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Theoretical and Numerical Methods for Modified Gravity

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Introduction

In the past century, two great discoveries revolutionized our understanding of the Universe. The first was the study of the NGC 3198 galaxy in the 80s [1]. Looking at the rotation velocity of the galaxy objects with respect to its center, the so-called *rotational curve of the galaxy*, an anomaly was found. The rotational curve did not seem to obey the known laws of physics as the velocities of objects far away from the center of NCG 3198 were too big with respect to any theoretical prediction. The explanation for these anomalies involves the presence of an additional unknown matter in the galaxies, called *dark matter*. An interesting property of dark matter is its interaction nature. Since we have not yet observed this matter with telescopes but only looked at its effect on galaxies objects, we believe dark matter interacts with standard matter (baryons, leptons, ...), radiation and neutrinos only gravitationally and not through electromagnetic interactions. In fact, up to now, dark matter has not been directly observed with ground detection experiments.

The second discovery came from the observation of type 1A supernovae emissions. Although we already knew that the Universe was expanding since the beginning of the 20^{th} century [2], at the end of the millennium, two independent experiments discovered that this expansion was accelerating [3, 4]. Within the theory of General Relativity, the acceleration can not be explained with the known standard matter, radiation, neutrinos, or even with a different spatial curvature. This contradiction led to the resolutive hypothesis that a new kind of matter, which throughout the whole history of the Universe has a constant density achieved with negative pressure, should be considered. This matter is called *dark energy*.

These two breakthroughs are the basis of the standard model of cosmology. However, even though this model has been proven astonishingly accurate in describing the history of the Universe, cosmologists still struggle with some fundamental questions about dark energy and dark matter. It is important to stress that both dark matter and dark energy are called "dark" to underline our ignorance about the fundamental nature of these additional matter types. We should think of them as a way to parametrize our ignorance about the actual nature of these two hypotheses rather than the solution of the two problems mentioned before. We know that there should be some matter with specific properties to explain the two aforementioned observational phenomena, and its inclusion in the theoretical model leads to satisfactory theory-observation accordance. However, we know nothing about the fundamental nature of dark matter and dark energy, nor any direct observation has proven their existence. Moreover, additional fundamental and mathematical questions arise when postulating dark matter and dark energy in the form proposed in the standard model.

In the decades after these discoveries, we are witnessing two phenomena in theoretical and observational cosmology. On one hand, experiments are becoming more accurate and precise in detecting information from the Universe. One of the most recent examples is the Planck experiment [5], whose space telescope observed the photons coming from a moment in the Universe's history called recombination, which happened 13 billions of years ago. At that moment, photons and electrons decoupled, letting the firsts travel freely and unscattered. This radiation is called Cosmic Microwave Background (CMB). We can collect these photons with a detector to create a snapshot of the photon intensity distribution at that time. This distribution is tightly linked with dark matter and dark energy properties, helping physicists to shed some light on the two dark components. See Figure 1 as an example. In general, the accuracy of new experiments puts very tight constraints on theoretical models.

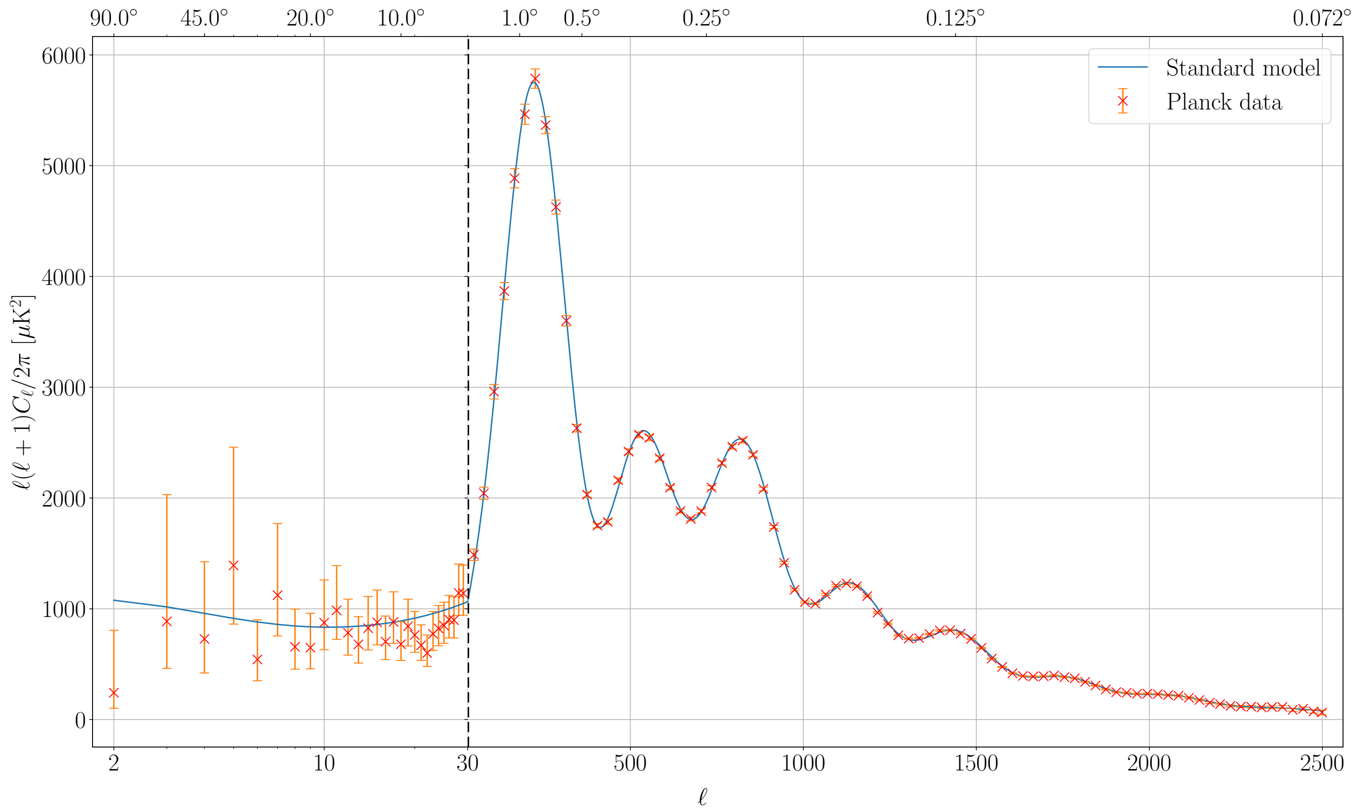


Figure 1: Plot of the Cosmic Microwave Background (CMB) power spectrum from Planck data [5] and the standard model prediction, here expressed with a normalized C_ℓ as a function of the angular distance between two incoming photons (upper x-axis). We can appreciate the precision of Planck data and the great accordance between the observation and the theory, which can be achieved only by including dark energy and dark matter contributions in the theoretical model. Alternative models without dark energy and dark matter can not fit the data.

On the other hand, many theoretical models have been proposed as alternatives to the standard model to solve the problems mentioned above. These models modify the General Relativity equations of motion, the Einstein equations, either replacing the dark matter and dark energy matter contents with respect to the standard model or modifying the geometry of spacetime. They achieve this by including additional dynamical quantities or degrees of freedom, whose evolution can explain the accelerated expansion acceleration or dark matter effects (or both). For instance, a scalar field can be considered [6], but other models with more complex additional degrees of freedom have been proposed. All these models are usually called *Modified Gravity* theories.

In the last few years, most of the modified gravity models have been under scrutiny due to increased observational data. For instance, the predictions of the CMB shown in Figure 1 might change when we consider modified gravity models for dark energy or dark matter, putting constraints on the theory parameters or ruling the model out. The data are becoming accurate enough to put very tight constraints on the modified gravity models.

Nevertheless, the analysis of the CMB power spectrum or similar observables is not an easy task. One of the main obstacles in checking the viability of the theoretical models against experimental data is the complexity of the theoretical study of these crucial observables. No analytical solution of the equations of motion valid at all times of the Universe's history can be found. For instance, Figure 1 has been obtained with complex software, called *Boltzmann solvers*, which computes the evolution of observables from the end of inflation to today, taking into account a multitude of thermodynamic and scattering effects that occurred during the Universe life. Moreover, additional degrees of freedom can increase the complexity of the evaluations for modified gravity models.

We should also consider that a single evaluation of the Universe's history is not enough to conclude anything about the viability of the model. When we compare a theoretical model with experiments, we should minimize the difference between the predictions and the data, varying the value of the theory parameters. This procedure usually needs an enormous number of evaluations that require significant computational power, even with the most efficient Monte Carlo algorithms.

Moreover, especially in the modified gravity context, it is also essential to distinguish the theory predictivity given by the new proposals' real physical and mathematical power rather than the simple addition of new degrees of freedom. It is easier to fit three points with a parabola with respect to a straight line at the price of adding a new parameter to the theory. However, is it always necessary? In physics, like in other fields, Occam's razor principle tells us that the most straightforward theory should always be preferred. With the introduction of the Bayesian probability, we can perform comparisons between models to find the ones that fit the data with fewer parameters. But, again, this procedure is computationally expensive.

Finally, we can ask ourselves if there is a way to parametrize the modified gravity models in a model-independent way. In other words, does it exist a way to write a general action or Lagrangian which can include all modified gravity models? The power of such a generalization would be undeniable: we would be able to compute the equations of motion from one single action and apply it for every modified gravity model. Such a theory, which we will call *Effective Field Theory (EFT) of Gravity*, has been developed, and it works for any theory with an additional degree of freedom with respect to General Relativity. The major drawback is that the general form of the EFT of Gravity does not provide an immediate physical interpretation of its Lagrangian terms, and therefore a mapping between a "standard" modified gravity theory and its EFT counterpart is always preferred.

Outline

This thesis firstly presents an overview of the General Relativity mathematical tools and some cosmology concepts, and briefly explains the main Universe periods. We also derive some crucial equations of the cosmological perturbation theory, which are the basis of the comparison between experimental data and theoretical models to compute observables like the CMB power spectrum in Figure 1. Moreover, we review the *Arnowitt–Deser–Misner* (ADM) theory, which can be thought of as the Hamiltonian formulation of General Relativity as opposed to the standard Lagrangian formulation.

In the second part, we show some modified gravity models and derive some results using the theoretical and numerical methods explained in the previous parts. In particular, we study two models. The first is the Horndeski class of models, which is the most general way to write a theory with one additional degree of freedom of General Relativity (a scalar field) retaining second-order derivatives equations of motion. The latter property is essential to avoid the so-called Ostrogradsky instabilities, which occur when the equations of motion are of third order in the derivatives, leading to un-physical predictions like the energy levels not bounded from below. Then we will show some results obtained with the mimetic class of models, which involves two additional degrees of freedom, one of which acts as a constraint for the value of the second through a Lagrange multiplier in the action.

The last part is dedicated to the study of the Effective Field Theory of Gravity. Firstly we introduce the standard Effective Field Theory concepts to compare them with the Effective Field Theory of Gravity. Then we will study the theory, derive its Lagrangian and the equations of motion. We also present an ADM formulation of this EFT and provide an example in the context of Horndeski gravity.

Finally, in the Appendix we present some of the numerical algorithms used in the thesis, such as Bayesian probability software as well as a tensor computer algebra extension of *Mathematica* called *xAct*.

Original results

The original results in the thesis are from [7, 8, 9, 10]. In [7] we discuss the existence of de Sitter solutions in some modified gravity theories. In particular, in section 5.6 we discuss the presence of de Sitter solution within the Horndeski gravity theories. We show that these solutions might not exist in general.

In section 6 we show and expand the discussion of [8, 9]. We firstly study a specific mimetic gravity, whose non-mimetic scalar field sector is a *broken* Horndeski to ensure a non-null sound speed of scalar perturbations, deriving the background and first order perturbation equations. Subsequently we perform a Bayesian parameter estimation the action parameters using the LIGO/Virgo collaboration observation of the event GW170817, produced by merger of a binary neutron star system [11], and the optical counterpart GRB170817A [12]. In particular, we use the speed of tensor perturbations to establish the order of magnitude of the action parameters.

In section 10.3 we study a dark matter modified gravity model firstly proposed in [13], whose linear perturbations numerical analysis has been performed in [10], as an example of the modified gravity standard approach and the Effective Field Theory introduced in the last part. We also perform an analysis of the perturbations, showing the presence of instabilities in the model.

Notation and units conventions

Unit of measurement system

The unit of measurement system we will consider has the following properties.

1. the Newton constant G will be explicitly written, while the speed of light c and the Planck constant are
$$c = \hbar = 1\,.$$

2. the scale factor is considered dimensionless and unitary today, i.e. $a(t_0) = 1$, where $t = t_0$ is the time today.

Metric signature

The signature of the metric considered is

$$\text{Sign}\,[g_{\mu\nu}] = (-, +, +, +)\,.$$

Symbols

The following symbols convention has been used

1. the Greek indices $\alpha, \beta, \ldots$ are used for spacetime indices, while Roman indices $i, j, \ldots$ are used for spatial indices;

2. the indices can be raised or lowered with the metric tensor. For instance spacetime indices can be raised/lowered with the covariant metric $V_\rho\, g^{\rho\mu} g_{\mu\nu} = V^\mu\, g_{\mu\nu} = V_\nu$;

3. the "," subscript or superscript followed by a tensor index denotes a partial derivative, i.e. if V^μ is a vector, $V^\mu{}_{,\nu} \equiv \partial_\nu V^\mu$;

4. the ";" subscript or superscript followed by a tensor index denotes a covariant derivative, i.e. if V^μ is a vector, $V^\mu{}_{;\nu} \equiv \nabla_\nu V^\mu$;

5. the round brakets "()" and square brakets "[]" as subscripts or superscripts respectively denotes symmetrization and anti-symmetrization operations on the enclosed indices. For instance, if $T_{\mu\nu}$ is a tensor, $T_{(\mu\nu)} \equiv (T_{\mu\nu} + T_{\nu\mu})/2$ and $T_{[\mu\nu]} \equiv (T_{\mu\nu} - T_{\nu\mu})/2$. The factor at the denominator is the factorial of the number of indices involved.

Fourier transform

Sometime we will use the Fourier transform of a function f as

$$f(\vec{k}) = \int d^3x\, e^{-i\vec{k}\cdot\vec{x}} f(\vec{x})\,,$$

and the anti-transform as

$$f(\vec{x}) = \int \frac{d^3k}{(2\pi)^3} \, e^{i\vec{k}\cdot\vec{x}} f(\vec{k}) \, .$$

Note that this leads to the following derivative conversion

$$\mathcal{F}\left[\frac{\partial f(\vec{x})}{\partial x_i}\right] = ik_i f(\vec{k}) \, .$$

Conversions

For future reference, we also show some common conversions.

$$1 \text{ pc} = 3 \times 10^{16} \text{ m} = 3.3 \text{ light years} \, .$$

Part I

General Relativity and Cosmology

Chapter 1

Introduction to General Relativity and Cosmology

This section introduces some of the key results of General Relativity, the standard theory that accurately describes gravitational interactions over fifteen orders of magnitude in length, from the smallest scales to cosmology. We will then focus on the evolution of a homogeneous and isotropic Universe used as a background to study the largest scales, and provide the relevant equations.

1.1 Summary of General Relativity

The theory of General Relativity is governed by the Einstein-Hilbert action

$$S = \frac{1}{16\pi G}\int d^4x\sqrt{-g}\left[R(g_{\mu\nu},\partial_\rho g_{\mu\nu},\partial_\sigma\partial_\rho g_{\mu\nu}) - 2\Lambda\right] + S_M\,, \tag{1.1}$$

where G is the Newton constant, $g_{\mu\nu}$ is the metric tensor, $\sqrt{-g} = \sqrt{-\det(g_{\mu\nu})}$, Λ is the so called *cosmological constant* and R is the Ricci scalar defined from the Riemann tensor $R^{\mu}{}_{\nu\rho\sigma}$. In fact, if we define the Ricci tensor

$$R_{\mu\nu} = R^{\rho}{}_{\mu\rho\nu} = \Gamma^{\alpha}_{\mu\nu,\alpha} - \Gamma^{\alpha}_{\mu\alpha,\nu} + \Gamma^{\alpha}_{\beta\alpha}\Gamma^{\beta}_{\mu\nu} - \Gamma^{\alpha}_{\beta\nu}\Gamma^{\beta}_{\mu\alpha}\,, \tag{1.2}$$

we can then define the Ricci scalar

$$R = g^{\mu\nu}R_{\mu\nu} = g^{00}R_{00} + g^{ij}R_{ij} + 2g^{0i}R_{0i}\,, \tag{1.3}$$

where the factor 2 in the last term comes from the symmetry of the Ricci tensor $R_{\mu\nu} = R_{\nu\mu}$ and of the metric $g_{\mu\nu} = g_{\nu\mu}$. Both the Ricci tensor $R_{\mu\nu}$ and the Ricci scalar R have a dependence on the Christoffel symbols of the metric*

$$\Gamma^{\sigma}_{\mu\nu} = \frac{1}{2}g^{\sigma\alpha}\left[g_{\mu\alpha,\nu} + g_{\nu\alpha,\mu} - g_{\mu\nu,\alpha}\right]\,. \tag{1.4}$$

Therefore the Ricci tensor is dependent on the metric and its first and second derivatives, although it is possible to integrate by parts to reduce the dependence on the metric and its first derivatives only.

The S_M part of the action contains all the matter sources. In the standard model of cosmology, the matter species that fill the Universe are baryons†, dark matter, photons, neutrinos. S_M is usually

* In principle, since we have three free spacetime indices, we would have to calculate 64 Christoffel symbols for each metric. The computation can be simplified exploiting the symmetry

$$\Gamma^{\sigma}_{\mu\nu} = \Gamma^{\sigma}_{\nu\mu}.$$

† This is an improper way of denoting all the standard matter species, including, e.g., also free electrons.

written from a Lagrangian

$$S_M = \int d^4x\sqrt{-g}\mathcal{L}_M(g_{\mu\nu})\,. \tag{1.5}$$

Using the variational principle on this action with respect to the metric $g_{\mu\nu}$, we find the *Einstein equations*

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi G T_{\mu\nu}\,. \tag{1.6}$$

These equations are covariant: all the quantities involved in the equations are invariant under local diffeomorphic coordinate transformations (diffeomorphisms). From a physical point of view, this means that we can freely change local coordinates without changing the experiment result at a given event x^μ.

The tensor $G_{\mu\nu}$ is the *Einstein tensor* defined as

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R\,, \tag{1.7}$$

and the tensor $T_{\mu\nu}$ on the right-hand side is called the *energy-momentum* (or *stress-energy*) tensor. It comes from the variation of the S_M part of the Einstein-Hilbert action, and is defined as

$$T^{\mu\nu} \equiv -\frac{2}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\mathcal{L}_M)}{\delta g_{\mu\nu}}\,, \tag{1.8}$$

where the $\delta f/\delta g_{\mu\nu}$ is the functional derivative of f with respect to the metric $g_{\mu\nu}$. The Einstein tensor has the important property of being divergenceless

$$\nabla^\mu G_{\mu\nu} \equiv G_{\mu\nu}{}^{;\mu} = 0\,. \tag{1.9}$$

Therefore, from the Einstein equation (1.6) we have that $T_{\mu\nu}$ must be divergenceless too.

The standard form of the equations of motion for a freely falling particle in spacetime (no forces on the particle) is

$$\frac{d^2x^\mu}{d\lambda^2} + \Gamma^\mu_{\rho\sigma}\frac{dx^\rho}{d\lambda}\frac{dx^\sigma}{d\lambda} = 0\,, \tag{1.10}$$

where Γ is the Christoffel symbol (1.4), and λ is a parameter that parametrizes the spacetime trajectory (world-line) $x(\lambda)$. These equations are called *geodesic equations*. If the parameter λ used to parametrize the trajectory gives the geodesic equations in the form (1.10), λ is called an *affine parameter*.

Finally, the metric can also be written in term of the *line element* (dx^μ is the infinitesimal displacement vector)

$$ds^2 \equiv g_{\mu\nu}\,dx^\mu dx^\nu\,, \tag{1.11}$$

which can be interpreted as the physical (observable) infinitesimal distance between two spacetime events defined by some fixed values of the spacetime coordinates x^μ. In fact, we can define the proper time as

$$\int_{\gamma(\lambda)} ds\,, \tag{1.12}$$

which can be rewritten with a change of variable

$$\int_{\gamma(\lambda)} ds = \int_{\gamma(\lambda)} d\lambda\left[-g_{\mu\nu}\frac{dx^\mu}{d\lambda}\frac{dx^\nu}{d\lambda}\right]^{1/2}\,. \tag{1.13}$$

The proper time is the time that would be measured with a clock following the world-line $\gamma(\lambda)$[‡]. From this definition, we can revisit the physical meaning of the geodesic as the world-line $\gamma(\lambda)$ which minimizes

[‡] More precisely, we need to consider a time-like world-line, i.e. a trajectory which obeys

$$-\,g_{\mu\nu}\frac{dx^\mu}{d\lambda}\frac{dx^\nu}{d\lambda} > 0\,. \tag{1.14}$$

the proper time. In fact, the variation of the proper time (1.12) with respect to the metric $g_{\mu\nu}$ gives the *geodesic equations* (1.10), which are therefore minimizing the physical distance between the starting and final point of $\gamma(\lambda)$. Therefore geodesics are usually considered the generalization of straight line trajectories in a Euclidean space.

1.2 Friedmann equations

The metric which describes an expanding flat, homogeneous and isotropic (smooth) Universe is called *Friedmann–Lemaître–Robertson–Walker* (FLRW). Written as a line element defined in equation (1.11), it has the following form

$$ds^2 = -dt^2 + a(t)^2 \left[\frac{dr^2}{1 - \kappa r^2} + r^2 \left(d\theta^2 + \sin^2\theta \, d\phi^2 \right) \right] . \tag{1.15}$$

The function $a = a(t)$ is called the *scale factor*, and describes the expansion of the Universe from the value of $a(0) = 0$ to the present, a conventionally fixed value of $a(t_0) = 1$ (t_0 is the present physical time, i.e., the age of the Universe). The scale factor is a monotonically increasing function of the proper time t, and for this reason, it can replace t to describe the evolution of the Universe. The κ parameter is called the *curvature* and describes the spatial curvature of the Universe. It is null if the Universe is spatially flat, negative if we have a spatially hyperbolic (open) Universe, and positive in the case of a spatially spherical (closed) Universe.

The FLRW metric does not contain any function with dependence on the spatial coordinates, and therefore it is correctly describing a smooth Universe, i.e., whose energy density is homogeneous and isotropic. This description of the Universe relies on the *Cosmological Principle*, which states that at sufficiently large scales ($\gtrsim$ 100 Mpc), the Universe is smooth. This principle can not be applied on small scales, where we know the matter clusters. However, for cosmological description purposes, these inhomogeneities are usually contained enough to be described as perturbations of the homogeneous and isotropic (background) Universe. In the following Chapters, we will see how this perturbation theory can be developed by modifying the FRWL metric.

The Einstein equations (1.6) evaluated on the FLRW metric, the so called *Friedmann equations*, are

$$\begin{aligned} H^2 &= \frac{8\pi G}{3}\rho + \frac{\Lambda}{3} - \frac{\kappa}{a^2} , \\ \dot{H} + H^2 &= -\frac{4\pi G}{3} \left(\rho + 3P \right) + \frac{\Lambda}{3} , \end{aligned} \tag{1.16}$$

where $\rho = \rho(t)$ is the *total energy density* of all components of the matter, $P = P(t)$ the *total pressure* and $H = (da/dt)/a = H(t)$ the *Hubble parameter*. We denote the derivative with respect to t with the upper dot, e.g. $\dot{H} \equiv dH/dt$. As expected from the form of the Einstein equations, we note that these differential equations are at most at second order in the time coordinate t, being

$$\dot{H}(t) = \frac{1}{a(t)} \frac{d^2 a(t)}{dt^2} - \frac{1}{a(t)^2} \left[\frac{da(t)}{dt} \right]^2 = \frac{1}{a(t)} \frac{d^2 a(t)}{dt^2} - H(t)^2 . \tag{1.17}$$

The Friedmann equations should be solved to find $a(t)$, which depends on the matter components considered through ρ and P. Some examples will be shown below.

We can also rewrite the second Friedmann equation as a conservation law

$$\frac{d\rho}{dt} + 3H \left(\rho + P \right) = 0 . \tag{1.18}$$

In cosmology, the fluids considered are usually *barotropic*, i.e. the pressure is a function of the density only

$$P = \omega \rho , \tag{1.19}$$

where the parameter ω is the *state parameter*, and has a constant value for the fluids considered: for a radiation fluid $\omega = 1/3$, while for standard matter $\omega = 0$. With this equation of state and the conservation equation (1.18) we find

$$\frac{\rho(t)}{\rho_0} = \left[\frac{a_0}{a(t)}\right]^{3(1+\omega)}, \tag{1.20}$$

from which we can derive the evolutions for radiation and standard matter fluid energy densities

$$\rho_r \propto \frac{1}{a^4} \qquad \text{and} \qquad \rho_m \propto \frac{1}{a^3}. \tag{1.21}$$

The inverse cubic dependence is not unexpected. The physical density must be defined with the physical volume $\propto D^{-3} \propto a^{-3}$ (ds gives the infinitesimal physical distance, which is proportional to a on the space coordinates). An additional $1/a$ is present for the radiation fluid, since the energy in the density ρ_r is defined as $\hbar\nu = 2\pi\hbar/\lambda$ and the physical wavelength λ of the photon increases as the Universe expands, i.e. $\lambda \propto a$, giving an additional scale factor on the denominator. Moreover, from equation (1.20) we see that an hypothetical component with constant density must have $\omega = -1$.

There is another way to write the Friedmann equations. We can rewrite the first Friedmann equation (1.16) in the form

$$H(t)^2 = \frac{8\pi G}{3}\rho(t), \tag{1.22}$$

where the density is given by the sum of the single component densities

$$\rho(t) = \rho_m(t) + \rho_r(t) + \rho_\Lambda(t) + \rho_k(t), \tag{1.23}$$

and

$$\rho_\kappa(t) \equiv -\frac{3}{8\pi G}\frac{\kappa}{a(t)^2}, \tag{1.24}$$

$$\rho_\Lambda(t) \equiv \frac{\Lambda}{8\pi G}. \tag{1.25}$$

The first is the effective energy density given by the spatial curvature, which, depending on the sign of the curvature parameter κ, might be negative. The latter is the effective energy density induced by the cosmological constant. Since it is constant, it can be interpreted as a matter component with an equation of state parameter $\omega_\Lambda = -1$.

If we divide (1.22) by $H(t)^2$, we obtain the equation

$$1 = \Omega_m(t) + \Omega_r(t) + \Omega_\Lambda(t) + \Omega_\kappa(t), \tag{1.26}$$

where Ω is called the *fractional energy density* of the i-th matter species and it is defined as

$$\Omega_i(t) \equiv \frac{8\pi G}{3}\frac{\rho_i(t)}{H^2(t)}. \tag{1.27}$$

This can be further rewritten in a more convenient form. Consider (1.22) at time t_0

$$H_0^2 \equiv H(t_0)^2 = \frac{8\pi G}{3}\rho(t_0) \equiv \frac{8\pi G}{3}\rho_{cr}, \tag{1.28}$$

where we define the *critical energy density* $\rho_{cr} \equiv \rho(t_0)$ to be the energy density today. Thus the fractional energy densities evaluated today, at $t = t_0$, are

$$\Omega_i^0 \equiv \Omega_i(t_0) = \frac{\rho_i(t_0)}{\rho_{cr}}. \tag{1.29}$$

Using the equation (1.20) for $\rho(t)$, we obtain the explicit equation for the energy density

$$\rho_m(t) = \frac{\rho_{cr}\Omega_m^0}{a(t)^3}\,, \qquad \rho_r(t) = \frac{\rho_{cr}\Omega_r^0}{a(t)^4}\,, \qquad \rho_\Lambda(t) = \rho_{cr}\Omega_\Lambda^0\,, \qquad \rho_\kappa(t) = \frac{\rho_{cr}\Omega_\kappa^0}{a(t)^2}\,, \tag{1.30}$$

and therefore

$$\Omega_m(t) \equiv \frac{H_0^2}{H(t)^2}\frac{\Omega_m^0}{a(t)^3}\,, \quad \Omega_r(t) \equiv \frac{H_0^2}{H(t)^2}\frac{\Omega_r^0}{a(t)^4}\,, \quad \Omega_\Lambda(t) \equiv \frac{H_0^2}{H(t)^2}\Omega_\Lambda^0\,, \quad \Omega_\kappa(t) \equiv \frac{H_0^2}{H(t)^2}\frac{\Omega_\kappa^0}{a(t)^2}\,. \tag{1.31}$$

In general, at any time t we can write

$$1 = \sum_{\text{species } i} \Omega_i(t)\,, \tag{1.32}$$

Finally, the Friedmann equation with this new notation is

$$H(t)^2 = \frac{8\pi G\rho_{cr}}{3}\left[\frac{\Omega_m^0}{a(t)^3} + \frac{\Omega_r^0}{a(t)^4} + \Omega_\Lambda^0 + \frac{\Omega_\kappa^0}{a(t)^2}\right]. \tag{1.33}$$

Therefore, once we have the value of the Hubble parameter at $t = t_0$ (in the ρ_{crit} definition) and the value of all the fractional energy densities today (minus one since one can be found from the others using (1.32)), we can obtain the value of the Hubble parameter $H(t)$ for any value of the scale factor $a(t)$. On the contrary, to obtain the value of the scale factor at a given time t we still need to solve the differential equation. We show the evolution of the fractional densities in Figure 2.5.

Finally, in standard cosmology, the spatial curvature is usually considered flat since the curvature parameter κ is experimentally compatible with 0 [5].

1.3 Definition of cosmological quantities

The cosmological time t, also called *proper time*, is not the only monotonically increasing or decreasing function that can be used to label the Universe time evolution. Some of these functions are:

(i) the *redshift* z, also defined as

$$1 + z \equiv \frac{1}{a}\,; \tag{1.34}$$

(ii) the *conformal time* η, whose infinitesimal definition is $d\eta = dt/a$. With this definition, the metric is

$$ds^2 = a(t)^2\left[-d\eta^2 + \frac{dr^2}{1-kr^2} + r^2\left(d\theta^2 + \sin^2\theta d\phi^2\right)\right]. \tag{1.35}$$

These coordinates (η, r, θ, ϕ) are called *comoving coordinates*. The conformal time η is the comoving distance the light travelled from the beginning of time to some given time t. To be more precise, considering an inflationary model, the definition of the conformal time is usually shifted and starts from the end of the inflation period, and is given by

$$\eta(t) \equiv \int_{t_e}^{t} \frac{dt'}{a(t')} = \int_{a_e}^{a} \frac{da'}{a'}\frac{1}{a'H(a')}\,, \tag{1.36}$$

where t_e is the proper time at the end of the inflation, and $a_e = a(t_e)$. For this reason, $\eta(t)$ is also called the *comoving horizon*;

(iii) the *photon temperature* $\propto 1/a$.

$$T = \frac{T_0}{a}\,, \tag{1.37}$$

where $T_0 = 2.7255$ K. This temperature have a very specific physical meaning as we will see in the next section.

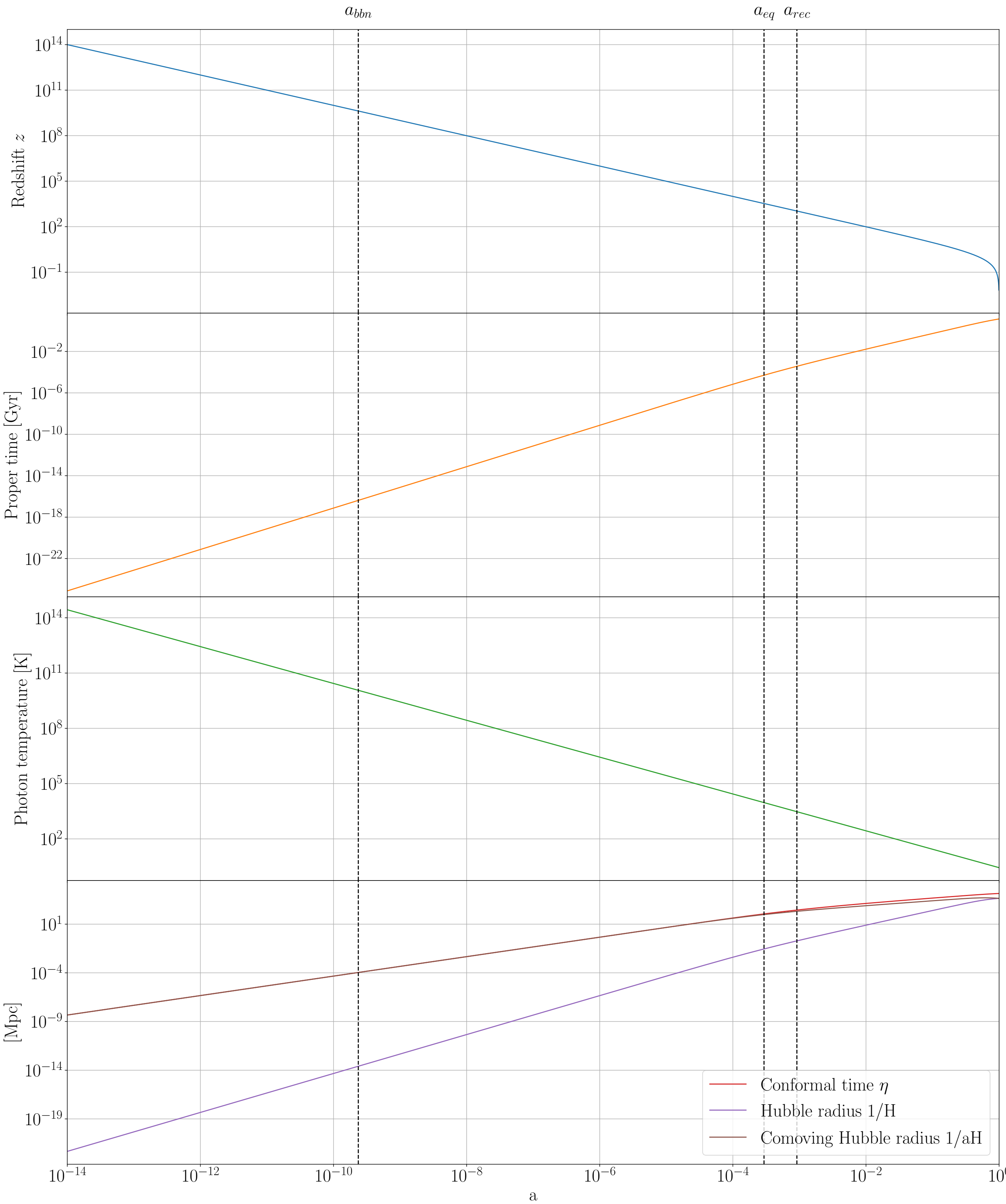


Figure 1.1: Plot of quantities used as time labels in cosmology. The lines are computed using the `CLASS` code with standard ΛCDM parameters [5].

Another important quantity is the *comoving Hubble radius*, which is defined as $1/aH$. Consider the physical space distance of an object from the Earth $D = ax$, where x is the comoving distance. The physical velocity of an object with no peculiar velocity dx/dt is given by

$$v = \frac{dD}{dt} = \frac{da}{dt}x + a\frac{dx}{dt} = \frac{da}{dt}x = Hax\,. \tag{1.38}$$

Suppose $x > 1/Ha$, the velocity v of the object receding from us is larger than the speed of light (in our units of measurement system, $c = 1$). In this case, not even a photon emitted by this object can reach us, and therefore the object is not causally connected to us. Note that the conformal time is not the same as the Hubble radius: the first is a more stringent horizon, since no particle outside the comoving horizon η_0 is or has ever been causally connected to us; the latter tells us about the causal connection with the object at a given time t. In fact, in Figure 1.1 we can see that the comoving Hubble radius is not a monotonically increasing function, and therefore an object now receding at speed greater than light might have been causally connected to us. Finally, note that the conformal time (1.36) is the integral of the Hubble radius with an additional a, and thus it must always be larger than the comoving Hubble radius.

From the equation of the physical velocity v (1.38) we can write the explicit version of the *Hubble law*

$$v = \frac{da}{dt}x = HD. \tag{1.39}$$

The physical velocity v of an object is then proportional to the physical distance of this object from the Earth. The proportionality constant is H_0, the Hubble parameter today, which is obtained from experiments. The value of H_0 in the Planck experiment is [5]§

$$H(t_0) = H_0 = (67.4 \pm 0.5)\ \text{km s}^{-1}\ \text{Mpc}^{-1} \equiv (100\ h \pm 0.5)\ \text{km s}^{-1}\ \text{Mpc}^{-1}\,. \tag{1.40}$$

In Figure 1.1 we plot the quantities defined above as functions of the scale factor. This plot is helpful to convert the cosmological quantities considered, providing a link with the more intuitive physical (proper) time t. For future reference, we also show some critical moment in the Universe evolution using data from the Planck data: the Big Bang nucleosynthesis at a_{bbn}, the matter-radiation equilibrium at a_{eq} and the recombination period a_* (or a_{rec}). In the following sections, we will briefly present an overview of these events.

1.4 Scalar-vector-tensor decomposition

In addition to the background, we can perturb the metric allowing for small deviations from background quantities. At linear order, the most general way is to consider

$$g_{\mu\nu} = g^{(0)}_{\mu\nu} + g^{(1)}_{\mu\nu}\,, \tag{1.41}$$

where $g^{(0)}_{\mu\nu}$ is the unperturbed metric, and $g^{(1)}_{\mu\nu}$ its perturbation metric.

It is common to separate the perturbation contributions as

$$g^{(1)}_{00} = -2\Psi\,, \tag{1.42}$$

$$g^{(1)}_{0i} = \omega_i\,, \tag{1.43}$$

$$g^{(1)}_{ij} = 2s_{ij} + 2\Phi\delta_{ij}\,, \tag{1.44}$$

§ The value of H_0 from the Planck experiment is not compatible with other experiments at lower redshifts, and therefore there is a tension between large and small scales observations. Since the problem is still under debate, we choose to consider the Planck experiment H_0, knowing that this choice might be considered incorrect in the future.

where Φ is computed from the trace of $g_{ij}^{(1)}$ and s_{ij} is the traceless part of $g_{ij}^{(1)}$, defined as

$$\Phi = -\frac{1}{6}\delta^{ij} g_{ij}^{(1)} \,, \tag{1.45}$$

$$s_{ij} = \frac{1}{2}\left(g_{ij}^{(1)} - \frac{1}{3}\delta^{kl} g_{kl}^{(1)} \delta_{ij} \right) \,. \tag{1.46}$$

Since we are at linear order, we can not admit terms like Ψ^2 in our expansion, nor crossed terms such as $\Phi\Psi$ in the associated equations of motion. We consider the (spatially flat) FLRW metric (1.15) for the background. The full perturbed metric $g_{\mu\nu}$ becomes

$$ds^2 = -(1+2\Psi)dt^2 + \omega_i a \left(dx^i dt + dt dx^i \right) + a^2 \left[(1+2\Phi)\,\delta_{ij} + 2 s_{ij} \right] dx^i dx^j \,. \tag{1.47}$$

It can be shown that the only propagating degrees of freedom, which is the number of dynamical quantities whose evolution defines the system's physical state, comes from s_{ij}, since Φ, Ψ and ω_i can be obtained from Einstein equations of the metric (1.47) that do not contain time derivatives [14].

We can further split the contributions from ω_i and s_{ij}. The first can be rewritten as

$$\omega^i = \omega^i_{\shortparallel} + \omega^i_{\perp} \,, \tag{1.48}$$

where the first term is the longitudinal part, which is curl-free; the second term is the transverse part of ω_i, which is divergence-less. In other words

$$\epsilon^{ijk}\partial_j \omega_{\shortparallel k} = 0 \qquad \text{and} \qquad \partial_i {\omega_\perp}^i = 0 \,, \tag{1.49}$$

where ϵ^{ijk} is the Levi-Civita tensor. Thus we can recast these terms respectively as

$$\omega_{\shortparallel i} = \partial_j \lambda \qquad \text{and} \qquad {\omega_\perp}^i = \epsilon^{ijk}\partial_j \xi_k \,. \tag{1.50}$$

From this form, we can clearly understand the decomposition of the ω^i, which is made of one scalar part (λ is a scalar degree of freedom) and a vector part (ξ^i is a vector degree of freedom). The scalar field λ represents one degree of freedom, while the vector field ξ^i contributes with two ($3-1$ due to the gauge freedom in the choice of ξ^i). The same procedure can be applied to the s_{ij} spatial tensor, separating the contributions as

$$s^{ij} = {s_{\shortparallel}}^{ij} + {s_S}^{ij} + {s_\perp}^{ij} \,. \tag{1.51}$$

Also in this case we have a longitudinal term ${s_{\shortparallel}}^{ij}$, whose divergence is longitudinal (curl-free), and a transverse term ${s_\perp}^{ij}$; moreover we add a solenoidal term ${s_S}^{ij}$, whose divergence is a transverse (divergence-less) vector. These properties can be written as

$$\epsilon^{jkl}\partial_j \partial_i {s_{\shortparallel}}^i{}_j = 0 \,, \qquad \partial_i \partial_j {s_S}^{ij} = 0 \qquad \text{and} \qquad \partial_i {s_\perp}^{ij} = 0 \,. \tag{1.52}$$

Therefore we can introduce again some additional fields to make more clear the nature of the degrees of freedom of s_{ij}

$$s_{\shortparallel ij} = \frac{1}{2}\left(\partial_i \partial_j - \frac{1}{3}\delta_{ij}\nabla^2 \right)\theta \qquad \text{and} \qquad s_{S\,ij} = \partial_{(i}\zeta_{j)} \,, \tag{1.53}$$

while the transverse part ${s_\perp}^{ij}$ can not be decomposed into vector or scalar fields. The longitudinal and solenoidal part contributes respectively with one scalar degree of freedom and two vector degrees of freedom; while the transverse part contributes with two tensor degrees of freedom (5 components of the traceless symmetric tensor ${s_\perp}^{ij}$ minus 3 from the condition $\partial_i {s_\perp}^{ij} = 0$).

Therefore this decomposition separates the contribution into 3 different *sectors*: scalar, vector, and tensor. The scalar part is given by Φ, Ψ, θ, and λ; the vector part by ξ_i and ζ_i; and the tensor part by $s_{\shortparallel ij}$ ¶. Therefore, we obtain a total of 10 degrees of freedom. However, it can be proven that, due to the gauge freedom (diffeomorphic invariance), each of these sectors actually contributes with only 2 physical degrees of freedom [15]. In other words, the gauge freedom allows to set to zero two out of four scalar fields Φ, Ψ, θ, and λ, and two components from the vector fields ξ_i and ζ_i.

Another advantage is that, at least at linear order, the three sectors can be studied independently, i.e., the equations of motion of the scalar sector do not depend on the vector and tensor perturbations, and similarly for the vector and tensor sectors. This is the so-called *decomposition theorem.*

In the following, we show some of the common gauge choices in cosmology. We neglect the vector perturbations as they are in general not interesting in cosmology since they decay rapidly.

1.4.1 Scalar perturbations

Consider only the scalar perturbations. The most general way of writing all the scalar contributions is

$$ds^2 = -(1+2\Psi)dt^2 + 2\partial_j\lambda\, a\, dx^j dt + a^2\left[(1+2\Phi)\,\delta_{ij} + \left(\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2\right)\theta\right] dx^i dx^j\,. \tag{1.54}$$

A possible gauge choice is the *Newtonian gauge*. It consists in considering $\lambda = \theta = 0$, obtaining

$$ds^2 = -\left[1+2\Psi(t,\vec{x})\right]dt^2 + a^2(t)\left[1+2\Phi(t,\vec{x})\right]\delta_{ij}dx^i dx^j\,. \tag{1.55}$$

Another possible choice is to consider $\Psi = \lambda = 0$, obtaining the *synchronous gauge* metric

$$ds^2 = -dt^2 + a^2(t)\left(\delta_{ij} + b_{ij}\right)dx^i dx^j\,, \tag{1.56}$$

where b_{ij} contains the contribution from Φ and θ.

1.4.2 Tensor perturbations

The tensor perturbations are encoded in the spatial tensor ${s_\perp}^{ij} = E^{ij}$. Since this tensor carries two degrees of freedom, we can rewrite the general tensor perturbation metric

$$ds^2 = -dt^2 + a^2(t)\left(\delta_{ij} + E_{ij}\right)dx^i dx^j\,, \tag{1.57}$$

where recall that $E_{ii} = 0$ and $\partial_i E^{ij} = 0$, as

$$ds^2 = -dt^2 + a(t)^2(1+E_+)dx^2 + 2a(t)^2\,E_\times dxdy + a(t)^2(1-E_+)dy^2 + a(t)^2dz^2\,. \tag{1.58}$$

This gauge choice is called TT-gauge, and it represents gravity waves travelling in the z direction [16]. The $E_+ = E_+(t,z)$ and $E_\times = E_\times(t,z)$ components are the $+$ and $\times$ polarizations of the gravity waves, i.e.,

$$E_{ij}(t,z) = \begin{pmatrix} E_+(t,z) & E_\times(t,z) & 0 \\ E_\times(t,z) & -E_+(t,z) & 0 \\ 0 & 0 & 0 \end{pmatrix}\,. \tag{1.59}$$

¶ This spatial tensor is usually denoted as h_{ij}, but in the following it will be denoted as E_{ij} to avoid definition ambiguities with the ADM induced metric h_{ij} which will be defined in Chapter 3.

Chapter 2

A brief history of the Universe

In this Chapter, we briefly describe the principal epochs of the history of the Universe. We present an overview of the events shown in Figure 2.1. The last dark energy domination era is the present epoch, which began only recently, at about $a \cong 0.7$ (or approximately three billion years ago).

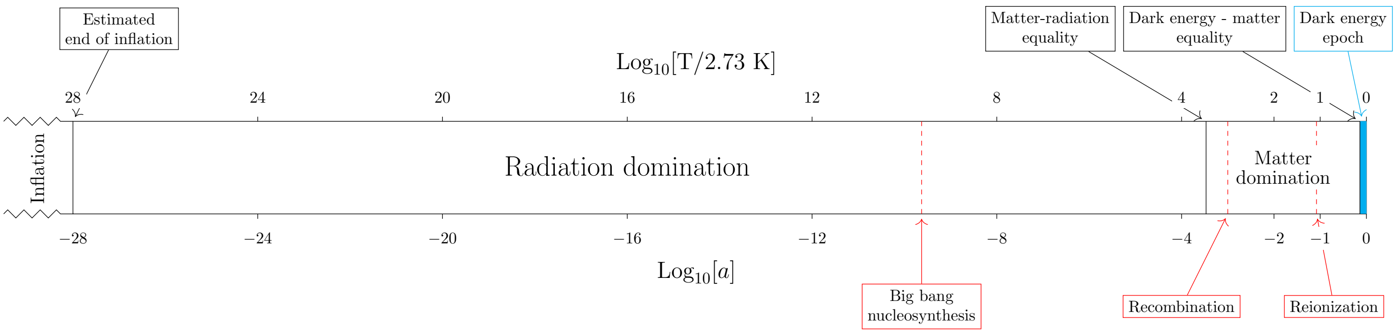


Figure 2.1: Timeline of the history of the Universe. The red lines are specific point in time defined by the Planck experiment results [5]. The black lines represent components equality instants, and are computed with `CLASS` in a ΛCDM model with Planck experiment results.

2.1 Inflation epoch

The first epoch in Figure 2.1 is called *inflation*, which stopped at about $a = 10^{-28}$ (or roughly 10^{-32} s after the Big Bang). The inflation mechanism has not been experimentally proven yet. However, inflation is widely accepted as the solution to a serious problem about the causality contact of photons and provides viable initial conditions for the evolution of fluctuations of the cosmic components.

Qualitatively, inflation provides a solution for the large angular distance isotropy problem of the photon distribution. We observe that all photons coming from the last scattering surface (when the photons started to freely move in the Universe without interacting with other matter, see Recombination section below) have the same temperature. If the Universe expanded from a radiation-dominated epoch, the distance between most of the observed photons when they were last scattered would have been larger than their comoving horizon at that time. This means that they were never in causal contact before the observation but still have the same temperature when observed today. A picture of this problem is shown in Figure 2.2.

The inflation accounts for this problem postulating a comoving Hubble radius $1/Ha$ larger than today and a comoving horizon $\int(1/aH)da/a$ such that distant photons were in causal contact before a vast accelerated expansion in a very early period (much earlier than the matter-radiation equality). Therefore during this expansion, the comoving Hubble radius decreased (while the comoving horizon increased), destroying the pre-existent causal contact between the photons. This explains why we see photons with the same temperature: they were in causal contact at very early times. Moreover, this justifies the definition of η as an integral starting from t_e instead of $t = 0$: η was prominent at the end of inflation (due to its large value before the accelerated expansion), and its value would be useless without this shift.

