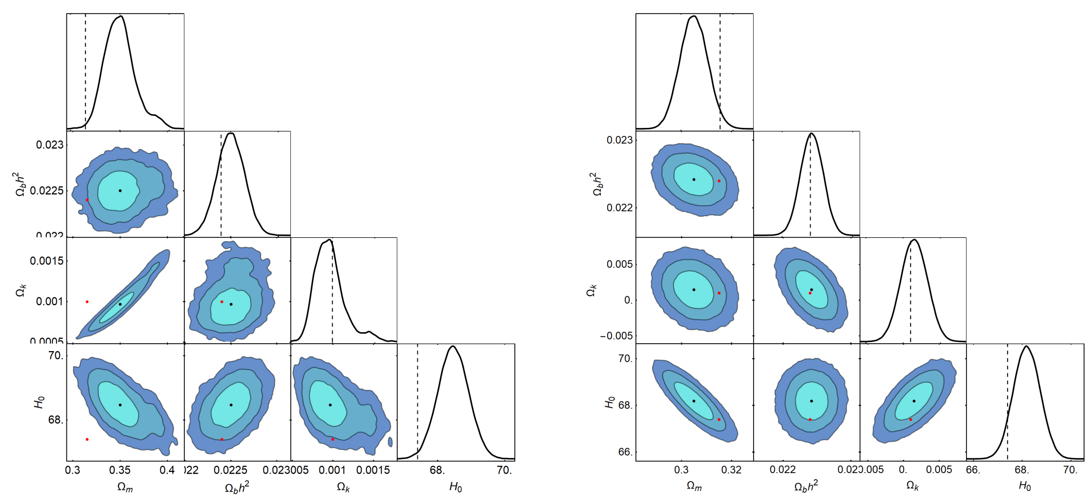

Figure B.6: The 68.3%, 95.5% and 99.7% confidence contours for the GREAT (left panel) and ΛCDM(right panel) models respectively, including all data and the TRGB prior on H_0. The red points/dashed lines correspond to the Planck best-fit $(\Omega_{m,0}, \Omega_{b,0}h^2, \Omega_{k,0}, H_0) = (0.315, 0.0224, 0.001, 67.4)$, where H_0 is given in units of $\mathrm{km\,s^{-1}\,Mpc^{-1}}$.

List of Figures

List of Tables

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