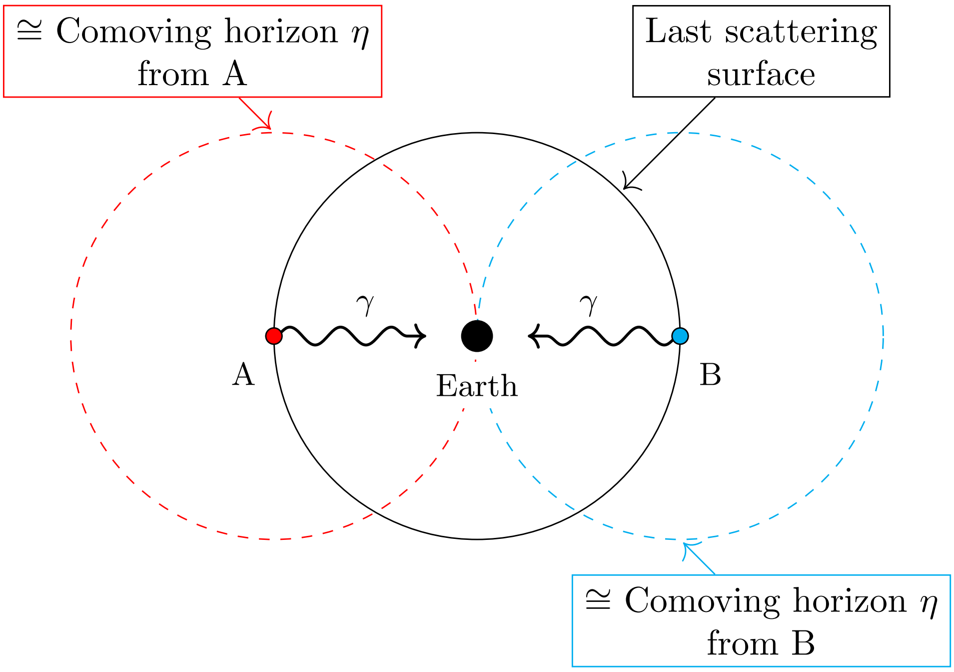


Figure 2.2: Picture of the large angular distance isotropy problem of the photon distribution. Two photons coming from opposite parts of the Universe A and B have comoving horizons (dashed circles) that do not overlap. Therefore, when they arrive on the Earth, they have never been in causal contact. Still, they have the same observed temperature. Note that dashed line is not the comoving horizon from the point of view of A and B, but the horizon (1.36) starting at $t \cong t_{rec}$ instead of $t = t_e$, and then all circles have the same radius.

Quantitatively, in order to have a decreasing comoving Hubble radius $1/aH$ we need to satisfy the following condition

$$\frac{d}{dt}[aH] = \frac{d}{dt}\left[a\frac{da}{dt}\frac{1}{a}\right] = \frac{d^2a}{dt^2} > 0\,, \tag{2.1}$$

that is also the condition for an accelerated expansion (positive acceleration of a).

As a very rough model, we can assume the Universe's expansion after the inflation as only radiation dominated. In this case, from the Friedman equation (1.33), the Hubble radius is proportional to a^{-2}, and therefore

$$\frac{a_0 H_0}{a_e H_e} \cong \frac{a_e}{a_0} = a_e\,, \tag{2.2}$$

where the subscript e refers to the end of inflation. From the timeline 2.1, we see that the end of inflation is estimated to happen at $a_e \cong 10^{-28}$ (or $T \cong 10^{28}$ K $\cong 10^{15}$ GeV). From equation (2.2) we can estimate the Hubble radius to be at least (remember the radiation domination after the inflation assumption) 10^{28} larger now than it was at the end of inflation. Thus to have a larger Hubble radius before inflation and then a causal contact for objects that are not in contact today, the Hubble radius decreased by at least a factor of 10^{28} during inflation.

One of the most common model for inflation considers a constant Hubble parameter H. Then, using the definition $(da/dt)/a = H$ we can write a simple time dependence for the scale factor

$$a(t) = a_e e^{H(t-t_e)} . \tag{2.3}$$

The question still open is: what is the matter source that makes this accelerated expansion of the Universe possible? We will see in section 2.4 that to have an acceleration (and then a decreasing Hubble radius), we need a matter species with an equation of state parameter $\omega < -1/3$, or the addition of a new scalar field ϕ (Modified Gravity Theories). Another way is to use a component with a constant energy density ($\omega = -1$), e.g., the already seen cosmological constant Λ, which gives precisely the scale factor's time dependence in equation (2.3).

2.2 Radiation epoch

The next period in the timeline 2.1 is an epoch of radiation (photons and relativistic neutrinos) domination in the history of the Universe. The radiation energy density ρ_r value is larger than matter and dark energy densities in this period. During this epoch, photons are highly coupled with the electrons due to the Compton scattering, and they constitute with good approximation a unique fluid. In other words, photons and electrons are in thermodynamic equilibrium.

During this epoch, the *Big Bang Nucleosynthesis* takes place at $a \cong 10^{-10}$ (or photon temperature $T \cong 1$ MeV, or $\cong 10$ s after the Big Bang). Before this event, nuclei were not produced since highly energetic photons (before nucleosynthesis $T \gtrsim 1$ MeV) would have destroyed them; also, neutrons and protons had the same abundance ensured by weak interactions like $p+e^- \to n+\nu_e$ (photons and neutrinos in this period have approximately the same temperature). As the Universe cooled down near $T = 1$ MeV, the Universe expanded, and the weak interaction was not efficient anymore, leading to the conversion of neutrons into protons. Moreover, photons lost energy due to the Universe's expansion, allowing the creation of stable nuclei. Initially, protons and neutrons made a fusion reaction into deuterium and ^{4}He. No heavier nuclei are produced in this epoch since the capture of a neutron or a proton in a helium-4 nucleus would have formed nuclei with $A = 5$, which are not stable. Moreover, deuterium and ^{4}He nuclei were insufficient to make fusion reactions between them possible. This fixed the abundance of helium to roughly a *mass factor* of

$$Y_{^4\text{He}} = \frac{4n_{^4\text{He}}}{n_b} \cong 0.22 \, , \tag{2.4}$$

where $n_{^4\text{He}}$ and n_b are respectively the number densities of Helium-4 nuclei and baryons (protons and neutrons), and the factor 4 comes from the fact that Helium-4 is 4 times massive than a proton/neutron. The other fractional density is made of protons and a tiny part of deuterium, helium-3 and lithium-7. Since further nucleosynthesis of heavier nuclei stopped until atoms (not nuclei) clustered together to form stars, $Y_{^4\text{He}}$ is roughly the same since the end of Big Bang nucleosynthesis. Therefore, since $Y_{^4\text{He}}$ is computed only with initial conditions set by the Big Bang, the accordance between this value with the experiments is valuable proof of the Big Bang existence.

Finally, the radiation epoch ended at $a = a_{eq}^{\Lambda} \cong 3 \times 10^{-4}$ (or $T \cong 10000K$, or about 50000 years after Big Bang). This moment has an important role in setting the matter energy density fluctuation from today's homogeneity. More generally, equating the matter and the radiation densities we find

$$a_{eq} = \frac{4.15 \times 10^{-5}}{\Omega_m h^2} \, . \tag{2.5}$$

2.3 Matter epoch

After the radiation domination era, the Universe entered an epoch of matter domination. During this period, two important events happened: recombination and reionization.

During the *recombination* at $a \cong 10^{-3} \equiv a_*$ (or $T \cong 3000K$, or about 400k years after the Big Bang), analogously to nucleosynthesis for nuclei, the temperature was low enough to make the creation of stable atom possible. We define the free electron fraction as

$$X_e = \frac{n_e}{n_e + n_H}, \tag{2.6}$$

where n_H and n_e are the hydrogen atom and electron number density. In Figure 2.3 we show the free electron fraction near recombination.

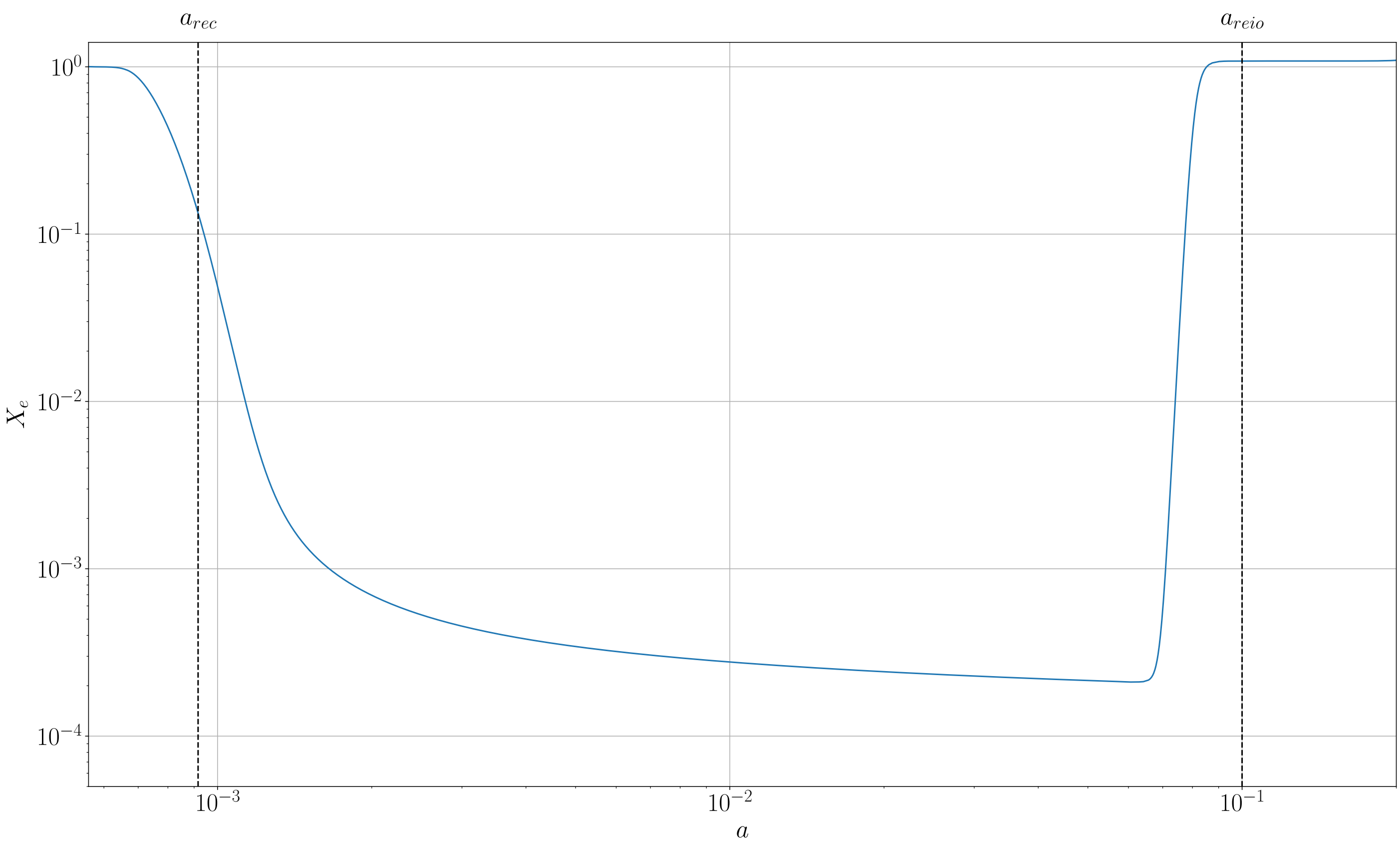


Figure 2.3: Plot of the free electron fraction X_e as a function of the scale factor a. The recombination point and the function is computed with `CLASS` with the standard ΛCDM parameters.

The electron fraction goes to zero after recombination, leading to the decoupling of the photons from the electron-photon fluid we had in the radiation epoch. The small fraction of electrons nuclei that have not been captured to form atoms is not enough to keep the electron-photon fluid at equilibrium. Therefore the photons decouple from electrons and can freely move without Compton scattering with electrons. This is why the recombination is usually considered coincident with the last scattering of the photons.* The sphere in the spacetime with radius given by η_* (recombination proper time) is called *last scattering surface* and is the surface from where the photons are freely travelling to our observation equipment. Due to the coupling with electrons, we can only receive photons from the scattering surface, and therefore before decoupling, the Universe was *opaque*. The spectrum of the photons coming to us is called *Cosmic Microwave Background* (CMB) and has the same form of a spectrum of black body radiation at $T = 2.73$ K. All the photons have approximately the same temperature regardless of the direction they are coming from. In Figure 2.4 we present the Planck analytical black body radiation spectrum and the data from the COBE experiment [17]. The analytical spectrum has been obtained

* But, although tightly connected, the two effects (recombination and decoupling of photons) are two different physical processes.

with the Planck formula using $T = 2.7255$ K. We also see the peak of the spectrum from which the CMB takes its name, which is at $\cong 200$ GHz, a microwave frequency.

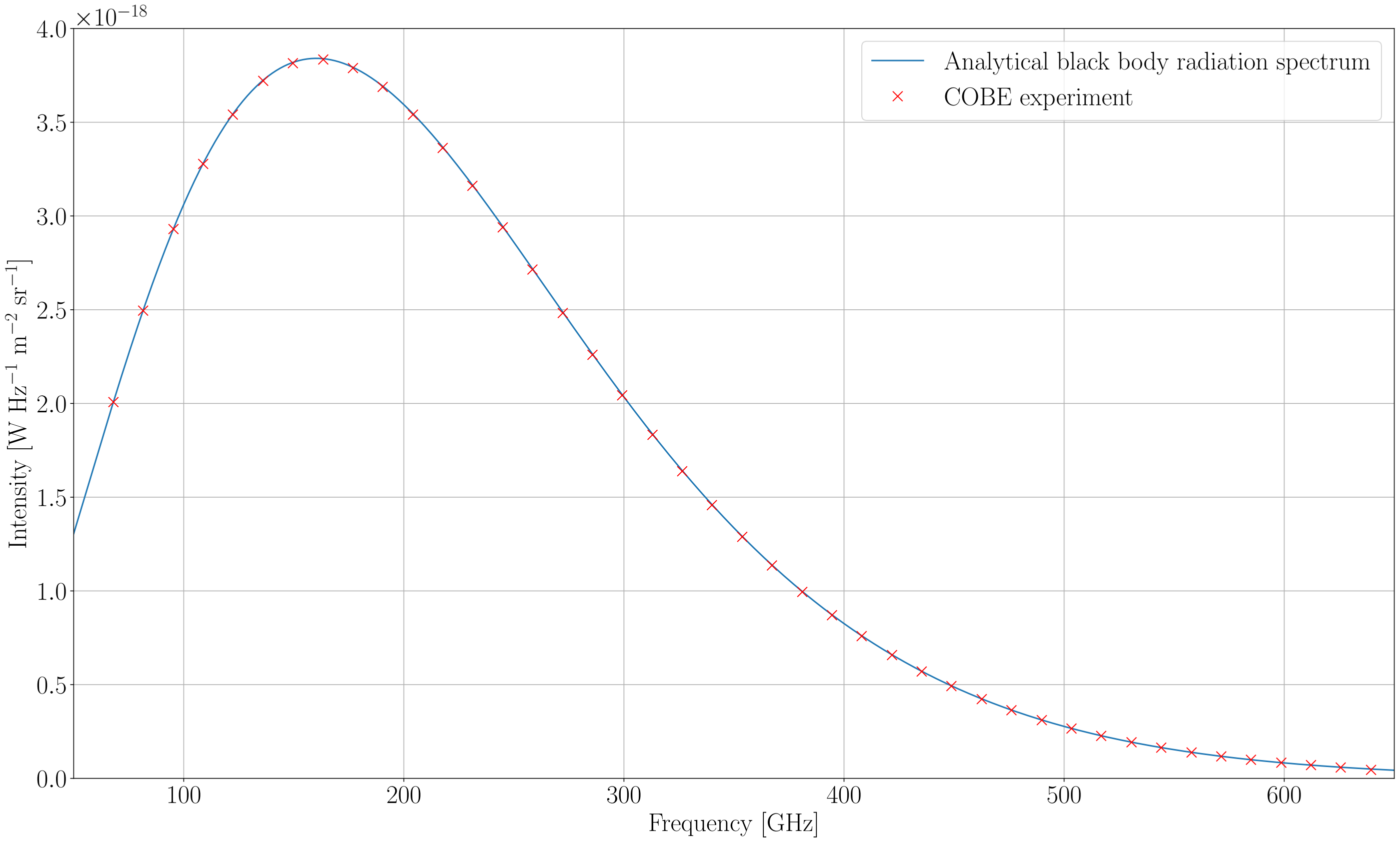


Figure 2.4: Plot of the Cosmic Microwave Background spectrum with respect to the frequency in the SI measure system. The error bars are so small (10^{-3} smaller in the scale of this plot) that cannot be seen. Data are taken from the public archive of the COBE experiment [17].

From Figure 2.3 we note that the free electron fraction X_e becomes non-negligible again, in an event called *reionization* (at $a \cong 0.1$, or $T \cong 30K$, or half a billion years after the Big Bang).

Finally, the matter domination period ended at $a \cong 0.8$ (or four billion years ago), followed by the dark energy epoch.

2.3.1 Dark Matter

During this epoch of matter domination, two main species with zero pressure ($\omega = 0$) are contributing. One is the standard matter composed of baryons, nuclei, atoms, ... The other is dark matter. This is a matter species that has been introduced in the standard model of cosmology to explain some observational phenomena that cannot be modelled with ordinary matter. Usually, this dark matter is considered *cold*, i.e., the velocity of dark matter is considered much smaller than $c = 1$. The standard model of cosmology considering Cold Dark Matter is called the CDM model.

The first evidence of the existence of dark matter came from the rotational curves of the galaxies [1], but there are now more reasons to believe that there must be non-standard matter, for instance, in the context of gravitational lensing [18] or galaxy clustering [19].

2.4 Dark energy epoch

A Universe composed only of matter and radiation would be very different from the one we observe, starting from the experimental evidence of the *accelerated* expansion of the Universe (the first experiments are [3, 4]). A way to explain this phenomenon is to add a new component, called *dark energy*, which must have particular properties to model this acceleration. Consider the condition for an accelerated expansion of the Universe

$$\frac{d^2a}{dt^2} > 0. \tag{2.7}$$

We can translate this condition into a condition on the pressure. Using the second Friedmann equation in (1.16), with ρ containing the cosmological constant as in equation (1.23), we find

$$\frac{dH}{dt} + H^2 = \frac{d^2a}{dt^2} = -\frac{4\pi G}{3}\left(\rho + 3P\right) , \tag{2.8}$$

from which we have

$$P < -\frac{\rho}{3} \qquad \text{i.e.} \qquad \omega < -\frac{1}{3}. \tag{2.9}$$

Thus an accelerated expansion needs a fluid with negative pressure and the state parameter smaller than $-1/3$. Standard matter and radiation cannot fulfil this requirement.

2.4.1 Constant dark energy density

The most immediate first candidate would be something with constant density or, equivalently, an object with an equation of state parameter $\omega = -1$. We already saw a component with constant energy density, that is, the one having $\rho = \rho_\Lambda$ coming from the cosmological constant Λ, and appearing the Friedmann equation (1.33). When the accelerated expansion of the Universe was first observed, considering the dark energy as a component with constant energy density given by the cosmological constant ($\rho_{de} = \rho_\Lambda$) was the first attempt at an explanation of the phenomenon.

In cosmology, ΛCDM is a model defined to have the dark energy coming only from the cosmological constant, i.e. $\rho_{de} = \rho_\Lambda$ is constant ($\omega_{de} = -1$). Contrarily, the model with no dark energy ($\rho_{de} = 0$) is called sCDM (standard CDM). In Figure 2.5 we present the evolution of the fractional densities with the sCDM and the ΛCDM models.

Moreover, there are some models where dark energy has a non-constant state parameter $\omega_{de}(t)$: this means that in these models $\rho_{de}(t)$ does not have a fixed dependence on $a(t)$, but the exponent of $1/a(t)$ in equation (1.20) changes in time.

One of the most compelling evidence of the existence of the dark energy is the discrepancy between the age of some of the oldest star we can see from Earth and the age of the Universe calculated without dark energy. We can see this from the Friedmann equation (1.33). In the following derivation we consider dark energy as a component with constant energy density coming from Λ. Rewriting this equation we obtain

$$\frac{1}{H_0}\frac{da}{dt} = a(t)\left[\frac{\Omega_m^0}{a(t)^3} + \frac{\Omega_r^0}{a(t)^4} + \Omega_\Lambda^0 + \frac{\Omega_k^0}{a(t)^2}\right]^{1/2} , \tag{2.10}$$

and then we find the equation for the age of the Universe

$$t_0 = \frac{1}{H_0}\int_0^1 da \frac{1}{a\left[\frac{\Omega_m^0}{a^3} + \frac{\Omega_r^0}{a^4} + \Omega_\Lambda^0 + \frac{\Omega_k^0}{a^2}\right]^{1/2}} . \tag{2.11}$$

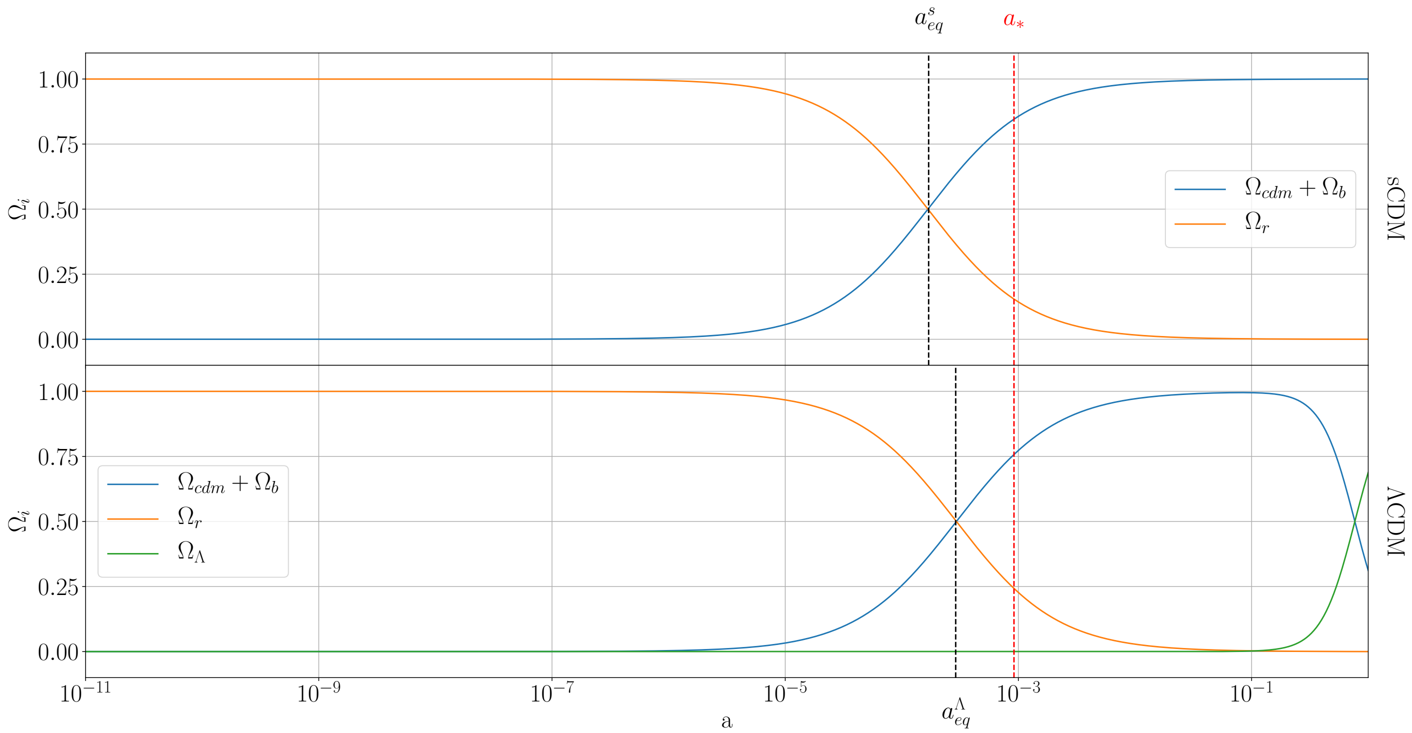


Figure 2.5: Plot of the fractional densities $\Omega(t)$ evolution. The sCMD lines have been computed using $\Omega_{de}(t_0) = 0$ and $\Omega_m(t_0) = 1$, while ΛCDM have the standard parameters. The recombination scale factor a_* is not the same in the two models, but in the scale of the plot the difference is barely visible. Note the different radiation-matter equality point a_{eq}, closer to a_* in the ΛCDM case.

To make this evaluation we consider the contribution from radiation negligible and a flat Universe with $\Omega_m^0 + \Omega_\Lambda^0 = 1$, obtaining the analytical solution

$$t_0 = \frac{1}{H_0} \frac{\log\left[\frac{2+2\sqrt{1-\Omega_m^0}-\Omega_m^0}{\Omega_m^0}\right]}{3\sqrt{1-\Omega_m^0}} \qquad (\Omega_m^0 + \Omega_\Lambda^0 = 1 \text{ and } \Omega_k^0 = \Omega_r^0 = 0)\,. \tag{2.12}$$

The plot of this function is in the Figure 2.6 (blue line).

In a matter dominated Universe today ($\Omega_m^0 \to 1$) we have

$$t_0 = \frac{2}{3}\frac{1}{H_0}. \tag{2.13}$$

Inserting an experimental value of H_0 we would find 8 Gyr $< t_0 <$ 10 Gyr, while observations of old stars requires an age larger than 12 Gyr. From Figure 2.6 (blue line), we see that increasing the dark energy fractional density (decreasing the matter fractional density) the age of the Universe increases: therefore, dark energy can be the solution for the age of the Universe problem. In fact, if we consider $\Omega_m^0 = 0.3$ (and then $\Omega_\Lambda^0 = 0.7$), we obtain from (2.12) $t_0 = 13.4$ Gyr, a value closer to experiment results.

Also, from the plot in Figure 2.6 (orange line) we see that if we try to solve the problem considering only curvature density ($\Omega_\Lambda^0 = 0$ and $\Omega_m^0 + \Omega_k^0 = 1$), we obtain $1/H_0$ as the maximum estimation of t_0. Nevertheless, this estimation of the Universe's age is smaller than experimental values, removing the possibility of considering non-negligible spacial curvature as the solution for the problem.

As a reference, we also show the result of Planck 2018 experiment [5]

$$t_0 = 13.796 \pm 0.020 \text{ Gyr} \qquad \text{(age of the Universe from Planck 2018 experiment)}, \tag{2.14}$$

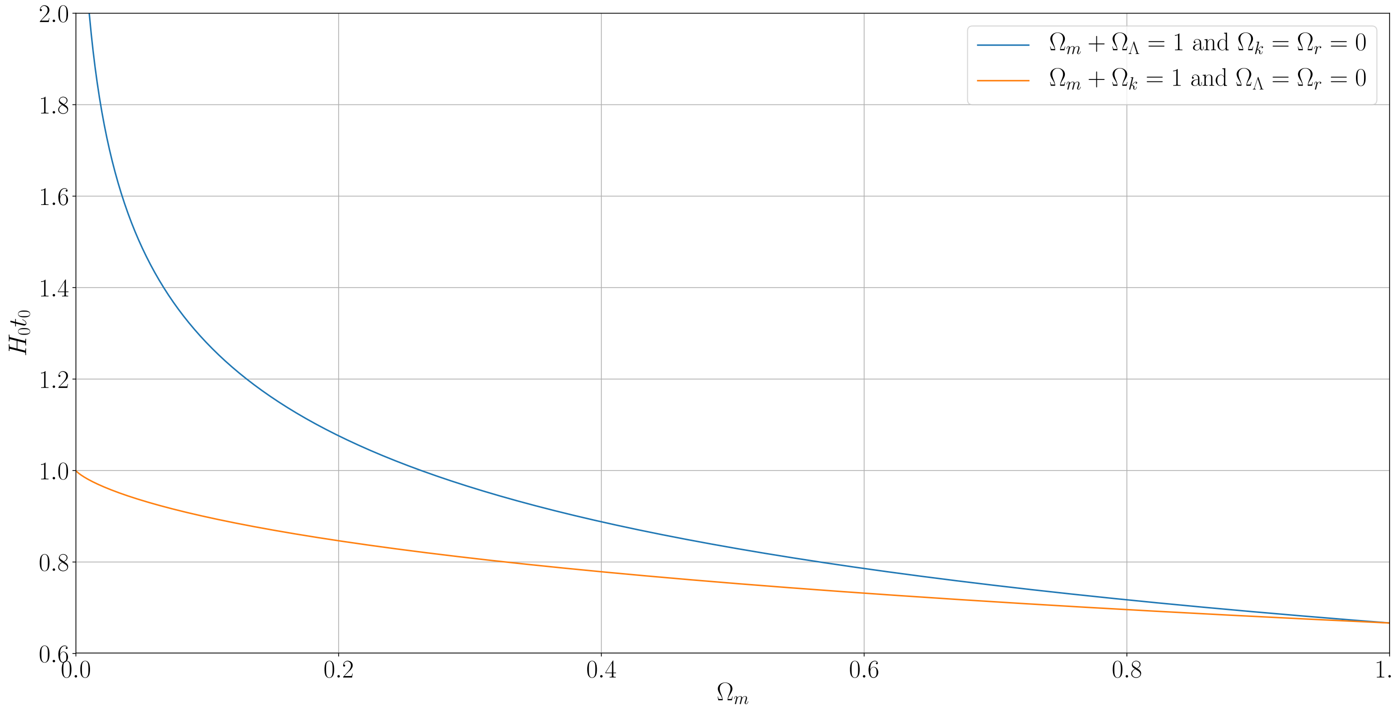


Figure 2.6: Plot of $t_0 H_0$. The blue line is the plot of equation (2.12) as a function of the fractional matter density. The orange line is the solution of the integral (2.11) without dark energy and considering the curvature.

which we will refer to as the **age of the Universe**.

Note that this value is not the **radius of the observable Universe** since an object that was 13.8 Gyr distant when it emitted a photon reaching us today is now much further away due to the Universe expansion. To find the observable Universe radius today we can start from the fact that $g_{\mu\nu} dx^\mu dx^\nu = 0$ for a photon. Thus $dt^2 = a^2 dx^2$, and then $dx = dt/a$. The comoving distance is defined as

$$\chi(t) \equiv \int_{t_i}^{t} \frac{dt'}{a(t')} = \int_{a_i}^{a} \frac{da'}{a} \frac{1}{a' H(a')} , \tag{2.15}$$

where t_i is the time of the emission of the photon. Note the additional a in the denominator with respect to the age of the Universe integral (2.11). The result is the physical observable Universe radius

$$\chi(t_0) \cong 45 \text{ billion light-years} \qquad \text{(observable Universe radius)} , \tag{2.16}$$

where we have used the fact that the comoving and the proper distance are the same at $t = t_0$, because $a(t_0) = 1$.† This quantity is also useful to make a very rough estimation of the ordinary matter in the observable Universe. Considering the critical density ρ_{cr} defined in equation (1.28) and using the volume of a sphere with the observable Universe radius $\chi(t_0)$ as radius we find

$$m_{ou} \cong 10^{54} \text{Kg} \qquad \text{(mass of ordinary matter in the observable Universe)} . \tag{2.17}$$

2.4.2 Non-constant dark energy density

Recent measurements of the CMB temperature and polarization anisotropies and their cross-correlations, in combination with geometrical measurements from Baryon Acoustic Oscillations and Supernovae Type-Ia luminosity distance measurements, suggest that the equation of state of dark energy is extremely close

† Incidentally, the fact that comoving and proper distances are the same at $t = t_0$ if $a_0 = 1$, is also the reason why a is conventionally fixed today at $a_0 = 1$.

to the cosmological constant value $\omega = -1$. But slight deviations from -1 are still allowed by data [5]. In particular, the 68% confidence level allowed region for the dark energy equation of state is given by [5]

$$-1.0051 < \omega_{\rm DE} < -0.961\,, \tag{2.18}$$

The $\omega < -1$ regime is called *phantom-like*, while $\omega > 1$ is called *quintessence-like*. In both regimes, the dark energy does not have a constant in time energy density. In the thesis, we will use these observational values to constraint some extensions of General Relativity.

2.5 Conclusion

In this section, we presented a brief history of the Universe, from which we can define the standard model of cosmology, called ΛCDM. Its definition is given in section 2.4, and can be summarised as follows:

- the dark matter is considered to be cold, i.e., only the over-density and the velocity are considered in the perturbation theory of this component;
- dark energy has a constant energy density and therefore the state parameter (1.19) is $\omega = -1$. This constant energy density comes from the cosmological constant Λ. Thus the dark energy density in this model is defined as $\rho_{de} \equiv \rho_\Lambda$, where ρ_Λ is defined in equation (1.23).

All parameters have been taken from the Planck 2018 experiment [5].

Chapter 3

Arnowitt–Deser–Misner formulation of General Relativity

In this Chapter, we present the main features of the Arnowitt–Deser–Misner (ADM) formulation of General Relativity, also called the Hamiltonian formulation of General Relativity. We derive the main equations of motions of General Relativity in this formulation, carefully showing some theoretical and technical passages that are usually neglected in the literature. This formulation will be one of the main tools to build the Effective Field Theory of Gravity, which will be introduced in Chapter 8. The discussion is based on the summary article [20] and the book [21], integrating it with additional explanations and examples.

3.1 Motivation

In General Relativity we consider the Einstein equations (1.6) (where we drop the cosmological constant contribution)

$$G_{\mu\nu} = 8\pi G T_{\mu\nu}\,, \tag{3.1}$$

which treat the metric tensor $g_{\mu\nu}$ as a unique object, ensuring that covariance is preserved. On the other hand, evaluating each of the Einstein equations we find that

- the time derivatives of the metric components g_{00} and g_{0i} do not appear in the Einstein equations due to the Riemann tensor symmetries;
- there are no second order time derivatives in the 00 (time-time) and $0i$ (time-space) equations;
- second order time derivatives of g_{ij} only appear in the ij (space-space) equations.

From these observations, it is clear that the dynamic is encoded only in g_{ij}. The ADM formulation provides a way to focus on these metric components with a receipt to split the time and space part of Einstein equations preserving covariance.

3.2 Geometrical tools

Before introducing the ADM formulation, we briefly revisit some geometric definitions and propositions used in this Chapter.

3.2.1 Congruence of curves

A congruence of curves through a region of spacetime (M, g) (M is a n-dimensional manifold and g the metric) is a collection of curves such that every point in the region lies on exactly one of the curves.

Every congruence naturally introduces an associated coordinate system (λ, y^i) $(i = 1, \dots, n-1)$ on the region, where λ is the parameter such that the vector $\partial_\lambda = t$ is tangent to the curve of the congruence at the point (λ, y^i). In other words, the coordinates y^i label the curves, and λ is the parameter along the curves.

We can also introduce the vector $\eta_i = \partial_{y^i}$, which are called *connecting vectors*.

3.2.2 Hypersurfaces

Beyond the splitting of time and space, there is the concept of hypersurfaces, which are defined as $n-1$ dimensions manifolds embedded in a $n-$dimensional ambient manifold, locally defined with a single implicit function $S(x^\mu)$. To characterize these hypersurfaces, we can introduce some entities.

Let $S(x^\mu)$ be a smooth function of spacetime coordinates x^μ, and consider a family of hypersurfaces $S(x^\mu) = \text{constant}$. We define the normal vector to $S(x^\mu)$ as

$$n^\mu = f(x^\mu) g^{\mu\nu} \partial_\nu S(x^\mu)\,, \tag{3.2}$$

where $f(x^\mu)$ is an arbitrary normalization function. The hypersurface is space-like if the normal vector is time-like everywhere on it, and vice-versa. Therefore if the hypersurface is space-like we can always find a normalization function $f(x^\mu)$ such that $n_\mu n^\mu = -1$ (or $n_\mu n^\mu = 1$ for time-like hypersurfaces). Moreover, when $n_\mu n^\mu = 0$ we have a null hypersurface.

3.2.3 Induced metric on a hypersurface

On any hypersurface Σ, embedded in the spacetime (M, g), we can define an induced metric as

$$h_{\mu\nu} = g_{\mu\nu} \pm n_\mu n_\nu\,, \tag{3.3}$$

where the $+$ is considered for space-like hypersurfaces, and the $-$ for time-like ones.

The induced metric h is a restriction of the embedding manifold metric g. In fact, while h is degenerate on the full tangent space at any point $p \in \Sigma$, it is positive definite for space-like Σ on the sub-space of the tangent space spanned by vectors tangent to curves in Σ, i.e. vectors v which satisfy $v_\mu n^\mu = 0$.

As an example we can consider a family of hypersurfaces given by $S(x^\mu) = \text{constant}$ in $3+1$ Minkowski space with coordinates $(t, \vec{x})$. Using the definition of the normal vector (3.2) we can compute $n^\mu = (1, 0, 0, 0)$, and the induced metric will be

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu = \text{diag}(-1, 1, 1, 1) + \text{diag}(1, 0, 0, 0) = \text{diag}(0, 1, 1, 1)\,. \tag{3.4}$$

Therefore the induced metric is positive definite on the 3-dimensional flat Euclidean space.

3.3 Time-space coordinates

This section introduces the coordinates we will use to rewrite the Einstein equation in the $3+1$ form. We start considering a scalar field $S(x^\mu) = t(x^\mu)$ such that we can define a family of non-intersecting space-like hypersurfaces $\Sigma(t)$ with $t = \text{constant}$. With this choice, we are considering a family of space-like hypersurfaces. In the following, we introduce the appropriate coordinates, build the induced metric and the induced covariant derivative.

Note that the introduction of a specific time coordinate for the foliation does not impair the general covariance of the theory under arbitrary coordinate transformations. The classic mechanics Hamiltonian case can be written in a parametrized form where time and energy can be seen as a conjugate pair coordinates of a new degree of freedom. Similarly we can think about foliated General Relativity as an "already-parametrized" theory, which is invariant under an arbitrary change of coordinates as the mechanics theory is invariant under an arbitrary re-parametrisation [20].

3.3.1 Induced coordinates and metric

We build the coordinates as follows. On each $\Sigma(t)$, we introduce the spatial coordinates y^i, and we connect different hypersurfaces with a congruence of curves that intersect these surfaces, using $\lambda = t$ as the parameter along the curves. Therefore, we are defining a mapping of events on different hypersurfaces, where y^i are spatial events intersected by the same curve. See Figure 3.1 for a pictorial representation of these coordinates.

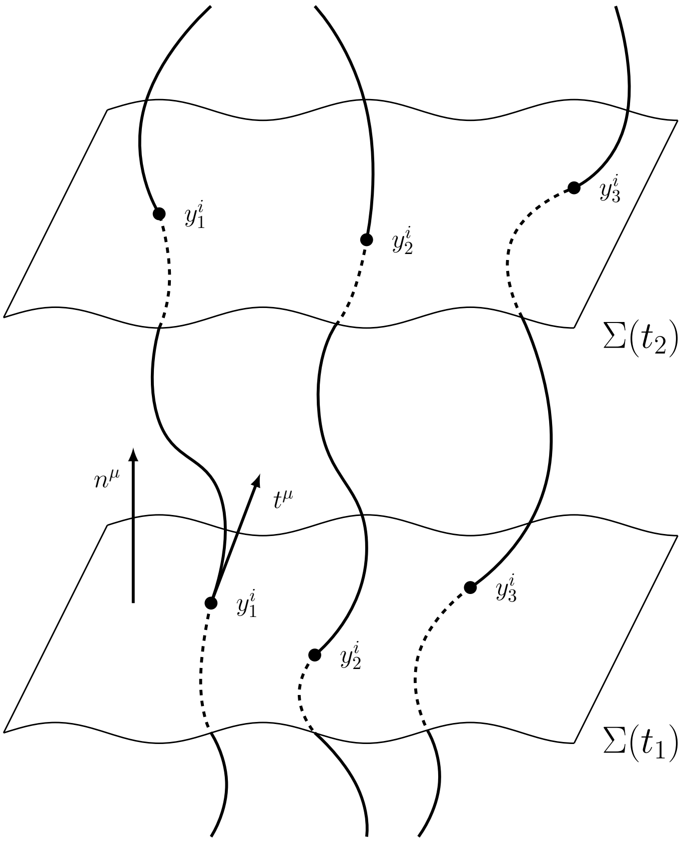


Figure 3.1: Representation of the hypersurfaces and the congruence of curves in the ADM formulation. The same coordinates y^i represent events intersected by the same curve.

Given the (t, y^i) coordinate system, we can define the following vectors:

- the normal to the hypersurfaces
$$n_\mu = -N\partial_\mu t\,, \tag{3.5}$$
where we used the definition (3.2). The N normalization factor is called *lapse* and it is set to obtain $n_\mu n^\mu = -1$. In particular, $n_0 = -N$ and $n_i = 0$;

- the *projection tetrad* to $\Sigma(t)$
$$e^\mu_i = \frac{\partial x^\mu}{\partial y^i}\,, \tag{3.6}$$

which are tangent to normal vectors, i.e. $n_\mu e_i^\mu = 0$;

- tangent vector to the curves
$$t^\mu = \frac{\partial x^\mu}{\partial t}\,, \tag{3.7}$$
which satisfies $t^\mu \partial_\mu t = 1$. We can decompose the tangent vector on the projection tetrad and the normal vector
$$t^\mu = N n^\mu + N^i e_i^\mu\,, \tag{3.8}$$
where N^i is the *shift* spatial vector.

From these definitions we can rewrite the dx^μ using the coordinate transformation $x^\mu = x^\mu(t, y^i)$

$$\begin{aligned} dx^\mu &= \frac{\partial x^\mu}{\partial t}dt + \frac{\partial x^\mu}{\partial y^i}dy^i = t^\mu dt + e_i^\mu dy^i = \\ &= \left(N n^\mu + N^i e_i^\mu\right) dt + e_i^\mu dy^i = (N dt)\, n^\mu + \left(dy^i + N^i dt\right) e_i^\mu\,, \end{aligned} \tag{3.9}$$

from which we can compute the line element

$$\begin{aligned} ds^2 &= dx_\mu dx^\mu = \\ &= \left[(N dt)\, n_\mu + \left(dy^j + N^j dt\right) e_{j\,\mu}\right]\left[(N dt)\, n^\mu + \left(dy^i + N^i dt\right) e_i^\mu\right] = \\ &= -N^2 dt^2 + \left(dy^i + N^i dt\right)\left(dy^j + N^j dt\right) e_{j\,\mu} e_i^\mu\,. \end{aligned} \tag{3.10}$$

Since the induced spatial coordinates on the hypersurfaces $\Sigma(t)$ are given by y^i, the induced metric will be the term multiplying $dy^i dy^j$. Therefore

$$h_{ij} = g_{\mu\nu} e_i^\mu e_j^\nu = g_{ij}\,. \tag{3.11}$$

From the results above, we can also obtain the whole form of the metric $g_{\mu\nu}$

$$g_{00} = -N^2 + N^i N_i\,, \qquad g^{00} = -N^2\,, \tag{3.12}$$
$$g_{0i} = N_i\,, \qquad g^{0i} = N^{-2} N^i\,, \tag{3.13}$$
$$g_{ij} = h_{ij}\,, \qquad g^{ij} = h^{ij} - N^{-2} N^i N^j\,. \tag{3.14}$$

The induced metric $h_{\nu\mu}$. Using (3.3) in the case of space-like hypersurfaces

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu\,, \tag{3.15}$$

we can also write the full version of the induced metric $h_{\mu\nu}$

$$h_{00} = N^i N_i \qquad h_{0i} = N_i \qquad h_{ij} = g_{ij}\,. \tag{3.16}$$

It is important to notice that, although h_{ij} is the metric on the 3−space, h_{00} and h_{0i} are not null because the non-diagonal terms of $g_{\mu\nu}$ are in general $g_{0i} \neq 0$. These non-zero terms of $h_{\mu\nu}$ are leftovers from the embedding of the hypersurfaces in a generic spacetime and are necessary to cancel out the effects of non-null g_{0i} in various physical scenarios.

Note that we can raise/lower indices with the induced metric if the vectors are purely spatial. In fact, consider a vector X_μ such that $n^\mu X_\mu = 0$. Applying the induced metric

$$h^{\mu\nu} X_\mu = \left(g^{\mu\nu} + n^\mu n^\nu\right) X_\mu = g^{\mu\nu} X_\mu = X^\nu\,. \tag{3.17}$$

Note that this is valid for any purely spatial tensor.

We can also compute the determinant transformation. The term $\sqrt{-g}\, d^4x$, where g is the determinant of the metric $g_{\mu\nu}$, is a scalar (i.e. it transforms convariantly under a generic smooth coordinate transformation) and therefore from (3.12)-(3.14) we obtain

$$\sqrt{-g}\, dx^4 = N\sqrt{h}\, dt\, d^3y\,, \tag{3.18}$$

where h is the determinant of the induced metric h_{ij}.

The projection tensor h^{ν}_{μ}. The tensor

$$h^{\nu}_{\mu} = \delta^{\nu}_{\mu} + n^{\nu} n_{\mu} \,, \tag{3.19}$$

where we used the induced metric definition (3.15), acts as a projection tensor onto the hypersurfaces $\Sigma(t)$. We can prove this starting from a generic vector decomposition

$$v^{\mu} = v^0 n^{\mu} + v^j e^{\mu}_j \,. \tag{3.20}$$

Applying the induced metric

$$\begin{aligned} h^{\nu}_{\mu} v^{\mu} &= \left(\delta^{\nu}_{\mu} + n^{\nu} n_{\mu}\right)\left(v^0 n^{\mu} + v^j e^{\mu}_j\right) = \\ &= v^0 n^{\nu} + v^j e^{\nu}_j - v^0 n^{\nu} = v^j e^{\nu}_j \,. \end{aligned} \tag{3.21}$$

From this result, we note that we can use the tetrad vectors e^{μ}_i to project covariant tensors directly on the hypersurface spatial coordinates (spatial indices). Another implication of this proposition is that the projection tensor maps spatial tensors into spatial tensors: applying the projection tensor to a spatial tensor X_{μ}, such that $n^{\mu} X_{\mu} = 0$, we obtain

$$h^{\mu}_{\nu} X_{\mu} = X_{\nu} \,, \tag{3.22}$$

which is consistent with the raise/lower operations in (3.17).

Finally, we can prove that applying a projection tensor on another projection tensor will simply generate a new projection tensor

$$\begin{aligned} h^{\rho}_{\mu} h^{\nu}_{\rho} &= \left(\delta^{\rho}_{\mu} + n^{\rho} n_{\mu}\right)\left(\delta^{\nu}_{\rho} + n^{\nu} n_{\rho}\right) = \\ &= \delta^{\nu}_{\mu} + n^{\nu} n_{\mu} + n^{\nu} n_{\mu} + n^{\rho} n_{\mu} n^{\nu} n_{\rho} = \\ &= \delta^{\nu}_{\mu} + n^{\nu} n_{\mu} = h^{\nu}_{\mu} \,, \end{aligned} \tag{3.23}$$

where we used $n_{\rho} n^{\rho} = -1$.

Properties of n^{μ}. Finally, we show some useful properties of the normal vector.

(i) From the definition of the projection tensor

$$h^{\mu}_{\nu} n^{\nu} = 0 \,. \tag{3.24}$$

(ii) The covariant derivative of the normal vector has the property

$$n^{\mu} \nabla_{\nu} n_{\mu} = 0 \,, \tag{3.25}$$

which can be proven starting from the constant normalization of the normal vector

$$0 = \nabla_{\nu}\left(n^{\mu} n_{\mu}\right) = 2 n^{\mu}\left(\nabla_{\nu} n_{\mu}\right) \,, \tag{3.26}$$

where in the second step we used $\nabla g_{\mu\nu} = 0$.

(iii) From the Frobenius theorem

$$n_{[\mu} \nabla_{\nu} n_{\sigma]} = 0 \,. \tag{3.27}$$

(iv) In our coordinate system, we can rewrite the normal vector as

$$n_{\mu} = -N \, \delta^0_{\mu} \,. \tag{3.28}$$

or the contravariant form

$$n^{\mu} = \frac{1}{N}\left(\delta^{\mu}_0 - N^{\mu}\right) \,, \tag{3.29}$$

where we define $N^{\mu} = (0, N^i)$.

3.3.2 Three-dimensional spatial covariant derivative

In this section we discuss the three-dimensional (3D) spatial derivative, which acts on the hypersurfaces $\Sigma(t)$. Consider the derivative acting on a vector X_μ tangent to $\Sigma(t)$, i.e $X_\mu n^\mu = 0$. The natural definition of the 3D derivative D_μ arises from projecting the four-dimensional covariant derivative Σ_μ on $\Sigma(t)$, using the tensor (3.19), as follows

$$D_\mu X_\nu \equiv h_\mu^\rho h_\nu^\sigma \nabla_\rho X_\sigma \,. \tag{3.30}$$

Similarly, we can define the 3D derivative acting on a scalar function $f(x^\mu)$ as

$$D_\mu f \equiv h_\mu^\nu \nabla_\nu f \,. \tag{3.31}$$

From these we can find how D_μ acts on a contravariant vector. Consider the 3D derivative of the product between two vectors X_μ and V^μ, both tangent to $\Sigma(t)$ ($X_\mu n^\mu = 0$ and $V^\mu n_\mu = 0$). We have

$$D_\mu \left(X_\nu V^\nu\right) = V^\nu D_\mu X_\nu + X_\nu D_\mu V^\nu \,. \tag{3.32}$$

The left hand side can be rewritten using the 3D derivative of a scalar (3.31)

$$h_\mu^\rho \nabla_\rho \left(X_\nu V^\nu\right) = h_\mu^\rho V^\nu \nabla_\rho X_\nu + h_\mu^\rho X_\nu \nabla_\rho V^\nu \,, \tag{3.33}$$

while the right hand side can be expanded using the 3D derivative of a covariant vector (3.30)

$$V^\nu D_\mu X_\nu + X_\nu D_\mu V^\nu = V^\nu h_\mu^\rho h_\nu^\sigma \nabla_\rho X_\sigma + X_\nu D_\mu V^\nu = V^\nu h_\mu^\rho \nabla_\rho X_\nu + X_\nu D_\mu V^\nu \,, \tag{3.34}$$

where we used the fact that, since $V^\mu n_\mu = 0$, $V^\nu h_\nu^\sigma = V^\sigma$. Inserting (3.33) and (3.34) back into (3.32), and simplifying one of the term appearing on both sides, we almost obtain the result we want

$$X_\nu D_\mu V^\nu = h_\mu^\rho X_\nu \nabla_\rho V^\nu \,. \tag{3.35}$$

Since $X_\nu n^\nu = 0$, X_ν is not a generic vector, we can not simplify X_ν on this equation. However, we can always consider $X_\nu = h_\nu^\rho Y_\rho$, where Y_ν is a generic vector. Therefore, simplifying Y_ν, we obtain

$$h_\nu^\rho D_\mu V^\nu = h_\mu^\sigma h_\nu^\rho \nabla_\sigma V^\nu \,. \tag{3.36}$$

Since, by construction, the spatial derivative maps spatial tensors into spatial tensors, the projection tensor on the left-hand side is redundant. Simplifying this, we obtain the definition

$$D_\mu V^\nu = h_\rho^\nu h_\mu^\sigma \nabla_\sigma V^\rho \,. \tag{3.37}$$

We can generalize this definition to any tensor, and the general rule is to project all free indices with the projection operators into $\Sigma(t)$. For instance,

$$D_\mu T_{\rho\sigma} = h_\mu^\alpha h_\rho^\beta h_\sigma^\gamma \nabla_\alpha T_{\beta\gamma} \,. \tag{3.38}$$

Finally, similarly to what happens to the four-dimensional metric property $\nabla_\rho g_{\mu\nu} = 0$, we can check that the induced metric obeys

$$D_\rho h_{\mu\nu} = 0 \,. \tag{3.39}$$

To prove this, we apply the definition of spatial derivative

$$\begin{aligned} D_\rho h_{\mu\nu} &= h_\rho^\alpha h_\mu^\beta h_\sigma^\gamma \nabla_\alpha h_{\beta\gamma} = \\ &= h_\rho^\alpha h_\mu^\beta h_\sigma^\gamma \nabla_\alpha \left(g_{\beta\gamma} + n_\beta n_\gamma\right) = \\ &= h_\rho^\alpha h_\mu^\beta h_\sigma^\gamma \nabla_\alpha \left(n_\beta n_\gamma\right) = \\ &= h_\rho^\alpha h_\mu^\beta h_\sigma^\gamma \left(n_\beta \nabla_\alpha n_\gamma + n_\gamma \nabla_\alpha n_\beta\right) = 0 \,, \end{aligned} \tag{3.40}$$

where we used the definition of the induced metric (3.15) and the normal vector property (3.24).

3.3.3 Lie derivative

Consider the definition of the Lie derivative of a generic tensor $T_{\mu\nu}$ with respect to a generic vector field ζ^μ

$$\begin{aligned}\pounds_\zeta T^\mu{}_\nu &= \zeta^\rho \partial_\rho T^\mu{}_\nu - T^\rho{}_\nu \partial_\rho \zeta^\mu + T^\mu{}_\rho \partial_\nu \zeta^\rho = \\ &= \zeta^\rho \nabla_\rho T^\mu{}_\nu - T^\rho{}_\nu \nabla_\rho \zeta^\mu + T^\mu{}_\rho \nabla_\nu \zeta^\rho \,, \end{aligned} \tag{3.41}$$

where the equality can be proven writing the covariant derivative in terms of partial derivatives and Christoffel symbols, and noting that the Christoffel symbols from the first term cancel exactly with the ones from the other terms. This is a general property of the Lie derivative: we can always switch between covariant and partial derivatives (provided we change them all).

In this section we want to prove that, given a purely spatial tensor $Q_{\mu\nu}$, i.e., $Q_{\mu\nu} n^\mu = Q_{\mu\nu} n^\nu = 0$, its Lie derivative with respect to the normal vector field can be written equivalently as

$$\pounds_n Q_{\mu\nu} = \frac{1}{N} \left(\frac{\partial Q_{\mu\nu}}{\partial t} - \pounds_N Q_{\mu\nu} \right) , \tag{3.42}$$

where the vectors written in coordinates are $n^\mu = N^{-1}(1, -N^i)$ and $N^\mu = (0, N^i)$. In particular, if the coordinate system has a shift vector with null components, i.e. $N^\mu = 0$ for all indices μ, the Lie derivative coincides with the time derivative

$$\pounds_n Q_{\mu\nu} = \frac{1}{N} \frac{\partial Q_{\mu\nu}}{\partial t} \qquad (N^\mu = 0 \text{ case}) \,. \tag{3.43}$$

Proof. Consider the definition of Lie derivative

$$\begin{aligned}\pounds_n Q_{\mu\nu} &= n^\rho \partial_\rho Q_{\mu\nu} + Q_{\rho\nu} \partial_\mu n^\rho + Q_{\mu\rho} \partial_\nu n^\rho = \\ &= n^\rho \partial_\rho Q_{\mu\nu} + \partial_\mu \left(n^\rho Q_{\rho\nu} \right) - n^\rho \partial_\mu Q_{\rho\nu} + \partial_\nu \left(n^\rho Q_{\mu\rho} \right) - n^\rho \partial_\nu Q_{\mu\rho} = \\ &= n^\rho \partial_\rho Q_{\mu\nu} - n^\rho \partial_\mu Q_{\rho\nu} - n^\rho \partial_\nu Q_{\mu\rho} \end{aligned} \tag{3.44}$$

Using the form of the normal vector written in coordinates (3.29) $n^\mu = \left(\delta^\mu_0 - N^\mu \right) / N$, we obtain

$$N \pounds_n Q_{\mu\nu} = \left(\delta^\rho_0 - N^\rho \right) \partial_\rho Q_{\mu\nu} - \left(\delta^\rho_0 - N^\rho \right) \partial_\mu Q_{\rho\nu} - \left(\delta^\rho_0 - N^\rho \right) \partial_\nu Q_{\mu\rho} \,. \tag{3.45}$$

We also note that, for a spatial vector $Q_{0\mu} = h^\nu_0 Q_{\mu\nu} = N^\nu Q_{\mu\nu}$, where the first equality comes from a proposition similar to (3.22), and the second from (3.16). Therefore

$$N \pounds_n Q_{\mu\nu} = \partial_0 Q_{\mu\nu} - N^\rho \partial_\rho Q_{\mu\nu} - \partial_\mu \left(N^\rho Q_{\rho\nu} \right) + N^\rho \partial_\mu Q_{\rho\nu} - \partial_\nu \left(N^\rho Q_{\mu\rho} \right) + N^\rho \partial_\nu Q_{\nu\rho} \,. \tag{3.46}$$

Using the Liebnitz rule on the third and fifth terms on the right-hand side, some terms cancel with the fourth and sixth terms. We are left with

$$N \pounds_n Q_{\mu\nu} = \partial_0 Q_{\mu\nu} - N^\rho \partial_\rho Q_{\mu\nu} - Q_{\rho\nu} \partial_\mu N^\rho - Q_{\mu\rho} \partial_\nu N^\rho \,. \tag{3.47}$$

But in the last terms are exactly the definition of the Lie derivative of the tensor $Q_{\mu\nu}$ with respect to the N^μ vector field

$$\pounds_N Q_{\mu\nu} = N^\rho \partial_\rho Q_{\mu\nu} + Q_{\rho\nu} \partial_\mu N^\rho + Q_{\mu\rho} \partial_\nu N^\rho \,. \tag{3.48}$$

Therefore we obtain the first result. The case $N^\mu = 0$ can be proven from the previous result noting that all $\pounds_N Q_{\mu\nu}$ terms contains N^μ components. □

3.3.4 Extrinsic curvature

In the previous sections we built the metric and the spatial derivative living on the spatial hypersurfaces $\Sigma(t)$. The next step is to identify a quantity which gives informations about how these hypersurfaces are embedded into the four-dimensional spacetime. Intuitively (see also Figure 3.1) we can retrieve these informations from how the the normal vector to $\Sigma(t)$ varies from one four-dimensional event to another. This intuition can be formalized with the definition of the *extrinsic curvature* of $\Sigma(t)$

$$K_{\mu\nu} \equiv -h^\alpha_\mu h^\beta_\nu \nabla_\alpha n_\beta \,. \tag{3.49}$$

Using the projection tensor equation (3.19), and the normal vector property (3.27), we can rewrite

$$h^\beta_\nu \nabla_\alpha n_\beta = \left(\delta^\beta_\nu + n^\beta n_\nu\right) \nabla_\alpha n_\beta = \nabla_\alpha n_\nu \,, \tag{3.50}$$

and therefore

$$K_{\mu\nu} \equiv -h^\alpha_\mu \nabla_\alpha n_\nu \,. \tag{3.51}$$

Therefore it is necessary to access the normal vector to the hypersurface to build the extrinsic curvature. In general, it is essential to distinguish between the extrinsic quantities like the extrinsic curvature, which can not be accessed by observers living on the hypersurface, and the intrinsic quantities such as the induced metric, which are accessible to *inhabitants* of the hypersurface. In practice, since we can access the whole four-dimensional spacetime through experiments, in the ADM theory we will consider the extrinsic and intrinsic quantities as different tools to characterize the embedding we are using to rewrite the Einstein equations in a $1+3$ form.

Properties of $K_{\mu\nu}$. The extrinsic curvature has the following properties.

(i) Using the normal vector property (3.25), we immediately find

$$n^\mu K_{\mu\nu} = n^\nu K_{\mu\nu} = 0 \,. \tag{3.52}$$

Therefore we can safely use the induced metric to raise/lower indices as in (3.17).

(ii) Since $n_j = 0$, the *contravariant* components of the extrinsic curvature are only spatial, i.e.

$$K^{0\nu} = 0 \,. \tag{3.53}$$

Proof. From the previous property we have

$$n_\mu K^{\mu\nu} = n_0 K^{0\mu} + n_j K^{j\mu} = n_0 K^{0\mu} \tag{3.54}$$

and since n_0 is not null, we have the property. □

Note that the same trick can not be applied to $n^\mu K_{\mu\nu}$ because n^j is in general not null, as can be seen from the normal vector definition (3.5).

(iii) The extrinsic curvature is symmetric under the exchange of its indices, i.e.

$$K_{\mu\nu} = K_{\nu\mu} \,. \tag{3.55}$$

Proof. Starting from the definition

$$K_{\mu\nu} = -h^\alpha_\mu \nabla_\alpha n_\nu = -\left(\delta^\alpha_\mu + n_\mu n^\alpha\right) \nabla_\alpha n_\nu = -\nabla_\mu n_\nu - n_\mu n^\alpha \nabla_\alpha n_\nu \,. \tag{3.56}$$

Consider the property of the normal vector (3.27), and the indices $\mu\alpha\nu$. Writing the property in a convenient and compact form $[\mu\alpha\nu] = 1/6\left(\mu\alpha\nu + \nu\mu\alpha + \alpha\nu\mu - \mu\alpha\nu - \nu\alpha\nu - \alpha\mu\nu\right) = 0$, where the last equality holds if these are the indices of the property (3.27). Thus we can rewrite the equation above as

$$\begin{aligned} -K_{\mu\nu} &= \nabla_\mu n_\nu + n^\alpha \left(-n_\alpha \nabla_\nu n_\mu - n_\nu \nabla_\mu n_\alpha + n_\mu \nabla_\nu n_\alpha + n_\nu \nabla_\alpha n_\mu + n_\alpha \nabla_\mu n_\nu\right) = \\ &= n_\nu \nabla_\mu + n^\alpha n_\nu \nabla_\alpha n_\mu = -K_{\nu\mu}, , \end{aligned} \tag{3.57}$$

where we repeatedly used the normalization $n_\mu n^\mu = -1$ and normal vector property (3.25). □

(iv) Inverting (3.56) we can rewrite the covariant derivative of the normal vector as

$$-\nabla_\nu n_\nu = K_{\mu\nu} + n_\mu \left(n^\alpha \nabla_\alpha n_\nu\right) \equiv K_{\mu\nu} + n_\mu a_\nu \,. \tag{3.58}$$

From (3.25) $n^\mu \nabla_\nu n_\mu = 0$, it is immediate to show that the acceleration a_μ is a spatial vector, i.e. $n^\nu a_\nu = 0$. Also note that the acceleration can be written in terms of the lapse as

$$a_\mu = \frac{1}{N} D_\mu N \,. \tag{3.59}$$

(v) From the property above, we can rewrite the spatial part of the extrinsic curvature as

$$K_{ij} = -\nabla_i n_j = -N\,\Gamma^0_{ij} \,, \tag{3.60}$$

where the first equality holds since the last part of (3.58) is normal to the hypersurfaces. The second equality comes from the definition of covariant derivative

$$\nabla_i n_j = \partial_i n_j - \Gamma^\alpha_{ij} n_\alpha = -\Gamma^0_{ij} n_0 = N \Gamma^0_{ij} \,, \tag{3.61}$$

where we used the definition of normal vector (3.5), namely $n_j = 0$ and $n_0 = -N$. With a further expansion of the Christoffel symbol in this definition, we obtain

$$K_{ij} = \frac{1}{2N} \left[D_i N_j + D_j N_i - \partial_0 h_{ij}\right] , \tag{3.62}$$

where $N_i = h_{ij} N^j$. Moreover, if we consider a coordinate system where the shift vector has null components, i.e. $N^\mu = 0$ for all μ,

$$K_{ij} = -\frac{1}{2N} \frac{\partial h_{ij}}{\partial t} \qquad (N^\mu = 0 \text{ case}) \,, \tag{3.63}$$

among which we can include the other component values

$$K_{0j} = K^{0j} = 0 \qquad \text{and} \qquad K_{00} = K^{00} = 0 \qquad (N^\mu = 0 \text{ case}) \,. \tag{3.64}$$

Therefore when the coordinate system has the property $N^\mu = 0$, K_{ij} (and not only K^{ij}) is purely spatial, and the non-zero components gives the time derivatives of the induced metric (which, from (3.16), it's purely spatial as well).

(vi) The extrinsic curvature is linked to the Lie derivative of the intrinsic metric with the relation

$$\pounds_n h_{\mu\nu} = -2K_{\mu\nu} \,. \tag{3.65}$$

This result highlights the physical meaning of the extrinsic curvature. Considering the definition of the Lie derivative, the case $\pounds_n h_{\mu\nu} = 0$ means that the intrinsic curvature is independent of the time coordinate t (the normal vector field in our coordinate system), and therefore $h_{\mu\nu}$ will be the same on all hypersurfaces $\Sigma(t)$. Since this also works in a general coordinate system, the Lie derivative of the induced metric can be considered as the generalization of the time derivative of the intrinsic metric. In other words, the normal vector field to these hypersurfaces will only carry the information about a "constant in time embedding". Intuitively, this situation also means that the extrinsic curvature, being the source of information about the embedding, should be constant as it can only carry the information about the trivial embedding. In fact, in this case, the normal vector field is constant in time and therefore, the extrinsic curvature, which is built from the covariant derivative of the normal vector, is 0. This qualitatively justifies why the Lie derivative quantifies the deviation from this limit case with the extrinsic curvature.

Proof. This can proved starting from the definition of the Lie derivative of a tensor

$$\pounds_n h_{\mu\nu} = n^\rho \nabla_\rho h_{\mu\nu} + h_{\rho\nu} \nabla_\mu n^\rho + h_{\rho\mu} \nabla_\nu n^\rho \,. \tag{3.66}$$

Using the intrinsic metric definition (3.15) $h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu$ and the normal vector property (3.24) $h^\mu_\nu n^\nu = 0$, we obtain

$$\begin{aligned}
\pounds_n h_{\mu\nu} &= n^\rho \nabla_\rho (n_\mu n_\nu) + g_{\rho\nu} \nabla_\mu n^\rho + g_{\rho\mu} \nabla_\nu n^\rho = \\
&= n^\rho n_\mu \nabla_\rho n_\nu + n^\rho n_\nu \nabla_\rho n_\mu + \nabla_\mu n^\nu + \nabla_\nu n^\mu = \\
&= \left(\delta^\rho_\mu + n^\rho n_\mu\right) \nabla_\rho n_\nu + \left(\delta^\rho_\nu + n^\rho n_\nu\right) \nabla_\rho n_\mu = \\
&= h^\rho_\mu \nabla_\rho n_\nu + h^\rho_\nu \nabla_\rho n_\mu = -K_{\mu\nu} - K_{\nu\mu} = -2K_{\mu\nu} \,.
\end{aligned} \tag{3.67}$$

□

3.4 Curvature equations

In this section, we derive the equations which link the curvature tensors of the hypersurface $\Sigma(t)$ and the extrinsic curvature to the tensors of the four-dimensional space.

3.4.1 Gauss–Codazzi equation

Analogously to the four-dimensional definition, we define the three-dimensional (spatial) Riemann tensor, applied to a spatial vector X_μ, as

$$^{(3)}R^\sigma{}_{\rho\mu\nu} X_\sigma = D_\nu D_\mu X_\rho - D_\mu D_\nu X_\rho \,. \tag{3.68}$$

The Gauss–Codazzi equation is

$$^{(3)}R_{\mu\nu\rho\sigma} = h^\alpha_\mu h^\beta_\nu h^\gamma_\rho h^\delta_\sigma R_{\alpha\beta\gamma\delta} + \epsilon \left(K_{\mu\rho} K_{\nu\sigma} - K_{\mu\sigma} K_{\nu\rho}\right) , \tag{3.69}$$

where

$$\epsilon = n_\mu n^\mu = \begin{cases} +1 & \text{for timelike } \Sigma(t) \\ -1 & \text{for spacelike } \Sigma(t) \end{cases} \,. \tag{3.70}$$

Therefore, it is essential to note that projecting the four-dimensional Riemann tensor is insufficient to obtain the curvature tensor on the hypersurface. For an inhabitant of the hypersurface, which has access only to the three-dimensional curvature tensors, it is impossible to obtain information about the four-dimensional spacetime. On the contrary, a four-dimensional spacetime inhabitant can recover information about the three-dimensional space curvature once he/she knows how the hypersurfaces have been embedded (extrinsic curvature).

Proof. We will prove the Gauss–Codazzi equation in the space-like hypersurfaces $\Sigma(t)$ case. We can start the proof from the definition of the spatial curvature tensor (3.68). In order to simplify the notation, exploiting the symmetry of the spatial curvature definition, we define $(\rho \leftrightarrow \sigma)$ as the part of the equation with ρ and σ indices exchanged. Using the spatial derivative definitions (3.30) and (3.38), we obtain

$$\begin{aligned} -{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu &= D_\rho D_\sigma X_\nu - D_\sigma D_\rho X_\nu = \\ &= h^\alpha_\rho h^\beta_\sigma h^\gamma_\nu \nabla_\alpha \left(h^\delta_\beta h^\eta_\gamma \nabla_\delta X_\eta\right) - (\rho \leftrightarrow \sigma) = \\ &= h^\alpha_\rho h^\beta_\sigma h^\gamma_\nu \left[h^\delta_\beta h^\eta_\gamma \nabla_\alpha \nabla_\delta X_\eta + \nabla_\alpha \left(h^\delta_\beta h^\eta_\gamma\right)\left(\nabla_\delta X_\eta\right)\right] - (\rho \leftrightarrow \sigma)\,. \end{aligned} \tag{3.71}$$

Using the projection tensor property (3.23) $h^\mu_\rho h^\rho_\nu = h^\mu_\nu$, we can simplify some tensors in the first term on the right hand side

$$-{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu = h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta + h^\alpha_\rho h^\beta_\sigma h^\gamma_\nu \left[h^\delta_\beta \nabla_\alpha h^\eta_\gamma + h^\eta_\gamma \nabla_\alpha h^\delta_\beta\right]\left(\nabla_\delta X_\eta\right) - (\rho \leftrightarrow \sigma)\,. \tag{3.72}$$

With the projection tensor definition (3.19), since the covariant derivative of the delta is null, we can simplify the ∇h terms

$$\begin{aligned} -{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu &= h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta + \\ &\quad + h^\alpha_\rho h^\beta_\sigma h^\gamma_\nu \left[h^\delta_\beta \nabla_\alpha \left(n_\gamma n^\eta\right) + h^\eta_\gamma \nabla_\alpha \left(n_\beta n^\delta\right)\right]\left(\nabla_\delta X_\eta\right) - (\rho \leftrightarrow \sigma) = \\ &= h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta + \\ &\quad + h^\alpha_\rho h^\beta_\sigma h^\gamma_\nu \left[h^\delta_\beta \left(n_\gamma \nabla_\alpha n^\eta + n^\eta \nabla_\alpha n_\gamma\right) + h^\eta_\gamma \left(n_\beta \nabla_\alpha n^\delta + n^\delta \nabla_\alpha n_\beta\right)\right]\left(\nabla_\delta X_\eta\right) + \\ &\quad - (\rho \leftrightarrow \sigma)\,. \end{aligned} \tag{3.73}$$

Some of the terms in the square brackets can be simplified with the normal vector property (3.24) $h^\mu_\nu n^\nu = 0$. The resulting terms can be rewritten in terms of the extrinsic curvature definition (3.51) and simplified with the projection tensor property (3.23) $h^\mu_\rho h^\rho_\nu = h^\mu_\nu$

$$\begin{aligned} -{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu &= h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta + \left(h^\alpha_\rho h^\delta_\sigma h^\gamma_\nu n^\eta \nabla_\alpha n_\gamma + h^\alpha_\rho h^\beta_\sigma h^\eta_\nu n^\delta \nabla_\alpha n_\beta\right)\left(\nabla_\delta X_\eta\right) - (\rho \leftrightarrow \sigma) = \\ &= h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta + \left[\left(-K_{\rho\nu}\right) h^\delta_\sigma n^\eta + \left(-K_{\rho\sigma}\right) h^\eta_\nu n^\delta \nabla_\delta X_\eta\right]\left(\nabla_\delta X_\eta\right) - (\rho \leftrightarrow \sigma)\,. \end{aligned} \tag{3.74}$$

We can use the symmetry $K_{\rho\sigma} = K_{\sigma\rho}$ to simplify the term with $K_{\rho\sigma}$ with the term coming from the $(\rho \leftrightarrow \sigma)$ part

$$-{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu = h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta - K_{\rho\nu} h^\delta_\sigma n^\eta \nabla_\delta X_\eta - (\rho \leftrightarrow \sigma)\,. \tag{3.75}$$

The vector X_μ we are considering is fully spatial. Therefore

$$0 = \nabla_\delta \left(n^\eta X_\eta\right) = X_\eta \nabla_\delta n^\eta + n^\eta \nabla_\delta X_\eta\,. \tag{3.76}$$

Substituting the equation above into (3.75) we obtain

$$-{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu = h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta + K_{\rho\nu} X^\eta h^\delta_\sigma \nabla_\delta n_\eta - (\rho \leftrightarrow \sigma) \tag{3.77}$$

Using again the extrinsic curvature definition

$$-{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu = h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta + K_{\rho\nu}\left(-K_{\sigma\eta}\right) X^\eta - (\rho \leftrightarrow \sigma) \tag{3.78}$$

$$= h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta - h^\alpha_\sigma h^\delta_\rho h^\eta_\nu \nabla_\alpha \nabla_\delta X_\eta - K_{\rho\nu} K_{\sigma\eta} X^\eta + K_{\sigma\nu} K_{\rho\eta} X^\eta\,. \tag{3.79}$$

We can rearrange the dummy indices and rewrite the equation as

$$\begin{aligned} -{}^{(3)}R_{\mu\nu\rho\sigma}X^\mu &= h^\alpha_\rho h^\delta_\sigma h^\eta_\nu \left(\nabla_\alpha \nabla_\delta X_\eta - \nabla_\delta \nabla_\alpha X_\eta\right) + \left(K_{\sigma\nu} K_{\rho\eta} - K_{\rho\nu} K_{\sigma\eta}\right) X^\eta \\ &= -h^\alpha_\rho h^\delta_\sigma h^\gamma_\nu\, R_{\eta\gamma\alpha\delta}\, X^\eta + \left(K_{\sigma\nu} K_{\rho\eta} - K_{\rho\nu} K_{\sigma\eta}\right) X^\eta\,. \end{aligned} \tag{3.80}$$

This is almost the result we want, because as we previously noted, X_μ is spatial vector, and therefore we can not simplify it as it was a generic vector in a covariant expression. But we can always rewrite $X^\mu = h^\mu_\nu Y^\nu$, where Y^ν is now a generic four-dimensional vector. We have

$$-{}^{(3)}R_{\mu\nu\rho\sigma} h^\mu_\beta Y^\beta = -h^\alpha_\rho h^\delta_\sigma h^\gamma_\nu\, R_{\eta\gamma\alpha\delta}\, h^\eta_\beta Y^\beta + \left(K_{\sigma\nu}K_{\rho\eta} - K_{\rho\nu}K_{\sigma\eta}\right) h^\eta_\beta Y^\beta \,. \tag{3.81}$$

We can now simplify Y^β and relabel some dummy indices

$${}^{(3)}R_{\beta\nu\rho\sigma} h^\beta_\mu = h^\alpha_\mu h^\beta_\nu h^\gamma_\rho h^\delta_\sigma\, R_{\alpha\beta\gamma\delta} + \left(K_{\rho\nu}K_{\sigma\eta} - K_{\sigma\nu}K_{\rho\eta}\right) h^\eta_\mu \,. \tag{3.82}$$

Since by definition (3.68) ${}^{(3)}R_{\beta\nu\rho\sigma}$ is a purely spatial tensor, we can use the projection tensor h^β_μ as a δ^β_μ. In other words, substituting on the left hand side the projection tensor h^β_μ with its definition (3.19), we obtain ${}^{(3)}R_{\beta\nu\rho\sigma}(\delta^\beta_\mu + n^\beta n_\mu)$, whose second term is null since the spatial curvature is a purely spatial tensor. Similarly, the last term on the left hand side can be simplified considering that the extrinsic curvature has the property (3.52) $K_{\mu\nu}n^\nu = 0$. □

3.4.2 Riemann tensor equations

The Gauss–Codazzi equation links the full projection of the four-dimensional Riemann tensor to $\Sigma(t)$ with the spatial Riemann tensor and the extrinsic curvature. In other words, in the Gauss–Codazzi equation, we projected all four indices of the Riemann tensor with projection tensors. In addition to this, we can also partially project the Riemann tensor, projecting only some indices on $\Sigma(t)$ and the others with the normal vector n^μ.

The equations we prove are the following

$$n^\sigma h^\mu_\alpha h^\nu_\beta h^\rho_\gamma R_{\mu\nu\rho\sigma} = -D_\alpha K_{\beta\gamma} + D_\beta K_{\alpha\gamma} \,. \tag{3.83}$$

$$h^\alpha_\mu n^\beta h^\gamma_\nu n^\delta R_{\alpha\beta\gamma\delta} = \pounds_n K_{\mu\nu} + K_{\beta\nu}K^{\beta\mu} + D_\mu a_\nu + a_\mu a_\nu \,. \tag{3.84}$$

All other different combinations of three or two projection tensors can be obtained using the symmetries of the Riemann tensor. Since the Riemann tensor is null if three or four indices are time indices due to its symmetries, there are no additional equations to prove.

The second equation (3.84) is also shown in the literature in a slightly different way. We can rewrite the second-last term using the alternative definition of acceleration (3.59)

$$D_\mu a_\nu = D_\mu\left(N^{-1}D_\nu N\right) = -\frac{1}{N^2}D_\mu N D_\nu N + \frac{1}{N}D_\mu D_\nu N = \frac{1}{N}D_\mu D_\nu N - a_\mu a_\nu \,, \tag{3.85}$$

and therefore the equation (3.84) becomes

$$h^\alpha_\mu n^\beta h^\gamma_\nu n^\delta R_{\alpha\beta\gamma\delta} = \pounds_n K_{\mu\nu} + K_{\beta\nu}K^{\beta\mu} + \frac{1}{N}D_\mu D_\nu N \,. \tag{3.86}$$

Proof of (3.83). We start from the definition of Riemann tensor written in the form

$$R_{\mu\nu\rho\sigma}n^\sigma = \nabla_\mu\nabla_\nu n_\rho - \nabla_\nu\nabla_\mu n_\rho = \nabla_\mu\left(-K_{\nu\rho} - n_\nu n^\delta \nabla_\delta n_\rho\right) - (\mu \leftrightarrow \nu) \,, \tag{3.87}$$

where we used (3.58) to substitute $\nabla_\nu n_\sigma$. Applying the remaining projection tensors, we obtain

$$\begin{aligned} n^\sigma h^\mu_\alpha h^\nu_\beta h^\rho_\gamma R_{\mu\nu\rho\sigma} &= -h^\mu_\alpha h^\nu_\beta h^\rho_\gamma\left[\nabla_\mu K_{\nu\rho} + \nabla_\mu\left(n_\nu n^\delta\right)\nabla_\delta n_\rho + n_\nu n^\delta \nabla_\mu\nabla_\delta n_\rho\right] - (\alpha\leftrightarrow\beta) = \\ &= -D_\alpha K_{\beta\gamma} - h^\mu_\alpha h^\nu_\beta h^\rho_\gamma\left(n^\delta\nabla_\mu n_\nu + n_\nu \nabla_\mu n^\delta\right)\left(\nabla_\delta n_\rho\right) - (\alpha\leftrightarrow\beta) = \\ &= -D_\alpha K_{\beta\gamma} - h^\mu_\alpha h^\nu_\beta h^\rho_\gamma\left(\nabla_\delta n_\rho\right) n^\delta \nabla_\mu n_\nu - (\alpha\leftrightarrow\beta) = \\ &= -D_\alpha K_{\beta\gamma} - h^\rho_\gamma\left(\nabla_\delta n_\rho\right) n^\delta K_{\alpha\beta} - (\alpha\leftrightarrow\beta) \,, \end{aligned} \tag{3.88}$$

where we repeatedly used the normal vector property (3.24) $h^\mu_\nu n^\nu = 0$ and the extrinsic curvature definition (3.51). We note that the second term on the right hand side is symmetric under the exchange of α and β, and therefore that term can be simplified with the same coming from $(\alpha \leftrightarrow \beta)$ with opposite sign. Therefore we obtain the result. □

Proof of (3.84). We start again from

$$\begin{aligned} R_{\mu\nu\rho\sigma}n^\sigma &= \nabla_\mu\nabla_\nu n_\rho - \nabla_\nu\nabla_\mu n_\rho = \\ &= \nabla_\mu\left(-K_{\nu\rho} - n_\nu n^\delta\nabla_\delta n_\rho\right) - \nabla_\nu\left(-K_{\mu\rho} - n_\mu n^\delta\nabla_\delta n_\rho\right) = \\ &= -\nabla_\mu\left(K_{\nu\rho} + n_\nu a_\rho\right) + \nabla_\nu\left(K_{\mu\rho} + n_\mu a_\rho\right) . \end{aligned} \tag{3.89}$$

We can add another normal vector and find

$$\begin{aligned} R_{\mu\nu\rho\sigma}n^\sigma n^\nu &= -n^\nu\nabla_\mu\left(K_{\nu\rho} + n_\nu a_\rho\right) + n^\nu\nabla_\nu\left(K_{\mu\rho} + n_\mu a_\rho\right) = \\ &= -n^\nu\nabla_\mu K_{\nu\rho} + n^\nu\nabla_\nu K_{\mu\rho} - n^\nu a_\rho\nabla_\mu n_\nu - n^\nu n_\nu\nabla_\mu a_\rho + n^\nu a_\rho\nabla_\nu n_\mu + n^\nu n_\mu\nabla_\nu a_\rho = \\ &= -n^\nu\nabla_\mu K_{\nu\rho} + n^\nu\nabla_\nu K_{\mu\rho} - n^\nu n_\nu\nabla_\mu a_\rho + a_\rho a_\mu + n^\nu n_\mu\nabla_\nu a_\rho = \\ &= -n^\nu\nabla_\mu K_{\nu\rho} + n^\nu\nabla_\nu K_{\mu\rho} + \left(\delta^\nu_\mu + n_\mu n^\nu\right)\nabla_\nu a_\rho + a_\rho a_\mu = \\ &= -n^\nu\nabla_\mu K_{\nu\rho} + n^\nu\nabla_\nu K_{\mu\rho} + h^\nu_\mu\nabla_\nu a_\rho + a_\mu a_\rho\,. \end{aligned} \tag{3.90}$$

Adding the remaining projection tensors we obtain

$$R_{\mu\nu\rho\sigma}n^\sigma n^\nu h^\mu_\alpha h^\rho_\beta = -h^\mu_\alpha h^\rho_\beta n^\nu\nabla_\mu K_{\nu\rho} + h^\mu_\alpha h^\rho_\beta n^\nu\nabla_\nu K_{\mu\rho} + h^\mu_\alpha h^\rho_\beta h^\nu_\mu\nabla_\nu a_\rho + h^\mu_\alpha h^\rho_\beta a_\mu a_\rho\,. \tag{3.91}$$

Since h^ν_μ maps spatial tensors into spatial tensors, $h^\mu_\alpha h^\rho_\beta h^\nu_\mu\nabla_\nu a_\rho = h^\mu_\alpha D_\mu a_\beta = D_\alpha a_\beta$. Moreover $h^\mu_\alpha a_\mu = \delta^\mu_\alpha a_\mu + n^\mu n_\alpha a_\mu = a_\alpha$, where in the last step we used the normal vector property (3.25) $n^\mu\nabla_\nu n_\mu = 0$ on $n^\mu a_\mu = n^\mu n^\nu\nabla_\nu a_\mu$. Therefore the equation becomes

$$R_{\mu\nu\rho\sigma}n^\sigma n^\nu h^\mu_\alpha h^\rho_\beta = -h^\mu_\alpha h^\rho_\beta n^\nu\nabla_\mu K_{\nu\rho} + h^\mu_\alpha h^\rho_\beta n^\nu\nabla_\nu K_{\mu\rho} + D_\alpha a_\beta + a_\alpha a_\beta\,. \tag{3.92}$$

The first term on the right hand side can be rewritten using the Leibnitz rule on the $n^\nu K_{\nu\rho}$, which is null for the extrinsic curvature property (3.52)

$$\begin{aligned} -h^\mu_\alpha h^\rho_\beta n^\nu\nabla_\mu K_{\nu\rho} &= -h^\mu_\alpha h^\rho_\beta\left[\nabla_\mu\left(n^\nu K_{\nu\rho}\right) + K_{\nu\rho}\nabla_\mu n^\nu\right] = \\ &= h^\mu_\alpha h^\rho_\beta K_{\nu\rho}\nabla_\mu n^\nu = h^\mu_\alpha K_{\nu\beta}\nabla_\mu n^\nu = -K_{\nu\beta}K^\nu_\alpha\,, \end{aligned} \tag{3.93}$$

where in the second-last step we used again the property $n^\rho K_{\nu\rho} = 0$.
The second term of (3.92) can be rewritten using the Lie derivative definition applied on the extrinsic curvature

$$\pounds_n K_{\mu\nu} = n^\rho\nabla_\rho K_{\mu\nu} + K_{\mu\rho}\nabla_\nu n_\rho + K_{\rho\nu}\nabla_\mu n_\rho\,, \tag{3.94}$$

and obtain

$$h^\mu_\alpha h^\rho_\beta n^\nu\nabla_\nu K_{\mu\rho} = h^\mu_\alpha h^\rho_\beta\left(\pounds_n K_{\mu\rho} - K_{\mu\gamma}\nabla_\rho n^\gamma - K_{\gamma\rho}\nabla_\mu n^\gamma\right) . \tag{3.95}$$

Note also that (again, since $n^\mu K_{\mu\nu} = 0$), we can also rewrite the Lie derivative of the extrinsic curvature as

$$\begin{aligned} \pounds_n K_{\alpha\beta} &= \pounds_n\left(h^\mu_\alpha h^\rho_\beta K_{\mu\rho}\right) = \\ &= h^\mu_\alpha h^\rho_\beta\pounds_n K_{\mu\rho} + h^\rho_\beta K_{\mu\rho}\pounds_n h^\mu_\alpha + h^\mu_\alpha K_{\mu\rho}\pounds_n h^\rho_\beta = \\ &= h^\mu_\alpha h^\rho_\beta\pounds_n K_{\mu\rho} + h^\rho_\beta K_{\mu\rho}\left(-2K^\mu_\alpha\right) + h^\mu_\alpha K_{\mu\rho}\left(-2K^\rho_\beta\right) = \\ &= h^\mu_\alpha h^\rho_\beta\pounds_n K_{\mu\rho} - 2K_{\mu\beta}K^\mu_\alpha - 2K_{\alpha\rho}K^\rho_\beta = \\ &= h^\mu_\alpha h^\rho_\beta\pounds_n K_{\mu\rho} - 4K_{\beta\mu}K^\mu_\alpha\,, \end{aligned} \tag{3.96}$$

where we used the Lie derivative of the intrinsic curvature (3.65). Inverting this equation

$$h^\mu_\alpha h^\rho_\beta\pounds_n K_{\mu\rho} = \pounds_n K_{\alpha\beta} + 4K_{\beta\mu}K^\mu_\alpha\,. \tag{3.97}$$

Therefore equation (3.95) becomes

$$\begin{aligned} h^\mu_\alpha h^\rho_\beta n^\nu \nabla_\nu K_{\mu\rho} &= \pounds_n K_{\alpha\beta} + 4K_{\beta\gamma}K^\gamma_\alpha - h^\mu_\alpha h^\rho_\beta \left(K_{\mu\gamma}\nabla_\rho n^\gamma + K_{\gamma\rho}\nabla_\mu n^\gamma\right) = \\ &= \pounds_n K_{\alpha\beta} + 4K_{\beta\gamma}K^\gamma_\alpha - K_{\alpha\gamma}K^\gamma_\beta - K_{\gamma\beta}K^\gamma_\alpha = \\ &= \pounds_n K_{\alpha\beta} + 2K_{\beta\gamma}K^\gamma_\alpha \,. \end{aligned} \tag{3.98}$$

Finally, inserting (3.93) and (3.98) in (3.92), we obtain

$$R_{\mu\nu\rho\sigma} n^\sigma n^\nu h^\mu_\alpha h^\rho_\beta = -K_{\nu\beta}K^\nu_\alpha + \pounds_n K_{\alpha\beta} + 2K_{\beta\gamma}K^\gamma_\alpha + D_\alpha a_\beta + a_\alpha a_\beta \tag{3.99}$$

which, after a trivial simplification, is exactly the result. □

3.4.3 Einstein tensor equations

In the previous sections we computed the ADM formulation equations involving the Riemann tensor. We can find analogous equations involving the Einstein tensor. The equations we want to prove are

$$2n^\mu n^\nu G_{\mu\nu} = -\epsilon\, {}^{(3)}R + \left(K^2 - K_{\mu\nu}K^{\mu\nu}\right) \,, \tag{3.100}$$

$$n^\rho h^\nu_\mu G_{\nu\rho} = n^\rho h^\nu_\mu R_{\nu\rho} = D_\mu K - D_\nu K^\nu_\mu \,, \tag{3.101}$$

where we define the spatial Ricci tensor and scalar as

$${}^{(3)}R \equiv h^{\mu\rho}\, {}^{(3)}R_{\mu\rho} \equiv h^{\mu\rho} h^{\nu\sigma} R_{\mu\nu\rho\sigma} \,. \tag{3.102}$$

Proof of (3.100). Consider the equation

$$\begin{aligned} h^{\mu\rho}h^{\nu\sigma}R_{\mu\nu\rho\sigma} &= \left(g^{\mu\rho} + n^\mu n^\rho\right)\left(g^{\nu\sigma} + n^\nu n^\sigma\right) R_{\mu\nu\rho\sigma} = \\ &= \left(g^{\mu\rho} + n^\mu n^\rho\right)\left(R_{\mu\rho} + n^\nu n^\sigma R_{\mu\nu\rho\sigma}\right) = \\ &= R + n^\nu n^\rho R_{\nu\rho} + n^\mu n^\rho R_{\mu\rho} + n^\mu n^\rho n^\nu n^\sigma R_{\mu\nu\rho\sigma} = \\ &= R + 2n^\nu n^\rho R_{\nu\rho} = \\ &= -g_{\mu\nu} n^\mu n^\nu R + 2n^\mu n^\nu R_{\mu\nu} = \\ &= 2n^\mu n^\nu G_{\mu\nu} \,, \end{aligned} \tag{3.103}$$

where we used the fact that $n^\mu n^\rho n^\nu n^\sigma R_{\mu\nu\rho\sigma} = 0$ because the Riemann tensor is null if three or four of its indices are time indices, and the definition of Ricci tensor (1.2), Ricci scalar (1.3), and Einstein tensor (1.7).

This equation can be combined with the Gauss-Codazzi equation (3.69). In fact, contracting the indices with the induced metric

$$\begin{aligned} h^{\mu\rho}h^{\nu\sigma}\, {}^{(3)}R_{\mu\nu\rho\sigma} &= h^{\mu\rho}h^{\nu\sigma}h^\alpha_\mu h^\beta_\nu h^\gamma_\rho h^\delta_\sigma R_{\alpha\beta\gamma\delta} - h^{\mu\rho}h^{\nu\sigma}\left(K_{\mu\rho}K_{\nu\sigma} - K_{\mu\sigma}K_{\nu\rho}\right) = \\ &= h^{\alpha\gamma}h^{\beta\delta}R_{\alpha\beta\gamma\delta} - \left(K^2 - K_{\mu\nu}K^{\mu\nu}\right) \,, \end{aligned} \tag{3.104}$$

where we used the fact that spatial tensors indices can be raised/lowered with the induced metric, see (3.17). The first term on the right hand side can be substituted with (3.103) to obtain the result. □

Proof of (3.101). We firstly prove the first equality. From the Einstein tensor definition

$$\begin{aligned} n^\mu h^\nu_\rho G_{\mu\nu} &= n^\mu h^\nu_\rho R_{\mu\nu} - \frac{1}{2} n^\mu h^\nu_\rho g_{\mu\nu} R = \\ &= n^\mu h^\nu_\rho R_{\mu\nu} - \frac{1}{2} n_\nu h^\nu_\rho R = \\ &= n^\mu h^\nu_\rho R_{\mu\nu} \,, \end{aligned} \tag{3.105}$$

because $n_\nu h^\nu_\rho = 0$.
In order to prove the second equality, consider the equation (3.83), and contract two indices with the induced metric

$$h^{\alpha\gamma} h^\mu_\alpha h^\rho_\gamma h^\nu_\beta n^\sigma R_{\mu\nu\rho\sigma} = -h^{\alpha\gamma} D_\alpha K_{\beta\gamma} + h^{\alpha\gamma} D_\beta K_{\alpha\gamma} \,, \tag{3.106}$$

$$h^{\gamma\mu} h^\rho_\gamma h^\nu_\beta n^\sigma R_{\mu\nu\rho\sigma} = -D_\alpha K^\alpha_\beta + D_\beta K \,, \tag{3.107}$$

$$h^{\mu\rho} h^\nu_\beta n^\sigma R_{\mu\nu\rho\sigma} = -D_\alpha K^\alpha_\beta + D_\beta K \,, \tag{3.108}$$

$$\left(g^{\mu\rho} + n^\mu n^\rho\right) h^\nu_\beta n^\sigma R_{\mu\nu\rho\sigma} = -D_\alpha K^\alpha_\beta + D_\beta K \,, \tag{3.109}$$

$$h^\nu_\beta n^\sigma g^{\mu\rho} R_{\mu\nu\rho\sigma} = -D_\alpha K^\alpha_\beta + D_\beta K \,, \tag{3.110}$$

where we repeatedly used the induced metric to raise/lower indices as in (3.17) and the fact that the Riemann tensor is null if three or four of its indices are time indices. From the last, using the definition of spatial Ricci tensor, we immediately obtain the result. □

3.4.4 Ricci tensor equations

Finally, we prove some equations involving the Ricci tensor

$$h^\rho_\mu h^\sigma_\nu R_{\rho\sigma} = {}^{(3)}R_{\mu\nu} + K K_{\mu\nu} - 2K^\sigma_\rho K_{\sigma\mu} - \pounds_n K_{\mu\nu} - N^{-1} D_\mu D_\nu N \,, \tag{3.111}$$

$$R = {}^{(3)}R + K_{\mu\nu}K^{\mu\nu} - K^2 - 2\nabla_\mu \left(n^\mu K + a^\mu\right) \,. \tag{3.112}$$

We also prove that the latter equation can be re-written as

$${}^{(3)}R = R + 2n_\mu n_\nu R^{\mu\nu} + K_{\mu\nu}K^{\mu\nu} - K^2 \,. \tag{3.113}$$

Proof of (3.111). Consider the Gauss–Codazzi equation, and contract two indices with the induced metric

$$h^{\nu\sigma}\, {}^{(3)}R_{\mu\nu\rho\sigma} = h^{\nu\sigma} h^\alpha_\mu h^\beta_\nu h^\gamma_\rho h^\delta_\sigma R_{\alpha\beta\gamma\delta} - h^{\nu\sigma}\left(K_{\mu\rho}K_{\nu\sigma} - K_{\mu\sigma}K_{\nu\rho}\right) \,, \tag{3.114}$$

Similarly to the proof of the previous equation, we obtain

$${}^{(3)}R_{\mu\rho} = h^\alpha_\mu h^\gamma_\rho h^{\beta\delta} R_{\alpha\beta\gamma\delta} - K_{\mu\rho}K + K^\nu_\mu K_{\nu\rho} \,, \tag{3.115}$$

and therefore

$${}^{(3)}R_{\mu\rho} = h^\alpha_\mu h^\gamma_\rho g^{\beta\delta} R_{\alpha\beta\gamma\delta} + h^\alpha_\mu h^\gamma_\rho n^\beta n^\delta R_{\alpha\beta\gamma\delta} - K_{\mu\rho}K + K^\nu_\mu K_{\nu\rho} \,. \tag{3.116}$$

Substituting the second term on the right-hand side with (3.86) we obtain the result. □

Proof of (3.112). Consider the definition of Riemann tensor applied on the normal vector

$$R_{\mu\nu\rho\sigma} n^\sigma = \nabla_\mu \nabla_\nu n_\rho - \nabla_\nu \nabla_\mu n_\rho \,. \tag{3.117}$$

Contracting two indices we get

$$\begin{aligned} g^{\mu\rho} R_{\mu\nu\rho\sigma} n^\nu n^\sigma = R_{\nu\sigma} n^\nu n^\sigma &= n^\nu \left(\nabla_\sigma \nabla_\nu n^\sigma - \nabla_\nu \nabla_\sigma n^\sigma\right) = \\ &= \nabla_\sigma \left(n^\nu \nabla_\nu n^\sigma\right) + \nabla_\sigma n^\nu \nabla_\nu n^\sigma - \nabla_\nu \left(n^\nu \nabla_\sigma n^\sigma\right) - \nabla_\nu n^\nu \nabla_\sigma n^\sigma \,. \end{aligned} \tag{3.118}$$

Using the extrinsic curvature property (3.58)

$$-\nabla_\nu n_\nu = K_{\mu\nu} + n_\mu a_\nu \,, \tag{3.119}$$

we can substitute the covariant derivatives of the normal vectors. We obtain

$$\begin{aligned} R_{\nu\sigma} n^\nu n^\sigma &= \nabla_\sigma a^\sigma - \left(K^\nu_\sigma + n_\sigma a^\nu\right)\left(K^\sigma_\nu + n_\nu a^\sigma\right) - \nabla_\nu\left(n^\nu K + n^\nu n_\sigma a^\sigma\right) + \left(K + n_\nu a^\nu\right)\left(K + n_\sigma a^\sigma\right) \\ &= \nabla_\sigma a^\sigma - K^\nu_\sigma K^\sigma_\nu - \nabla_\nu\left(n^\nu K\right) + K^2 \\ &= \nabla_\nu\left(a^\nu + n^\nu K\right) - K_{\mu\nu}K^{\mu\nu} + K^2\,, \end{aligned} \tag{3.120}$$

where we repeatedly used the fact that $n_\mu a^\mu = 0$. But we can also write

$$R = -R g_{\mu\nu} n^\mu n^\nu = 2\left(G_{\mu\nu} - R_{\mu\nu}\right) n^\mu n^\nu \tag{3.121}$$

and use (3.100)

$$2n^\mu n^\nu G_{\mu\nu} = -\epsilon\, {}^{(3)}R + \left(K^2 - K_{\mu\nu}K^{\mu\nu}\right)\,, \tag{3.122}$$

to finally obtain

$$R = {}^{(3)}R + \left(K^2 - K_{\mu\nu}K^{\mu\nu}\right) - 2\nabla_\nu\left(a^\nu + n^\nu K\right) + 2K_{\mu\nu}K^{\mu\nu} - 2K^2\,. \tag{3.123}$$

After some trivial simplifications, we get the first result. The second equation be easily obtained substituting (3.122) into (3.121). □

3.5 Einstein equations

In the previous sections, we derived the equations that are needed to write the Einstein equations (1.6) (without cosmological constant, which can be added in the stress-energy tensor)

$$G_{\mu\nu} = 8\pi G T_{\mu\nu} \tag{3.124}$$

in the ADM formulations, i.e. in the $(3+1)$ form, in the presence of matter modelled with the stress-energy tensor $T_{\mu\nu}$. For completeness, although they will not be used in the thesis, we will introduce these equations and state how they can be solved in practice. The equations we derive are compatible with (3.15) in the ADM summary paper [20].

3.5.1 Constraint equations

Considering the reasoning in the introduction, we do not expect to find any contribution to the dynamics in the Einstein equations with at least one time index. In other words, these equations will only involve the presence of at most first-order time derivatives. Since we also have second-order derivatives in time in the space-space components, these equations will only act on the first-time derivatives as a constraint on the initial conditions.

Time-time component. This component can be computed as the projection of both indices of the Einstein equations (3.124) with the normal vectors. We already computed the left hand side in equation (3.100). Therefore we obtain

$$2n^\mu n^\nu G_{\mu\nu} = -\epsilon\, {}^{(3)}R + \left(K^2 - K_{\mu\nu}K^{\mu\nu}\right) = 16\pi G\, n^\mu n^\nu T_{\mu\nu}\,, \tag{3.125}$$

Time-space component. Applying a similar procedure, considering one index projected with the normal vector and one with the projection tensor, whose resulting equation right hand side is given by (3.101), we obtain

$$n^\rho h^\nu_\mu G_{\nu\rho} = D_\mu K - D_\nu K^\nu_\mu = 8\pi G\, n^\rho h^\nu_\mu T_{\nu\rho}\,. \tag{3.126}$$

Note that in both equations, the first time derivative is hidden in the definition of the extrinsic curvature, as can be explicitly seen in equation (3.62).

3.5.2 Equations of motion

The remaining space-space components are the ones carrying the dynamics. We will prove that the dynamics can be written in terms of two main equations

$$\partial_0 h_{ij} - \pounds_N h_{ij} = -2NK_{ij}\,, \tag{3.127}$$

$$\partial_0 K_{ij} - \pounds_N K_{ij} = N\,{}^{(3)}R_{ij} + N\left(KK_{ij} - 2K_i^r k_{rj}\right) - D_i D_j N - 16\pi G h_i^\alpha h_j^\beta \left(T_{\alpha\beta} - \frac{1}{2} g_{\alpha\beta} T\right)\,, \tag{3.128}$$

where $T = T_\alpha^\alpha$. Note that we decide to substitute the Lie derivative of the normal vector with equation (3.42)

$$\pounds_n Q_{\mu\nu} = \frac{1}{N}\left(\frac{\partial Q_{\mu\nu}}{\partial t} - \pounds_N Q_{\mu\nu}\right)\,, \tag{3.129}$$

because we want to explicit the time derivative of the dynamical quantities h_{ij} and K_{ij}.

Proof of (3.127). From equation (3.65)

$$\pounds_n h_{\mu\nu} = -2K_{\mu\nu}\,, \tag{3.130}$$

and substituting the Lie derivative of the normal vector with (3.42) we immediately obtain the result. To get the spatial indices, we can project the equations with e_i^μ and e_j^ν (see equation (3.21) and its discussion). □

Proof of (3.128). Consider the left hand side of (3.128). Using (3.42) and (3.111)

$$h_\mu^\rho h_\nu^\sigma R_{\rho\sigma} = {}^{(3)}R_{\mu\nu} + KK_{\mu\nu} - 2K_\rho^\sigma K_{\sigma\mu} - \pounds_n K_{\mu\nu} - N^{-1} D_\mu D_\nu N\,. \tag{3.131}$$

we can write

$$N \pounds_n K_{\mu\nu} = \partial_0 K_{ij} - \pounds_N K_{ij} = N\,{}^{(3)}R_{\mu\nu} + N\left(KK_{\mu\nu} - 2K_\rho^\sigma K_{\sigma\mu}\right) - D_\mu D_\nu N - h_\mu^\rho h_\nu^\sigma R_{\rho\sigma}\,. \tag{3.132}$$

But from the trace of the Einstein equations (3.124)

$$8\pi G\, T = g^{\mu\nu} R_{\mu\nu} - \frac{1}{2} g^{\mu\nu} g_{\mu\nu} R = -R\,, \tag{3.133}$$

where we used the fact that $g^{\mu\nu} g_{\mu\nu} = 4$. Therefore, again from the Einstein equations

$$R_{\mu\nu} = 8\pi G\, T_{\mu\nu} + \frac{1}{2} g_{\mu\nu} R = 8\pi G \left(T_{\mu\nu} - \frac{1}{2} g_{\mu\nu} T\right)\,. \tag{3.134}$$

Inserting this result in (3.132) we obtain the result with covariant indices. To get the spatial indices, we can project the equations with e_i^μ and e_j^ν. □

3.5.3 Solving procedure

Given the equations just found, the procedure is the following

(i) introduce a foliation of the spacetime, which should be completely arbitrary and contain the four functions $N(x^\mu)$ and $N^i(x^\mu)$;

(ii) choose initial values of h_{ij} and K_{ij} consistent with the constraint equations

$$ {}^{(3)}R + K^2 - K_{\mu\nu} K^{\mu\nu} = 16\pi G\, n^\mu n^\nu T_{\mu\nu}\,, \tag{3.135}$$

$$D_i K - D_j K_i^j = 8\pi G\, n^\rho h_i^\nu T_{\nu\rho}\,; \tag{3.136}$$

(iii) evolve the system with the dynamical equations

$$\partial_0 h_{ij} - \pounds_N h_{ij} = -2NK_{ij}\,, \tag{3.137}$$

$$\begin{aligned}\partial_0 K_{ij} - \pounds_N K_{ij} = N\,{}^{(3)}R_{ij} + N\left(KK_{ij} - 2K_i^r k_{rj}\right) - D_i D_j N - \\ - 16\pi G h_i^\alpha h_j^\beta \left(T_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}T\right)\,.\end{aligned} \tag{3.138}$$

Note that we can entirely and uniquely determine the metric components from the dynamical equations provided we specify initial conditions compatible with the constraint equations.

Moreover, it is important to note that the Einstein equations in the $(3+1)$ form are covariant by definition but foliation dependent. These equations implicitly depend on the form of the normal vector field $n^\mu(x^\mu)$, which describes how the spacetime is foliated.

3.6 Action

Another way to obtain the equations of motion is to use the action principle. We can vary the Einstein-Hilbert action with respect to N, N^μ and $h_{\mu\nu}$, and obtain the Einstein equations in the $(3+1)$ form we found in the previous section. In this section, we will provide the action written in a convenient way for the variation and explore its properties.

Consider the usual Einstein–Hilbert action (without the cosmological constant) (1.1)

$$S = \frac{1}{16\pi G}\int d^4x\sqrt{-g}R\,. \tag{3.139}$$

We can rewrite it with the previous result (3.112)

$$R = {}^{(3)}R + K_{\mu\nu}K^{\mu\nu} - K^2 - 2\nabla_\mu\left(n^\mu K + a^\mu\right)\,. \tag{3.140}$$

Therefore we can define the ADM action as

$$S_{\text{ADM}} = \frac{1}{16\pi G}\int dtd^3x\, N\sqrt{h}\,\mathcal{L}_{\text{ADM}} - \frac{1}{8\pi G}\int d^4x\sqrt{-g}\nabla_\mu\left(n^\mu K + a^\mu\right) \equiv S_{\text{ADM}} + S_{\text{surf}}\,, \tag{3.141}$$

where the ADM Lagrangian is

$$\mathcal{L}_{\text{ADM}} \equiv {}^{(3)}R + K_{\mu\nu}K^{\mu\nu} - K^2\,. \tag{3.142}$$

The second term S_{surf} is a covariant derivative, and therefore it does not contribute to the equations of motion once we vary the total action.

The first term S_{ADM} is the main ADM action, which gives the constraint equations (3.135) and (3.126) when we variate respectively with respect to N and N^i; and the dynamical equations (3.137) and (3.138) when varying with respect to $h_{\mu\nu}$. Note that S_{ADM} is quadratic in the time derivative of the dynamical variable $h_{\mu\nu}$, providing proper dynamical equations when we variate with respect to $h_{\mu\nu}$. In fact, as already mentioned, these time derivatives are hidden in the definition of the extrinsic curvature, as we can explicitly see in (3.62)

$$K_{ij} = \frac{1}{2N}\left[D_i N_j + D_j N_i - \partial_0 h_{ij}\right]\,. \tag{3.143}$$

From the latter equation, we can find another essential property of this action. The lapse appears only in the determinant $N\sqrt{h}$ factor, and as N^{-1} in the definition of the extrinsic curvature, while the shift can be found only in the definition of the extrinsic curvature. Moreover none of these two appears differentiated in time. This fact will be of great importance when we introduce the Hamiltonian formulation in the next section.

3.7 Hamiltonian formulation

Finally, we have all the theoretical tools to introduce the Hamiltonian formulation. In this formulation, even at a Newtonian mechanics level, the Lagrangian coordinates (q and $\dot{q}$ of classical mechanics) are replaced by the Hamiltonian *canonical coordinates* (q and p of classical mechanics). Moreover, in the previous section, we introduced the ADM Lagrangian, from which the equations are computed. In this section, we will compute the analogous function, the ADM Hamiltonian, from which the equations of motion, the Hamilton equations, are computed.

3.7.1 Legendre transform

Analogously to the canonical momenta $p = \partial\mathcal{L}/\partial\dot{q}$ of classical mechanics, we can define the canonical momenta for the quantities appearing in our action from the action by means of the Legendre transform. As we mentioned in the previous section, since $\dot{N}$ and $\dot{N}^i$ do not appear in the Lagrangian, the canonical momenta of N and N^i

$$\frac{\partial}{\partial\dot{N}}\left[\sqrt{-g}\mathcal{L}_{\text{ADM}}\right] \qquad \text{and} \qquad \frac{\partial}{\partial\dot{N}^i}\left[\sqrt{-g}\mathcal{L}_{\text{ADM}}\right] \tag{3.144}$$

are identically null, and therefore it is not necessary to define them. Moreover, the equations coming from the variations of the action with respect of N and N^i

$$\frac{\partial S_{\text{ADM}}}{\partial N} = 0 \qquad \text{and} \qquad \frac{\partial S_{\text{ADM}}}{\partial N^i} = 0 \tag{3.145}$$

act as constraints, and these two variables do not participate in the real evolution.

The real dynamic is instead given by h_{ij} and the canonical variables of h_{ij} we are about to define. The canonical momenta of h_{ij} is defined as in classical mechanics as

$$p^{ij} \equiv \frac{\partial}{\partial\dot{h}_{ij}}\left[\sqrt{-g}\mathcal{L}_{\text{ADM}}\right]. \tag{3.146}$$

But, as we previously noted, the time derivative of h_{ij} comes only from the extrinsic curvature, and therefore we can write

$$p^{ij} = \frac{\partial K_{rs}}{\partial\dot{h}_{ij}}\frac{\partial}{\partial K_{rs}}\left[\sqrt{-g}\mathcal{L}_{\text{ADM}}\right]. \tag{3.147}$$

If we rewrite the $\mathcal{L}_{\text{ADM}}$ as

$$\begin{aligned}\sqrt{-g}\mathcal{L}_{\text{ADM}} &= \frac{\sqrt{h}N}{16\pi G}\left[\,^{(3)}R + K_{ij}K^{ij} - K^2\right] = \\ &= \frac{\sqrt{h}N}{16\pi G}\left[\,^{(3)}R + h^{is}h^{jr}\left(K_{ij}K_{sr} - K_{is}K_{sr}\right)\right] = \\ &= \frac{\sqrt{h}N}{16\pi G}\left[\,^{(3)}R + \left(h^{is}h^{jr} - h^{ij}h^{sr}\right)K_{ij}K_{sr}\right],\end{aligned} \tag{3.148}$$

we can easily compute the canonical momenta as

$$\begin{aligned}16\pi G\, p^{ij} &= \frac{\partial K_{mn}}{\partial\dot{h}_{ij}}\sqrt{h}N\frac{\partial}{\partial K_{mn}}\left\{\left[\left(h^{is}h^{jr} - h^{ij}h^{sr}\right)K_{ij}K_{sr}\right]\right\} = \\ &= \left(-\frac{1}{2N}\right)\sqrt{h}N\left[2\left(h^{is}h^{jr} - h^{ij}h^{sr}\right)K_{sr}\right] = \\ &= -\sqrt{h}\left[\left(K^{ij} - h^{ij}K\right)\right] \equiv \pi^{ij},\end{aligned} \tag{3.149}$$

where we have computed $\partial K_{rs}/\partial\dot{h}_{ij}$ using the extrinsic curvature equation (3.62). The factors 2 in the second line comes from the redefinition of dummy indices in the summations. The variables π^{ij}

are sometime used instead of the extrinsic curvature K^{ij} due to their immediate interpretation in the Hamiltonian formulation (see for instance [20]).

Note that the K_{ij} implicitly contains the dependence on the canonical variables through

$$K^{ij} = -\frac{16\pi G}{\sqrt{h}}\left(p^{ij} - \frac{1}{2}p\, h^{ij}\right) = -\frac{1}{\sqrt{h}}\left(\pi^{ij} - \frac{1}{2}\pi\, h^{ij}\right), \tag{3.150}$$

where p and π are respectively the trace of p^{ij} and π^{ij}. This can be easily proven starting from (3.149) and its trace

$$16\pi G\, p = 2K\sqrt{h}\,, \tag{3.151}$$

and substituting everything to obtain K^{ij}.

3.7.2 Hamiltonian

The Hamiltonian density is given by the usual equation

$$\mathcal{H}_{\mathrm{ADM}} = \frac{\partial}{\partial \dot{h}_{ij}}\left[\sqrt{-g}\mathcal{L}_{\mathrm{ADM}}\right]\dot{h}_{ij} - \sqrt{-g}\mathcal{L}_{\mathrm{ADM}} = p^{ij}\dot{h}_{ij} - \sqrt{-g}\mathcal{L}_{\mathrm{ADM}}\,. \tag{3.152}$$

Again, in principle we should also add the derivatives of the Lagrangian with respect to $\dot{N}$ and $\dot{N}^i$, because N and N^i are valid action variables. But in this formulation, terms like $\partial(\sqrt{-g}\mathcal{L}_{\mathrm{ADM}})/\partial\dot{N}^i$ are null.

We can explicitly compute the ADM Hamiltonian density

$$\begin{aligned}
16\pi G\,\mathcal{H}_{\mathrm{ADM}} &= \sqrt{h}\left(K^{ij} - h^{ij}K\right)\left(2NK_{ij} - D_iN_j - D_jN_i\right) - \sqrt{h}N\left[{}^{(3)}R + K_{ij}K^{ij} - K^2\right] = \\
&= \sqrt{h}\left(2NK^{ij}K_{ij} - 2NK^2 - 2K^{ij}D_iN_j + 2Kh^{ij}D_iN_j\right) - \sqrt{h}\,N\left[{}^{(3)}R + K_{ij}K^{ij} - K^2\right] = \\
&= \sqrt{h}\,N\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) - \sqrt{h}\left[2K^{ij} - 2h^{ij}K\right]D_iN_j = \\
&= \sqrt{h}\,N\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) - \\
&\quad - \sqrt{h}D_i\left[\left(2K^{ij} - 2h^{ij}K\right)N_j\right] + \sqrt{h}D_i\left(2K^{ij} - 2h^{ij}K\right)N_j\,,
\end{aligned} \tag{3.153}$$

where in the first equality we used (3.62) to substitute $\dot{h}_{ij}$ in terms of the extrinsic curvature, and exploited several times the symmetry of the extrinsic curvature $K_{ij} = K_{ji}$. We can neglect the total derivative term (a total derivative in the three-dimensional hypersurface), and write the Hamiltonian as

$$H_{\mathrm{ADM}} \equiv \int_\Sigma d^3y\,\mathcal{H} = \int_\Sigma d^3y\,\frac{\sqrt{h}}{16\pi G}\left[N\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) + 2D_i\left(K^{ij} - h^{ij}K\right)N_j\right]. \tag{3.154}$$

From the Hamiltonian theory, we know that we can write the action as

$$S_H = \int_{t_1}^{t_2} dt\left\{\int_\Sigma d^3y\, p^{ij}\dot{h}_{ij} - H_{\mathrm{ADM}}\right\}, \tag{3.155}$$

which is called Hamiltonian action. Our canonical coordinates are h_{ij} and p_{ij}, among with the coordinates N and N^i. Since in the action they only appear linearly in H_{ADM}, N and N^i can be considered as Lagrange multipliers. In fact, although $\dot{h}_{ij}$ seems to have a definite dependence to N^i given by (3.62), in applying the variational principle we should interpret $\dot{h}_{ij}(t)$ as the time derivative of a generic $h_{ij}(t)$ which is set by the variation procedure.

Before proceeding further, we should make a comment about the coordinate invariance of the Hamiltonian density $\mathcal{H}$. In fact, it is known (also in Newtonian mechanics) that the Hamiltonian is not a scalar, and it does not remain the same if we perform a change of Hamiltonian coordinates. In fact, consider the Hamiltonian coordinates transformation of the *spatial* sector, namely h_{ij} and p^{ij}, on the constant time hypersurface $\Sigma(t)$. A general transformation of our Hamiltonian variables which preserves the Hamilton equations is in the form

$$t' = t + c \tag{3.156}$$
$$h'_{ij} = h'_{ij}(t, h_{ij}) \tag{3.157}$$
$$p'^{ij} = \frac{\partial h_{kh}}{\partial h'_{ij}} p^{hk}\,, \tag{3.158}$$

where c is a constant. The transformation is the natural transformation for a canonical variable p^{ij} given a scalar (on the three-dimensional hypersurface) Lagrangian $\mathcal{L}_{\rm ADM}$ where the canonical variables transform as usual

$$t' = t + c \tag{3.159}$$
$$h'_{ij} = h'_{ij}(t, h_{ij}) \tag{3.160}$$
$$\dot{h}'_{ij} = \frac{\partial h'_{ij}}{\partial h_{hk}} \dot{h}_{hk} + \frac{\partial h'_{ij}}{\partial t}\,. \tag{3.161}$$

In other words, the latter transformation has the form of a *defined* total derivative (we can not really consider it a total derivative because the Lagrangian h_{ij} and $\dot{h}_{ij}$ are independent coordinates). It is straightforward to show that, under the general coordinate transformation of Hamiltonian coordinates on the three-dimensional hypersurfaces, the Hamiltonian in the new coordinates will be

$$\mathcal{H}' = \mathcal{H} + \frac{\partial h'_{ij}}{\partial t} p'^{ij} = \mathcal{H} + \frac{\partial h_{ij}}{\partial t'} p^{ij}\,. \tag{3.162}$$

It can also be proven that the condition (3.162) ensures that the Hamiltonian equations in both the coordinate systems h_{ij} - p^{ij} and h'_{ij} - p'^{ij} are the same. The Lagrangian is invariant under such a change of Lagrangian coordinates.

From this equation, we see that, once the foliation of spacetime is fixed, and therefore we are considering transformations only on the three-dimensional hypersurfaces, in general, the Hamiltonian will change on the hypersurface under a change of spatial Hamiltonian coordinates only if the transformation is time-dependent.

3.7.3 Hamilton equations

In order to find the equations of motion, in the absence of matter, we can proceed varying the action with respect to the coordinates h_{ij}, p^{ij}, N and N^i. The equations we found are the usual Hamilton equations

$$\frac{dh_{ij}}{dt} = \frac{\delta H_{\rm ADM}}{\delta p^{ij}} \equiv Q_{ij}\,, \tag{3.163}$$
$$\frac{dp^{ij}}{dt} = -\frac{\delta H_{\rm ADM}}{\delta h_{ij}} \equiv P^{ij}\,, \tag{3.164}$$

and the two constraint equations

$$C \equiv \frac{\delta H_{\rm ADM}}{\delta N} = 0\,, \tag{3.165}$$
$$C_i \equiv \frac{\delta H_{\rm ADM}}{\delta N^i} = 0\,. \tag{3.166}$$

As already mentioned, the latter constraint equations can be found noticing that we can interpret N and N^i as Lagrange multipliers (see equation (3.155) and the discussion below). Again, the dynamics will be included in P^{ij} and Q_{ij} equations, while the variations with respect to N and N^i provide constraint equations for the initial conditions.

C equation. Starting from the definition, we notice again that N only appears as a Lagrange multiplier (no N is hidden in the definition of K_{ij})

$$C \equiv \frac{\delta H_{\text{ADM}}}{\delta N} = K_{ij}K^{ij} - K^2 - {}^{(3)}R = 0\,, \tag{3.167}$$

which is exactly the time-time component of the Einstein equations (3.135).

C_i equation. Analogously to the previous constraint equation, we obtain

$$C_i \equiv \frac{\delta H_{\text{ADM}}}{\delta N^i} = 2D_j\left(K_i^j - \delta_i^j K\right) = 2D_jK_i^j - 2D_iK = 0\,, \tag{3.168}$$

which is exactly the time-space component of the Einstein equations (3.126).

Q_{ij} equation. We omit the lengthy computation which only involves the substitution of K_{ij} and K respectively with (3.150) and (3.151). We obtain

$$Q_{ij} \equiv \frac{\delta H_{\text{ADM}}}{\delta p^{ij}} = \frac{32\pi G}{\sqrt{H}}N\left(p_{ij} - \frac{p}{2}h_{ij}\right) + 2D_{(i}N_{j)} = \frac{dh_{ij}}{dt}\,. \tag{3.169}$$

P^{ij} equation. Also in this case, we omit the computation, which involves the same substitutions as for Q_{ij}, among with the substitution of the spatial Ricci scalar with (3.112), to obtain the Einstein tensor G^{ij}. We obtain

$$\begin{aligned} P^{ij} \equiv \frac{\delta H_{\text{ADM}}}{\delta h_{ij}} &= N\sqrt{h}\,G^{ij} - \frac{N}{2\sqrt{h}}\left(p_{rs}p^{rs} - \frac{p^2}{2}\right)h^{ij} + \frac{2N}{\sqrt{h}}\left(p_r^i p^{rj} - \frac{p}{2}p^{ij}\right) - \\ &- \sqrt{h}\left(D^iD^jN - h^{ij}D^rN_r\right) - \sqrt{h}D_r\left(\frac{1}{\sqrt{h}}p^{ij}N^r\right) + 2p^{r(i}D_rN^{j)} = \frac{dp^{ij}}{dt}\,. \end{aligned} \tag{3.170}$$

The latter equations correspond respectively to the Lagrangian equations (3.137) and (3.138). Since the Hamiltonian variation principle is equivalent to the Lagrangian one, the equations should be the same, up to the substitution of the appropriate coordinates with the Legendre transformation.

3.8 Conclusion

In this section, we introduced an alternative covariant way to formulate General Relativity which splits the time and space part of the Einstein equations in an arbitrary spacetime (provided you can foliate it with space-like hypersurfaces) and rewrote the Einstein equations in a $(3+1)$ form. Moreover, the problem can be rethought with the Hamiltonian formulation, obtaining equivalent equations of motion. The advantage of this procedure is to have a better picture of what are the dynamical quantities, the spatial components, and what are just constraints on the initial conditions.

We will apply this formulation on a general theory for modified gravity models with one additional degree of freedom, the Effective Field Theory, in Chapter 9.

Part II

Modified gravity

Chapter 4

Introduction

In this Chapter, we introduce some extensions of the General Relativity action (1.1), which might be considered to explain some experimental effects at large scales, namely dark energy and dark matter. We introduce some theoretical problems of the cosmological problem solution of dark energy. Regarding the dark matter, although its presence is necessary to explain some phenomena (see section 2.3), no experiment has made a direct observation of it. This justifies the possibility of searching for alternatives to ΛCDM also for dark matter.

Finally, we also list some of the necessary mathematical conditions for viable alternative models of gravity at *large scales*. We stress that General Relativity at *small scales* (Solar System scales) is still the paradigm theory as no deviations from it have been found with experiments.

4.1 Dark Energy

In section 2.4 we have seen some pieces of evidence for the presence of dark energy, namely the age of the universe and the accelerated expansion problems. The simplest solution is to introduce a cosmological constant as the source of dark energy (see Chapter 1). In this section, we want to show the limit of this choice in the context of cosmology.

4.1.1 Fine tuning

In this section we explain the *fine-tuning* problem as presented by S. Weinberg [22]. Consider the Einstein equations (1.6), where the stress-energy tensor $T_{\mu\nu}$ includes the matter components of the universe. From Quantum Field Theory (QFT) we know that the vacuum has its own energy, and contributes to the stress-energy tensor with a constant energy density term

$$T_{\text{vac},\,\mu\nu} = -\rho_{\text{vac}} g_{\mu\nu} \,. \tag{4.1}$$

The value of the vacuum energy density from QFT is given by the sum over all possible zero-point energy of the scalar field

$$\rho_{\text{vac}} = \int^{\bar{k}} \frac{4\pi dk}{(2\pi)^3} \frac{k^2}{2} \sqrt{k^2 + m^2} \cong \frac{\bar{k}^4}{16\pi^2} \,, \tag{4.2}$$

where $\bar{k}$ is the cut-off momentum of the theory, and we consider that large k dominate in the integral. If the cut-off is at the Planck mass (expected limit of validity of General Relativity), we find $\rho_{\text{vac}} = 10^{71}$ Gev^4.

The vacuum part of the stress-energy tensor (4.1) indeed behaves like the cosmological constant Λ in the Einstein–Hilbert action, since it is proportional to the metric. If we consider the vacuum energy density as a contribution to Λ, we can rewrite the Einstein equations as

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = G_{\mu\nu} - \tilde{\Lambda} g_{\mu\nu} - 8\pi G T_{\text{vac},\,\mu\nu} = 8\pi G T_{\mu\nu} \,, \tag{4.3}$$

where $\tilde{\Lambda}$ is a the bare cosmological constant that does not contains the vacuum energy contribution, i.e., $\Lambda = 8\pi G\rho_{\rm vac} - \tilde{\Lambda}$. We also know that the value of ρ_Λ is given by (1.30), which if computed with experimental data is

$$\rho_\Lambda \equiv \frac{\Lambda}{8\pi G} = \rho_{cr}\Omega_\Lambda^0 = \frac{3H_0^2}{8\pi G}\Omega_\Lambda^0 \cong 10^{-47}\ \text{GeV}^4\,. \tag{4.4}$$

Therefore the bare constant $\tilde{\Lambda}$ should satisfy

$$\rho_\Lambda = \rho_{\rm vac} - \rho_{\tilde{\Lambda}} \qquad \Rightarrow \qquad |\rho_{\tilde{\Lambda}} - \rho_{\rm vac}| \cong 10^{-47}\ \text{GeV}^4\,. \tag{4.5}$$

This means that $\rho_{\tilde{\Lambda}}$ and $\rho_{\rm vac}$ must cancel with a precision of 121 significant figures. This huge precision needed in the definition of the cosmological constant is the essence of the fine-tuning problem.

Moreover, we know that the cosmological constant is related to the fractional density with $\Lambda = 3H_0^2\Omega_\Lambda^0$. Therefore even a slight modification of Λ changes not only the cosmic evolution of dark energy coming from the cosmological constant but also the evolution of the other components (because all the fractional densities must obey (1.32), i.e., they must sum to 1). This is another face of the fine-tuning problem: the value of Λ must be fine-tuned to match the observed cosmic evolution.

4.1.2 Coincidence problem

Another problem arises when we analyse the time when the dark energy starts to be non-negligible. Consider the matter-dark energy equality condition

$$\rho_\Lambda = \rho_m. \tag{4.6}$$

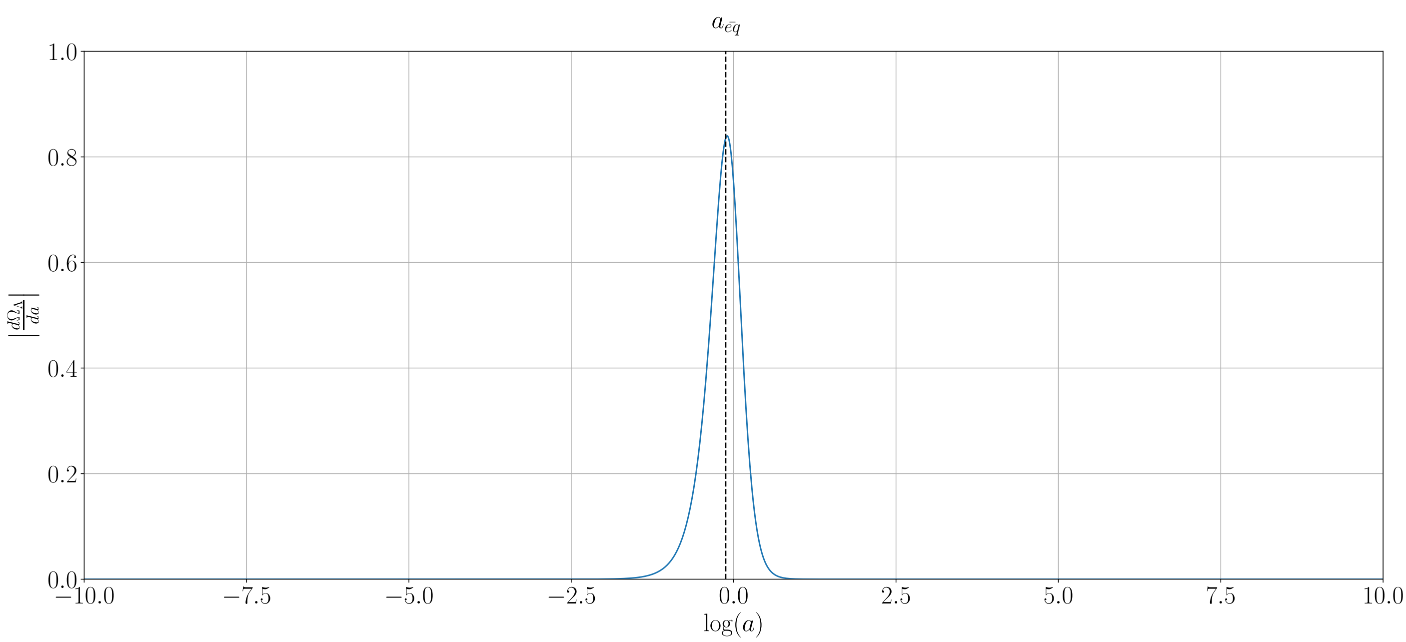


Figure 4.1: Plot of the derivative of Ω_Λ with respect to the scale factor a. The spike is at the value of $a_{\bar{eq}}$ computed with $\Omega_\Lambda = 0.7$.

Using the definitions in equation (1.30), and $\Omega_m^0 = 1-\Omega_\Lambda^0$ since we are neglecting other contributions, we find the matter-dark energy scale factor

$$a_{eq} = \sqrt[3]{\frac{1-\Omega_\Lambda^0}{\Omega_\Lambda^0}}\,. \tag{4.7}$$

If we consider $\Omega_\Lambda^0 = 0.7$, we obtain $a_{eq} \cong 0.75$, very close to the value of the scale factor today $a = 1$. Also, the derivative of the cosmological constant fractional density with respect to the scale factor a

$$\frac{d\Omega_\Lambda}{da} = -\frac{3a^2}{(a^3+1)^2}, \tag{4.8}$$

is shown in Figure 4.1. We immediately see that today ($\log(a) = 0$) is the only moment where the derivative has a maximum. This is the essence of the *coincidence problem*. In fact, if the densities of the matter and the cosmological constant were different, we would see a different behaviour.

4.2 Extensions of General Relativity

For the problems mentioned above, the theory of General Relativity seems not to be the definitive theory of gravity at large scales. An alternative is to consider some extension theories, which usually add new degrees of freedom to General Relativity.* However, such theories have a downside: they can be complicated to solve analytically, as we will see in the following Chapters.

We can generalize the Einstein–Hilbert action (1.1) as

$$S = \int d^4x\sqrt{-g}f(R, R_{\mu\nu}, R_{\mu\nu\rho\sigma}, \phi, V^\mu, T^{\mu\nu}, \dots), \tag{4.9}$$

where ϕ, V^μ and $T^{\mu\nu}$ are generic scalar, vector and tensor fields that we add as new degrees of freedom. Note that this generalization includes not only models with *minimally coupled* matter, i.e., models where the matter and gravity sectors of the action are independent, and the matter part depends on gravity only through the presence of the metric.

In general, we have an infinite arbitrariness in choosing the type and the number of additional degrees of freedom we can add to a theory. In practice, several constraints should be taken into account. In this section, we will list *some* of the main mathematical conditions the modified gravity models should satisfy to be viable for cosmology, i.e., a theory free of mathematical instabilities.

4.2.1 Ostrogradsky instabilities

The Ostrogradsky instabilities appear when the equations of motions have a differential order higher than two. We firstly revisit the standard *stable* second-order differential equations case and then analyse the third-order case.

Second-order systems. In a general second-order in time physics theory, we consider a Lagrangian

$$\mathcal{L} = \mathcal{L}\left(t, q^k(t), \dot{q}^k(t)\right), \tag{4.10}$$

where t is the time coordinate, q^k and $\dot{q}^k$ are the Lagrangian coordinates, and $k \in [0, n]$ denotes the Lagrangian coordinate. The coordinates are independent from each others, i.e., $\dot{q}$ is not $dq(t)/dt$ at this point.

Using the variational principle, we can derive the Euler–Lagrange equations

$$\begin{cases} \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{q}^k} - \frac{\partial\mathcal{L}}{\partial q^k} = 0 \\ \dot{q}^k = \frac{dq^k}{dt} \end{cases}, \tag{4.11}$$

* Although we will not deal with this problem in the thesis, it is important to stress that the addition of new degrees of freedom to a theory should always be done carefully. Only quantitative treatments with statistical methods, such as Bayesian model comparison, can assess if experimental data favour them with respect to General Relativity. In fact, following Occam's razor principle, it is pointless to add new degrees of freedom if a theory with less has already the same accordance with data.

where we consider for simplicity a system completely described by the Lagrangian $\mathcal{L}$ (i.e. all the Lagrangian components $\mathcal{Q}_k = 0$). We can further expand the first equation and obtain

$$\frac{d\dot{q}^s}{dt}\frac{\partial^2\mathcal{L}}{\partial\dot{q}^s\partial\dot{q}^k} + \frac{dq^s}{dt}\frac{\partial^2\mathcal{L}}{\partial q^s\partial\dot{q}^k} - \frac{\partial\mathcal{L}}{\partial q^k} = 0\,, \tag{4.12}$$

from which we should require the invertibility of the $\partial^2\mathcal{L}/\partial\dot{q}^s\partial\dot{q}^k$ coefficients matrix if we want to isolate the *accelerations*. In other words, we should request the non-degeneracy of the Lagrangian ($\partial\mathcal{L}/\partial\dot{q}^k \neq 0$ for each k), or analogously

$$\det\left(\frac{\partial^2\mathcal{L}}{\partial\dot{q}^s\partial\dot{q}^k}\right) \neq 0\,. \tag{4.13}$$

Provided the condition above is satisfied, also using the second equation, we can rewrite the system of equations in a normal form

$$\frac{d^2q^k}{dt^2} = F\left(t, q^k, \frac{dq^k}{dt}\right)\,, \tag{4.14}$$

which ensures there are no *ambiguities* in the results. To solve this differential equation as a Cauchy problem, the normal form in addition to the $2n$ (n for q^k and n for its time derivative) initial conditions are required to satisfy the Cauchy theorem hypothesis and obtain the existence and uniqueness of the differential equation's solution.

We can then use the Legendre transform to obtain the canonical coordinates (Hamilton coordinates) using

$$\begin{cases} t' = t + c \\ q'^k = q^k \\ p_k = \frac{\partial\mathcal{L}}{\partial\dot{q}^k}\,, \end{cases} \tag{4.15}$$

where c is a constant. From the last equation, since the Lagrangian is non-degenerate, we can also write the inverse transform in order to obtain $\dot{q}^k = \dot{q}^k(t, q^k, p_k)$. Therefore we can write the Hamiltonian as

$$\mathcal{H}(t, q^k, p_k) = p_k\dot{q}^k(t, q^k, p_k) - \mathcal{L}(t, q^k, \dot{q}^k, (t, q^k, p_k))\,. \tag{4.16}$$

where $\dot{q}^k = \dot{q}^k(t, q^k, p_k)$ in the canonical space is not a variable any more, but a function of the Hamilton coordinates. The Jacobi theorem states that the Hamiltonian coincides with the mechanical energy of the system if and only if it does not explicitly depend on time, i.e. $\partial\mathcal{H}/\partial t = 0$. Another theorem ensures that a system evolving with the Euler–Lagrange equations, after the Legendre transformation, evolves with the Hamilton equations

$$\begin{cases} \frac{dq^k}{dt} = \frac{\partial\mathcal{H}}{\partial p_k} \\ \frac{dp_k}{dt} = -\frac{\partial\mathcal{H}}{\partial q^k}\,. \end{cases} \tag{4.17}$$

This system of differential equations is at first order, and each canonical variable should have an initial condition for a total of $2n$ initial conditions. Therefore the number of canonical coordinates should be equal to the number of initial conditions.

Third-order systems. Consider the following Lagrangian[†]

$$\mathcal{L} = \mathcal{L}\left(t, q^k(t), \dot{q}^k(t), \ddot{q}^k(t)\right)\,, \tag{4.18}$$

where, with respect to (4.10), we add a dependence to the coordinates $\ddot{q}^k$, and update the definition of non-degeneracy on the higher order coordinate, i.e. $\partial\mathcal{L}/\partial\ddot{q}^k \neq 0$ for each k. As in the previous case, we

[†] This is a more detailed discussion of [23, 24].

should consider all the Lagrangian coordinates independent. The Euler–Lagrange equations are

$$\begin{cases} \frac{d^2}{dt^2}\frac{\partial \mathcal{L}}{\partial \ddot{q}^k} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}^k} + \frac{\partial \mathcal{L}}{\partial q^k} = 0 \\ \dot{q}^k = \frac{dq^k}{dt} \\ \ddot{q}^k = \frac{d^2 q^k}{dt^2} \, . \end{cases} \tag{4.19}$$

In other words, the equations of motion are in the form

$$q^{k\,(4)} = F\left(t, q^k, \frac{dq^k}{dt}, \frac{d^2q^k}{dt^2}, \frac{d^3q^k}{dt^3}\right) \tag{4.20}$$

which means that the solutions of these differential equations will depend on four initial conditions for each k, i.e. $4n$ initial conditions. The number of canonical coordinates should then be $4n$, since each of them generates a first order differential equations and needs an initial condition.

The analogous of the Legendre transformation proposed by Ostrogradsky is

$$\begin{cases} t' = t + c \\ q'^k = q^k \\ \dot{q}'^k = \dot{q}^k \\ p_k^1 = \frac{\partial \mathcal{L}}{\partial \dot{q}^k} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \ddot{q}^k} \\ p_k^2 = \frac{\partial \mathcal{L}}{\partial \ddot{q}^k} \, , \end{cases} \tag{4.21}$$

where the last two comes from the definition of canonical momentum once we define q'^k and $\dot{q}'^k$. For instance, when the Lagrangian does not depend on q^k, from the Euler–Lagrange equations (4.19), we obtain that the conserved quantity is exactly p_k^1.

Moreover, from this transformation we can justify the non-degeneracy condition as $\partial\mathcal{L}/\partial\ddot{q}^k \neq 0$ for each k. In fact, this is the condition needed to invert the Legendre transformation and obtain $\ddot{q}^k = \ddot{q}^k(t, q^k, \dot{q}^k, p_k^1, p_k^2)$ as functions of the canonical coordinates from the p_k^2 equation above

$$p_k^2 = \frac{\partial \mathcal{L}\left(t, q^k, \dot{q}^k, \ddot{q}^k\right)}{\partial \ddot{q}^k} \, . \tag{4.22}$$

However, the Lagrangian depends only on three Lagrangian coordinates for each k, and therefore also the inverse function should be a function of only three canonical coordinates. Thus we can remove the dependence on one conjugate momentum, for instance $\ddot{q}^k = \ddot{q}^k(t, q^k, \dot{q}^k, p_k^2)$.

We do not explicitly need $\partial\mathcal{L}/\partial\dot{q}^k \neq 0$ in order to find $\dot{q}'^k = \dot{q}'^k(t, q^k, \dot{q}^k, p_k^1, p_k^2)$, because we already have by definition that $\dot{q}'^k = \dot{q}^k$. With these we can then write the analogous of Hamiltonian (4.16) as

$$\begin{aligned} \mathcal{H} = \sum_{i=1}^{2} q^{k\,(i)}(t, q^k, \dot{q}^k, p_k^1, p_k^2)p_k^i - \mathcal{L}\left(t, q^k, \dot{q}^k, \ddot{q}^k(t, q^k, \dot{q}^k, p_k^1, p_k^2)\right) = \\ = p_k^1\dot{q}^k + p_k^2\ddot{q}^k(t, q^k, \dot{q}^k, p_k^2) - \mathcal{L}\left(t, q^k, \dot{q}^k, \ddot{q}^k(t, q^k, \dot{q}^k, p_k^2)\right) \, , \end{aligned} \tag{4.23}$$

where we removed the dependence of $\ddot{q}^k$ on one of the conjugate momenta, see discussion around (4.22), and therefore the Hamiltonian depends only linearly on p_1^k. In this case $\dot{q}^k$ is a canonical variable, while $\ddot{q}^k$ is a function of 3 out of 4 canonical variables. We can also find the analogous of the Hamilton equations, similarly to (4.17), i.e. considering

$$\begin{cases} \frac{dq^k}{dt} = \frac{\partial \mathcal{H}}{\partial p_k^1} \\ \frac{d\dot{q}^k}{dt} = \frac{\partial \mathcal{H}}{\partial p_k^2} \\ \frac{dp_k^1}{dt} = -\frac{\partial \mathcal{H}}{\partial q^k} \\ \frac{dp_k^2}{dt} = -\frac{\partial \mathcal{H}}{\partial \dot{q}^k} \, . \end{cases} \tag{4.24}$$

Omitting the $\dddot{q}^k$ dependence on the canonical variables to simplify the notation, we can evaluate these equations. The first equation is

$$\frac{dq^k}{dt} = \frac{\partial \mathcal{H}}{\partial p_k^1} = \dot{q}^k\,; \tag{4.25}$$

the second is

$$\frac{d\dot{q}^k}{dt} = \frac{\partial \mathcal{H}}{\partial p_k^2} = \ddot{q}^k + p_l^2 \frac{\partial \ddot{q}^l}{\partial p_k^2} - \frac{\partial \mathcal{L}}{\partial \ddot{q}^l}\frac{\partial \ddot{q}^l}{\partial p_k^2} = \ddot{q}^k\,; \tag{4.26}$$

the third is

$$\frac{dp_k^1}{dt} = -\frac{\partial \mathcal{H}}{\partial q^k} = -p_l^2 \frac{\partial \ddot{q}^l}{\partial q^k} + \frac{\partial \mathcal{L}}{\partial q^k} + \frac{\partial \mathcal{L}}{\partial \ddot{q}^l}\frac{\partial \ddot{q}^l}{\partial q^k} = \frac{\partial \mathcal{L}}{\partial q^k}\,; \tag{4.27}$$

and the last is

$$\frac{dp_k^2}{dt} = -\frac{\partial \mathcal{H}}{\partial \dot{q}^k} = -p_k^1 - p_l^2 \frac{\partial \ddot{q}^l}{\partial \dot{q}^k} + \frac{\partial \mathcal{L}}{\partial \dot{q}^k} + \frac{\partial \mathcal{L}}{\partial \ddot{q}^l}\frac{\partial \ddot{q}^l}{\partial \dot{q}^k} = -p_k^1 + \frac{\partial \mathcal{L}}{\partial \dot{q}^k}\,. \tag{4.28}$$

From these equations, it is apparent that the Hamiltonian (4.23) can generate a non-trivial evolution of all the defined Hamiltonian coordinates. Therefore it might be tempting to use higher order derivative theories to describe systems that can not be described by second-order differential equations in time. However, the Hamiltonian (4.23) is linear in one of the conjugate momenta, and this has vast implications on stability. A linear momentum dependence means no bound on the energy, and the system energy can indefinitely decrease. This instability is called Ostrogradsky instability, taking the mathematician's name who first formalized the Hamiltonian formulation of higher-order derivative theories. The same procedure can also be applied to higher order systems, obtaining equivalent instabilities. This means that no theory can be formulated with higher-order derivatives if we want to avoid these instabilities.

It is important to stress that this derivation was carried out starting from the Lagrangian, and therefore the Ostrogradsky instabilities appear at the background level. These are different from instabilities that might appear when we perturb the background as done in AppendixA (in the case of additional degrees of freedom, as perturbations in plain General Relativity are stable). We discuss these instabilities in the next section.

Finally, a comment about the non-degeneracy of the Lagrangian is in order. If the determinant (4.13) is null, there will be an *ambiguity* in the results, as the solution is not unique (if it exists). For instance, this is the case of gauge degrees of freedom, which introduce arbitrary functions of time to the results and create a mathematical ambiguity. The core of this *mathematical* ambiguity is that, although a physical state is uniquely determined given a set of q^k and p_k values, the converse is not true, since more than one set of values q^k and p_k represent a given physical state. In other words, the whole set of canonical coordinates q^k and conjugate momenta p_k overly describe the physical state: some of these are redundant in the description of the physical state. Even if taken into account, the lack of non-degeneracy does not change the general conclusions about the presence of Ostrogradsky instabilities. However, some theories exploit the gauge freedom which comes from the degeneracy of the Lagrangian to obtain ad-hoc higher order derivatives equations of motion which circumvent the Ostrogradky instabilities problem (see for instance Beyond Horndeski in Section 5.7).

4.2.2 Gradient and ghost instabilities

Another category of mathematical instability describes gradient and ghost instabilities. While Ostrogradsky's instabilities are general, the gradient and ghost ones might appear when we compute the perturbations.

These instabilities are linked to the so-called quadratic action, which is computed perturbing the action at the quadratic order in perturbations, i.e. retaining all the terms quadratic in the perturbation quantities. As an example, we consider the perturbations over a FLRW background, with the metric (1.55) for the scalar perturbations sector and the metric (1.57) for the tensor part. Moreover, we add a scalar field $\varphi(t,\vec{x}) = \varphi_0(t) + \delta\varphi(t,\vec{x})$ not coupled with the matter (the standard matter part of the action S_m remains unmodified), where φ_0 is the background value of the scalar field and $\delta\varphi(t,\vec{x})$ a small (compared to the background) perturbation. The quadratic action is usually in the form

$$\begin{aligned} S_{\rm S}^{(2)} = \int d^4x \, \Big\{ & Q_s(t) \left[\dot{\Phi}^2 - \frac{c_s^2(t)}{a^2} \Phi_{,k} \, \Phi^{,k} + \dots \right] \\ & + Q_T(t) \left[\dot{E}_{ij} \dot{E}^{ij} - \frac{c_T^2(t)}{a^2} E_{ij,k} \, E^{ij,k} + \dots \right] \\ & + Q_\varphi(t) \left[\dot{\delta\varphi}^2 - \frac{c_\varphi^2(t)}{a^2} \delta\varphi_{,k} \, \delta\varphi^{,k} + \dots \right] \Big\} \,, \end{aligned} \tag{4.29}$$

where Φ is the gravitational potential appearing in the perturbed metric (1.55) in the scalar sector, E_{ij} is the tensor perturbation matrix defined in (1.57), and ... denote terms that are not important for this discussion. For instance, the dots might include terms like $\delta\varphi\delta\dot{\varphi}$ which do not affect stability, or the velocity of the perfect fluid. Moreover, the parts for the velocity of the perfect fluid standard matter are missing, since we know from General Relativity they are stable. The last part is related to the scalar field, and therefore if there are more scalar fields or different tensors, this part should be replaced with the appropriate ones.

The perturbation functions Q_s, Q_T, c_s^2, and c_T^2 are functions of time only. In fact, the quantities Φ^2 and h^2 in the quadratic action (4.29) are at second order, and, in the settings we are considering, only perturbations quantities are carrying space dependencies (for instance the background is $1+\Psi(t,\vec{x})$). Therefore Q_s, Q_T, c_s^2, and c_T^2 should be only functions of time. Otherwise, any spatial contributions inside this function would increase the order of the action from the quadratic order.

In the scalar field theories, the scalar field and the gravitational field perturbations can be studied together using the unitary gauge, which is defined as the gauge where we gauge fix the scalar perturbations $\delta\varphi$ as null. In this case, the problem is simplified since we can study the standard scalar and tensor perturbations (Φ and E_{ij} parts) conditions. The unitary gauge will be discussed in details in section 8.2.1.

The stability is ensured if the quadratic action has

(i) the *correct kinetic sign*, i.e. the *kinetic part* of the perturbation denoted with the square of the time derivative of the perturbation appear with a positive sign. Therefore the Q_i functions should be positive, i.e.

$$Q_i(t) > 0 \qquad \forall t \,, \tag{4.30}$$

where i is an index that goes trough all possible perturbation degrees of freedom. This is similar to what happen in the Ostrogradsky instabilities case, where the *energy* of the perturbations is not bounded from below. If a Q function is negative, the instabilities that might occur are called *ghost instabilities*;

(ii) the correct sign in the perturbation equations, i.e. a positive *sound speed* c_i^2

$$c_i^2(t) > 0 \qquad \forall t \,. \tag{4.31}$$

If the sign is negative, it means that the perturbations equations, which are usually in an harmonic oscillator like form

$$\delta\dot{\varphi} + \frac{k^2 c_s^2}{a^2} \delta\phi + \dots = 0 \,, \tag{4.32}$$

are exponentially growing, breaking the perturbation assumption of some of the quantities. In this case the instabilities are called *gradient instabilities*.

Therefore, a mathematically stable theory also requires these two sets of conditions.

Note that while the ghost instabilities are hard to tame, the gradient instabilities are sometimes considered milder. It is possible to create theories that accept negative sound speeds in some epochs if the period needed for the exponential perturbations to grow is much larger than the time where the additional degrees of freedom (with respect to General Relativity) are non-negligible.

4.3 Conclusions

In this Chapter, we presented some problems of the ΛCDM model, where the dark energy comes from the cosmological constant, namely the fine-tuning and coincidence problems. We also argued that, since no experiment has yet found any direct evidence of dark matter presence, it is worthy of exploring alternatives also for this dark sector.

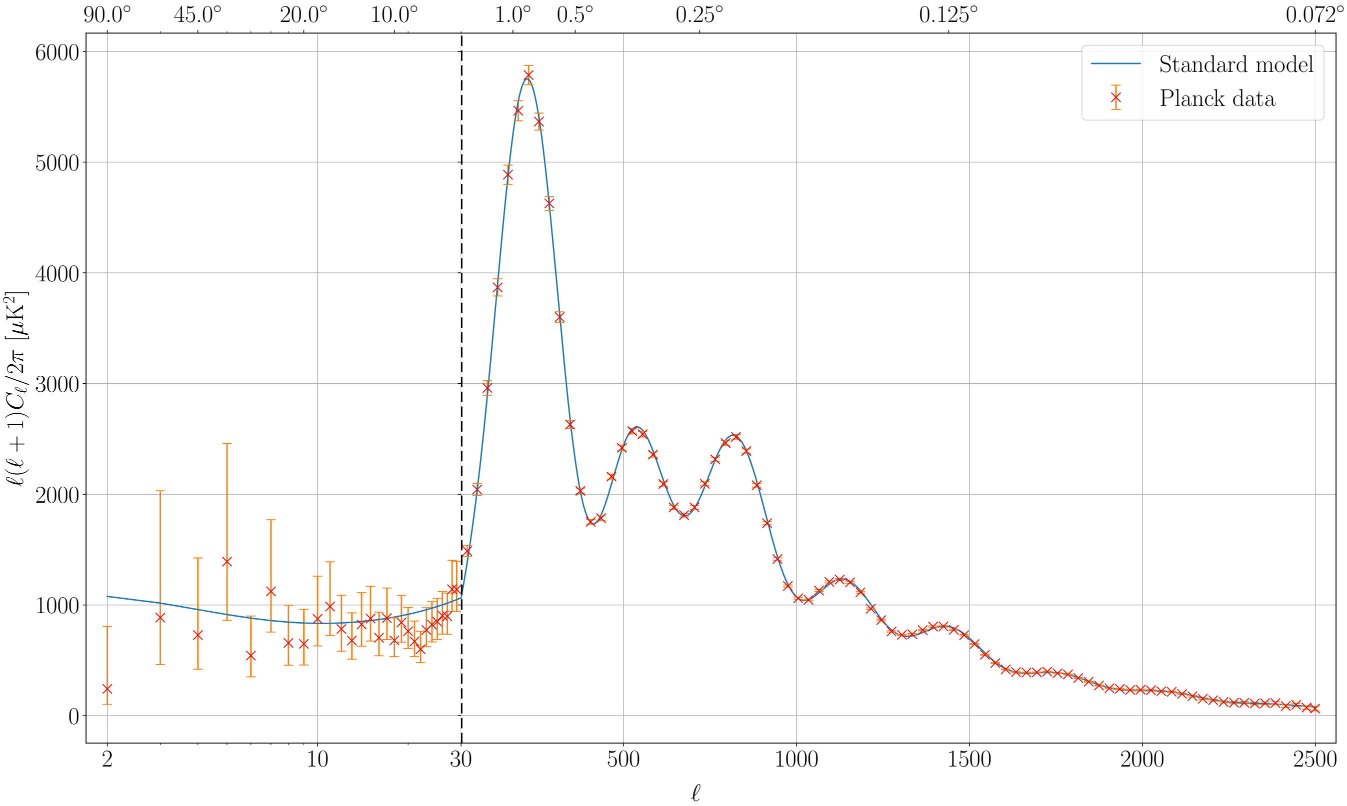


Figure 4.2: Plot of the Planck data of the Cosmic Microwave Background (CMB) power spectrum [5] and the standard model prediction, here expressed with a normalized intensity C_ℓ as a function of the angular distance between two incoming photons (upper x-axis). We can appreciate the precision of Planck data and the great accordance between the observation and the theory, which can be achieved only by including dark energy and dark matter contributions in the theoretical model. Alternative models without dark energy and dark matter can not fit the data.

A general way to extend the current theory of gravity is to modify the Einstein–Hilbert action as

$$S = \int d^4x \sqrt{-g} f(R, R_{\mu\nu}, R_{\mu\nu\rho\sigma}, \phi, V^\mu, T^{\mu\nu}, \dots) \,, \tag{4.33}$$

where we considered a generic function of additional degrees of freedom from different sources. While this approach can introduce an infinite arbitrariness in the choice of these extensions, we should always have in mind the mathematical stability conditions in order to avoid background instabilities coming from the introduction of differential equations of time order bigger than two (Ostrogradsky instabilities), and perturbation instabilities (*ghost* and *gradient* instabilities).

Checking the lack of the instabilities mentioned above does not grant the physical viability of the model. Both at the background and the perturbations level, there are many data that constraint the possible models we can propose. For instance, the CMB data from the Planck experiment has severely constrained the perturbation data [5], as we can see from Figure 4.2. Moreover, this experiment confirmed the need for dark energy and dark matter once again since the plot in the Figure can fit the data only if we consider these components.

Chapter 5

Horndeski theory

In this Chapter, we introduce *Horndeski gravity*. This theory was at first obtained by Horndeski [6], and recently rediscovered in [25]. In the following, we will also use parametrization of the Horndeski theories proposed in [26]. In this section is also discussed the original work about de Sitter solutions in Horndeski gravity [7].

5.1 Action

The Horndeski gravity is a modified general relativity theory with the following action

$$S[g_{\mu\nu},\phi] = \frac{1}{8\pi G}\int d^4x\sqrt{-g}\sum_{i=2}^{5}\mathcal{L}_i[g_{\mu\nu},\phi] + S_M[g_{\mu\nu}], \tag{5.1}$$

where the four Lagrangian parts $\mathcal{L}_i$ are defined as

$$\mathcal{L}_2 = G_2[\phi,X] \tag{5.2}$$
$$\mathcal{L}_3 = -G_3[\phi,X]\Box\phi \tag{5.3}$$
$$\mathcal{L}_4 = G_4[\phi,X]R + G_{4X}[\phi,X]\left[(\Box\phi)^2 - \phi_{;\mu\nu}\phi^{;\mu\nu}\right] \tag{5.4}$$
$$\mathcal{L}_5 = G_5[\phi,X]G_{\mu\nu}\phi^{;\mu\nu} - \frac{1}{6}G_{5X}[\phi,X]\left[(\Box\phi)^3 - 3(\Box\phi)\phi_{;\mu\nu}\phi^{;\mu\nu} + 2\phi_{;\mu}{}^{\nu}\phi_{;\nu}{}^{\alpha}\phi_{;\alpha}{}^{\mu}\right]. \tag{5.5}$$

The $G_i[\phi,X]$ are four arbitrary functions of a scalar field ϕ and $X = \partial_\mu\phi\partial^\mu\phi$. Moreover, $\Box = \nabla_\mu\nabla^\mu$, while the subscript ϕ or X on the G_i functions represent respectively the derivative with respect to ϕ and X, e.g. $G_{iX} \equiv \partial G_i/\partial X$ and $G_{i\phi} \equiv \partial G_i/\partial\phi$.

The main feature of this Lagrangian is that the equations of motion are second-order differential equations. This is achieved by a careful cancellation of higher order terms given by the structure of the action. It can be proved that this is the most general theory of General Relativity with one additional scalar degree of freedom (with respect to General Relativity) with second-order differential equations [6]. As we explain in section 4.2, this property is essential to avoid the presence of Ostrogradsky instabilities.

The action of General Relativity is obtained considering

$$G_2[\phi,X] = -\Lambda,\ G_4[\phi,X] = \frac{M_{\rm Pl}^2}{2} \text{ and } G_3[\phi,X] = G_5[\phi,X] = 0. \qquad (\Lambda\text{CDM model}) \tag{5.6}$$

Note that in this formulation, there is no coupling in the Horndeski gravity action between the matter part $S_M[g_{\mu\nu}]$ and the scalar field.

5.2 Equations of motion

Varying the action (5.1) and imposing the FLRW metric

$$ds^2 = -dt^2 + a(t)^2(dx^2 + dy^2 + dz^2)\,, \tag{5.7}$$

we obtain the equations of motion

$$H^2 = \frac{8\pi G}{3M_\bullet^2}\left(\rho + \rho_\phi\right) \tag{5.8}$$

$$\dot{H} + H^2 = -\frac{4\pi G}{3M_\bullet^2}\left(\rho + \rho_\phi + 3P + 3P_\phi\right) \tag{5.9}$$

where ρ and P are the energy density and pressure of standard matter, as defined in (1.16), and ρ_ϕ and P_ϕ are the energy density and pressure of the scalar field, defined as

$$\begin{aligned}\frac{8\pi G}{3}\rho_\phi = &-\frac{1}{3}G_2 + \frac{2}{3}X\left(G_{2X} - G_{3\phi}\right) - \frac{2H^3\dot{\phi}X}{3}\left(7G_{5X} + 4XG_{5XX}\right) \\ &+ H^2\left[1 - M_\bullet^2\left(1-\alpha_B\right) - 4X\left(G_{4X} - G_{5\phi}\right) - 4X^2\left(2G_{4XX} - G_{5\phi X}\right)\right],\end{aligned} \tag{5.10}$$

$$\begin{aligned}\frac{8\pi G}{3}P_\phi = &\frac{1}{3}G_2 - \frac{2}{3}X\left(G_{3\phi} - 2G_{4\phi\phi}\right) + \frac{4H\dot{\phi}}{3}\left(G_{4\phi} - 2XG_{4\phi X} + XG_{5\phi\phi}\right) - \frac{\ddot{\phi}}{3\dot{\phi}}HM_\bullet^2\alpha_B \\ &- \frac{4}{3}H^2X^2G_{5\phi X} - \left(H^2 + \frac{2\dot{H}}{3}\right)\left(1 - M_\bullet^2\right) + \frac{2H^3\dot{\phi}}{3}XG_{5X}.\end{aligned} \tag{5.11}$$

The dot denotes a derivative with respect to the cosmological time t. In these definitions, we introduce some new functions, namely $M_\bullet^2$ and α_B. These are part of a set of functions of time that can specify the Horndeski gravity model considered, which is equivalent to specify the G_i functions *at the perturbations level* (not at the action level, because the G_i functions are covariant, while the α functions are not). The α functions are usually used in place of the G_i functions to describe the perturbations as they have an immediate physical interpretation (see the following list), and they allow a simpler form for the perturbation equations. The complete set is given by:

(i) the *cosmological strength of gravity*, defined as the normalization of the kinetic term of gravitons. In the language of the G_i functions, this is*

$$M_\bullet^2 \equiv 2\left[G_4 - 2XG_{4X} + XG_{5\phi} - H\dot{\phi}XG_{5X}\right]. \tag{5.12}$$

Moreover, the time derivative of $M_\bullet^2$

$$\alpha_M \equiv \frac{d\ \ln\ M_\bullet^2}{d\ \ln\ a} = \frac{1}{H}\frac{d\ \ln\ M_\bullet^2}{dt}\,, \tag{5.13}$$

is called the *Planck-mass run rate*. This function is used for large-scale structure computations, which are sensitive only to variations of the Planck mass.

(ii) the *kineticity*, which is the coefficient of the kinetic term for the scalar field, is defined as

$$\begin{aligned}H^2M_\bullet^2\alpha_K \equiv\ &2X\left[G_{2X} + 2XG_{2XX} - 2G_{3\phi} - 2XG_{3\phi X}\right] \\ &+ 12H\dot{\phi}X\left[G_{3X} + XG_{3XX} - 3G_{4\phi X} - 2XG_{4\phi XX}\right] \\ &+ 12H^2X\left[G_{4X} - G_{5\phi} + X\left(8G_{4XX} - 5G_{5\phi X}\right) + 2X^2\left(2G_{4XXX} - G_{5\phi XX}\right)\right] \\ &+ 4H^3\dot{\phi}X\left[3G_{5X} + 7XG_{5XX} + 2X^2G_{5XXX}\right];\end{aligned} \tag{5.14}$$

* The symbol for the cosmological strength of gravity here is different from the standard one. We are considering different functions to distinguish the *constant* M_*^2 that will appear in the EFT action (8.81) and the cosmological strength *function* $M_\bullet^2$, as defined in [26].

(iii) the *braiding*, which is usually interpreted as the strength of a fifth force between massive particles. This operator gives rise to a new mixing of the scalar field and metric kinetic terms for the propagating degree of freedom. It is defined as

$$HM_\bullet^2\alpha_B \equiv 2\dot{\phi}\left[XG_{3X} - 2G_{4\phi} - 2XG_{4\phi X}\right] + 8HX\left[G_{4X} + 2XG_{4XX} - G_{5\phi} - XG_{5\phi X}\right] + 2H^2\dot{\phi}X\left[3G_{5X} + 2XG_{5XX}\right]\,; \tag{5.15}$$

(iv) the *tensor excess*, that is the difference between the speed of light and the propagation speed of the gravitational waves, i.e. $\alpha_T = 1 - c_T^2$. Using the G_i functions, α_T is

$$M_\bullet^2\alpha_T \equiv 4X\left[G_{4X} - G_{5\phi}\right] - 2\left[\ddot{\phi} - H\dot{\phi}\right]XG_{5X}\,. \tag{5.16}$$

We will refer to this set of four functions as the α-functions from now on. Moreover, from (5.6) and the definitions above we find that the General Relativity theory has the following α functions definitions

$$M_\bullet^2 = 1 \qquad \text{and} \qquad \alpha_M = \alpha_K = \alpha_B = \alpha_T = 0\,, \qquad (\Lambda\text{CDM model}) \tag{5.17}$$

together with the evolution of the Hubble parameter H given by the standard Friedmann equations.

We can also define the state parameter ω_ϕ for the scalar field with the usual definition

$$\omega_\phi = \frac{\rho_\phi}{P_\phi}\,. \tag{5.18}$$

5.3 Linear Perturbations

Since the Horndeski gravity action (5.1) has no coupling between the standard matter term S_m and the scalar field ϕ, the standard matter perturbation equations are the same. We consider the perturbed metric in Newtonian gauge(1.55)

$$ds^2 = -\left[1 + 2\Psi(t,\vec{x})\right]dt^2 + a^2(t)\left[1 + 2\Phi(t,\vec{x})\right]\delta_{ij}dx^i dx^j\,. \tag{5.19}$$

The equations to be modified are the ones coming from the Einstein equations because the presence of another component from ϕ does not change the standard matter stress-energy tensor $T^{\mu\nu}$. Moreover, since we have a new dynamical degree of freedom given by the scalar field, we need to introduce a new equation for ϕ perturbations, usually called the perturbation Klein–Gordon equation. For the perturbations of the scalar field, we will use the gauge-invariant variable [26]

$$v_X = -a\frac{\delta\phi}{\dot{\phi}}\,. \tag{5.20}$$

The analogous of the tt Einstein equation (A.4) is

$$\frac{k^2\Phi}{a^2} + \frac{3}{2}\left(2 - \alpha_{\rm B}\right)H\dot{\Phi} - \frac{1}{2}\left(6 - \alpha_{\rm K} - 6\alpha_{\rm B}\right)H^2\Psi + \frac{1}{2}\left(\alpha_{\rm K} + 3\alpha_{\rm B}\right)H^2\dot{v}_X + \frac{1}{2}\left[\alpha_{\rm B}\frac{k^2}{a^2} - 3\dot{H}\alpha_{\rm B} + 3\left(2\dot{H} + \tilde{\rho}_{\rm m} + \tilde{p}_{\rm m}\right)\right]Hv_X = \frac{4\pi Ga^2}{M_*^2}\delta\rho\,, \tag{5.21}$$

while the analogous of the longitudinal traceless part of the ij Einstein equation (A.7) is

$$k^2\left[\Psi + \left(1 + \alpha_{\rm T}\right)\Phi - \left(\alpha_{\rm M} - \alpha_{\rm T}\right)Hv_X\right] = 12\pi Ga^2\Sigma\,, \tag{5.22}$$

The equation for the scalar field perturbations v_X

$$
\begin{aligned}
&-3H\alpha_{\rm B}\ddot{\Phi} + H^2\alpha_{\rm K}\ddot{v}_X + 3\left[\left(2\dot{H} + \tilde{\rho}_{\rm m} + \tilde{p}_{\rm m}\right) - H^2\alpha_{\rm B}\left(3+\alpha_{\rm M}\right) - \frac{d}{dt}\left(\alpha_{\rm B}H\right)\right]\dot{\Phi} \\
&\quad + \left(\alpha_{\rm K} + 3\alpha_{\rm B}\right)H^2\dot{\Psi} + 2\left(\alpha_{\rm M} - \alpha_{\rm T}\right)H\frac{k^2}{a^2}\Phi - \alpha_{\rm B}H\frac{k^2}{a^2}\Psi - \\
&\quad + \Big[3\left(2\dot{H} + \tilde{\rho}_{\rm m} + \tilde{p}_{\rm m}\right) - \dot{H}(2\alpha_{\rm K} + 9\alpha_{\rm B}) - \\
&\qquad - H\left(\dot{\alpha}_{\rm K} + 3\dot{\alpha}_{\rm B}\right) - H^2\left(3+\alpha_{\rm M}\right)\left(\alpha_{\rm K}+3\alpha_{\rm B}\right)\Big] H\Psi + \\
&\quad + \left[2\dot{H}\alpha_{\rm K} + \dot{\alpha}_{\rm K}H + H^2\alpha_{\rm K}\left(3+\alpha_{\rm M}\right)\right]H\dot{v}_X + H^2M^2v_X + \\
&\quad + \left[-\left(2\dot{H} + \tilde{\rho}_{\rm m} + \tilde{p}_{\rm m}\right) + 2H^2\left(\alpha_{\rm M} - \alpha_{\rm T}\right) + H^2\alpha_{\rm B}\left(1+\alpha_{\rm M}\right) + \frac{d}{dt}\left(\alpha_{\rm B}H\right)\right]\frac{k^2}{a^2}v_X = 0\,, \qquad (5.23)
\end{aligned}
$$

where

$$
H^2M^2 \equiv 3\dot{H}\left[\dot{H}\left(2-\alpha_{\rm B}\right) + \tilde{\rho}_{\rm m} + \tilde{p}_{\rm m} - H\dot{\alpha}_{\rm B}\right] - 3H\alpha_{\rm B}\left[\ddot{H} + \dot{H}H\left(3+\alpha_{\rm M}\right)\right]. \qquad (5.24)
$$

In addition to the equations of the standard matter density and velocity perturbations, we have the complete set of equations we can solve to obtain the perturbations functions.

5.4 Stability

In principle, by choosing different forms of G_i, we can create an infinite number of new models. Nevertheless, as explained in section 4.2, we should check that some stability conditions are satisfied to have stable perturbations. Once computed, using the unitary gauge where the perturbations of the scalar field are null, the quadratic action has indeed the form (4.29)

$$
S_{\rm S}^{(2)} = \int d^4x \left\{ Q_S(t,\vec{x})\left[\dot{\Phi}^2 - \frac{c_s^2(t,\vec{x})}{a^2}\Phi_{,k}\,\Phi^{,k}\right] + Q_T(t,\vec{x})\left[\dot{h}_{ij}\dot{h}^{ij} - \frac{c_T^2(t,\vec{x})}{a^2}h_{ij,k}\,h^{ij,k}\right]\right\} + \ldots\,, \qquad (5.25)
$$

where we omit the uninteresting terms for stability. Note that with respect to (4.29), the scalar field part is missing since we are in unitary gauge. The stability functions are defined as

$$
Q_s \equiv \frac{2M_\bullet^2 D}{(2-\alpha_B)^2} > 0\,, \qquad (5.26)
$$

$$
c_s^2 \equiv \frac{1}{D}\left[(2-\alpha_B)\left(-\frac{\dot{H}}{H^2} + \frac{1}{2}\alpha_B\left(1+\alpha_T\right) + \alpha_M - \alpha_T\right) - \frac{(\rho_m + P_m)}{H^2M_*^2} + \frac{\dot{\alpha}_B}{H}\right] > 0\,, \qquad (5.27)
$$

$$
Q_T \equiv \frac{M_\bullet^2}{8} > 0\,, \qquad (5.28)
$$

$$
c_T^2 \equiv 1 + \alpha_T > 0\,, \qquad (5.29)
$$

where ρ_m and P_m are respectively the energy density and the pressure of all matter (radiation, baryons, etc) without the scalar field contribution, and $D \equiv \alpha_K + 3\alpha_B^2/2$.

5.5 Horndeski gravity after GW170817/GRB170817A

In 2017, the LIGO/Virgo collaboration observed the event GW170817, produced by the merger of a binary neutron star system [11]. Thereafter, several counterparts across the electromagnetic (EM) spectrum were observed. In particular, the optical counterpart of the GW170817, the short gamma-ray burst event GRB170817A, was observed by the *Fermi* Gamma-ray Burst Monitor and the Anti-Coincidence Shield onboard the International Gamma-Ray Astrophysics Laboratory (*INTEGRAL*) spectrometer [12]. The optical counterpart GRB170817A was detected within a time-delay of $\delta t = (1.734 \pm 0.054)\,s$ from GW170817. Most of the time delay is dominated by astrophysical contributions, associated with the collapse of the hypermassive neutron star formed during the merger, and the final gravitational waves speed c_T is extremely close to the speed of light: $c_T \approx 1$.

This astonishingly simple observation has already placed severe constraints on several theories of modified gravity: any modified gravity model predicting $c_T \neq 1$ must now be seriously reconsidered, and several previously viable theories of gravity are now excluded [27, 28, 29, 30, 31] (see [32, 33] for earlier important work).

In the context of Horndeski gravity, the velocity of gravitational waves is described by the equation of α_T (5.16) as

$$c_T^2 \equiv 1 + \alpha_T \,, \tag{5.30}$$

where

$$\alpha_T \equiv \frac{4X}{M_\bullet^2}\left[G_{4X} - G_{5\phi}\right] - \frac{2X}{M_\bullet^2}\left[\ddot{\phi} - H\dot{\phi}\right] G_{5X} \,. \tag{5.31}$$

Looking at this equation, there are a couple of ways to obtain a $c_T^2 \approx 1$ (or $\alpha_T \approx 0$)

(i) one trivial solution is to consider some of the Horndeski functions in the action (5.1) null, i.e., $G_4 = 0$ and $G_5 = 0$. From these functions definitions (5.4) and (5.5), this condition eliminates all scalar field terms coupling with the Ricci scalar and with the Einstein tensor, in addition to quadratic and cubic derivative terms in $\mathcal{L}_4$ and $\mathcal{L}_5$. In particular, the first means that the scalar field could couple with gravity only minimally. However, we can relax the condition on G_4 since it only appears differentiated by X. Therefore the necessary condition to obtain a $c_T^2 = 1$ can be summarized as

$$G_{4X} = 0 \qquad \text{and} \qquad G_5 = 0 \,. \tag{5.32}$$

Or, in other words, G_4 can be only a function of the scalar field ϕ but not of its kinetic term X, $G_4(\phi, X) = G_4(\phi)$.

(ii) another way to approach the problem is to allow for a G_4 dependence on X and a non-null G_5. The condition is

$$G_{4X} = G_{5\phi} \qquad \text{and} \qquad G_{5X} = 0 \,. \tag{5.33}$$

(iii) finally, a very large cosmological strength of gravity $M_\bullet^2$ (5.12) can be considered. But, since this quantity is modifying effectively the Newton constant, a large $M_\bullet^2$ might be a very unlikely scenario.

Therefore, when we consider a Horndeski model, we should always check that at least one of these conditions is respected if we want to use it for late Universe cosmological applications.

Finally, we note that in principle, one could also imagine models where the dispersion relation of GWs is modified only outside the experiment conditions. For instance, we can create Horndeksi models with $c_T = 1$ today, but not on other periods. Alternatively, in non-Horndeski models (higher derivative models), we can propose models with $c_T = 1$ only for the range of wavelengths detectable by the LIGO/Virgo experiment.

5.6 de Sitter solutions

In this Chapter, we will explore the possibility of obtaining de Sitter solutions using the Horndeski gravity action. The discussion is based on [7].

5.6.1 Spherically symmetric space

Before considering the de Sitter solutions, we review some essential facts about Spherically Symmetric Space-times (SSS), of which the D-dimensional Friedmann-Lemaitre-Robertson-Walker space-times are examples. We follow the discussion in [34, 35].

The generic SSS metric reads

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = \gamma_{ab}(x)dx^a dx^b + r^2(x)dS^2_{D-2}\,, \tag{5.34}$$

where $a, b = 0, 1$ and r is a scalar quantity, while S^2_{D-2} is the $D-2$ dimensional sphere. Other relevant scalar quantities on SSS are

$$\chi = \gamma^{ab}\partial r_a \partial r_b\,, \tag{5.35}$$

and

$$\Phi = \nabla^2_\gamma r\,, \tag{5.36}$$

where ∇^2_γ is the two dimensional Laplacian on the two dimensional normal space-time whose metric is γ_{ab}.

For example, in a non-flat FLRW space-time with a metric

$$ds^2 = -dt^2 + a(t)^2\left(\frac{d\rho^2}{1-k\rho^2} + \rho^2 dS^2_{D-2}\right)\,, \quad k = 0, \pm K_0\,, \tag{5.37}$$

we obtain $x = (t, \rho)$, $r = a(t)\rho$, $\gamma_{ab} = \mathrm{diag}\left[-1, a^2/(1-k\rho^2)\right]$. Therefore the first scalar (5.35) becomes

$$\chi = \gamma^{ab}\partial r_a \partial r_b = 1 - r^2 J^2\,, \quad J^2 = H^2 + \frac{k}{a^2}\,. \tag{5.38}$$

The other invariant (5.36) reads

$$\Phi = \nabla^2_\gamma r = -(J^2 + Q^2)r\,, \quad Q^2 = H^2 + \dot{H}\,. \tag{5.39}$$

Thus J^2 and Q^2 are confirmed to be scalar quantities in a generic SSS. Moreover, the Ricci scalar can be obtained from these two scalar quantities as

$$R = 6\left[J^2 + Q^2\right]\,. \tag{5.40}$$

Another example is the de Sitter (dS) space-time. Besides the static patch

$$ds^2 = -(1 - H_0^2 r^2)dt^2 + \frac{dr^2}{1 - H_0^2 r^2} + r^2 dS^2\,, \tag{5.41}$$

where the Hubble parameter $H = H_0$ is a constant, dS space-time admits three FLRW space-times patches.

The first one is flat FLRW patch with $k = 0$,

$$ds^2 = -dt^2 + e^{2H_0 t}\left(d\rho^2 + \rho^2 dS_2^2\right)\,, \tag{5.42}$$

where $a(t) = e^{H_0 t}$, and $H = H_0$. From equation (5.38), we obtain $J^2 = H_0^2 = Q^2$.

The second is the $k > 0$ patch. With a set of new coordinates (T, R) it can be written as

$$ds^2 = -dT^2 + \cosh^2 H_0 T\left(\frac{dR^2}{1 - H_0^2 R^2} + R^2 dS_2\right)\,. \tag{5.43}$$

Here, $a(T) = \cosh H_0 T$, $k = H_0^2$ and $H = H_0 \sinh H_0 T/\cosh H_0 T$. We still have $J^2 = H_0^2 = Q^2$, as in the flat case.

Finally, we have the $k < 0$ dS patch. With another set of coordinates (τ, σ) we obtain,

$$ds^2 = -d\tau^2 + \sinh^2 H_0 \tau\left(\frac{d\sigma^2}{1 + H_0^2\sigma^2} + \sigma^2 dS_2\right)\,, \tag{5.44}$$

where $a(\tau) = \sinh H_0\tau$, $k = -H_0^2$ and $H = H_0 \cosh H_0\tau/\sinh H_0\tau$. Again, we have $J^2 = H_0^2 = Q^2$. In all dS patches, the Ricci scalar is constant and reads $R = 12H_0^2$

5.6.2 Example

In this section, we will investigate only a reduced sector of Horndeski in the vacuum. Consider the following Horndeski action

$$S = \int d^4x\sqrt{-g}\left[\frac{R}{2} + \alpha G^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - V(\phi)\right] , \tag{5.45}$$

where $G_5 = 4\pi G\alpha\phi$ and $G_2 = X + V(\phi)$, and the other G's are null. Note that, in order to obtain the same form of the (5.1), we should perform an integration by parts on the G_5 term. For simplicity, we consider $8\pi G = 1$ in this section. This model has been studied without the potential in Refs. [13, 10].

The generalized Friedmann equation can be found with `xAct` using the `FLCurved` metric option, see discussion around equation (A.1). Converting the result with the (5.38) and (5.39) scalar definitions, we obtain

$$3J^2 - 3\alpha\dot{\phi}^2\left(J^2 + 2H^2\right) = \frac{1}{2}\dot{\phi}^2 + V(\phi)\,. \tag{5.46}$$

Similarly, we can obtain the equation of motion associated with ϕ,

$$\frac{d}{dt}\left[a^3(1 + 6\alpha J^2)\dot{\phi}\right] = -a^3\frac{dV}{d\phi}\,. \tag{5.47}$$

The above equations agree with the non-flat FLRW Hordenski equations in Ref. [36]. Also, note that we can also obtain the second generalized Friedmann equation. However, this equation simply follows from the two above equations (5.46) and (5.47).

When the potential is constant, i.e. $V = V_0$, we have

$$\dot{\phi} = \frac{C}{a^3\left[1 + 6\alpha J^2\right]}\,, \tag{5.48}$$

where C is a constant of integration.

We want to investigate the existence of dS solution. Firstly, we consider the $k = 0$ case (5.42), and make the ansatz $a(t) = e^{H_0 t}$. The equation of motion of ϕ becomes

$$\dot{\phi} = \frac{C}{1 + 6\alpha H_0^2}e^{-3H_0 t}\,. \tag{5.49}$$

Inserting the same ansatz in the modified Friedmann equation (5.46), we obtain

$$3H_0^2 = \frac{C^2}{2}\frac{1 + 18\alpha H_0^2}{\left(6\alpha H_0^2 + 1\right)^2}\,e^{-6H_0 t} + V_0\,. \tag{5.50}$$

If we consider a constant scalar field, i.e., $C = 0$, we can choose $H_0^2 = V_0/3$ and obtain a flat dS-like solution. On the other hand, if $C \neq 0$, we can still find a solution for equation (5.50), imposing $\alpha < 0$ and fixing

$$H_0^2 = -\frac{1}{18\alpha} \qquad V_0 = \frac{1}{6\alpha}\,. \tag{5.51}$$

Therefore, in the flat case, we can find a dS solution.

Consider the non-flat case with $k \neq 0$. In the $k > 0$ case (5.43), we have the ansatz $a(t) = \cosh H_0 t$ and $k = H_0^2$. The equation we obtain is

$$3H_0^2 = C^2\,\frac{1 - 6\alpha H_0^2 + (18\alpha H_0^2 + 1)\cosh(2H_0 t)}{4\left(6\alpha H_0^2 + 1\right)^2}\,\mathrm{sech}^8(H_0 t) + V_0\,. \tag{5.52}$$

If $C = 0$, we obtain again $H_0^2 = V_0/3$, and therefore making the same H_0 choice as in the flat case we have a dS solution. However, in the non-trivial case $C \neq 0$, the situation is more complex, as we can not find a unique choice of constant H_0 and V_0 to solve this equation. This means that we can not find a $k > 0$ dS solution for this model. A similar analysis can be carried on in the $k < 0$ case, obtain a similar result.

5.6.3 Conclusion

In this section, we proved that we should be careful if we wish to consider de Sitter solutions within Horndeski's theory. As we showed in the example above, it is possible to find at least one case where the de Sitter solution can not be found for all patches (flat and non-flat patches). In general, the ad-hoc rule to follow is to check the equations of motion. If we can rewrite them in terms of the scalars J^2 and Q^2, it should be possible to find a de Sitter solution of all patches. On the contrary, if there are other time functions (as an additional H^2 in the equation of motion (5.46) of the example above), these will inevitably prevent the de Sitter solution.

Note that this problem is not only related to Horndeski's theory, since, as we showed in [7], also other modified gravity models are affected. In general, we should be cautious if the equations of motion can not be written in terms of the scalars J^2 and Q^2.

5.7 Beyond Horndeski

The Horndeski theory, as already mentioned, is one of the most studied alternatives to General Relativity since it is the most general theory with one scalar field with second-order differential equations. Therefore it lacks the Ostrogradsky instabilities presented in section 4.2. However, a new theory has been recently proposed that, although it posses higher order derivatives, it does not feature Ostrogradsky-like instabilities [37, 38]. The main feature of this theory is the presence of matter sound speed modifications even if the matter is minimally coupled to gravity.

As the name suggests, the theory is an extension of Horndeski (5.1), with additional functions in the Lagrangian. The action is still in the form

$$S[g_{\mu\nu},\phi] = \frac{1}{8\pi G}\int d^4x\sqrt{-g}\sum_{i=2}^{5}\mathcal{L}_i[g_{\mu\nu},\phi] + S_M[g_{\mu\nu}]\,, \tag{5.53}$$

where the four Lagrangian $\mathcal{L}_i$ are defined as

$$\mathcal{L}_2 = G_2[\phi, X] \tag{5.54}$$

$$\mathcal{L}_3 = -G_3[\phi, X]\Box\phi \tag{5.55}$$

$$\begin{aligned}\mathcal{L}_4 = {} & G_4[\phi, X]R + G_{4X}[\phi, X]\left[(\Box\phi)^2 - \phi_{;\mu\nu}\phi^{;\mu\nu}\right] + \\ & + F_4[\phi, X]\epsilon^{\mu\nu\rho}{}_{\sigma}\epsilon^{\mu'\nu'\rho'\sigma}\phi_{;\mu}\phi_{;\mu'}\phi_{;\nu\nu'}\phi_{;\rho\rho'}\end{aligned} \tag{5.56}$$

$$\begin{aligned}\mathcal{L}_5 = {} & G_5[\phi, X]G_{\mu\nu}\phi^{;\mu\nu} - \frac{1}{6}G_{5X}[\phi, X]\left[(\Box\phi)^3 - 3(\Box\phi)\phi_{;\mu\nu}\phi^{;\mu\nu} + 2\phi_{;\mu}{}^{\nu}\phi_{;\nu}{}^{\alpha}\phi_{;\alpha}{}^{\mu}\right] + \\ & + F_5[\phi, X]\epsilon^{\mu\nu\rho\sigma}\epsilon^{\mu'\nu'\rho'\sigma'}\phi_{;\mu}\phi_{;\mu'}\phi_{;\nu\nu'}\phi_{;\rho\rho'}\phi_{;\sigma\sigma'}\,.\end{aligned} \tag{5.57}$$

where $\epsilon_{\mu\nu\rho\sigma}$ is the totally anti-symmetric Levi–Civita tensor. We can recover the *Horndeski limit* considering

$$F_4[\phi, X] = 0 \qquad \text{and} \qquad F_5[\phi, X] = 0 \qquad \text{(Horndeski limit)}\,. \tag{5.58}$$

In general, this theory generates third-order differential equations. Therefore, following the reasoning of section 4.2, it should be affected by Ostrogradsky instabilities. However, it can be proven that the theory is free of such instabilities. The crucial point is that, as in General Relativity, the ADM Lagrangian of the theory is degenerate (contrarily to the assumption we made in the discussion of Ostrogradky instabilities), i.e., $\partial\mathcal{L}/\partial\dot{q}^k = 0$ for some canonical coordinates q^k, where, for instance, the q^k in General Relativity are N and the three shift spatial vector components N^i. This degeneracy creates Hamiltonian constraints that reduce the number of degrees of freedom of the theory. Moreover, the Ostrogradsky instabilities are effectively generated by the presence of additional degrees of freedom introduced in the Lagrangian (for instance, compare the number of Hamiltonian coordinates in (4.15) and (4.21) necessary to have a complete description of the system). The F_4 and F_5 functions are defined in such a way to generate constraints that reduce the number of scalar degrees of freedom to the ones of General Relativity, plus only one scalar degree of freedom coming from the addition of a dynamical scalar field to the theory as in plain Horndeski.† In particular, F_4 and F_5 functions are arranged in a way to prevent the appearance of $\dot{N}$ in the Lagrangian, which would promote N to a dynamical variable. Therefore there is no room for additional degrees of freedom with respect to Horndeski, preventing the appearance of Ostrogradsky instabilities. Again, we stress that this theory is not a counter-example of the Ostrogradsky instabilities theorem. While in the discussion we considered a non-degenerate Lagrangian, in this case, the Lagrangian is degenerate, and the constraints can be used to remove the additional degrees of freedom coming from the presence of higher-order coordinates in the Lagrangian.

5.8 Conclusion

In this Chapter, we introduced the most general theory with second-order differential equations and one additional degree of freedom with respect to General Relativity, Horndeski gravity. We defined the action and showed the equations of motion of the background and the linear perturbations, among their stability conditions. We also argued that we could rewrite the Horndeski theory on a FLRW space-time using the (non-covariant) α functions, which are defined in such a way to provide a better physical understanding of the proposed models. For instance, we can immediately understand from $c_T^2 = 1 + \alpha_T$ which models modify the speed of gravitational waves to constrain them with the Ligo/Virgo observation $c_T \approx 1$.

We also showed with a simple example that we should be careful while considering some solutions in Horndeski gravity, as some models might not support all the de Sitter patches. As a general rule, if we wish to consider spatially curved de Sitter solutions, we should check that the resulting equations of motions can be re-casted in terms of the scalars $J^2 = H^2 + k/a^2$ and $Q^2 = H^2 + \dot{H}$ only, e.g., without the presence of H^2 terms that can not be rewritten with other terms as J^2 or Q^2.

Finally, we discuss an extension of Horndeski, called Beyond Horndeski, which admits higher-order equations of motion without introducing Ostrogradsky instabilities. This is achieved with a careful definition of extended Horndeski functions, which avoids the appearance of higher-order canonical coordinates in the Lagrangian.

† The appearance of the additional degree of freedom from the scalar field addition can also be interpreted in the ADM formulation as follows. As already mentioned, in General Relativity the Hamiltonian constraints (3.167) and (3.168) are generators of gauge transformations, removing two degrees of freedom from the physical degrees of freedom counting (first-class constraints [39]). However, in second-order theories with one additional degree of freedom (such as Horndeski), the presence of the scalar field changes the N constraint, which is not a generator of a gauge transformation anymore (second class constraint). Therefore, it removes only one degree of freedom.

Chapter 6

Mimetic gravity

In this Chapter, we introduce mimetic gravity, a theory made of two independent scalar fields, one of which effectively acts as a Lagrange multiplier, generating a constraint on the evolution of the second scalar field. In particular, we will evaluate a particular model of mimetic gravity based on a "broken" Horndeski sector for the constrained scalar field, studying the background evolution and the perturbations equations. Similar to what we did in Horndeski gravity, we compute the velocity of tensor waves, and we use this result to constraint the action parameter performing a Bayesian estimation. The experimental value used for the Bayesian analysis (likelihood) is the unique GW170817 Ligo/Virgo observation [11] and its electromagnetic counterpart [12].

This Chapter is based on the original work publications [8, 9].

6.1 Introduction

An exciting theory of modified gravity is mimetic gravity, proposed by Chamseddine and Mukhanov [40]. In the original work, the conformal degree of freedom of gravity was isolated in a covariant way, through a reparametrization of the physical metric $g_{\mu\nu}$ in terms of an auxiliary metric $\tilde{g}_{\mu\nu}$ and the mimetic scalar field ϕ:

$$g_{\mu\nu} = -\tilde{g}_{\mu\nu}\tilde{g}^{\alpha\beta}\partial_\alpha\phi\partial_\beta\phi\,. \tag{6.1}$$

It is easy to show that, for consistency, the following condition has to be satisfied:

$$g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi = -1\,. \tag{6.2}$$

In [40], it was shown that the equations of motion resulting from the reparametrization of (6.1) mimic a pressure-less fluid on cosmological scales, which can be identified with dark matter. Subsequently, it was realized that the theory is related to GR via a non-invertible disformal transformation involving the mimetic field ϕ, thus explaining why the dynamics of the theory are modified with respect to GR [41, 42, 43]. In [44] a simple extension of the original model featuring a potential for the mimetic field, $V(\phi)$, has also been shown to be able to mimic dark energy and provide an early-time inflationary era, as well as some allowing for bouncing solutions.

A particularly appealing variant of the original mimetic theory starts from a "seed" Horndeski action rather than the Einstein-Hilbert one. In other words, the mimetic constraint (6.2) is enforced on the scalar degree of freedom of Horndeski gravity through a Lagrange multiplier term in the action. The resulting mimetic Horndeski theory has been proposed in [45]. On a cosmological background, the theory features a fluid mimicking dark matter. However, at the perturbative level, this theory features some problems. The mimetic constraint removes the wave-like parts of the Horndeski scalar degree of freedom and removes the theory's scalar degree of freedom. This implies that the speed of scalar perturbations (the sound speed c_s) vanishes. It is worth clarifying that a vanishing sound speed is problematic only if one wishes to perform inflation with the mimetic field because the resulting perturbations would fail in explaining structure formation, as explained in [44]. In fact, if $c_s = 0$, perturbations of the mimetic field do not propagate in space. Quantizing such a field and consequently generating vacuum quantum fluctuations is problematic for many reasons (for instance, it would be hard to satisfy the appropriate commutation relation with the conjugate momentum). This in turn hinders the generation of perturbations which will then grow under gravitational instability to form the large-scale structure, one of the most important outcomes of successful inflation. Perhaps more importantly, a vanishing sound speed of the inflaton is also problematic from the observational point of view. In fact, measurements of the CMB temperature and polarization anisotropies from the *Planck* satellite (and in particular the absence of detection of primordial non-Gaussianity) favour a speed of sound for the inflaton $c_s = 1$, with a 95% confidence level lower bound of $c_s > 0.024$ [5]. This result excludes $c_s = 0$ at high significance. We wish to stress that a vanishing speed of sound is strictly speaking only a problem if one wishes to perform inflation with the mimetic field, and not if one is only aiming at describing dark matter (for which $c_s = 0$ is instead quite natural).

At any rate, it is worth considering modifications to the original mimetic scenario, which allow for a non-vanishing sound speed. An obvious way to address this issue is to break the Horndeski structure of the theory, thereby removing the special tuning guaranteeing that the equations of motion are at most of second order. Nonetheless, the presence of the mimetic constraint prevents the appearance of higher-than-second-order derivatives in the equations of motion, and therefore Ostrogradsky instabilities as seen in section 4.2. In this Chapter, we shall follow this procedure and consider the mimetic model proposed in [46], obtained by breaking the Horndeski structure of a starting mimetic Horndeski model, thus allowing for a non-zero sound speed.

As already discussed in Horndeski theory (section 5.5), the LIGO/Virgo collaboration observation of the event GW170817, produced by merger of a binary neutron star system [11], and the optical counterpart GRB170817A [12], found the gravitational waves speed c_T to be extremely close to the speed of light: $c_T \approx 1$. In the last part of this Chapter, we will use this result to place constraints on the action parameters of the mimetic model considered, performing an analysis with Bayesian probability.

6.2 Background equations

We consider the mimetic theory defined by the following action

$$S = \int d^4x \sqrt{-g}\Big[R(1+2\alpha X) - \frac{\gamma}{2}(\Box\phi)^2 + \frac{\beta}{2}(\nabla_\mu\nabla_\nu\phi)^2 - \frac{\lambda}{2}(2X+1) - V + \mathcal{L}_m\Big]\,, \tag{6.3}$$

where for simplicity we set $16\pi G = 1$ (G is Newton's constant), $\mathcal{L}_m$ is the matter part of the action, that in this model we consider to be made of standard matter and radiation, ϕ is the mimetic field, $V \equiv V(\phi)$ is a potential for the mimetic field, and $X \equiv (1/2)g_{\mu\nu}\nabla^\mu\phi\nabla^\nu\phi$ is the kinetic term of the field. The Lagrangian multiplier λ is introduced to enforce the mimetic constraint (6.2) on the mimetic field, while $\alpha\,,\beta\,,\gamma$ are constant parameters.

The model involves the presence of "broken" G_2 (5.2) and G_4 (5.2) functions: the coefficients of the terms $R\,X$, $(\Box\phi)^2$ and $(\nabla_\mu\nabla_\nu\phi)^2$ are arbitrary and in general different from each others, while the Horndeski form requires γ and β to be G_{4X}. In fact when $\beta = \gamma = 4\alpha$ we recover a mimetic Horndeski model as in (5.1). Breaking of the Horndeski structure of the action is necessary for scalar perturbations to propagate [46, 47]. However, we will see that, on a Friedmann-Lemaître-Robertson-Walker (FLRW) background, the model preserves the solutions of the corresponding mimetic Horndeski Lagrangian up to a (constant) rescaling of the effective Plank mass of the theory. Note that when $\beta = \gamma = 4\alpha$ we recover a mimetic Horndeski model as in (5.1).

The equations of motion of our mimetic model are obtained by varying the action with respect to the metric, the Lagrange multiplier, and the mimetic field. Varying the action with respect to the metric we get

$$(1+2\alpha X)G_{\mu\nu} + \nabla_\mu\phi\nabla_\nu\phi\left(\alpha R - \frac{\lambda}{2}\right) - \frac{1}{2}g_{\mu\nu}\left[\frac{\beta}{2}\phi_{;\rho\sigma}\phi^{;\rho\sigma} - \frac{\gamma}{2}(\Box\phi)^2 - \frac{\lambda}{2}(2X+1) - V\right] +$$
$$+2\alpha(g_{\mu\nu}\Box X - \nabla_\mu\nabla_\nu X) - \frac{\beta}{2}g^{\rho\sigma}\left[\nabla_\rho(\phi_{;\mu\sigma}\nabla_\nu\phi) + \nabla_\rho(\phi_{;\nu\sigma}\nabla_\mu\phi) - \nabla_\rho(\phi_{;\mu\nu}\nabla_\sigma\phi)\right] + \beta\phi^{;\rho}{}_{\mu}\phi_{;\rho\nu} +$$
$$+\frac{\gamma}{2}\left[\nabla_\nu\phi\nabla_\mu(\Box\phi) + \nabla_\mu\phi\nabla_\nu(\Box\phi) - g_{\mu\nu}g^{\rho\sigma}\nabla_\rho(\Box\phi\nabla_\sigma\phi)\right] = \frac{1}{2}T_{\mu\nu}\,, \tag{6.4}$$

where in this theory we consider $T_{\mu\nu}$ as the stress-energy tensor of ordinary baryonic matter and radiation. Variation of the action with respect to the field ϕ yields

$$(\lambda - 2\alpha R)(\nabla_\mu\nabla^\mu\phi) + (\nabla_\mu\phi)(\nabla^\mu\lambda) - 2\alpha(\nabla_\mu R)(\nabla^\mu\phi) + \beta(\nabla_\nu\nabla_\mu\nabla^\nu\nabla^\mu\phi) -$$
$$-\gamma(\nabla_\mu\nabla^\mu\nabla_\nu\nabla^\nu\phi) - \frac{\partial V(\phi)}{\partial\phi} = 0\,. \tag{6.5}$$

Finally, variation with respect to the Lagrange multiplier λ enforces the mimetic constraint

$$X = -\frac{1}{2}\,. \tag{6.6}$$

In this Chapter, we work within a spatially flat FLRW space-time (1.15). Evaluating the mimetic constraint on this space-time, we can immediately identify the field with the cosmological time (up to a constant)

$$\phi = t\,. \tag{6.7}$$

With this identification, from the $(0,0)$ and $(1,1)$ components of (6.4) we obtain the equations of motion

$$(-6\gamma + 24\alpha)\dot{H} + (36\alpha + 9\gamma + 12 - 9\beta)H^2 - 2V - 2\lambda - 2\rho_{\rm m} = 0\,, \tag{6.8}$$
$$3H^2 + 2\dot{H} = \frac{2V - 2P_{\rm m}}{4 - 4\alpha - \beta + 3\gamma}\,, \tag{6.9}$$

where $\rho_{\rm m}$ and $P_{\rm m}$ correspond to the usual combined energy density and pressure of radiation and baryonic matter. The density $\rho_{\rm m}$ does not contain dark matter nor dark energy, as the mimetic gravity fields will mimic them.

The Klein-Gordon equation of the field (6.5), evaluated on the FLRW space-time and taking into account the mimetic constraint (6.7), becomes

$$\frac{1}{a^3}\frac{d}{dt}\left[a^3\left(\lambda + (3\beta - 24\alpha)H^2 + (3\gamma - 12\alpha)\dot{H}\right)\right] = -\frac{dV}{dt}\,, \tag{6.10}$$

while the continuity equation $\nabla_\mu T^{\mu\nu} = 0$ for baryonic matter and radiation assumes the standard form

$$\dot{\rho}_{\rm m} + 3H(\rho_{\rm m} + P_{\rm m}) = 0\,. \tag{6.11}$$

Note that when the Horndeski structure for the ϕ sector of the action (6.3) is recovered, i.e. when $\gamma = 4\alpha$, the $\dot{H}$ term in (6.10) disappears, leaving a second order differential equation.

Given the equation of state of the matter fluid (6.11), once the form of the potential V is chosen, the system of equations (6.8)-(6.9) can be solved with respect to the scale factor $a(t)$ and the scalar field $\lambda(t)$. Alternatively, we can use (6.10) with one of (6.8) or (6.9). In the latter case, if we define a *dark fluid* energy density $\rho_{\rm df}$, i.e. the energy density of the mimetic gravity scalar field, as

$$\rho_{\rm df} := \lambda + V + (3\beta - 24\alpha)H^2 + (3\gamma - 12\alpha)\dot{H}\,, \tag{6.12}$$

from (6.10) we obtain its evolution

$$\rho_{\rm df}(t) = \frac{C}{a(t)^3} + \frac{3}{a(t)^3}\int^t V(t')a(t')^3H(t')dt' \,, \tag{6.13}$$

where $C > 0$ is an integration constant which sets the amount of mimetic dark matter, as the corresponding contribution to the energy density decays as a^{-3}, as expected for a pressure-less component, in accordance with (1.20). Defining also a *dark fluid* pressure as

$$P_{\rm df} := -V \,, \tag{6.14}$$

using equation (6.10), we obtain a continuity equation similar to the one holding for the standard matter (6.11), namely

$$\dot\rho_{\rm df} + 3H(\rho_{\rm df} + P_{\rm df}) = 0 \,. \tag{6.15}$$

Rearranging the equations (6.8) and (6.9) we obtain

$$\begin{aligned} 6H^2 &= \frac{4}{4-\beta+3\gamma-4\alpha}\left(\rho_{\rm df}+\rho_{\rm m}\right) \,, \\ -4\dot H - 6H^2 &= \frac{4}{4-\beta+3\gamma-4\alpha}\left(P_{\rm df}+P_{\rm m}\right) \,. \end{aligned} \tag{6.16}$$

We recognize the above as being Friedmann-like equations, with the Planck mass $1/\sqrt{8\pi G}$ rescaled by a factor $(4-\beta+3\gamma-4\alpha)/4$. The quantity by which the Planck mass is rescaled determines the effective Newton constant. Enforcing a positive effective Newtonian constant rescaling, we obtain a constraint on the action parameter

$$4-\beta+3\gamma-4\alpha > 0 \,. \tag{6.17}$$

Notice that for $\alpha = \beta = 0$ we recover the results of [44], which extended the original mimetic action by a term proportional to $(\Box\phi)^2$.

We immediately see that a constant potential V in (6.12)-(6.14) can be exploited to model dark matter and dark energy through the corresponding fluid. For more complex potentials, given in the action as functions of ϕ (and therefore of t due to the mimetic constraint), the dark fluid will model various types of fluids while leaving the dark matter sector unchanged.

6.3 Perturbations on a FLRW background

As mentioned above, one of the main problems in mimetic gravity is the vanishing sound speed, implying the non-propagation of scalar perturbations. The problem persists even in mimetic Horndeski gravity. We have seen that by breaking the Horndeski form of the ϕ sector, we can find a non-vanishing sound speed [47, 46]. However, this comes at the risk of modifying the speed of gravitational waves c_T, which in the original mimetic gravity model is identically equivalent to the speed of light, $c_T = 1$. Enforcing that c_T remains equal to the speed of light when considering the mimetic model of (6.3), to satisfy the experimental GW170817/GRB17081A constraint will strongly constrain the Lagrangian parameters. We will discuss these issues in detail and begin by computing the sound speed c_s and the gravitational wave speed c_T.

6.3.1 Scalar perturbations

In this section, we derive the scalar perturbations around a flat FLRW line element. We consider the Newtonian gauge, and therefore the metric form (1.55)

$$ds^2 = -\left[1+2\Psi(t,\vec x)\right]dt^2 + a(t)^2\left[1+2\Phi(t,\vec x)\right]\delta_{ij}dx^idx^j \,. \tag{6.18}$$

We perturb the mimetic field and the Lagrange multiplier field as follows

$$\phi = t + \delta\phi(t,\vec{x})\,, \quad \lambda = \lambda_0(t) + \lambda_1(t,\vec{x})\,, \tag{6.19}$$

where $|\delta\phi/t|\,, |\lambda_1/\lambda| \ll 1$. The mimetic constraint yields

$$\Psi = \delta\dot{\phi}\,, \tag{6.20}$$

and the $i \neq j$ components of the perturbed field equations (6.4) give

$$(1-\alpha)\Phi + \frac{\beta}{2}H\delta\phi - \left(\alpha - \frac{\beta}{2} - 1\right)\delta\dot{\phi} = 0\,. \tag{6.21}$$

By substituting this result into any of the tj components of (6.4) leads to

$$\delta\ddot{\phi} + H\delta\dot{\phi} + \left[\dot{H} + \frac{c_s^2(\rho_{\rm m} + P_{\rm m})}{\beta - \gamma}\right]\delta\phi - \frac{c_s^2}{a^2}\nabla^2\delta\phi = -\frac{ac_s^2}{\beta-\gamma}(\rho_{\rm m} + P_{\rm m})v_{\rm m}\,, \tag{6.22}$$

where $v_{\rm m}$ is the matter velocity, and the squared speed of sound

$$c_s^2 = \frac{2(\beta-\gamma)(\alpha-1)}{(2\alpha-\beta-2)(4-4\alpha-\beta+3\gamma)}\,, \tag{6.23}$$

Recall that we defined $\rho_{\rm m}$ and $P_{\rm m}$ to include both the baryonic matter and radiation components, although, in principle, one could separate them in the above discussion. In fact, the term $(p_{\rm m} + \rho_{\rm m})v_{\rm m}$ should really be considered as a sum over the baryonic matter and radiation contributions. Notice also that in the limit $\alpha = 0, \beta = 0$ and $\gamma \to -2\gamma$ we find the results of [44]. Notice finally that these results are independent of the choice of the field potential V.

The computation has been carried on with `xAct`, with the methods explained in Appendix A. The only additional step is to enforce the mimetic constraint (6.20). This can be done creating a rule with the `MakeRule` command, and automatically enforcing the rule with `AutomaticRules`

```
MimeticConstraint=MakeRule[{ϕh [LI[1],LI[0]], φ[LI[1], LI[1]]}]
AutomaticRules[ϕh,MimeticConstraint]
```

Note that we should do the same also for the second derivative $\delta\ddot{\varphi}$

```
MimeticConstraint2=MakeRule[{ϕh[LI[1],LI[1]], φ[LI[1], LI[2]]}]
AutomaticRules[ϕh,MimeticConstraint2]
```

In both cases, for each object, the first `LI[1]` denotes the order of perturbation, while the second is the order of the time derivative applied to the object. To substitute the occurrences of the background field ϕ, we can proceed the same way or use the Mathematica rule at the end of the computation, i.e., `/.` commands.

6.3.2 Tensor perturbations

Consider the tensor perturbations. The line-element we consider is the TT-gauge metric (1.57)

$$ds^2 = -dt^2 + a(t)^2(1+E_+)dx^2 + 2a(t)^2E_\times dxdy + a(t)^2(1-E_+)dy^2 + a(t)^2dz^2\,. \tag{6.24}$$

By inserting this into the Einstein equations and by using the unperturbed equations, we find the perturbed equation at the first order, where $E = E_\times$ or $E = E_+$

$$\ddot{E} + 3H\dot{E} - \frac{2(1-\alpha)}{2-2\alpha+\beta}\frac{1}{a(t)^2}\frac{\partial^2 E}{\partial z^2} = 0\,. \tag{6.25}$$

From the above, we read off the squared gravitational wave speed

$$c_T^2 = \frac{2(1-\alpha)}{2-2\alpha+\beta}\,. \tag{6.26}$$

The gravitational wave speed is, in general, different from the speed of light. Notice furthermore that the tensor perturbations are not affected by the presence of standard matter.

We see that to satisfy the recent constraint from GW170817 /GRB17081A, which enforces $c_T^2 \simeq 1$, we have to consider $|\beta| \ll 1$. In fact, the requirement that $c_T \equiv 1$ forces b to be identically 0. We will consider further implications of these findings in the next sections.

6.3.3 Ghost and gradient instabilities

In this section, we compute the quadratic action (using `xAct`) to study the possible ghost and gradient instabilities of the theory. The analysis of the stability is performed following the discussion in section 4.2. As shown, for instance, in [48], a similar mimetic model has unavoidable scalar gradient instabilities while ghost instabilities disappear in certain areas of the parameter space. Our case, however, is more complicated because of the non-minimal coupling to the gravity of the kinetic term X, see (6.3). The effects of the non-minimal coupling can be spotted by inspecting (6.22), where the speed of sound c_s^2 is modulated by the factor $(\beta-\gamma)^{-1}$, but only in the matter sector, i.e. an effective sound speed $c_{s,\text{eff}}^2 = c_s^2/(\beta-\gamma)$ appears. If $\beta = 0$ and $\gamma > 0$ we see that c_s^2 and $c_{s,\text{eff}}^2$ have always opposite signs.

To shed further light on the behaviour of perturbations, we consider the action to quadratic order in both scalar and tensor perturbations. For the scalar sector, we obtain

$$S_{\rm S}^{(2)} = 2(1-\alpha)\int d^4x\, a^4 H^2\left[-\frac{1}{c_s^2}\dot{\delta\phi}^2 + \frac{1}{a^2}\left(\partial_k\delta\phi\right)\left(\partial^k\delta\phi\right)+\ldots\right], \tag{6.27}$$

where $\ldots$ stands for terms proportional to $\delta\phi\delta\phi$ and $\delta\phi\dot{\delta\phi}$ which are not important for the stability analysis. For the tensor sector we obtain

$$S_{\rm T}^{(2)} = \frac{1}{4}(1-\alpha)\int d^4x\, a^3\left[\frac{\dot{E}^2}{c_T^2} - \frac{1}{a^2}\left(\frac{\partial E}{\partial z}\right)^2\right]. \tag{6.28}$$

From (6.28), one sees that for tensor perturbations to not suffer from instabilities, we must set $\alpha < 1$, so that both terms on the right-hand side of the quadratic action for tensor perturbations appear with the right sign. However, this choice leads, as can be straightforwardly seen from (6.27), to gradient instability in the scalar sector and, depending on the sign of c_s^2, also to ghost instability. When $\beta = \alpha = 0$, we recover the same result of [48], up to some irrelevant normalisation factors. Thus, as suggested also in this work, the only way to avoid ghost instabilities is to choose $c_s^2 < 0$*. By combining (6.16) and (6.23) we see that, for $\beta = 0$, c_s^2 and γ must have opposite signs. Thus, the conditions $\alpha < 1$ and $\gamma > 0$ guarantee that the theory is free from ghost instabilities in both the scalar and tensor sectors, although gradient instabilities are still present in the scalar sector.

However, as discussed above, the instability might be tamed by the fact that $c_{s,\text{eff}}^2 = c_s^2/(\beta-\gamma) > 0$ when $c_s^2 < 0$ and $\gamma > 0$ in the limit where $\beta \to 0$, i.e., the effective sound speed in the presence of matter non-minimally coupled to gravity might be positive.

6.4 Late-time cosmological evolution

The main goal of this section is to find solutions mimicking dark matter and/or dark energy in the late Universe while respecting observational bounds on the speed of scalar and tensor perturbations. To

* In [48] the quantity $(2-3\gamma)/\gamma$ corresponds to our c_s^{-2}.

simplify the discussion, we will force the gravitational wave speed c_T to be identically equal to the speed of light, $c_T = 1$: as we have seen previously, this implies setting the Lagrangian parameter β to 0. In other words, a term of the form $\nabla^\mu\nabla^\nu\phi\nabla_\mu\nabla_\nu\phi$ is forbidden from appearing in the action, Eq. (6.3).

6.4.1 Vacuum case

We begin by considering the idealized case of vacuum, where no cosmological matter is present. From the first equation in (6.16), combined with (6.12) and imposing $\beta = 0$, we get

$$6H(t)^2 = \frac{4}{4+3\gamma-4\alpha}\left[\frac{C}{a(t)^3} + \frac{3}{a(t)^3}\int^t V(t')a(t')^3 H(t')dt'\right] . \tag{6.29}$$

Thus given a specific form for the scale factor $a(t)$, and therefore a specific form for the Hubble parameter $H(t)$, it is possible to reconstruct from (6.29) the potential V as a function of t and therefore of ϕ.

The equation of state parameter of the dark fluid can be defined similarly to the standard matter definition (1.19). Using (6.12) and (6.14) we obtain

$$\omega_{\rm df} := \frac{P_{\rm df}}{\rho_{\rm df}} = \frac{-V}{V+\lambda-24\alpha H^2+(3\gamma-12\alpha)\dot{H}} . \tag{6.30}$$

Since, as we already mentioned earlier, the future evolution of the Universe is expected to be dominated by dark energy, we consider the far-future evolutionary history where we neglect the contribution of the dark matter, setting $C = 0$ in (6.29). In this scenario, the $\omega_{\rm df}$ is the equation of state parameter of a dark energy-like component, which we can constraint with the Planck experiment observation [5], in particular with the values in (2.18).

To describe all the three possible regimes of $\omega_{\rm df}$ (cosmological constant-like, quintessence-like, and phantom-like), we will consider the following choices for the scale factor

$$a(t) = \mathrm{e}^{H(t-t_0)} \qquad \omega_{\rm df} = -1 , \tag{6.31}$$

$$a(t) = \left(\frac{t}{t_0}\right)^{\frac{2}{3(1+\omega_{\rm df})}} \qquad \omega_{\rm df} > -1 , \tag{6.32}$$

$$a(t) = \left(\frac{t^*-t}{t^*-t_0}\right)^{\frac{2}{3(1+\omega_{\rm df})}} \qquad \omega_{\rm df} < -1 , \tag{6.33}$$

where t_0 is the present time for which $a(t_0) = 1$, while $t^*, t < t^*$ is the time of the Big Rip [49] (which emerges within phantom cosmologies, but which can be avoided if a de Sitter Universe is asymptotically reached [50], or in certain modified gravity theories [51]). Furthermore, we note that the Hubble parameter H in the case $\omega = -1$ is a constant.

Potential for $\omega_{\rm df} = -1$

Consider the scale factor (6.31), where H is constant. By choosing the constant potential:

$$V(t) = 2\Lambda , \tag{6.34}$$

where Λ is the cosmological constant, from (6.29) we obtain:

$$6H^2 = \frac{4}{4+3\gamma-4\alpha}(2\Lambda) , \tag{6.35}$$

which is the solution one would expect for a Λ-dark energy dominated universe (up to the Newton constant rescaling factor). Notice that from (6.30) a constant $\lambda = 24\alpha H^2$ is needed in order to have $\omega_{\rm df} = -1$.

Potentials for $-1 < \omega_{\rm df}$

Consider an equation of state in the quintessence region. Using the quintessence potential

$$V(t) = V_0 \left(\frac{t_0}{t}\right)^2 = V_0 \left(\frac{\phi_0}{\phi}\right)^2 , \tag{6.36}$$

where $\phi_0 = \phi(t_0)$ and V_0 a constant, we recover the scale factor evolution (6.32). The constant V_0 follows from (6.29) and reads

$$V_0 t_0^2 = -\frac{2\,\omega_{\rm df}}{3(1+\omega_{\rm df})^2}(4+3\gamma-4\alpha)\,. \tag{6.37}$$

We see that α is positive when $\omega_{\rm df} < 0$. More specifically, the constraint (2.18) leads to:

$$420\,(4+3\gamma-4\alpha) \lesssim V_0 t_0^2 < +\infty\,, \tag{6.38}$$

where $\omega_{\rm df} = -1$ corresponds to the limit $V_0 \to +\infty$.

Potentials for $\omega_{\rm df} < -1$

Finally, we consider the case where the equation of state is phantom. Similarly to the previous case, we can use a potential of the form

$$V(t) = \tilde{V}_0 \left(\frac{t_* - t_0}{t_* - t}\right)^2 = \tilde{V}_0 \left(\frac{\phi_* - \phi_0}{\phi_* - \phi}\right)^2 , \tag{6.39}$$

where $\phi_* = \phi(t_*)$ and $\phi_0 = \phi(t_0)$, in order to find the scale factor evolution (6.33). From (6.29) we find that the constant $\tilde{V}_0$ reads

$$\tilde{V}_0 (t_* - t_0)^2 = -\frac{2\,\omega_{\rm df}}{3(1+\omega_{\rm df})^2}(4+3\gamma-4\alpha)\,, \tag{6.40}$$

and therefore

$$25800\,(4+3\gamma-4\alpha) \lesssim \tilde{V}_0 (t_* - t_0)^2 < +\infty\,, \tag{6.41}$$

where we used (2.18) and $\omega_{\rm df} = -1$ corresponds to the limit $\tilde{V}_0 \to +\infty$.

6.4.2 Adding radiation, baryons, and dark matter

In this section we numerically solve the system of equations given by the continuity equations for the cosmological matter (6.11) and the dark fluid (6.15), as well as the second Friedmann equation in (6.16), using the constant potential $V(t) = 2\Lambda$, as in (6.34). The numerical analysis has been performed with the software we coded specifically for this model [52]. We consider the action parameter $\beta = 0$ for in order to ensure $c_T = 1$ and hence agreement with GW170817/GRB170817A, and we take $\alpha < 1$ and $\gamma > 0$ (from the requirements on the stability for $\beta \approx 0$) as free parameters. We further impose that the Planck mass is rescaled to a positive quantity, considering the condition (6.17).

We plot the fractional densities defined as

$$\Omega_i(t) = \frac{4}{4+3\gamma-4\alpha}\,\frac{\rho_i(t)}{6H(t)^2}\,, \tag{6.42}$$

where the index i can correspond to r (radiation), b (baryonic matter) or *df* (dark fluid), where the dark fluid will include dark energy and dark matter, since in general $C \neq 0$ in Eq. (6.13). The factor in front of the density is needed if we require the fractional densities of all the components (radiation, baryonic matter, and dark fluid) to sum to one at any time t. With this definition, we expect the Ω's to not depend on the action parameters α and γ.

As initial conditions we set $\Omega_r(t_0) = 8 \times 10^{-5}$ and $\Omega_b(t_0) = 0.0486$, in agreement with [5], and compute the remaining dark fluid density through $1 - \Omega_r(t_0) - \Omega_b(t_0)$. We evolve the system from a scale factor $a = 10^{-5}$ (radiation era) to $a = 1$ (present time).

The evolution we obtain is depicted in Figure 6.1. The fractional densities behave exactly like the ones of ΛCDM, with the dark fluid corresponding to the cold dark matter and dark energy of ΛCDM. As already mentioned, we obtain the same fractional densities for every value of γ and α.

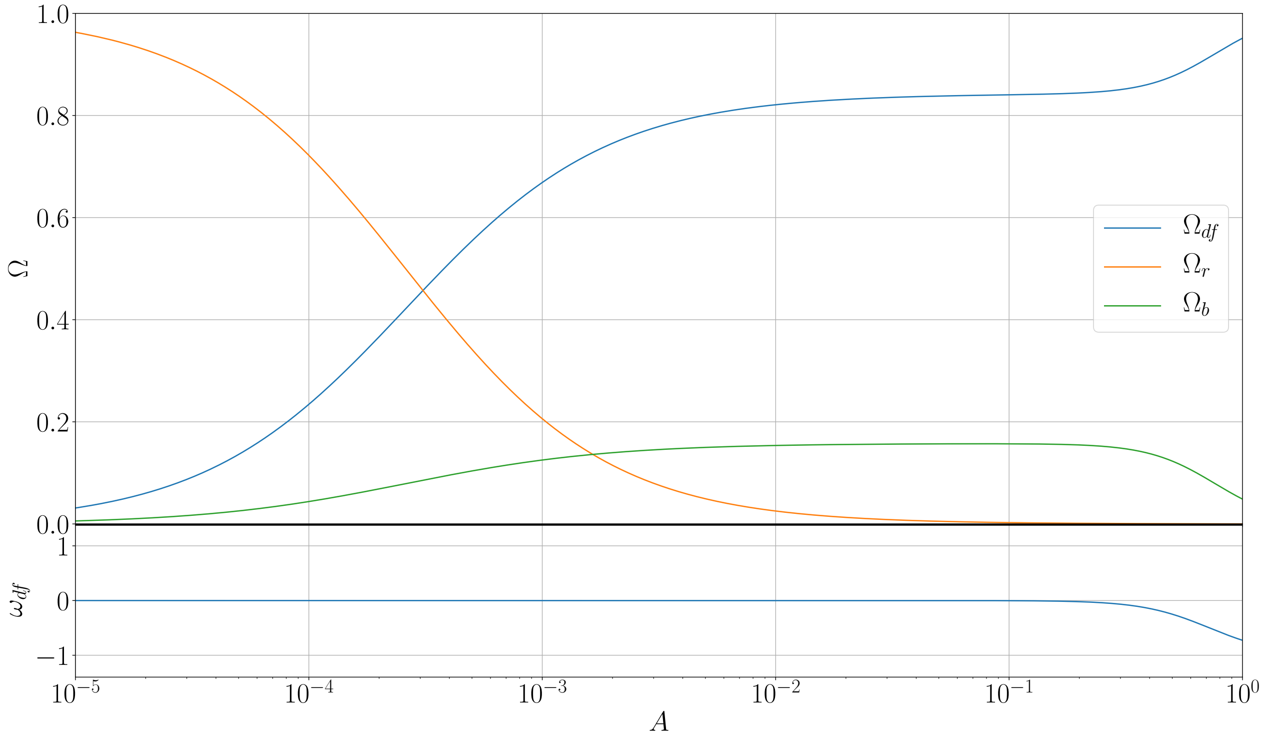


Figure 6.1: Plot of the evolution of the fractional densities Ω, defined in equation (6.42), for the cosmological matter components (baryonic matter and radiation) and the dark fluid, and the equation of state parameter $\omega_{\rm df}$, as functions of the scale factor a.

Let us further analyse how varying α and γ affects the age of the Universe, which is given by

$$t_0 \equiv \int_0^1 \frac{da}{aH(a)} = \sqrt{\frac{4+3\gamma-4\alpha}{4}} \int_0^1 \frac{da}{aH_0\sqrt{\frac{1}{6}\sum_i \Omega_i(a)}}\,, \tag{6.43}$$

where $H_0 = H(t_0)$, and we have written the integral as a function of the fractional densities as they do not depend on α and γ. Since the factor in front of the integral is 1 if the action parameters satisfy the condition $4\alpha = 3\gamma$ (and therefore also in the case of GR $\alpha = \gamma = 0$), we expect the value of the age of the Universe to be different from 1 with a dependence on the action parameters given by

$$t_0 = \sqrt{\frac{4+3\gamma-4\alpha}{4}}\, t_0|_{4\alpha=3\gamma} \equiv \Gamma\, t_0|_{4a=3c}\,. \tag{6.44}$$

Notice that the parameter Γ is always real because of the condition imposed in Eq. (6.17). We show some results in Tab. 6.1, where we confirm that Eq. (6.44) is consistent with our numerical results from [52]. The conclusion is that, although the evolution of the fractional densities of the dark fluid corresponds to the one expected in ΛCDM, the age of the Universe we predict will, in general, be different unless $4\alpha = 3\gamma$. In addition to the constraint on β from the speed of gravitational waves, constraints on the Universe's age can, in principle, be used further to constrain α and γ.

α	γ	t_0 numerical [Gyr]	Γ
0	0	13.818	1
0.75	1	13.818	1
0.075	0.1	13.818	1
0.1	0.1	13.644	$0.99 = 13.644/13.818$
0.5	0.1	10.478	$0.76 = 10.478/13.818$
0	1	18.280	$1.32 = 18.280/13.818$

Table 6.1: Age of the universe, as function of the action parameters α and γ. The factor Γ is defined in equation (6.44).

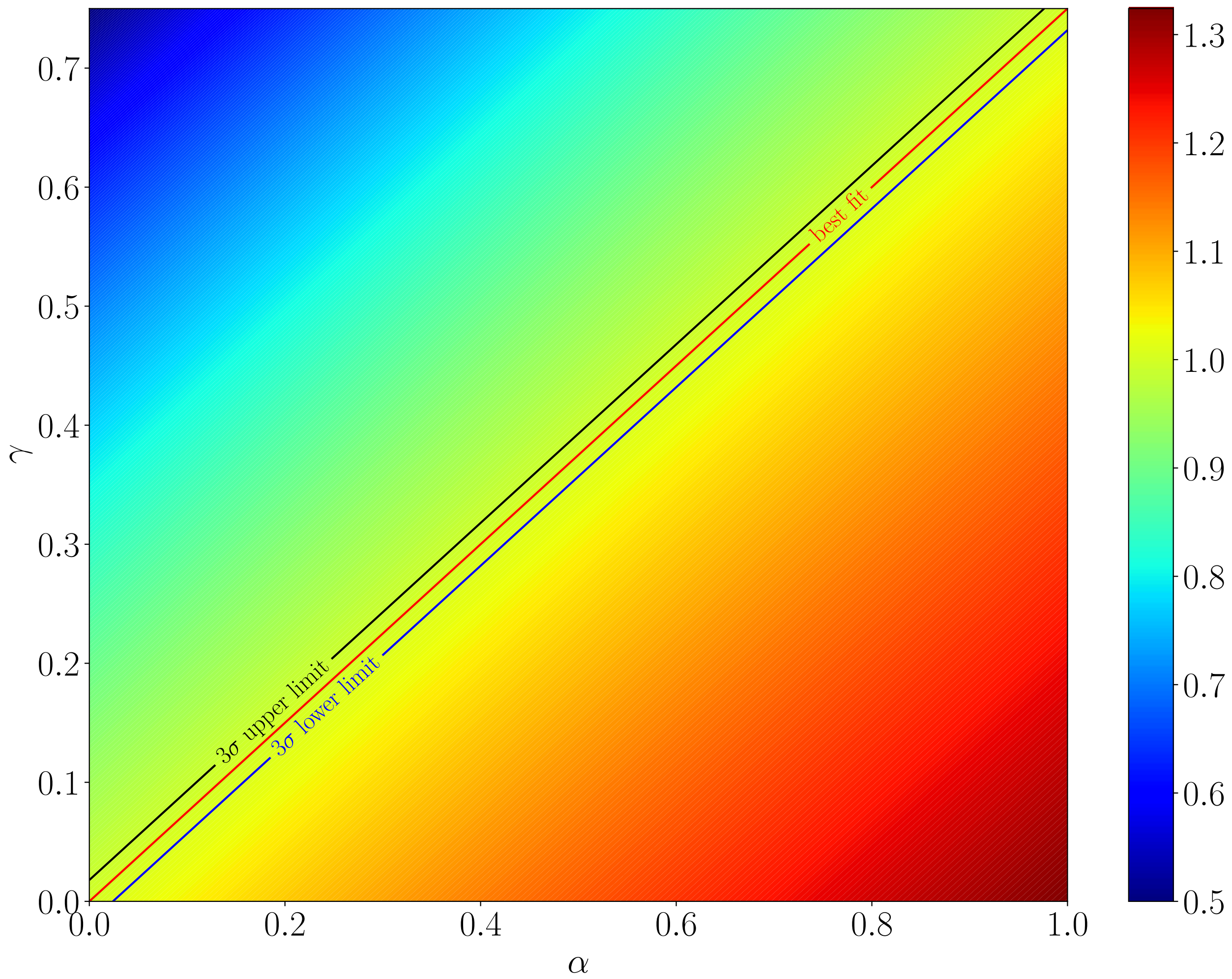


Figure 6.2: Contour-plot of $\Gamma = \sqrt{(4+3\gamma-4\alpha)/4}$ in the α-γ parameter space, focusing for definiteness on the region of parameter space where $\alpha\,,\gamma \lesssim \mathcal{O}(1)$. The black, red, and blue lines correspond to contours of constant $\Gamma = 1.009$, $\Gamma = 1.000$, and $\Gamma = 0.991$. These values approximately correspond to the 3σ upper limit, best fit, and 3σ lower limit on Γ respectively, given the constraint $\Gamma = 1.000 \pm 0.003$ which we derive from the 0.3% determination of the age of the Universe from Planck [5]. Notice that the contours lie along lines of constant $4\alpha - 3\gamma$, as expected given the functional form of Γ.

To get a rough feeling for how constraints on the age of the Universe can restrict the viable α-γ parameter space, we note that the $\approx 0.3\%$ determination of the age of the Universe from Planck [5] can in turn be used to constrain Γ, leading to the approximate requirement $\Gamma = 1.000 \pm 0.003$. This requirement can be used to set bounds on α and γ. Focusing for definiteness on the region of parameter space where $\alpha\,,\gamma \lesssim \mathcal{O}(1)$, in Figure 6.2 we show a contour-plot of $\Gamma = \sqrt{(4+3\gamma-4\alpha)/4}$ as a function of α and γ, along with the contours corresponding to $\Gamma = 1.009$, $\Gamma = 1.000$, and $\Gamma = 0.991$. These values approximately correspond to the 3σ upper limit, best fit, and 3σ lower limit on Γ respectively, arising from the constraint $\Gamma = 1.000 \pm 0.003$. These contours lie along lines of constant values of the linear combination $4\alpha - 3\gamma$. Moreover, as expected, we see that limits on the age of the Universe do not constrain the parameters α and γ *per se*, but rather the "orthogonal" linear combination $4\alpha - 3\gamma$ (in this sense, the combination $4\alpha - 3\gamma$ can be thought of as a principal component of the system), as is clear from the functional form of Γ.

6.5 Parameter estimation

In this section, we study the implications of the GW170817/GRB170817A bound for mimetic gravity and confirm that in the original setting of the theory, GWs propagate at the speed of light, hence ensuring agreement with the recent multi-messenger detection. Performing a Bayesian statistical analysis where we compare the predictions of the higher-order mimetic model for the speed of GWs against the observational bound from GW170817/GRB170817A, we derive constraints on the three free parameters of the theory. Imposing the absence of both ghost instabilities and superluminal propagation of scalar and tensor perturbations, we find very stringent 95% confidence level upper limits of $\sim 7 \times 10^{-15}$ and $\sim 4 \times 10^{-15}$ on the coupling strengths of Lagrangian terms of the form $\nabla^\mu\nabla^\nu\phi\nabla_\mu\nabla_\nu\phi$ and $(\Box\phi)^2$ respectively, with ϕ the mimetic field. We finally discuss the implications of the obtained bounds for mimetic theories. This work presents the first-ever robust comparison of a mimetic theory to observational data.

6.5.1 Scalar and tensor perturbations

We recall the results from the perturbation analysis of the previous sections (6.23) and (6.26) which will be the theoretical predictions to be used in the Bayesian analysis. They are

$$c_s^2 = \frac{2(\beta-\gamma)(\alpha-1)}{(2\alpha-\beta-2)(4-4\alpha-\beta+3\gamma)}\,, \tag{6.45}$$

$$c_T^2 = \frac{2(1-\alpha)}{2(1-\alpha)+\beta}\,. \tag{6.46}$$

Again, from (6.46) it is clear that $\beta \neq 0$ is a necessary condition for obtaining $c_T \neq 1$. We see that bounds on the GW speed from GW170817 will constrain the parameters α and β, whereas further information on the sound speed is necessary in order to put constraints on γ. Notice also that, when $\alpha = \beta = \gamma = 0$, we recover $c_s^2 = 0$ and $c_T^2 = 1$, in agreement with expectations from the original mimetic gravity model [40], and in full agreement with the GW170817/GRB170817A detection [11].

Moreover, we also found from the quadratic actions (6.27) and (6.28) that the theory is free of ghosts only when choosing $\alpha < 1$ and $\gamma > 0$. Heretofore, we shall impose these conditions to ensure the theoretical consistency of the model. In addition to these conditions ensuring the absence of ghosts, stability arguments impose the conditions $0 \leq c_s^2 \leq 1$ and $0 \leq c_T^2 \leq 1$. The upper limit of 1 on c_s^2 and c_T^2 enforces the absence of superluminal propagation of scalar and tensor modes.

The recent near-simultaneous detection of GW170817 [11] and its optical counterpart GRB170817A [12], has placed very stringent constraints on δc_T, the fractional deviation of the GW speed from the speed of light. As already discussed in section 5.5 for the Horndeski theory, following [29], we will consider the following bound

$$|\delta c_T| < 5 \times 10^{-16}\,. \tag{6.47}$$

The bound in (6.47) provides a very stringent constraint on deviations of c_T from the speed of light. Imagine for a moment to *fix* the requirement $c_T = 1$. In the context of the mimetic model considered

(6.3), from (6.46) it follows that $c_T \equiv 1$ instead imposes the *very stringent* constraint $\beta = 0$. This implies that a term of the form $\nabla^\mu\nabla^\nu\phi\nabla_\mu\nabla_\nu\phi$ is prohibited from appearing in the action. In the remaining part of the work, we will entertain the possibility of a tiny violation of the constraint $c_T \equiv 1$, in accordance with the the bounds on c_T provided by (6.47), and explore the implications of this bound on the parameters of the model.

6.5.2 Analysis methodology

We perform a standard Bayesian statistical analysis, explained in Appendix B (in particular, see Appendix B.5 about the parameter estimation method), to constrain the three parameters of the extended mimetic model $\mathcal{M}$ (with parameters α, β, and γ) in light of the near-simultaneous GW170817/GRB170817A detection. The constraint on δc_T of (6.47) can only be used to provide bounds on α and β (6.46). The first part of our analysis is therefore concerned with determining the joint and marginalized posterior probability distributions of α and β, in light of observational data $\boldsymbol{d}$ given the constraint on δc_T of (6.47).

We begin by considering the parameters $\boldsymbol{\theta} \equiv (\alpha, \beta)$. To proceed, we need to construct the likelihood $\mathcal{L}(\boldsymbol{\theta})$, consisting of the probability of observing the data $\boldsymbol{d}$ given a choice of model parameters $\boldsymbol{\theta}$: $\mathcal{L}(\boldsymbol{\theta}) = P(\boldsymbol{d}|\boldsymbol{\theta})$. Following (6.47), we model the likelihood as an univariate Gaussian in δc_T, centered around $\delta c_T = 0$

$$\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta}, \mathcal{M}) \equiv \mathcal{L}(\boldsymbol{\theta}) \equiv \mathcal{L}(\alpha, \beta) = \exp\left\{-\frac{[\delta c_T(\alpha,\beta)]^2}{2\sigma^2_{\delta c_T}}\right\}, \tag{6.48}$$

where $\delta c_T(\alpha, \beta)$, following (6.46), is given by

$$\delta c_T(\alpha, \beta) = \sqrt{\frac{2(1-\alpha)}{2-2\alpha+\beta}} - 1\,. \tag{6.49}$$

In (6.48), $\sigma_{\delta c_T}$ denotes the uncertainty on δc_T, which we estimate as $\sigma_{\delta c_T} = 5 \times 10^{-16}$ following (6.47). Note that from this equation we will omit to explicitly write the model $\mathcal{M}$ in the probabilities.

Using Bayes theorem (B.22), we construct the joint posterior distribution of α and β as the product of the likelihood (6.48) and the prior probability distributions we assign to α and β. The choice of prior is dictated by a combination of theoretical and phenomenological considerations. Following our previous discussion, we firstly impose the requirement of subluminality of tensor perturbations: $c_T^2(\alpha, \beta) \leq 1$.

In the action (6.3), the term multiplying the Riemann tensor is $1+\alpha\, g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi = 1+2\,\alpha\, X = 1-\alpha$. As this term controls the strength of the effective Newton constant, we must impose its non-negativity, which implies $\alpha < 1$. Notice that, as already discussed in section 6.3.3, requiring the absence of ghosts led to the condition $\alpha < 1$. In addition, guided by perturbativity arguments, we expect $|\alpha| \lesssim \mathcal{O}(1)$, as in general, it could be problematic to embed a coupling constant $|\alpha| \gg \mathcal{O}(1)$ in the context of a UV-complete theory of gravity. Guided by these considerations, we choose for simplicity to impose a top-hat (flat) prior on α within the range $[-1, 1]$. We assess a posteriori that our results are only mildly affected by other choices of flat prior as long as the upper and lower limits are $\sim \mathcal{O}(1)$ in modulo.

Concerning β, we already know that this parameter is required to be $\ll \mathcal{O}(1)$, for the bound in (6.47) to be satisfied. Moreover, we see from (6.46) that for $\beta < 0$, one would obtain $c_T^2 > 1$, which violates the subluminality requirement. Based on these arguments, we impose a top-hat prior on β within the range $[0, 1]$. In conclusion, the joint posterior distribution of α and β we sample from is given by

$$P(\alpha, \beta|\boldsymbol{d}) = \exp\left\{-\frac{[\delta c_T(\alpha,\beta)]^2}{2\sigma^2_{\delta c_T}}\right\}\Theta(c_T^2)\Theta(1-c_T^2)\Theta(1+\alpha)\Theta(1-\alpha)\Theta(\beta)\Theta(1-\beta)\,, \tag{6.50}$$

where $\Theta(x)$ denotes the Heaviside step function.

In the second part of the analysis, we include the parameter γ as well, which requires additional information to be taken into account beyond the constraint on δc_T of (6.47). Since γ enters in the expression for the sound speed c_s (6.45), we additionally impose the subluminality of scalar perturbations †. In addition, as already discussed in section 6.3.3, requiring the absence of ghosts leads to the condition $\gamma > 0$. Therefore, guided by considerations on the absence of ghosts and perturbativity as per our previous discussion, we impose a top-hat prior on γ within the range $[0, 1]$. We will later anyway see that data require $\gamma \ll \mathcal{O}(1)$. In this case, the joint posterior distribution of α, β, and γ, given the data $\boldsymbol{d}$, is given by

$$P(\alpha, \beta, \gamma|\boldsymbol{d}) = \exp\left\{-\frac{[\delta c_T(\alpha,\beta)]^2}{2\sigma^2_{\delta c_T}}\right\}\Theta(1+\alpha)\Theta(1-\alpha)\Theta(\beta)\Theta(1-\beta)\Theta(\gamma)\Theta(1-\gamma)\times$$
$$\times\,\Theta(c_T^2)\Theta(1-c_T^2)\Theta(c_s^2)\Theta(1-c_s^2)\,. \tag{6.51}$$

To sample the posterior distributions (6.50) and (6.51), we make use of Markov Chain Monte Carlo (MCMC) methods, by implementing the Metropolis-Hastings algorithm introduced in Appendix B.6.2. We use two methods: a novel software we specifically coded for this analysis [54], and the cosmological MCMC sampler `Montepython` [55], configured to act as a generic sampler. In the following, since we confirmed that the two methods give the same results, we will show the `Montephyton` results. We monitor the convergence of the MCMC chains using the Gelman and Rubin parameter $\hat{R}-1$, introduced in Section B.6.3, which we require to be < 0.01 for the chains to be considered converged.

6.5.3 Results

We first sample the joint α-β posterior distribution given by (6.50). We show the results in the triangular plot of Fig. 6.3, whose diagonal contains the marginalized probability distributions of the two parameters.

We find $\alpha < 0.55$ at 95% confidence level (C.L.), while the marginalized posterior of β is, as expected, peaked at $\beta = 0$ and falls rapidly as β increases, indicating $\beta < 5.11 \times 10^{-15}$ at 95% C.L.. The reason for these very tight bounds is readily found by inspecting Eq. (6.46). As β moves away from 0 (at fixed α), c_T^2 rapidly moves away from 1, and hence the probability density of the given point in (α, β) parameter space decreases.

Although deviations of c_T from 1 are controlled mainly by β, the parameter α does nonetheless play a role. In fact, from the orientation of the joint α-β posterior distribution (lower left panel in Figure 6.3), we see that the two parameters exhibit a mild negative correlation (also referred to as parameter degeneracy). That is, it is possible to increase/decrease one parameter and correspondingly decrease/increase the other, and still maintain consistency with the GW170817 bound on c_T. This observation can be rigorously shown by Taylor expanding δc_T in the limit of small $\beta/(2-2\alpha)$

$$\delta c_T = \left(1 + \frac{\beta}{2-2\alpha}\right)^{-\frac{1}{2}} - 1 \underset{\frac{b}{2-2\alpha}\to 0}{\longrightarrow} -\frac{\beta}{4(1-\alpha)}\,. \tag{6.52}$$

From (6.52), we see that the more β increases, the more c_T deviates from 1. Moreover, the smaller α is, the larger the term $4(1-\alpha)$ in Eq. (6.52) is, implying that it is consequently possible to "tolerate" larger values of β and still be consistent with the deviation of c_T from 1 allowed by GW170817/GRB170817A. This explains the mild negative correlation between α and β. From our MCMC chains, we estimate the correlation coefficient between the two parameters to be ≈ -0.40.

† There exist upper limits on the sound speed of dark matter from observations of the CMB and large-scale structure, which suggest $c_s^2 \lesssim 10^{-10.7}$ [53]. However, these bounds are not entirely model-independent: the analysis should be re-performed in our case by solving the relevant Einstein-Boltzmann equations. Moreover, the propagating scalar mode in our model does not exclusively mimic dark matter, but a combination of dark matter and dark energy (see [8]). To be conservative, we have decided not to impose these upper limits on c_s.

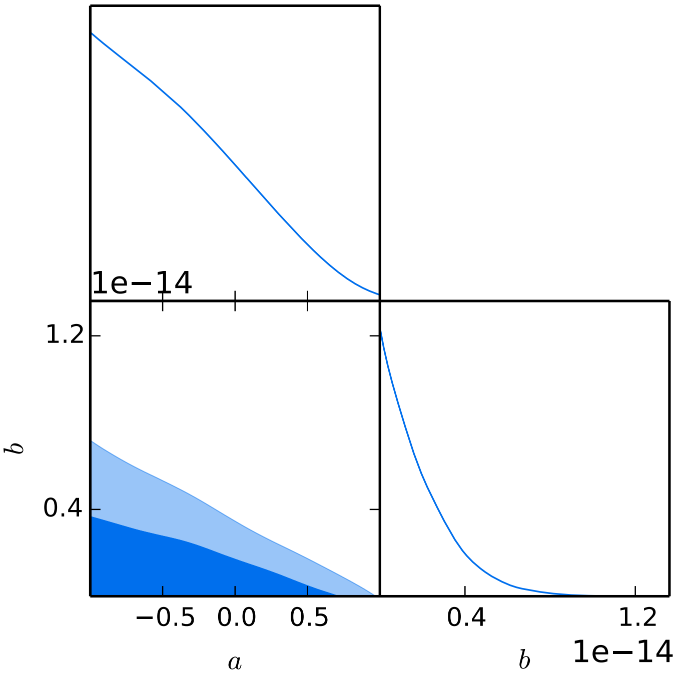


Figure 6.3: Triangular plot showing joint and marginalized posterior probability distributions of the parameters $a = \alpha$ and $b = \beta$, in light of the joint GW170817/GRB170817A detection, and imposing the subluminality of tensor perturbations and absence of ghosts. The blocks along the diagonal (upper left and lower right) contain the 1D marginalized posterior distributions of α and β (since the quantity plotted is a *normalizable* probability distribution, the overall scale of these plots is irrelevant, which is the reason why the y-axes are unit-less). The remaining block (lower left) shows the joint 2D α-β posterior distribution, with 68% C.L. and 95% C.L. credible regions corresponding to the light and dark blue areas respectively.

Next, we sample the joint α-β-γ posterior probability distribution given by (6.51). We show the results in the triangular plot of Figure 6.4. Quoting all 95% C.L. upper bounds, we find $\alpha < 0.27$, $\beta < 7.18 \times 10^{-15}$, and $\gamma < 4.68 \times 10^{-15}$. [‡] To explain the results we find, it is useful to consider the expression for the sound speed squared, Eq. (6.45), and the combinations of the three parameters α, β, and γ necessary to keep this quantity positive. It is then quite easy to see that, in the limit where $\beta \ll \alpha$ and $\gamma > 0$, it is possible to keep $c_s^2 \geq 0$ by requiring that γ be smaller than β, i.e. $\gamma \lesssim \beta \sim O(10^{-15})$, while also having $1 - \alpha \gg O(10^{-15})$ (i.e. α is sufficiently far from 1). In this limit, the sound speed is approximately given by

$$c_s^2(\alpha, \beta, \gamma) \approx \frac{(\beta - \gamma)}{4 - 4\alpha - \beta + 3\gamma} \,, \tag{6.53}$$

where the condition $\gamma \lesssim \beta \sim O(10^{-15})$ now ensures that the numerator of Eq. (6.53) is positive, while the condition $(1 - \alpha) \gg O(10^{-15})$ ensures that there are no "accidental cancellations" between the terms $4(1 - \alpha)$ and $3\gamma - \beta$ in the denominator which might otherwise make it negative, i.e. that the denominator is approximately given by $4(\alpha - 1)$ and hence is always positive since $\alpha < 1$. This discussion

[‡] Although there appears to be a mild peak in the posterior distribution of β, we find that the distribution is consistent with $\beta = 0$ at $\sim 2\sigma$. Therefore, as is standard practice in the field, we only quote an upper limit for β instead of a "detection" of non-zero β. Recall also that we had chosen the upper and lower limits for our priors based on perturbativity considerations. We have checked that our results, and in particular the upper limits on β on γ, are only very marginally affected (within the same order of magnitude) by other choices for the upper and lower limits of the prior, which still are $\mathcal{O}(1)$ in modulo. We, therefore, consider our results relatively robust against the choice of prior.

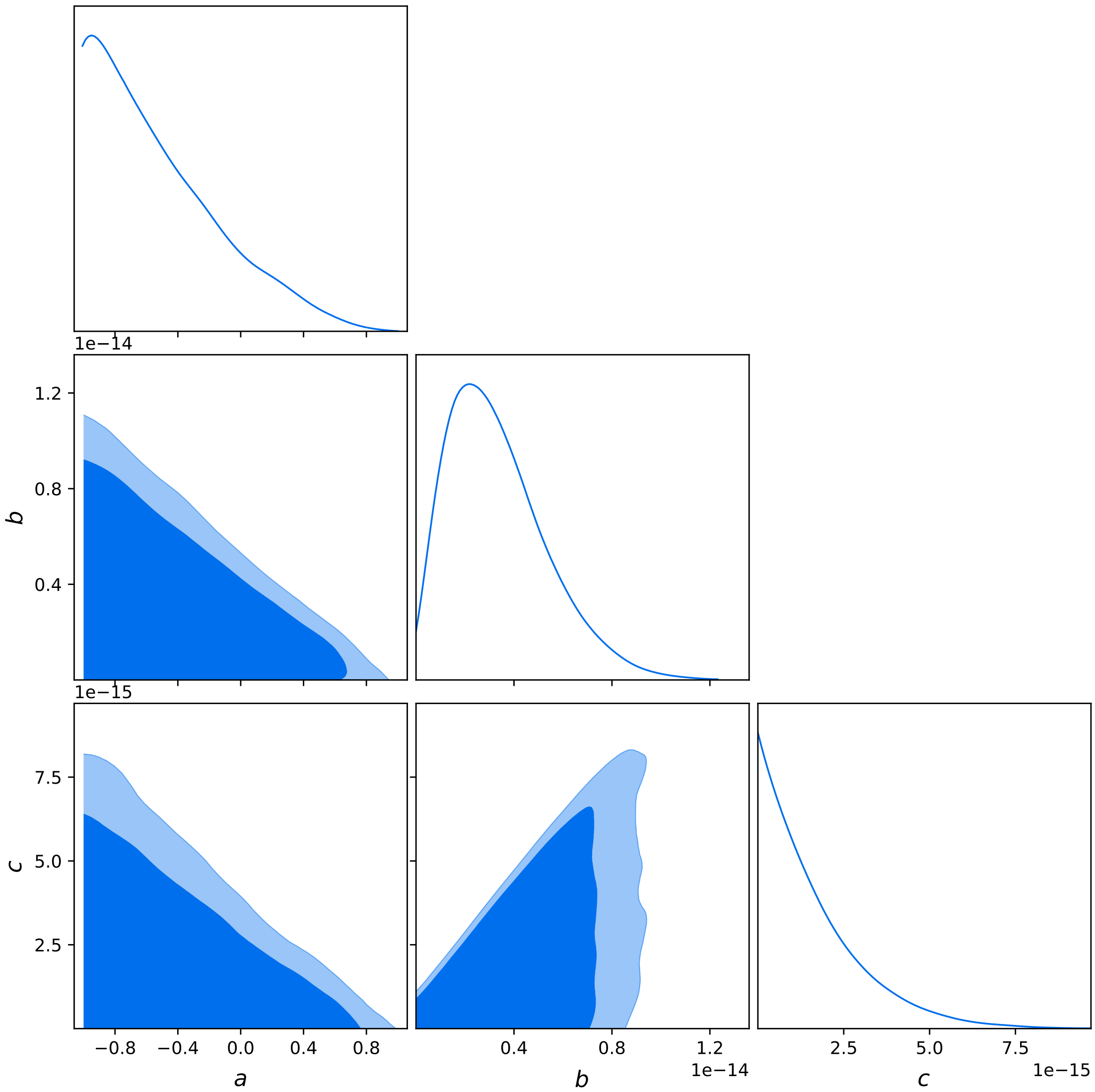


Figure 6.4: As in Figure 6.3, with the addition of the parameter $c = \gamma$ and the further imposition of subluminality of scalar perturbations.

explains why the upper limit on γ is approximately of the same order as the upper limit on β, i.e., of order 10^{-15}, since γ is required to be positive (to avoid ghosts) but smaller than β (to have $c_s^2 \geq 0$).

The above discussion also suggests that we can expect a strong positive correlation between β and γ (since increasing γ requires increasing β to keep the numerator of (6.53) positive). We find a correlation coefficient of 0.66 between β and γ, which is stronger than the already strong correlation we previously found between γ and β. On the other hand, we find a weaker correlation between α and γ, with a correlation coefficient of -0.28, induced by the mutual correlations of these two parameters with β. The negative correlation between α and γ, and the positive one between β and γ, explain why introducing the parameter γ has respectively tightened and loosened the upper limits we previously derived on α and β when only considering these two parameters (recall that the upper limit shifted from 0.55 to 0.27 for α, and from 5.11×10^{-15} to 7.18×10^{-15} for β). We plot a heatmap of the correlation coefficients between the three parameters in Figure 6.5, where it is clear that the strongest correlation is that between β and γ, for reasons already discussed previously.

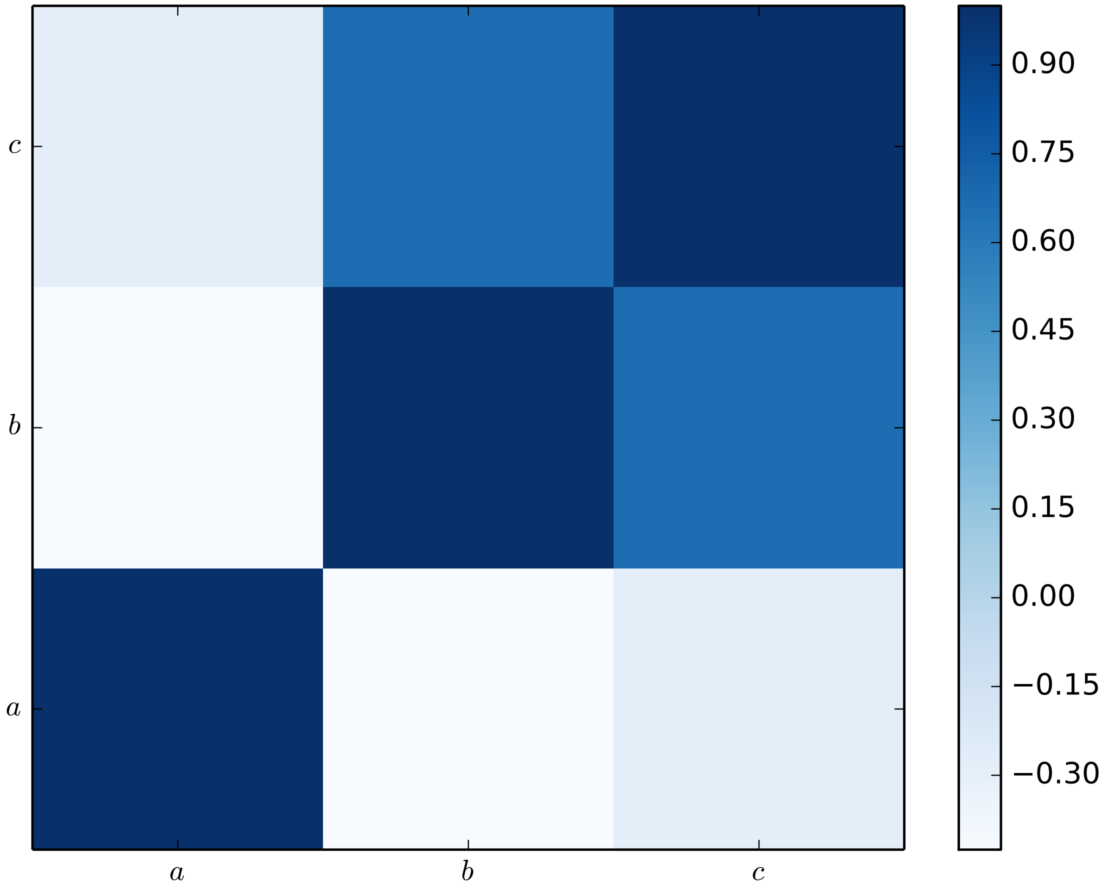


Figure 6.5: Heatmap of the correlation matrix between the 3 parameters ($a = \alpha$, $b = \beta$, and $c = \gamma$) we are examining. We visually see that the strongest correlation is that between β and γ, resulting from the necessity of avoiding ghost instabilities (which requires $\gamma > 0$) while needing $c_s^2 \geq 0$ (which requires $\gamma < \beta$), as discussed in the text.

6.6 Summary

In this Chapter, we have studied a mimetic model constructed in [46] by breaking the Horndeski structure of a starting mimetic Horndeski model to achieve a non-zero sound speed. We explored the model in light of the recent near-simultaneous detection of GW170817/GRB170817A, which implies that the speed of tensor perturbations c_T is extremely close to the speed of light. In light of this constraint, we then showed how the model could closely mimic dark matter and dark energy evolution.

In this first part, we have found that the stringent constraint on the speed of gravitational waves, equal to the speed of light up to deviations of order 1 part in 10^{15} [12], severely constrains the Lagrangian parameter β, which controls the strength of a term of the form $\nabla^\mu \nabla^\nu \phi \nabla_\mu \nabla_\nu \phi$ in the action (6.3). In the limit where we force c_T to be identically equal to the speed of light, $\beta = 0$ is required. We have found that the other two Lagrangian parameters α and γ lead to a constant rescaling of the Planck mass, where the unscaled Planck mass of GR is recovered for $3\gamma = 4\alpha$.

By considering the addition of radiation and baryonic matter, we have numerically solved the modified Friedmann equation and shown that the system can closely mimic an evolutionary history of the Universe consistent with the standard ΛCDM one at the background level: that is, the mimetic model in question with $\beta = 0$ (to comply with constraints from G170817/GRB170817A) can mimic, at the background level, dark matter and dark energy consistently with observations. We computed the Universe's age and found that the ΛCDM value for this quantity is recovered when $3\gamma = 4\alpha$ (which leads to an unscaled Planck mass) as well as for the trivial case where $\alpha = \gamma = 0$. Therefore, we expect the approximate relation $3\gamma \simeq 4\alpha$ to hold.

A consideration concerning the stability of the theory is necessary. We have shown that to avoid ghost instabilities, we need a negative squared sound speed c_s^2 together with $\gamma > 0$. However, gradient instabilities are still present in the scalar sector, but these might be mildened because of the matter field contributions. The stability issue has been studied in many recent papers, see e.g. [56, 48, 57, 58, 59, 60, 61, 62, 63, 64]. While definitive consensus on the matter is yet to be reached, we notice that these issues are likely to affect our model as well, thus undermining its theoretical viability. Nonetheless, solutions to these issues have been proposed, involving direct couplings between higher derivatives of the mimetic field and curvature, for instance of the form $f(\Box\phi)$ or $\nabla^\mu\nabla^\nu R_{\mu\nu}$ [59, 60, 64]. Of course, such terms would be expected to modify the prediction for c_T we derived in (6.26) and could conflict with the GW170817/GRB170817A detection.

Finally, in the last section, we have examined, performing quantitative analysis, the status of mimetic gravity in light of the recent near-simultaneous detection of the GW event GW170817 [11] and its optical counterpart, the short γ-ray burst GRB170817A [12]. Entertaining the possibility of a tiny violation of the $c_T \equiv 1$ constraint, in agreement with experimental constraints from GW170817/GRB170817A [12], we have performed a Bayesian statistical analysis to derive observational constraints on the three free parameters of the model. In particular, we have found that β and γ, the coefficients of the terms $\nabla^\mu\nabla^\nu\phi\nabla_\mu\nabla_\nu\phi$ and $(\Box\phi)^2$ in the action respectively (with ϕ the mimetic field), are subject to the very stringent constraints $0 \leq \beta < 7.18 \times 10^{-15}$ and $0 \leq \gamma < 4.68 \times 10^{-15}$ at 95% confidence level. In light of these very tight limits, it is tempting to conclude that, to avoid incurring fine-tuning and naturalness issues, both parameters should be 0. In this case, the gravitational wave speed is identically equivalent to the speed of light, while the sound speed squared is $1/4(1-\alpha)$ and always positive as long as $\alpha < 1$, which is required to avoid ghost instabilities. We stress that this work is the *first* that derives that robust observational constraints are placed on a mimetic theory.

We conclude with a comment on the smallness of the parameter β, which might lead to a fine-tuning problem. When integrated by parts, the relevant term in the action, $\nabla^\mu\nabla^\nu\phi\nabla_\mu\nabla_\nu\phi$, leads to a term proportional to $\phi\,\Box^2\phi$. In [65] (see also [66, 67]), it was argued that such a term appears when considering 1-loop corrections to the cubic Galileon action. While the analysis of [65] is not directly applicable to our model, the results tempt us to speculate that the smallness of β might be due to the relevant term being a quantum correction, with the bare parameter being $\beta = 0$. However, a detailed analysis of the issue is well beyond the scope of this paper, and hence we defer it to future work.

Part III

Effective Field Theory for Gravity

Chapter 7

Introduction to the Effective Field Theories

In this Chapter, we explain the main properties and features of the standard Effective Field Theory. In the next Chapter, we will use some of the tools developed in this part, in the context of building an Effective Field Theory of Gravity.

7.1 Definition

A rough but immediate definition of an Effective Field Theory (EFT) is the following.

> *The Effective Field Theory is a method to study physics at low energies without worrying about what happens at higher energy scales.*

Usually, the low energy regime is called the infrared (IR) regime, while the high energy one is called the ultra-violet (UV) regime. The latter high energy scale is described by a constant λ, i.e. the energy E of the processes we are interested in satisfies the relation $E \ll \lambda$. This provides a natural expansion parameter E/λ, and the physical processes are computed with an expansion in powers of E/λ. Therefore, provided the energy of the process always satisfies $E \ll \lambda$, higher order terms are increasingly negligible. Note that the same argument can be rephrased in terms of the length scale L instead of the energy E, with an expansion in $(L\lambda)^{-1}$.

A more formal explanation involves the path integrals and the degrees of freedom of the theory. If we have a known UV theory (ideally the complete theory with all possible degrees of freedom, which provides a description at any energy scale), we might be interested in the behaviour at low energies without having to solve the complete theory equations (and usually more complicated) of the UV theory. To study the IR regime, we can thus use the Effective Field Theory, which prescribes to "integrate out" the heavy degrees of freedom from the path integral. Formally, if $S_{\text{UV}}[\phi_i, \Psi_j]$ is the UV theory action as a function of the fields ϕ_i and Ψ_j, respectively the low and heavy degrees of freedom, the EFT action is

$$e^{iS_{\text{EFT}}[\phi_i]} = \int \prod_j \mathcal{D}\Psi_j \; e^{iS_{\text{UV}}[\phi_i, \Psi_j]} \, . \tag{7.1}$$

Note that the UV theory can be known (e.g. in the case of electrodynamic, where the UV theory is the Quantum Electrodynamic), but also unknown as it happens for gravity. In the following sections, we will consider some examples of how to build an Effective Field Theory using a different approach with respect to the path integral one.

7.2 Electromagnetism

As a first example, we consider Electromagnetism in flat space. We will use the convention $c = G = 1$. As already mentioned, in this case, the UV theory is Quantum Electrodynamic (QED), which involves two fields: the Dirac field and the gauge (Maxwell) field A_μ. The first field is associated with a fermion, while the second one describes the photons. The fermion we consider is the electron, which has a mass m. We can use this mass to define an EFT energy scale. Since we conventionally fixed $c = 1$, the energy scale is given by $\lambda = m$. Therefore, if the energy E of a process satisfies $E < \lambda = m$, we can neglect the presence of the electrons. This is the first step in building an EFT.

The question which immediately arises now is: how can we find the action (and thus the equations of motion) of such an EFT?

In the case of Electromagnetism, we can start from the standard classical Maxwell term, i.e.

$$S_0[A_\mu] = \int d^4x \left(-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}\right) \qquad \text{where} \qquad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \,. \tag{7.2}$$

Performing the variation of this action we obtain the equations of motion at the zeroth order, the Maxwell equations

$$\frac{\delta S_0}{\delta A_\mu} = \partial_\rho F^{\rho\mu} \,, \tag{7.3}$$

where $\partial_\rho = \partial/\partial x^\rho$. This is not enough if we want to describe the interactions between the photons at low energies. The *scattering of light by light* can be introduced by adding terms with an increasing number of the gauge field A_μ. For example, we can add a term $(F_{\mu\nu}F^{\mu\nu})^2$, which respects the symmetries of the UV theory (Lorentz invariance, parity). Indeed we want the UV theory to reduce to the EFT theory as we lower the energy, and therefore the addition of terms with the same symmetries of the UV theory can be promoted to be the golden rule to build an EFT.

> **R1.** *The Effective Field Theory is built with all the terms which respect the symmetries of the underlying UV theory.*

In the case of Electromagnetism, it turns out that another term respects the symmetries mentioned, leading to the action

$$S_{\text{EFT}} = \int d^4x \left[-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + a\,(F_{\mu\nu}F^{\mu\nu})^2 + b\left(F_{\mu\nu}\tilde{F}^{\mu\nu}\right)^2 + \cdots\right] , \tag{7.4}$$

where $\tilde{F}_{\mu\nu} = \epsilon_{\mu\nu\rho\sigma}F^{\rho\sigma}$ ($\epsilon_{\mu\nu\rho\sigma}$ is the totally antisymmetric Levi-Civita symbol).

Some additional questions arise from this expression: how can we choose the value of the coefficients a and b? Since in principle the number of terms we can add to the action are infinite, which terms are dominant?

The first question can be answered considering again the fact that the UV theory should become the EFT in the limit of low energies. Therefore

> **R2.** *The coefficients of the Effective Field Theory should assume a value such that the Effective Field Theory is a viable limit of the UV theory in the low energy regime.*

Performing this computation for this example, we can find the value of the coefficients in terms of the fine structure constant $\alpha = e^2/4\pi$, where e is the charge of the electron. They are

$$a = \frac{\alpha^2}{90m^4} \qquad \text{and} \qquad b = \frac{7\alpha^2}{360m^4} \,. \tag{7.5}$$

The second question answer lies in the expansion in terms of E/λ we mentioned in the previous section. In fact, consider the dimensionality of the objects we have in our theory. Since $c = \hbar = 1$, the mass scale is the inverse of a length scale, i.e. $L \backsim m^{-1}$. Therefore the dimensionality of a Lagrangian is

$$[\mathcal{L}] = L^{-4} \backsim E^4 \,. \tag{7.6}$$

This means that

$$[F] = L^{-2} \qquad \text{and therefore} \qquad [A] = L^{-1} \,. \tag{7.7}$$

Moreover

$$\left[(FF)^2\right] = L^{-8} \qquad \text{and therefore} \qquad [a, b] = L^4, \tag{7.8}$$

which is consistent with the values of a and b in equation (7.5). In general, any object X which contains p field tensors $F_{\mu\nu}$ and n derivatives of $F_{\mu\nu}$ (the derivatives have a dimensionality of $L^{-1} \backsim m$) has a dimensionality

$$[X] = L^{-2p-n} \,. \tag{7.9}$$

These objects, in order to be added to the action, must be adjusted in their dimensionality with a coefficient a_X such that (the only possible mass scale is given by the electron mass, i.e. $\lambda = m$)

$$[a_X] = L^{2p+n-4} \backsim m^{4-2p-n} \,. \tag{7.10}$$

Therefore:

> **R3.** *The terms with a large number of field tensors and its derivatives, i.e. large p and n, are suppressed, and they are less important in a E/m expansion.*

The last fact we want to prove is that the action (7.2) is the most general EFT action for the order m^{-4} of the coefficients, in the case of electromagnetism.

Firstly note that there is no $(F_{\mu\nu}\tilde{F}^{\mu\nu})^1$ term, because $F_{\mu\nu}\tilde{F}^{\mu\nu}$ is odd under parity, while the QED is even. In general, any $(F_{\mu\nu}\tilde{F}^{\mu\nu})^{2n+1}$ with $n \in \mathbb{N}$ is incompatible with the parity symmetry and therefore cannot be added to the EFT action. However, terms with even exponents, e.g., $(F_{\mu\nu}\tilde{F}^{\mu\nu})^2$ in action (7.4), can be considered.

Secondly, although they are of order L^6 (and therefore dominant with respect to the FF terms of order m^8 we kept), we can neglect terms like $\partial F \partial F$. In fact these terms can be eliminated by means of a field redefinition. For instance, consider a candidate term (with the coefficient with the appropriate dimensionality, i.e. β adimensional)

$$\frac{\beta}{m^2}\partial^\mu F_{\mu\sigma}\partial^\rho F_\rho{}^\sigma \,. \tag{7.11}$$

It is possible to redefine the gauge field as

$$A_\mu = A'_\mu - \frac{\beta}{m^2}\partial^\rho F'_{\rho\mu}, \tag{7.12}$$

where $F'_{\mu\nu}$ is the field tensor defined as $F_{\mu\nu}$, but with the redefined field A'_μ instead of A_μ. Transforming this term we obtain

$$S_0[A] + \frac{\beta}{m^2}\partial^\mu F_{\mu\sigma}\partial^\rho F_\rho{}^\sigma = S_0[A'] - \frac{\beta}{m^2}\frac{\delta S_0}{\delta A_\mu}\partial^\rho F_{\rho\mu} + \frac{\beta}{m^2}\partial^\mu F_{\mu\sigma}\partial^\rho F_\rho{}^\sigma \,. \tag{7.13}$$

But the last two terms on the right-hand side of the equation cancel exactly due to the equations of motion (7.3). This is an example of a more general property:

> **R4.** *We can eliminate from the Effective Field Theory action all the terms proportional to the zeroth-order equations of motion with a field redefinition.*

The cases discussed include all the possible additions to the action up to the m^{-4} order in the coefficients. Therefore the action (7.2) with the coefficients defined in equation (7.5) and without additional terms ("without the dots") is the most general EFT theory of order m^{-4} in the coefficients.

Finally, note that the rules we have explained in this section are general of any Effective Field Theory consistent with its underlying UV theory. In the next section, we will apply these rules to another theory for which we do not know the underlying UV theory: General Relativity.

7.3 Gravity

In this section, we will consider the gravity theory. In this context, the EFT can be used as a framework to parametrize possible deviations from General Relativity.

As already mentioned, we have no high energy (UV) theory for gravity. This means that we can not proceed as in the previous example, where the UV theory was very well known. However, we can still use the rules derived for the Electromagnetism case: we need to identify a low energy degree of freedom (and thus an energy scale) and write down the most general Lagrangian which is consistent with the symmetries we might expect for the theory (**R1**). It is reasonable to assume diffeomorphism invariance (covariance) and parity will be the symmetries of the UV theory.

We will also exploit the third rule **R3** and write the Lagrangian as an expansion in terms with increasing mass dimension such that the lower order terms in this expansion are dominant with respect to the higher ones. This is valid only if we want to describe a system that involves energies smaller than the UV scale λ. For instance, if the aim is to study the gravitational waves, the UV scale can be set to be $\lambda^{-1} \cong 1$ km. However, the UV scale is usually the Planck mass, i.e. $\lambda \cong M_p = 1/8\pi G$.

With these rules, we can write the Lagrangian with no matter terms as

$$S_{\text{EFT}} = \int d^4x\sqrt{-g}\left[\frac{M_p^2}{2}\left(R - 2\Lambda\right) + aR^2 + bR_{\mu\nu}R^{\mu\nu} + c\,\mathcal{G} + \dots\right], \tag{7.14}$$

where Λ is a constant, and the dots stand for terms of order (in the curvature tensors) higher than two. The $\mathcal{G}$ is the Gauss–Bonnet term defined as

$$\mathcal{G} = R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma}\,. \tag{7.15}$$

Therefore, the action (7.14) involves the presence of all the curvature tensors, which are covariant and even under parity. These terms are all the possible terms that can be added that have four derivatives. Note also that the Weyl tensor can be added to this action with a suitable combination of the terms in the action, i.e. choosing a, b, and c. The zeroth-order equations of motion are given by the Einstein vacuum equations in the presence of a cosmological constant

$$R_{\mu\nu} = \Lambda g_{\mu\nu}\,. \tag{7.16}$$

To find the order of the terms in the action in terms of the energy scale λ, we can start again from the dimensionality of the Lagrangian (7.6)

$$[\mathcal{L}] = L^{-4}\,. \tag{7.17}$$

Since by definition the Ricci scalar contains two derivatives (each with dimensionality λ), i.e.

$$[R] = L^{-2}\,, \tag{7.18}$$

from the first term we can find the metric dimensionality as

$$[g_{\mu\nu}] = L^{0}\,. \tag{7.19}$$

Moreover, the second order terms in the curvature tensors have

$$\left[R^2\right] = L^{-4}\,, \tag{7.20}$$

and therefore the coefficients a, b and c are dimensionless. Terms with three curvature tensors would have a coefficient energy scale of λ^{-2}. We will consider the energy scale $\lambda = M_p^2$.

When $\Lambda = 0$, from the second rule **R2**, we can eliminate the terms R^2 and $R_{\mu\nu}R^{\mu\nu}$ with a field redefinition, as they are proportional to the equations of motion. The same cancellation can occur when $\Lambda \neq 0$, allowing for a redefinition of the constant and the Planck mass M_p.

Therefore, the only remaining term at the second order in the curvature tensors is the Gauss–Bonnet term. But the variation of the Gauss–Bonnet term with respect to the metric

$$\frac{1}{\sqrt{-g}}\frac{\delta\left(\sqrt{-g}\mathcal{G}\right)}{\delta g_{\mu\nu}} = \text{total derivative}\,, \tag{7.21}$$

and therefore $\mathcal{G}$ does not contribute to the equations of motion.

Therefore, with a field redefinition, we can eliminate all terms at second order in the curvature tensor (terms with four derivatives). Thus the only EFT contribution should come from terms with three curvature tensors (six derivatives), with a suppression of λ^{-2}. Is there a way to avoid this conclusion?

One way might be to consider a space-time dimension $d > 4$, which introduces a new contribution to the equations of motion coming from the Gauss–Bonnet term. In fact, the Gauss-Bonnet variation with respect to the metric is a total derivative only for $d \leq 4$. Note that, due to the Lovelock theorem, the equations of motion will still be at 2^{nd} order.

Another way in $d = 4$ is to add matter (which we neglected in the previous discussion), in terms of a scalar field ϕ. The EFT action (up to a field redefinition) is

$$S_{\text{EFT}} = S_2 + S_4\,, \tag{7.22}$$

$$S_2 \equiv \int d^4x\sqrt{-g}\left[\frac{M_p^2}{2}R - X - V(\phi)\right]\,, \tag{7.23}$$

$$S_4 \equiv \int d^4x\sqrt{-g}\left[f(\phi)X^2 + g(\phi)\mathcal{G}\right]\,, \tag{7.24}$$

where $X \equiv \partial^\mu\phi\partial_\mu\phi$. The actions S_2 and S_4 contain respectively terms with 0 or 2 derivatives and terms with 4 derivatives. The equations of motion of this theory will be at second order. Note that the Gauss-Bonnet term, even if we are in $d = 4$, contributes to the equations of motion due to the non-constant coupling $g(\phi)$.

7.4 Conclusion

The Effective Field Theory is a powerful tool to study the properties of a physical system at a low energy regime, without considering the high energy effects. The practical rules are summarized here.

> **R1.** *The Effective Field Theory is built with all the terms which respect the symmetries of the underlying UV theory.*
>
> **R2.** *The coefficients of the Effective Field Theory should assume a value such that the Effective Field Theory is a viable limit of the UV theory in the low energy regime.*
>
> **R3.** *The terms with a large number of field tensors and their derivatives, i.e. large p and n, are suppressed, and they are less important in a E/m expansion.*
>
> **R4.** *We can eliminate from the Effective Field Theory action all the terms proportional to the zeroth-order equations of motion with a field redefinition.*

In the next Chapter, we introduce an Effective Field Theory useful for cosmological applications such as dark energy and inflation phenomena. We will argue that this effective field theory since it follows the aforementioned rules.

Chapter 8

The Effective Field Theory of Gravity

In this Chapter we introduce the Effective Field Theory of Gravity (EFT) using a non-covariant approach, that consists in breaking the time diffeomorphism of standard general relativity theories. This procedure allows us to build an effective Lagrangian given a certain energy scale that depends on the problem (e.g., inflation or late universe evolution). With this theory, we introduce a model-independent way to describes Modified Gravity deviations from General Relativity in the context of cosmology. This approach can therefore be efficiently applied for numerical evaluations of linear and non-linear perturbations. You can then map the *covariant* Modified Gravity model (in the sense of the previous Part) into the EFT to constraint it, without the need to perform a new analysis.

We firstly introduce the concept of spontaneous symmetry breaking in a simple case using a toy model. Then, we will build the effective Lagrangian using this tool. The derivation resembles the one in [68, 69, 70, 71].

8.1 Spontaneous symmetry breaking

In this section we introduce the spontaneous symmetry breaking, starting from an example. We introduce the Lagrangian for a complex scalar field ϕ with the addition of a massless U(1) gauge field A_μ

$$\mathcal{L} = -(\partial_\mu + ieA_\mu)\phi^*(\partial^\mu - ieA^\mu)\phi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - V(\phi)\,, \tag{8.1}$$

where $F_{\mu\nu}$ is the standard electromagnetic tensor defined as

$$F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu\,, \tag{8.2}$$

and the potential is the so-called "Mexican hat" potential

$$V(\phi) = -\mu^2 |\phi|^2 + \lambda |\phi|^4\,. \tag{8.3}$$

Note that for $\mu^2 < 0$, the potential is a standard parabola. From now on we will consider only the case $\mu^2 > 0$.

In the Lagrangian (8.1), with respect to a photon-free theory (e.g. the Lagrangian $\mathcal{L} = -\partial_\mu\phi^*\partial^\mu\phi - V(\phi\phi^*)$ of a single complex scalar field) the partial derivative seems to be substituted by $\partial_\mu + ieA_\mu$. This term is usually called the covariant derivative of the gauge theory and has the same function of counterpart of General Relativity, that is, to eliminate unpleasant terms which arise when we differentiate the coefficient of a coordinate transformation.

The Lagrangian (8.1) is invariant under U(1) symmetry of both the scalar and the gauge field. Explicitly, the transformation is

$$\phi \to e^{i\alpha(x)}\phi \qquad\qquad A_\mu \to A_\mu + \frac{1}{e}\partial_\mu\alpha(x)\,, \tag{8.4}$$

where $\alpha(x)$ is a generic function of the spacetime coordinate x^μ, and therefore this is a *local transformation*. This symmetry is also a *gauge symmetry* because applying the transformation we go to another physical state that is mathematically equivalent to the starting one., i.e. the states connected by a gauge symmetry are physically the same. This translates into a mathematical redundancy of the description of the physical reality. This feature of gauge transformations gives us the freedom to *fix the gauge*, in a procedure called *gauge fixing*, where we choose one representative from the set of physically equivalent states. The definition of the gauge fixing condition becomes part of the theory itself, at the price of breaking the gauge symmetry in the theory. But, again, since the gauge symmetry is only a mathematical symmetry, the physical description does not lose generality. Notable examples are the Coulomb or Lorentz gauges in the theory of electromagnetism. In our example, gauge fixing requires to specify the transformation function $\alpha(x)$ in (8.4).

The Mexican hat potential (8.3) has one unstable state for $\phi(x) = 0$, and a continuous set of stable states defined by the minimum of the potential, that is at

$$\phi\phi^* = \frac{\mu^2}{2\lambda} \equiv v\,. \tag{8.5}$$

Therefore this theory has an infinite number of possible vacuum states, and each of them has the same probability to be the ground state. This is the core of symmetry breaking: we are forced to a ground state that does not have the symmetry of $\phi(x) = 0$.

We can expand the field around the ground state v

$$\phi(x) \equiv [\pi(x) + v]\, e^{i\theta(x)}, \tag{8.6}$$

where $\theta(x)$ is a scalar field associated to the degree of freedom associated with the rotation of the vacuum state, that does not require any energy: $\pi(x)$ is a scalar field associated to the oscillation around the vacuum state in the direction orthogonal to the one of θ, which requires energy.

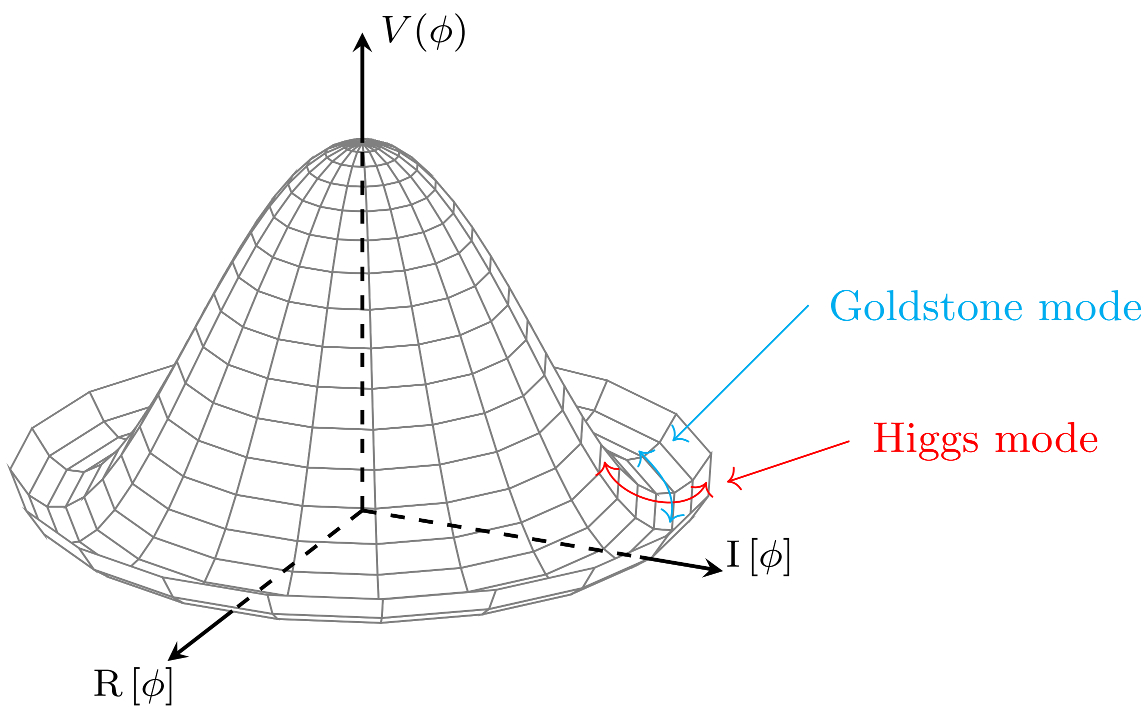


Figure 8.1: Plot of the Mexican hat potential (8.3). The Higgs mode is the mode $\pi(x)$ that also climbs the potential, and therefore its motion requires energy. On the contrary, the $\theta(x)$ mode has a motion that does not require energy since is on an equipotential line (the minimum of the hat). Therefore we expect the first to be a massive mode, and the latter to be massless.

Substituting this form of the field in the Lagrangian (8.1), we obtain at quadratic order

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - v^2\partial_\mu\theta\partial^\mu\theta - \partial_\mu\pi\partial^\mu\pi - 4\lambda v^2\pi^2 + e^2v^2A_\mu^2 - 2ev^2\partial_\mu\theta\partial^\mu\pi + \text{higher order terms}. \quad (8.7)$$

In this Lagrangian we note that:

- the scalar field π appears in the Lagrangian with a mass $2v\sqrt{\lambda}$ given by the fourth term of $\mathcal{L}$. This massive boson is usually called **Higgs boson**;
- the scalar field θ is a massless field, since in the Lagrangian we have only the kinetic term $v^2\partial_\mu\theta\partial^\mu\theta$. When a symmetry is broken, the Goldstone theorem ensures that a massless boson must always appear. Because of this, θ is called **Goldstone boson**. We will see in a moment that this particle (in this case) is not physical, and can be removed from the theory fixing the gauge;
- the photon has acquired a mass (fifth term of $\mathcal{L}$), that comes from the interaction between the photon and the constant part of ϕ.

It is worth stressing that the appearance of a mass for the photon is, up to now, only a feature of the field redefinition. Therefore, a question might arise naturally: how is it possible to give photons a mass with just a mathematical trick? If the photons were described by a Lagrangian with a scalar field ϕ governed by a Mexican hat potential (8.3), this would be the case. In practice, symmetry breaking is used to give mass to other gauge fields such as the $W^\pm$ and Z^0 bosons from electroweak theory. From the theoretical point of view, we are only redefining the fields and adjusting our physical interpretation of them. Although we always write about symmetry breaking, a more correct definition would be hidden symmetry, since the new Lagrangian (8.7) is still invariant under U(1) symmetry (8.4), but the latter is hidden in the redefinition of the fields.

The next step is to fix the gauge, which shows that the Goldstone boson is non-physical. If we consider the gauge fixing condition $\alpha = -\theta$ we obtain the following gauge fixed transformation

$$\phi \to e^{-i\theta(x)}\phi \qquad\qquad A_\mu \to A_\mu - \frac{1}{e}\partial_\mu\theta(x)\,. \quad (8.8)$$

This is the same as considering $\theta(x) = 0$, as can be easily seen applying the gauge fixed transformation (8.8) to the field definition (8.6). This gauge, where the Goldstone boson disappears, is usually called the **unitary gauge**. It removes the U(1) symmetry from the Lagrangian (8.7), together with the scalar field $\theta(x)$. So, the gauge-fixed Lagrangian is

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \partial_\mu\pi\partial^\mu\pi - 4\lambda v^2\pi^2 + e^2v^2A_\mu^2 + \text{higher order terms}\,. \quad (8.9)$$

The removal of the Goldstone boson, while the massive boson is still present, is called **Higgs mechanism**. This is the reason why this process is usually explained as the Goldstone boson being "eaten" to give the photon a mass. Explicitly, we are converting the scalar degree of freedom of the Goldstone boson with the new longitudinal degree of freedom of the photon, arising from the appearance of mass.

There is a way to restore the symmetry, that we have removed with the unitary gauge, that is to force the inverse (8.8) transformation, i.e. by performing the transformation

$$\phi \to e^{i\theta(x)}\phi \qquad\qquad A_\mu \to A_\mu + \frac{1}{e}\partial_\mu\theta(x) \quad (8.10)$$

on the Lagrangian (8.9). The Lagrangian symmetry U(1) is restored, and the Goldstone boson $\theta(x)$ reappears. This procedure is called **Stueckelberg trick**.

Another interesting similar case happens when we are dealing with a Lagrangian without a photon, e.g., $\mathcal{L}$ (8.1) without A_μ

$$\mathcal{L} = -\partial_\mu\phi^*\partial^\mu\phi - V(\phi)\,. \tag{8.11}$$

This is invariant only under the global U(1) gauge transformation

$$\phi \to e^{i\omega}\phi, \tag{8.12}$$

where ω is a constant (compare with the local transformation (8.4), where the exponent is a function of spacetime position). The minimum of the potential is instead the same of the previous case.

In this case, using the same redefinition of the field ϕ (8.6), we obtain the Lagrangian

$$\mathcal{L} = -v^2\partial_\mu\theta\partial^\mu\theta - \partial_\mu\pi\partial^\mu\pi - 4\lambda v^2\pi^2 - 2ev^2\partial_\mu\theta\partial^\mu\pi + \text{higher order terms}\,. \tag{8.13}$$

This Lagrangian is now non-reducible in the sense that we do not have any gauge symmetry to fix to remove the Goldstone boson. The ω is a constant and therefore it can not eliminate $\theta(x)$, for every x^μ, as happened with the gauge condition $\alpha(x) = -\theta(x)$ in the previous case. Therefore, the Goldstone boson in this case is a physical degree of freedom.

From this example, we can appreciate the difference between global and local symmetries. The Higgs mechanism can occur only in the presence of a local gauge[*] symmetry.

In Figure 8.2 we show a scheme of the spontaneous symmetry breaking mechanism.

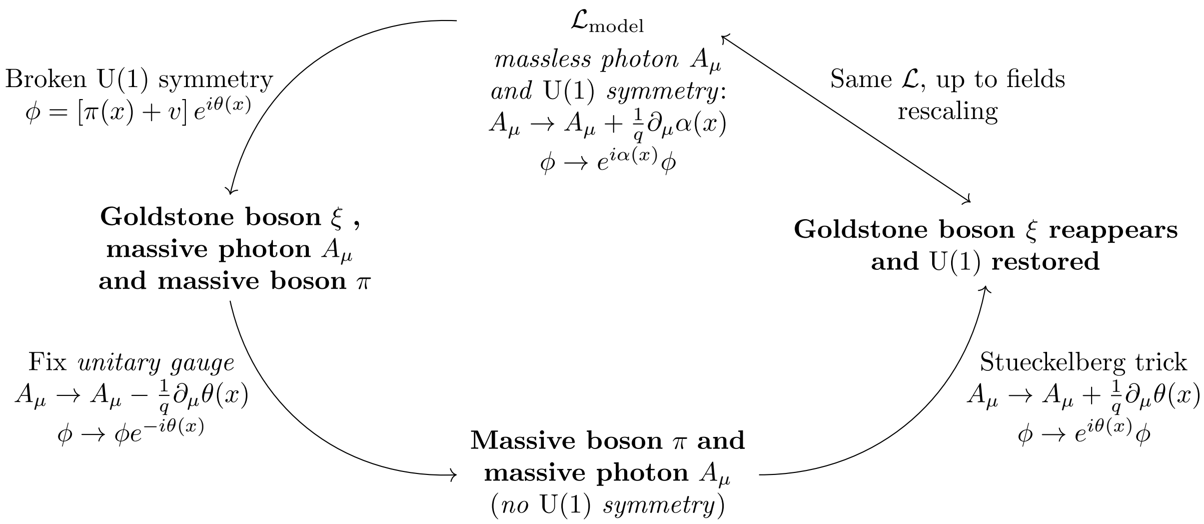


Figure 8.2: Scheme of the spontaneous symmetry breaking mechanism. The *field rescaling* we are considering is the inverse procedure needed to go from the Lagrangian (8.7) to (8.1).

8.2 Towards an Effective Field Theory of Gravity

In this section, we proceed towards the definition of the action of the non-covariant Effective Field Theory of Gravity. We call it non-covariant because we spontaneously break the space-time diffeomorphism in the time sector only, leaving the space diffeomorphism unbroken. With this procedure, we generate a

[*] The gauge adjective for a local symmetry is redundant. To be physically viable, local symmetries must always be gauge symmetries. This can be easily seen considering a generic action: if we perform a local symmetry far from the extremal points, the path (field) connecting these points changes, and the field that extremized the action might not be the one that extremized the transformed one. But, if the local symmetry is a gauge symmetry, we are connecting fields that are physically the same, and therefore all the transformed fields will extremize the action, retaining the determinism of the theory. This does not happen with global symmetries, because in that case the whole field is shifted, and therefore also the extremal points.

theory where we can isolate the terms preserving the remaining spatial translation symmetry, which are relevant in the description of linear and higher order perturbations. Then, we can then apply an EFT approach (using the rules of the previous section 7) to build the Lagrangian of the theory as a series of terms whose order is proportional to their importance at small scales.

We proceed differently with respect to the previous section 8.1. Consider the scheme 8.3, starting from the upper $\mathcal{L}_{\text{eff}}$: we firstly build the already broken action $\mathcal{L}_{\text{eff}}$, considering all the terms that preserve the space translation symmetry using the ADM formalism, and then provide the "top-down" procedure to go from a covariant action $\mathcal{L}$ to the effective one. Then we apply the Stueckelberg trick to restore time diffeomorphism and work with the Goldstone boson.

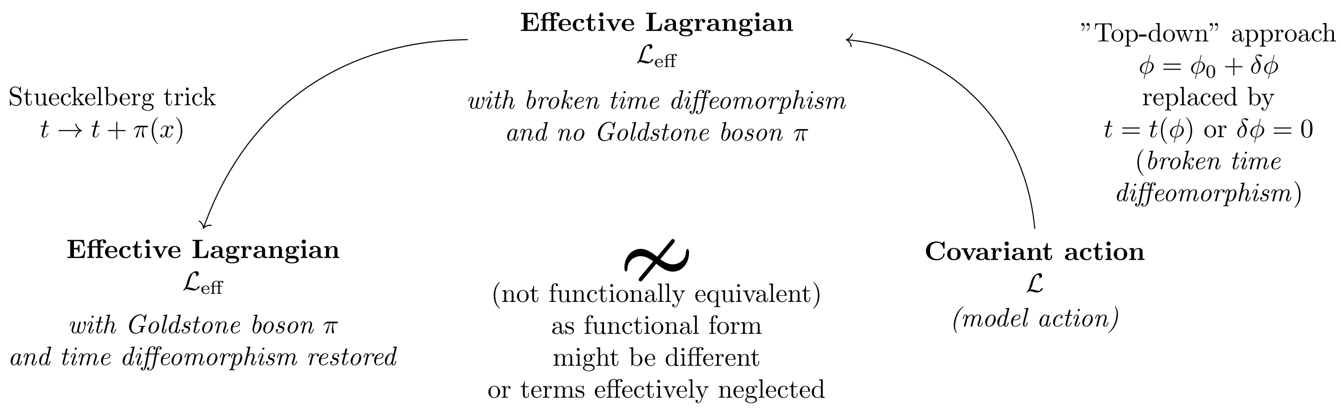


Figure 8.3: Scheme of the procedure we adopt to build the effective action.

8.2.1 Breaking time shift symmetry

Before building the action, we break time shift-invariance (or time diffeomorphism). We start from analysing a scalar degree of freedom (that might be the scalar field of a scalar-tensor theory). We usually perturb the background solution of a scalar field $\phi_0(t)$, to let it describe inhomogeneities and anisotropies, as

$$\phi(t, \vec{x}) = \phi_0(t) + \delta\phi(t, \vec{x})\,. \tag{8.14}$$

Under time diffeomorphism

$$t \to t + \xi^0(t, \vec{x})\,, \tag{8.15}$$

the scalar field perturbation $\delta\phi$ transforms as

$$\delta\phi(t, \vec{x}) \to \delta\phi(t, \vec{x}) - \xi^0 \partial_t \phi_0(t)\,. \tag{8.16}$$

Proof. Consider the definition (we omit to write the $\vec{x}$ dependence to simplify the notation)

$$\delta\phi(t + \xi^0) = \phi(t + \xi^0) - \phi_0(t + \xi^0) = \phi(t) - \phi_0(t) - \xi^0 \partial_t \phi_0 = \delta\phi(t) - \xi^0 \partial_t \phi_0\,, \tag{8.17}$$

where in the second equality we use the fact that ϕ is a scalar and we stop at first order since we are considering an infinitesimal transformation. □

Therefore, $\delta\phi$ is not a scalar under time diffeomorphism. But we can choose the gauge where $\delta\phi = 0$ for every space-time point, that is, $\phi(t, \vec{x}) = \phi_0(t)$. This procedure is very similar to the example in the previous section, where we set the Goldstone boson to be null (unitary gauge). Therefore, we call this gauge where $\delta\phi = 0$ the unitary gauge. The whole analogy is summarized in Table 8.1.

	Section 8.1	Gravity
Symmetry	U(1)	$t \to t + \xi^0$
Gauge fixing condition	$\alpha(x) = -\theta(x)$	$\delta\phi(t) = \xi^0 \partial_t \phi_0$
Goldstone boson	$\theta(x)$	$\delta\phi(t, \vec{x})$
"Photon"	A_μ	$g_{\mu\nu}$

Table 8.1: Table showing the analogy between the model considered in the previous section and the one we are building for Gravity.

But, how can we say if a theory is spontaneously broken? In the previous section, we had a spontaneously broken symmetry only with a certain potential. Similarly, in our case, we need to find theories where we can break the time diffeomorphism. We know that every symmetry of the metric $g_{\mu\nu}$ in curved space-time (remember that $g_{\mu\nu}$ is analogous to the photon in the previous case) is generated by a Killing vector, which gives the direction of the symmetry. More precisely, we are interested in time-like Killing vectors, to have a physically walkable direction. With a coordinate transformation, we can rotate this Killing vector in the time direction, and exploit the symmetry breaking mechanism. Notable examples are FRW and de Sitter, which are not time translation invariant but leaves space translations untouched.

Therefore, with the unitary gauge we set to zero the perturbation of one scalar field, and we are left with $\phi(\vec{x}, t) = \phi_0(t) = \phi(t)$. We can build a slicing of spacetime with hypersurfaces Σ: $\phi(t) = \text{constant}$. But, since ϕ is now only a function of time, we can consider a more simple Σ: $t = \text{constant} = t(\phi)$. Thus, using this slicing with the gauge $\delta\phi = 0$, we can build an action where the only fluctuations are the ones of the metric $g_{\mu\nu}$. In other words, we build an action where the only degrees of freedom left is given by the metric. In the next section, we will build this Lagrangian.

8.2.2 Which frame?

A question still under debate in cosmology (not only for the Effective Field Theory action) is whether we should use the Jordan Frame (JF) or the Einstein Frame (EF) to write the action. A possible explanation on why we might prefer the JF can be found in [72], and we briefly summarize here the discussion.

We define the JF to be the one in the form

$$S_{\rm J} = \int d^4x\sqrt{-g}\left[\frac{f(\phi)}{16\pi G}R + F\left(\phi, g_{\mu\nu}\right)\right] + S_m\left[g_{\mu\nu}\right] , \tag{8.18}$$

where ϕ is a scalar field, f is a generic function of ϕ, while F is a function also of the metric, and can contain its derivatives. The matter part of the action S_m couples only to the metric $g_{\mu\nu}$. We can find a transformation of the metric from JF to EF. This transformation is usually conformal, i.e. a transformation $g_{\mu\nu} \to \tilde{g}_{\mu\nu} = \Omega(\phi)^2 g_{\mu\nu}$ which preserves causality (e.g. if the vector is timelike, after the conformal transformation it is still timelike). The EF is defined as the frame with an action in the form

$$S_{\rm E} = \int d^4x\sqrt{-g}\left[\frac{1}{16\pi G}\tilde{R} + \tilde{F}\left(\phi, \tilde{g}_{\mu\nu}\right)\right] + \tilde{S}_m\left[\phi, \tilde{g}_{\mu\nu}\right] , \tag{8.19}$$

where the $\sim$ quantities are in EF; $\tilde{F}$ is still a function of the scalar field and the EF metric, but does not contain the Ricci scalar, i.e., we separate the $R/16\pi G$ of standard General Relativity from the other parts of the action. This feature of EF can greatly simplify the computation of the equation of motion, because the standard General Relativity term gives always the Einstein tensor $G_{\mu\nu}$ when we vary the action with respect to $\tilde{g}$. Note that due to the transformation from JF to EF, the matter action might acquire a ϕ dependence.

The latter difference with respect to JF is crucial in describing the matter components. In the EF the matter fields couple with the scalar field, and their equations of motion will not be independent to

ϕ. This is the reason why the JF is usually considered the physical one: the matter in JF is only coupled with the metric and evolves independently to ϕ.

As an example in cosmology [72], consider the standard metric as the one in Einstein frame $d\tilde{s}^2 = -d\tilde{t}^2 + \tilde{a}(\tilde{t})^2 d\tilde{x}^2$. We can go to JF with a conformal transformation $\tilde{g}_{\mu\nu} \to g_{\mu\nu} = \Omega(\phi)^2 \tilde{g}_{\mu\nu}$. Therefore, the new metric is given by $ds^2 = -dt^2 + a(t)^2 dx^2$, where $a(t) = \Omega(\phi)\tilde{a}(t)$. Therefore, also the Hubble constant $H = 1/a\, da/dt$ will be different in the EF. In the JF, photons are not coupled with the scalar field ϕ, and therefore we expect the usual redshift definition $1 + z = 1/a$ to hold only with the scale factor of JF. Therefore, we must confront the result of experiments with z computed in JF. Similarly, the Hubble constant we must compare with experiments is the one computed in JF.

For the reasons above, we will use the JF as the physical frame during the construction of the effective action. This means that in general there will be a function of time (instead of a function of the field, because $\phi = \phi(t)$ in unitary gauge) in front of the Ricci scalar. However, it is important to note that, at least at the classical non-quantum level, if the EF to JF transformation (and vice versa) is conformal, the two frames must describe the system equivalently.

8.3 Building the Effective Lagrangian

In this section, we build an action with broken time diffeomorphism, i.e., the $\mathcal{L}_{\text{eff}}$ in the top middle of the scheme in Figure 8.3. We can add to the Lagrangian all quantities that are invariant under the unbroken symmetries, that are the spatial diffeomorphisms. Firstly, we study the background action (at zero and first order in perturbations) adding all the terms which are not redundant, i.e., that cannot be written in terms of other quantities. Then we add higher order terms in the fluctuations of the quantities from the background.

The background part of a tensor T is written as its value evaluated on the background $T^{(0)}$, and the perturbation part (out of its background value) as δT, i.e. $T = T^{(0)} + \delta T$. A general rule, given the contraction of two generic tensors G and T

$$\begin{aligned} TG &= (T^{(0)} + \delta T)(G^{(0)} + \delta G) = \\ &= T^{(0)}G^{(0)} + T^{(0)}\delta G + G^{(0)}\delta T + \delta G \delta T = \\ &= T^{(0)}(G^{(0)} + \delta G) + G^{(0)}(T^{(0)} + \delta T) + \delta T \delta G - T^{(0)}G^{(0)} = \\ &= \delta T \delta G + T^{(0)} G + T G^{(0)} - T^{(0)} G^{(0)} \,. \end{aligned} \tag{8.20}$$

8.3.1 Background

Action

We start with the background of a flat FRW cosmology, and write the more general time shift (not necessarily constant) broken action. Some background values are the following

$$g^{(0)}_{00} = -1 \,, \tag{8.21}$$

$$R^{(0)}_{\mu\nu} = 2H^2 h_{\mu\nu} - (H^2 + \dot{H})(3 n_\mu n_\nu - h_{\mu\nu}) \,, \tag{8.22}$$

$$R^{(0)} = 6\left(2H^2 + \dot{H}\right) \,, \tag{8.23}$$

$$K^{(0)}_{\mu\nu} = -H h_{\mu\nu} \,. \tag{8.24}$$

Due to the symmetries of the FRW metric, every background tensor can be written in terms of the induced metric $h_{\mu\nu}$, the normal vector n_μ and t.

To build the action, we consider the following arguments.

(i) In general, every four-dimensional diffeomorphism invariant quantity is by definition invariant under spatial diffeomorphism (R, $R_{\mu\nu}$, $R^{\mu}{}_{\nu\rho\sigma}$, $g_{\mu\nu}$). This means we can always add spacetime tensors to the action. Moreover, since any function of time is by definition invariant under space diffeomorphism, we can add functions of time in front of any part of the action. The simplest part we can add is a Ricci scalar multiplied by a function of time (see the previous discussion on Jordan-Einstein frames to know why this function is needed). A trivial observation is that, since we are building a scalar, we must avoid free indices, and thus we need these tensors to be contracted with themselves.

(ii) We can also add terms that are the purely time components of four-dimensional tensors. In fact, we can define a vector normal to the $S(x^\mu) =$ constant hypersurfaces at any spatial point, defined as usual as (3.2)

$$n_\mu \equiv -N\partial_\mu S(x^\nu)\,. \tag{8.25}$$

When we choose the unitary gauge, and we slice the spacetime with $t =$ constant (i.e. $S(x^\nu) = t =$ constant) hypersurfaces, the normal vector becomes

$$n_\mu = -\frac{\delta^0_\mu}{\sqrt{-g^{00}}}\,. \tag{8.26}$$

Therefore we can always multiply four-dimensional tensors with n_μ to project the four-dimensional tensors into their time components. For instance, the metric can be written as $n_\mu n_\nu g^{\mu\nu} = g^{00}$. Since we are building a scalar, the action, we contract every free index with the normal vector and transform it to a 0 index.

We also recall the definition of the induced metric (3.15) on the three-dimensional hypersurfaces

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu\,, \tag{8.27}$$

and the fact that $h_{ij} = g_{ij}$.

(iii) Other spatial diffeomorphism invariant quantities are the ADM tensors that we defined in Chapter 3. Among these, there is the extrinsic curvature (3.51)

$$K_{\mu\nu} = -h^\sigma_\mu \nabla_\sigma n_\nu\,. \tag{8.28}$$

Any contraction of $K_{\mu\nu}$ with the normal vector n_μ is null due to the extrinsic curvature property (3.52). Therefore it is unnecessary to add $n_\mu n_\nu K^{\mu\nu}$ terms to the action. Moreover, the trace of the extrinsic curvature[†]

$$K \equiv K^\nu{}_\nu = -g^{\mu\nu} h^\sigma_\mu \nabla_\sigma n_\nu = -g^{\mu\nu}(\delta^\sigma_\mu + n_\mu n^\sigma)\nabla_\sigma n_\nu = -\nabla^\nu n_\nu\,, \tag{8.29}$$

is also redundant. We can prove this from the integral

$$\begin{aligned}\int d^4x\sqrt{-g}f(t)K &= -\int d^4x\sqrt{-g}f(t)\nabla_\nu n^\nu \\ &= \int d^4x\sqrt{-g}\,n^\nu\partial_\nu f(t) = \int d^4x\sqrt{-g}\sqrt{-g^{00}}\,\partial_t f(t)\,,\end{aligned} \tag{8.30}$$

where in the second equality we integrate by parts, and in he last equality we use the definition of n^μ (8.26). Then we can expand the square root of g^{00} in terms of the perturbation of the metric from the FRW background value $\delta g^{00} \equiv 1 + g^{00}$, and thus we can include the K term in a non-background term.

[†] In the derivation, we have used the fact that $h^\sigma_\mu = \delta^\sigma_\mu + n_\mu n^\sigma$ and $n^\nu\nabla_\sigma n_\nu = 0$.

Another ADM tensor which is purely spatial is the 3-dimensional Riemann tensor, i.e. the curvature tensor defined on the constant time hypersurfaces (3.68)

$$- {}^{(3)}R^{\sigma}{}_{\rho\mu\nu}\, X_\sigma = D_\mu D_\nu X_\rho - D_\nu D_\mu X_\rho \,, \tag{8.31}$$

where D_μ is the three-dimension covariant derivative defined in (3.30). If X_ρ in the definition above is a purely spatial tensor, i.e. $X_\mu n^\mu = X^\mu n_\mu = 0$, it can be shown that we can rewrite the three-dimensional derivative in the three-dimensional hypersurface Σ (and thus using only spatial indices) as

$$D_i X_j = \partial_i X_j - {}^{(3)}\Gamma^k_{ij} X_k \;, \tag{8.32}$$

where the three-dimensional Christoffel symbols are defined using the induced metric on the three-dimensional hypersurface Σ, h_{ij}, instead of $g_{\mu\nu}$, i.e.,

$${}^{(3)}\Gamma^k_{ij} = \frac{1}{2} h^{ks} \left(\partial_i h_{sj} + \partial_j h_{is} - \partial_s h_{ij} \right) \,. \tag{8.33}$$

However, we can substitute the three-dimensional Riemann tensor with the Gauss-Codazzi equation (3.69)

$${}^{(3)}R_{\mu\nu\rho\sigma} = h^{\mu'}_{\mu} h^{\nu'}_{\nu} h^{\rho'}_{\rho} h^{\sigma'}_{\sigma} R_{\mu'\nu'\rho'\sigma'} + n_\mu n^\mu (K_{\mu\rho}K_{\nu\sigma} - K_{\mu\sigma}K_{\nu\rho}) \,, \tag{8.34}$$

with tensors that we already discussed.

(iv) We might want to include $R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma}$, $R_{\mu\nu}R^{\mu\nu}$ or R^2 terms to the background action. However we can re-write the contribution of the first term using the Gauss-Bonnet invariant

$$\mathcal{G} \equiv R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma} \,. \tag{8.35}$$

Another way is to substitute $R_{\mu\nu\rho\sigma}$ with the Weyl tensor, which has the useful property to be null at the background.

We are left with terms like $R_{\mu\nu}R^{\mu\nu}$ and R^2. The first can be rewritten using the rule (8.20)

$$R_{\mu\nu}R^{\mu\nu} = \delta R_{\mu\nu} \delta R^{\mu\nu} + 2R^{(0)}_{\mu\nu} R^{\mu\nu} - R^{(0)}_{\mu\nu} R^{(0)\,\mu\nu}. \tag{8.36}$$

The first term is manifestly at second order in perturbation quantities, and therefore it should not appear in the background action. The last term can be rewritten using the background value of the Ricci tensor (8.22)

$$R^{(0)}_{\mu\nu} R^{(0)\,\mu\nu} = 12 \left(3H^4 + \dot{H}^2 + 3H^2\dot{H} \right) , \tag{8.37}$$

and therefore it will contribute as a function of time, that will appear in the action, not multiplied by any tensor. The second term of (8.36) is given by, using again (8.22),

$$\begin{aligned} R^{(0)}_{\mu\nu} R^{\mu\nu} &= 2H^2 h_{\mu\nu} R^{\mu\nu} - (H^2 + \dot{H})(3n_\mu n_\nu - h_{\mu\nu}) R^{\mu\nu} \\ &= 2H^2 (g_{\mu\nu} + n_\mu n_\nu) R^{\mu\nu} - (H^2 + \dot{H})(2n_\mu n_\nu - g_{\mu\nu}) R^{\mu\nu} \\ &= -2\dot{H} n_\mu n_\nu R^{\mu\nu} + (3H^2 + \dot{H}) R \,. \end{aligned} \tag{8.38}$$

The last term contributes to the function in front of the Ricci scalar. The first term can be rearranged using the equation (3.120)

$$\frac{R^{00}}{-g^{00}} = R^{\mu\nu} n_\mu n_\nu = \nabla_\mu (K n^\mu + a^\mu) - K_{\mu\nu}K^{\mu\nu} + K^2 \,. \tag{8.39}$$

The first two terms can be integrated by parts to give

$$\int d^4x\sqrt{-g}f(t)\nabla_\mu(Kn^\mu) = -\int d^4x\sqrt{-g}\partial_\mu f(t)Kn^\mu\,, \tag{8.40}$$

$$\int d^4x\sqrt{-g}f(t)\nabla_\mu a^\mu = -\int d^4x\sqrt{-g}\partial_\mu f(t)a^\mu = 0\,, \tag{8.41}$$

where in the last equation we use $n_\mu a^\mu = 0$ and $\partial_\mu f(t) \propto n_\mu$ (being $f(t)$ a purely spatial function). But we previously showed that the trace can be transformed into a term proportional to δg^{00}; and the term $K_{\mu\nu}K^{\mu\nu}$ can be rewritten using the rule (8.20)

$$K_{\mu\nu}K^{\mu\nu} = \delta K_{\mu\nu}\delta K^{\mu\nu} + 2K^{(0)}_{\mu\nu}K^{\mu\nu} - K^{(0)}_{\mu\nu}K^{(0)\,\mu\nu}\,. \tag{8.42}$$

Again, the first term is at second order, and using (8.24) we find that the last term can be included in a function of time. The term in the middle is given by $K^{(0)}_{\mu\nu}K^{\mu\nu} = -a^2Hh_{\mu\nu}K^{\mu\nu} = -a^2HK$, that is proportional to the trace K.

The last term to consider is R^2, and using the rule (8.20) it is trivial to find that

$$R^2 = \delta R^2 + 2R^{(0)}R - R^{(0)}R^{(0)}. \tag{8.43}$$

Due to (8.23), the last term goes into a function of time; δR^2 is at second order; and $R^{(0)}R$ is an additional contribution to the function of time in front of the Ricci scalar.

Finally, note that R^{00} is also a redundant term, because of (8.39).

Combining all the arguments above, we write the background action as

$$S^{(0)} = \int d^4x\sqrt{-g}\left[\frac{M_*^2}{2}f(t)R - \Lambda(t) - c(t)g^{00}\right] + S_m, \tag{8.44}$$

where M_* is a constant[‡]. The function $\Lambda(t)$ also includes all the terms coming from $T^{(0)}T^{(0)}$ terms (e.g. $R^{(0)}R^{(0)}$). The additional S_m contains all the standard matter fields, which, since we are in Jordan frame, are independent from the scalar field ϕ.

Note that this action is not at zero order in the perturbed quantities, because g^{00} contains also the first order δg^{00} term. However, the discussion above proves that this is the most general action at zero and first order in the perturbed quantities.

Variation of the action

We want to obtain an expression for the functions c and Λ on a FLRW background. Therefore, when needed, we will use the background values of the quantities considered. We start varying the action with respect to the metric $g^{\mu\nu}$. In order to do this computation, consider for notation simplicity the following Lagrangian from $S^{(0)}$

$$\mathcal{L} = \left[\frac{M_*^2}{2}f(t)R - \Lambda(t) - c(t)g^{00}\right] + \mathcal{L}_m\,. \tag{8.45}$$

During the computation we will also use

$$\frac{\delta\sqrt{-g}}{\delta g^{\mu\nu}} = -\frac{\sqrt{-g}}{2}g_{\mu\nu}\,. \tag{8.46}$$

[‡] This constant does not necessarily need to be the reduced Planck mass $\sqrt{\hbar c/(8\pi G)}$ at this point. Also note that this quantity is not the strength of gravity in the α parametrization of Horndeski theories [26].

The functional derivative of $\mathcal{L}$ with respect to the metric is

$$\begin{aligned}\frac{\delta\left[\sqrt{-g}\mathcal{L}\right]}{\delta g^{\mu\nu}} &= \frac{\delta\sqrt{-g}}{\delta g^{\mu\nu}}\left[\frac{M_*^2}{2}f(t)R - \Lambda(t) - c(t)g^{00}\right] + \\ &+ \sqrt{-g}\frac{\delta}{\delta g^{\mu\nu}}\left[\frac{M_*^2}{2}f(t)R - \Lambda(t) - c(t)g^{00}\right] + \frac{\delta\left[\sqrt{-g}\mathcal{L}_m\right]}{\delta g^{\mu\nu}}\,, \end{aligned} \tag{8.47}$$

and therefore

$$\frac{2}{\sqrt{-g}}\frac{\delta\mathcal{L}}{\delta g^{\mu\nu}} = -g_{\mu\nu}\left[\frac{M_*^2}{2}f(t)R - \Lambda(t) - c(t)g^{00}\right] - 2c(t)\delta^0_\mu\delta^0_\nu + M_*^2 f(t)\frac{\delta R}{\delta g^{\mu\nu}} - T_{\mu\nu}. \tag{8.48}$$

Evaluating the last uncomputed term we find

$$\begin{aligned}M_*^2 f(t)\frac{\delta R}{\delta g^{\mu\nu}} &= M_*^2 f(t)\frac{\delta}{\delta g^{\mu\nu}}\left[g^{\rho\sigma}R_{\rho\sigma}\right] = \\ &= M_*^2 f(t)R_{\mu\nu} + M_*^2 f(t)g^{\rho\sigma}\frac{\delta}{\delta g^{\mu\nu}}\left[R_{\rho\sigma}\right]\,. \end{aligned} \tag{8.49}$$

The last term of (8.49) can be re-written using a standard General Relativity result.

$$g^{\mu\nu}\delta R_{\mu\nu} = g^{\mu\nu}g^{\rho\sigma}\left[\delta g_{\nu\sigma;\mu\rho} - \delta g_{\mu\nu;\sigma\rho}\right]\,. \tag{8.50}$$

Thus the second term of (8.49) is

$$\begin{aligned}M_*^2 f(t)g^{\rho\sigma}\delta R_{\rho\sigma} &= M_*^2 f(t)g^{\mu\nu}g^{\rho\sigma}\left[\delta g_{\nu\sigma;\mu\rho} - \delta g_{\mu\nu;\sigma\rho}\right] \\ &= -M_*^2 f(t)\left[\delta g^{\nu\sigma}{}_{;\nu\sigma} - g_{\mu\nu}\delta g^{\mu\nu;\rho}{}_{\rho}\right]\,, \end{aligned} \tag{8.51}$$

where we used the relations $g^{\mu\nu}g^{\rho\sigma}\delta g_{\mu\sigma;\nu\rho} = -\delta g^{\nu\sigma}{}_{;\nu\sigma}$ and $g_{\mu\nu}\delta g^{\mu\nu} = -g^{\mu\nu}\delta g_{\mu\nu}$. Remember that the Lagrangian is integrated, and therefore we can make an integration by parts and obtain

$$\frac{\sqrt{-g}}{2}M_*^2 f(t)g^{\rho\sigma}\delta R_{\rho\sigma} = \frac{\sqrt{-g}}{2}M_*^2 f(t)\left[g_{\mu\nu}\delta g^{\mu\nu;\rho}{}_{\rho} - \delta g^{\nu\sigma}{}_{;\nu\sigma}\right] \to -\frac{\sqrt{-g}}{2}M_*^2\delta g^{\nu\sigma}\left[f_{;\nu\sigma} - g_{\nu\sigma}f^{;\rho}{}_{\rho}\right]\,. \tag{8.52}$$

Setting $\delta\mathcal{L}/\delta g^{\mu\nu} = 0$ and merging the results (8.48), (8.49) and (8.52) we obtain the equations of motion

$$\left(fG_{\mu\nu} - \nabla_\mu\nabla_\nu f + g_{\mu\nu}\Box f\right)M_*^2 + \left(cg^{00} + \Lambda\right)g_{\mu\nu} - 2c\delta^0_\mu\delta^0_\nu = T_{\mu\nu}\,. \tag{8.53}$$

We can find the equations for c and Λ by taking the 00 component of (8.53). We consider the standard results

$$G_{00} = 3H^2, \qquad R = -G^\mu_\mu = 12H^2 + 6\dot{H}, \qquad \nabla_\mu\nabla_\nu f = \partial_\mu\partial_\nu f - \Gamma^0_{\mu\nu}\dot{f}, \qquad \Box f = -\ddot{f} - 3H\dot{f}\,. \tag{8.54}$$

The last two equations are obtained from the background quantities as follows

$$\begin{aligned}\Box f &= g^{\mu\nu}\nabla_\mu\nabla_\nu f = g^{\mu\nu}\nabla_\mu\partial_\nu f \\ &= g^{\mu\nu}\partial_\mu\partial_\nu f - g^{\mu\nu}\Gamma^\sigma_{\mu\nu}\partial_\sigma f \\ &= -\ddot{f} - g^{ij}\Gamma^0_{ij}\dot{f} \\ &= -\ddot{f} - a^{-2}\delta^i_i a^2 H\dot{f} \\ &= -\ddot{f} - 3H\dot{f}\,. \end{aligned} \tag{8.55}$$

It is also possible to see that $\nabla_\mu\nabla_\nu f = \partial_\mu\partial_\nu f - \Gamma^0_{\mu\nu}\dot{f}$. Moreover, we define $T_{\mu\nu}$ to be the perfect fluid energy tensor defined as

$$T_{\mu\nu} = \left(\rho_m + P_m\right)u_\mu u_\nu + P_m g_{\mu\nu} \qquad \text{with} \qquad u_\mu = (1,0,0,0)\,, \tag{8.56}$$

that is equivalent to say $T^{\nu}_{\mu} = \mathrm{diag}(-\rho_m, P_m, P_m, P_m)$. Since we are in Jordan frame, we also have the continuity equation

$$\dot{\rho}_m + 3H(\rho_m + P_m) = 0\,. \tag{8.57}$$

Using these results we find respectively the 00 component and the trace of the equations of motion (8.53)

$$3M_*^2\left(H^2 f + H\dot{f}\right) - c - \Lambda = \rho_m\,, \tag{8.58}$$

$$M_*^2\left(-3\ddot{f} - 9H\dot{f} - 6f\dot{H} - 12H^2 f\right) - 2c + 4\Lambda = -\rho_m + 3P_m\,, \tag{8.59}$$

where we use $g^{\mu}_{\mu} = \delta^{\mu}_{\mu} = 4$, $g^{\mu\nu}\delta^0_\mu\delta^0_\nu = g^{00} = -1$. By solving the first equation (8.58) for Λ and substituting the result into the second equation (8.59), and by doing the same solving (8.58) for c, we obtain respectively

$$c = -\frac{1}{2}\left(\rho_m + P_m\right) - M_*^2 f\left(\frac{1}{2}\frac{\ddot{f}}{f} - \frac{1}{2}\frac{\dot{f}}{f}H + \dot{H}\right)\,, \tag{8.60}$$

$$\Lambda = -\frac{1}{2}\left(\rho_m - P_m\right) + M_*^2 f\left(\frac{1}{2}\frac{\ddot{f}}{f} + \frac{5}{2}\frac{\dot{f}}{f}H + \dot{H} + 3H^2\right)\,. \tag{8.61}$$

Equations of motion of the scalar fluid

We can also recast (8.60) and (8.61) into two Friedmann like equations

$$H^2 = \frac{1}{3}\frac{1}{M_*^2 f}\left[\rho_m + c + \Lambda - 3M_*^2\dot{f}H\right]\,, \tag{8.62}$$

$$\dot{H} = -\frac{1}{2}\frac{1}{M_*^2 f}\left[\rho_m + P_m + 2c + M_*^2\left(\ddot{f} - \dot{f}H\right)\right]1,. \tag{8.63}$$

The first can be obtained from (8.61) substituting P_m obtained from (8.60), the second using only (8.60).

Making the comparison with the standard Friedmann equations

$$H^2 = \frac{1}{3}\rho \qquad \text{and} \qquad \dot{H} = -\frac{1}{2}(\rho + P)\,, \tag{8.64}$$

we can define the density and the pressure of the scalar fluid as

$$\rho_d \equiv c + \Lambda - 3M_*^2\dot{f}H\,, \tag{8.65}$$

$$P_d \equiv -\Lambda + M_*^2(\ddot{f} + 2\dot{f}H) + c\,, \tag{8.66}$$

and obtain the Friemann equations

$$H^2 = \frac{1}{3}\frac{1}{M_*^2 f}\left(\rho_m + \rho_d\right)\,, \tag{8.67}$$

$$\dot{H} = -\frac{1}{2}\frac{1}{M_*^2 f}\left(\rho_m + P_m + \rho_d + P_d\right)\,. \tag{8.68}$$

The scalar field fluid, as defined in equations (8.65) and (8.66), does not satisfy an homogeneous continuity equation as the standard matter fluid. Starting from the definitions (8.65) and (8.66), substituting c and Λ with the equations (8.60) and (8.61), and eliminating the standard matter density and pressure with equation (8.57), we indeed find that the left hand side of the following equation is given by

$$\dot{\rho}_d + 3H(\rho_d + P_d) = 3M_*^2 H^2 f\,. \tag{8.69}$$

Finally, we can rewrite c and Λ with ρ_d and P_d

$$c = \frac{1}{2}(\rho_d + P_d) + \frac{1}{2}M_*^2(-\ddot{f} + \dot{f}H)\,, \tag{8.70}$$
$$\Lambda = \frac{1}{2}(\rho_d - P_d) + \frac{1}{2}M_*^2(\ddot{f} + 5\dot{f}H)\,, \tag{8.71}$$

and therefore the functions of time c and Λ are fixed, up to the function $f(t)$ and its derivatives.

Another possibility is to consider an alternative definition of the energy density and pressure of the scalar field such that the continuity equation is homogeneous. In fact, if we consider

$$\rho_d \equiv c + \Lambda - 3M_*^2\dot{f}H + 3H^2M_*^2\,(1-f)\;, \tag{8.72}$$
$$P_d \equiv c - \Lambda + M_*^2(\ddot{f} + 2\dot{f}H) - M_*^2(2\dot{H} + 3H^2)(1-f)\,, \tag{8.73}$$

we can write the Friedmann-like equations as

$$H^2 = \frac{1}{3}\frac{1}{M_*^2}\,(\rho_m + \rho_d)\,, \tag{8.74}$$
$$\dot{H} = -\frac{1}{2}\frac{1}{M_*^2}\,(\rho_m + P_m + \rho_d + P_d)\;. \tag{8.75}$$

and we can verify that the continuity equation is indeed

$$\dot{\rho}_d + 3H(\rho_d + P_d) = 0\,. \tag{8.76}$$

Moreover c and Λ with this definitions are

$$c = \frac{1}{2}(\rho_d + P_d) + \frac{1}{2}M_*^2(-\ddot{f} + \dot{f}H), \tag{8.77}$$
$$\Lambda = \frac{1}{2}(\rho_d - P_d) + \frac{1}{2}M_*^2(\ddot{f} + 5\dot{f}H)\,. \tag{8.78}$$

The f at the denominator vanishes in equations (8.74) and (8.75), with respect to the equations (8.67) and (8.68) where we consider the alternative definition of the energy density and pressure of the scalar field. Finally, if not otherwise stated, we will use these latter definitions for the energy density and pressure of the scalar field.

8.3.2 Higher order action

The next part in the construction of an effective action is to include higher order terms with an expansion in perturbation quantities. These quantities are summarized in Table 8.2.

Perturbation quantity δT	Background value $T^{(0)}$
δg^{00}	-1
δR	$6(2H^2 + \dot{H})$
$\delta K_{\mu\nu}$	$-Hh_{\mu\nu}$
δK	$-3H$
$\delta^{(3)}R = {}^{(3)}R$	0

Table 8.2: Table of the perturbation quantities introduced in the action at higher order with respect to the background. The definition of a perturbation quantity is $\delta T = T - T^{(0)}$.

We will consider 3-dimensional quantities because they do not contain higher time derivatives. We can always transform 4-dimensional quantities into 3-dimensional quantities using the Gauss-Codazzi equation (8.34). Moreover, the 3-dimensional Ricci scalar ${}^{(3)}R$ is null for the background, and thus it is already a perturbation quantity.

We can then write the general second-order action as

$$S^{(2)} = \int d^x \sqrt{-g} F^{(2)} \left[\delta g^{00}, \delta K_{\mu\nu}, \delta K, {}^{(3)}R, t\right] , \tag{8.79}$$

where $F^{(2)}$ is a function at second order in perturbation quantities that is usually written as

$$\begin{aligned} F^{(2)} = & \frac{M_2^4(t)}{2}(\delta g^{00})^2 - \frac{m_3^3(t)}{2}\delta K \delta g^{00} - m_4^2(t)(\delta K^2 - \delta K^\mu{}_\nu \delta K^\nu{}_\mu) + \\ & + \frac{\tilde{m}_4^2(5)}{2}\, {}^{(3)}R \delta g^{00} - \bar{m}_4^2(t)\delta K^2 + \frac{\bar{m}_5(t)}{2}\, {}^{(3)}R \delta K + \frac{\bar{\lambda}(t)}{2}\, {}^{(3)}R\,. \end{aligned} \tag{8.80}$$

8.3.3 Summary

Finally, we explicitly write the total effective action we have constructed in the previous sections as

$$\begin{aligned} S = S_m + \int d^4x \sqrt{-g} \Bigg[& \frac{M_*^2}{2} f(t) R - \Lambda(t) - c(t) g^{00} + \\ & + \frac{M_2^4(t)}{2}(\delta g^{00})^2 - \frac{m_3^3(t)}{2}\delta K \delta g^{00} - m_4^2(t)(\delta K^2 - \delta K^\mu{}_\nu \delta K^\nu{}_\mu) + \frac{\tilde{m}_4^2(t)}{2}\, {}^{(3)}R \delta g^{00} + \\ & - \bar{m}_4^2(t)\delta K^2 + \frac{\bar{m}_5(t)}{2}\, {}^{(3)}R \delta K + \frac{\bar{\lambda}(t)}{2}\, {}^{(3)}R^2 + m_2^2(t) h^{\mu\nu}\partial_\mu g^{00}\partial_\nu g^{00} + \\ & + \text{higher order terms} \Bigg] , \end{aligned} \tag{8.81}$$

where c and Λ are respectively in equations (8.60) and (8.61).

The first line gives the background of the theory, that evolves with the background equations (8.67) and (8.68). The scalar fluid (e.g. the one describing dark energy at late times) is defined with the equations for its density (8.65) and pressure (8.66). The second and third lines do not contribute to the background, but only to the linear perturbations. The third line contains higher order spatial derivatives with respect to the first and the second line, and, as we will see, contributes with terms proportional to k^2, introducing higher order deviations from the standard linear $\omega = c_s k$. Note that, if $m_4^2 \neq \tilde{m}_4^2$, higher order derivatives can also appear from the second line with terms like $k^2\partial_t$. The additional terms of higher order give higher order perturbations.

The action is sometimes also written in another form, where some terms are collected with a newly defined function of time (the number of functions of time must be the same)

$$\begin{aligned} S = S_m + \int d^4x \sqrt{-g} \Bigg[& \frac{M_*^2}{2} f(t) R - \Lambda(t) - c(t) g^{00} + \\ & + \frac{M_2^4(t)}{2}(\delta g^{00})^2 - \frac{\bar{M}_1^3(t)}{2}\delta K \delta g^{00} - \bar{M}_2^2(t)\delta K^2 - \bar{M}_3^2(t)\delta K^\mu{}_\nu \delta K^\nu{}_\mu + \frac{\hat{M}^2(t)}{2}\, {}^{(3)}R \delta g^{00} + \\ & + \frac{\bar{m}_5(t)}{2}\, {}^{(3)}R \delta K + \frac{\bar{\lambda}(t)}{2}\, {}^{(3)}R^2 + m_2^2(t) h^{\mu\nu}\partial_\mu g^{00}\partial_\nu g^{00} + \\ & + \text{higher order terms} \Bigg] . \end{aligned} \tag{8.82}$$

Different models (i.e., with different starting covariant actions) are defined by different functions of time $f(t), M_2^4(t)$, ...

8.4 Top-down construction

Up to now, we built the effective action in the form of (8.82). We must show how to find the functions of time appearing in the effective Lagrangian. In other words, we want to find how we can specify the functions of time given a standard covariant action, that is, the right part of the scheme in Figure 8.3.

The key of the procedure is to use the time shift breaking equations. We set $\delta\phi(t,\vec{x}) = 0$ (unitary gauge), and the time coordinate to be the a function of the field ϕ. In this way, we have that only the metric degrees of freedom must appear in the action. The procedure consists in:

- writing the explicit dependence on the metric of the terms in the covariant action $\mathcal{L}$;
- considering ϕ as a function of time only $\phi(t)$ (unitary gauge);
- expanding the terms in the perturbations of the quantities appearing.

A trivial example is the kinetic term of a Quintessence field. The procedure consists in

$$-\frac{1}{2}\partial_\mu\phi(x^\nu)\,\partial^\mu\phi(x^\nu) \to -\frac{1}{2}g^{\mu\nu}\partial_\mu\phi_0(t)\,\partial_\nu\phi_0(t) = -\frac{1}{2}g^{00}\partial_t\phi_0(t)\,\partial_t\phi_0(t) = -\tilde{c}(t)g^{00}\,, \tag{8.83}$$

where in the first expression we consider $\phi(x^\nu) = \phi_0(t) + \delta\phi(t,\vec{x})$, and with the right arrow we go to the unitary gauge. The function $\tilde{c}(t)$ is only one possible contribution to the $c(t)$ function appearing in the action (8.82). Moreover, g^{00} might be expanded in its fluctuations using $g^{00} = -1 + \delta g^{00}$. Another example can be the coupling between the Ricci tensor and the kinetic term of a scalar field ϕ, that under this procedure becomes as follow

$$\begin{aligned}\partial_\mu\phi(x^\nu)\,\partial^\mu\phi(x^\nu)R \to g^{\mu\nu}\partial_\mu\phi_0(t)\,\partial_\nu\phi_0(t)R &= g^{00}\dot{\phi}_0^2(t)R \\ &= (-1+\delta g^{00})\dot{\phi}_0^2(t)(R^{(0)}+\delta R) \\ &= \dot{\phi}_0^2\left[-R^{(0)} - \delta R + \delta g^{00}\delta R^{(0)} + \delta g^{00}\delta R\right] \\ &= \dot{\phi}_0^2\left[-R + \delta g^{00}\delta R + R^{(0)} + g^{00}R^{(0)}\right]\,,\end{aligned} \tag{8.84}$$

where: the $\dot{\phi}_0^2 g^{00}R^{(0)}$ term also contributes to $c(t)$; $\dot{\phi}_0^2 R^{(0)}$ to $\Lambda(t)$; $\dot{\phi}_0^2 = f(t)$; and $\dot{\phi}_0^2\delta g^{00}\delta R$ is a second order term. Other examples will be discussed in the next sections.

8.5 Stueckelberg trick

In order to restore the time diffeomorphism and be able to write the equation of motion for the perturbation part of the scalar degree of freedom (here called π), we can use the Stueckelberg trick (see the left part of the scheme in Figure 8.3). As in section 8.1, we need to force the action to go under the inverse transformation with respect to the gauge fixing. In our case, we want to force the following transformation

$$t \to \bar{t} = t + \pi(x^\mu) \qquad x^i \to \bar{x} = x^i\,, \tag{8.85}$$

which can be written in a more compact form

$$x^\mu \to \bar{x}^\mu = x^\mu + \delta^\mu_0\pi(x)\,. \tag{8.86}$$

Under this transformation, a generic function of time transforms as

$$f(t) \to f(t+\pi(x)) = f(t) + \partial_t f(t)\pi(x) + \ldots\,. \tag{8.87}$$

On the contrary, a scalar quantity (e.g. Ricci scalar R) does not change under this transformation. For a generic tensor G we apply the usual transformations rule

$$G^{\mu\nu} \to \bar{G}^{\mu'\nu'} = \frac{\partial \bar{x}^{\mu'}}{\partial x^{\mu}} \frac{\partial \bar{x}^{\nu'}}{\partial x^{\nu}} G^{\mu\nu} = \left(\delta^{\mu'}_{\mu} + \delta^{\mu'}_{0} \partial_{\mu}\pi\right) \left(\delta^{\nu'}_{\nu} + \delta^{\nu'}_{0} \partial_{\nu}\pi\right) G^{\mu\nu} \,, \tag{8.88}$$

$$G_{\mu\nu} \to \bar{G}_{\mu'\nu'} = \frac{\partial x^{\mu}}{\partial \bar{x}^{\mu'}} \frac{\partial x^{\nu}}{\partial \bar{x}^{\nu'}} G_{\mu\nu} = \left(\delta^{\mu}_{\mu'} - \delta^{\mu}_{0} \partial_{\mu'}\pi\right) \left(\delta^{\nu}_{\nu'} - \delta^{\nu}_{0} \partial_{\nu'}\pi\right) G_{\mu\nu} \,. \tag{8.89}$$

For example, the transformed metric at first order is

$$\begin{aligned} g^{\mu\nu} \to \bar{g}^{\mu'\nu'} &= \left(\delta^{\mu'}_{\mu} + \delta^{\mu'}_{0} \partial_{\mu}\pi\right) \left(\delta^{\nu'}_{\nu} + \delta^{\nu'}_{0} \partial_{\nu}\pi\right) g^{\mu\nu} = \\ &= g^{\mu'\nu'} + \delta^{\mu'}_{0} g^{\alpha\nu'} \partial_{\alpha}\pi + \delta^{\nu'}_{0} g^{\alpha\mu'} \partial_{\alpha}\pi \,, \end{aligned} \tag{8.90}$$

$$\begin{aligned} g_{\mu\nu} \to \bar{g}_{\mu'\nu'} &= \left(\delta^{\mu}_{\mu'} - \delta^{\mu}_{0} \partial_{\mu'}\pi\right) \left(\delta^{\nu}_{\nu'} - \delta^{\nu}_{0} \partial_{\nu'}\pi\right) g_{\mu\nu} = \\ &= g_{\mu'\nu'} - g_{0\nu'} \partial_{\mu'}\pi - g_{0\mu'} \partial_{\nu'}\pi \,. \end{aligned} \tag{8.91}$$

The partial derivatives transforms with the following rule

$$\bar{\partial}_{\sigma'} \equiv \frac{\partial}{\partial \bar{x}^{\sigma'}} = \frac{\partial x^{\sigma}}{\partial \bar{x}^{\sigma'}} \frac{\partial}{\partial x^{\sigma}} = \left(\delta^{\sigma}_{\sigma'} - \delta^{\sigma}_{0} \partial_{\sigma'}\pi\right) \frac{\partial}{\partial x^{\sigma}} \,. \tag{8.92}$$

In particular, from equations (8.90)-(8.92) we obtain the transformations

$$g^{00} \to g^{00} + 2 g^{\alpha 0} \partial_{\alpha}\pi \,, \tag{8.93}$$

$$g^{ij} \to g^{ij} \,, \tag{8.94}$$

$$g_{ij} \to g_{ij} - g_{0j} \partial_{i}\pi - g_{0i} \partial_{j}\pi \,, \tag{8.95}$$

$$g_{i0} \to g_{i0} - g_{i0} \partial_{0}\pi - g_{00} \partial_{i}\pi \,, \tag{8.96}$$

$$\partial_{0} \to \left(1 - \partial_{0}\pi\right) \partial_{0} \,, \tag{8.97}$$

$$\partial_{i} \to \left(\delta^{\sigma}_{i} - \delta^{\sigma}_{0} \partial_{i}\pi\right) \partial_{\sigma} = \partial_{i} - (\partial_{i}\pi) \partial_{0} \,. \tag{8.98}$$

The hypersurfaces quantities (e.g. $K_{\mu\nu}$) do not change covariantly under this transformation. If we change the time coordinate, we should adjust the foliation of space-time accordingly, and the hypersurfaces where these quantities are defined change. This means that the transformations of $K_{\mu\nu}$ and ${}^{(3)}R$ do not obey respectively the tensor transformation (8.89) and the scalar transformations rules, but we need to derive their form explicitly.

8.5.1 Transformations

We can apply these transformations to the quantities we have in our theory.

Ricci scalar. Consider the Ricci scalar. Since it is a scalar, it does not change under the transformation, i.e. $R(t) \to R(\bar{t}) = R(t)$. But its fluctuation $\delta R(t)$ does transform non-trivially. In fact, consider

$$\delta R(t) \to \delta R(t+\pi) = R(t+\pi) - R^{(0)}(t+\pi) = R(t) - R^{(0)}(t) - \pi \partial_t R^{(0)}(t) = \delta R(t) - \pi \dot{R}^{(0)}(t) \,, \tag{8.99}$$

where we have used (8.87) on $R^{(0)}$ in the second equality.

Extrinsic Curvature. The extrinsic curvature $K_{\mu\nu}$ does not transform covariantly, and therefore we must compute the transformed $K_{\mu\nu}$ explicitly. We begin from the extrinsic curvature property (3.58)

$$-\nabla_\mu n_\nu = K_{\mu\nu} + n_\mu a_\nu \,, \tag{8.100}$$

i.e., the covariant derivative of the normal vector to the hypersurfaces Σ can be decomposed into a part which is tangential to Σ (the $K_{\mu\nu}$ term, because $n^\mu K_{\mu\nu} = 0$) and a part normal to Σ (given by $n_\mu a_\nu$, since $n^\mu n_\mu a_\nu = -a_\mu$). Therefore

$$K_{ij} = -\nabla_i n_j = -\partial_i n_j + \Gamma^\sigma_{ij} n_\sigma = -\frac{1}{\sqrt{-g^{00}}}\Gamma^0_{ij} \,, \tag{8.101}$$

where we have used the definition of the normal vector (8.26). But

$$K_{ij} = -\frac{1}{\sqrt{-g^{00}}}\Gamma^0_{ij} = -\frac{1}{2\sqrt{-g^{00}}} g^{0\sigma}\left(g_{i\sigma,j} + g_{j\sigma,i} - g_{ij,\sigma}\right) = \frac{1}{2}\sqrt{-g^{00}}\left(g_{ij,0} - g_{i0,j} - g_{j0,i}\right) \,, \tag{8.102}$$

where the second equality comes from the fact that terms like $g^{0k} g_{ik,j}$ are at second order, because the metric is diagonal and does not depend on space coordinates on the background. From (8.93)-(8.98) we have

$$\begin{aligned} K_{ij} \to & \frac{1}{2}\sqrt{-g^{00} - 2g^{\alpha 0}\partial_\alpha \pi}\,\left[(1-\partial_0\pi)\,\partial_0(g_{ij} - g_{0j}\partial_i\pi - g_{0i}\partial_j\pi) + \right.\\ & \left. -\left(\partial_j - (\partial_j\pi)\partial_0\right)\left(g_{i0} - g_{i0}\partial_0\pi - g_{00}\partial_i\pi\right) - \left(\partial_i - (\partial_i\pi)\partial_0\right)\left(g_{j0} - g_{j0}\partial_0\pi - g_{00}\partial_j\pi\right)\right] \,. \end{aligned} \tag{8.103}$$

Since we want an expression at first order, knowing that g^{0i} and π are small quantities (e.g., in the sum $g^{\alpha 0}\partial_\alpha\pi$ the only term at first order is $g^{00}\partial_0\pi$), we can expand the square root at first order

$$\sqrt{-g^{00}} \to \sqrt{-g^{00} - 2g^{\alpha 0}\partial_\alpha\pi} \simeq \sqrt{-g^{00}}\sqrt{1 + 2\partial_0\pi} \simeq \sqrt{-g^{00}}\,(1 + \dot\pi) \,, \tag{8.104}$$

and simplify the expression

$$\begin{aligned} K_{ij} \to & \frac{1}{2}\sqrt{-g^{00}}\,(1+\dot\pi)\left[(1-\dot\pi)\,\partial_0 g_{ij} - \partial_j\left(g_{i0} - g_{00}\partial_i\pi\right) - \partial_i\left(g_{j0} - g_{00}\partial_j\pi\right)\right] = \\ = & \frac{1}{2}\sqrt{-g^{00}}\,(1+\dot\pi)\left[(1-\dot\pi)\,\partial_0 g_{ij} - \left(\partial_j g_{i0} + \partial_j\partial_i\pi\right) - \left(\partial_i g_{j0} + \partial_i\partial_j\pi\right)\right] = \\ = & \frac{1}{2}\sqrt{-g^{00}}\left[\partial_0 g_{ij} - \partial_j g_{i0} - \partial_i g_{j0}\right] - \partial_i\partial_j\pi = \\ = & K_{ij} - \partial_i\partial_j\pi \,, \end{aligned} \tag{8.105}$$

where in the first equality we use the fact that $g^{00} = -1$ at first order, while in the second equality we commute the partial derivatives.

The trace K can be computed tracing the transformed extrinsic curvature (8.105). We obtain

$$K = g^{ij}K_{ij} \to K - g^{ij}\partial_i\partial_j\pi \cong K - \frac{1}{a^2}\partial^2\pi \,, \tag{8.106}$$

where we consider (8.94), defined $\partial^2 \equiv \partial^i\partial_i$. In the last equality we use the background value $g^{(0)\,ij}$ instead of the complete value of $g^{ij} = g^{(0)\,ij} + \delta g^{ij}$ because π is already at first order. We will repeatedly use this trick in the next computations, omitting to specify its use every time. Using the transformation of the Hubble parameter

$$H(t) \to H(t+\pi) = H(t) + \dot H(t)\pi \,, \tag{8.107}$$

computed using equation (8.87), we can find the transformation of the extrinsic curvature tensor K_{ij}

$$\begin{aligned}\delta K_{ij}(t) = K_{ij}(t) - K_{ij}^{(0)}(t) = K_{ij}(t) + H(t)h_{ij} &\rightarrow K_{ij}(t+\pi) + H(t+\pi)h_{ij}\\ &= K_{ij}(t) - \partial_i\partial_j\pi + H(t)h_{ij} + \dot{H}\pi h_{ij}\\ &= \delta K_{ij}(t) + \dot{H}\pi h_{ij} - \partial_i\partial_j\pi\,, \end{aligned} \tag{8.108}$$

where we also use the fact that at first order the $h_{ij} = g_{ij}$ transforms in itself, as we can see from equation (8.95). Similarly to what we did for the Ricci scalar fluctuations in (8.99), the extrinsic curvature trace fluctuations transform as

$$\begin{aligned}\delta K(t) = K(t) - K^{(0)}(t) &\rightarrow K(t+\pi) - K^{(0)}(t+\pi)\\ &= K(t+\pi) - K^{(0)}(t) - \pi\partial_t K^{(0)}(t)\\ &= K(t) - K^{(0)}(t) - \frac{1}{a^2}\partial^2\pi + 3\pi\dot{H}\\ &= \delta K(t) - \frac{1}{a^2}\partial^2\pi + 3\pi\dot{H}\,. \end{aligned} \tag{8.109}$$

Normal vector. Consider the normal vector general definition (8.25),

$$n_\mu = -\frac{\partial_\mu S(x^\nu)}{\sqrt{-g^{\rho\sigma}\partial_\rho S(x^\nu)\partial_\sigma S(x^\nu)}}\,, \tag{8.110}$$

where we explicitly write the normalization term N. The normal vector transforms as

$$n_\mu \rightarrow \bar{n}_\mu = -\frac{\bar{\partial}_\mu S(\bar{x}^\nu)}{\sqrt{-\bar{g}^{\rho\sigma}\bar{\partial}_\rho S(\bar{x}^\nu)\bar{\partial}_\sigma S(\bar{x}^\nu)}} = \frac{\partial x^\nu}{\partial \bar{x}^\mu}\left[n_\nu(1-\dot{\pi}) - \partial_\nu\pi\right]\,, \tag{8.111}$$

where we used the equations (8.87) (for $S(x^\nu) = S(t) = t$), (8.90) and (8.92). The result is the same as in [73].

Three-dimensional Ricci scalar. Consider (3.113) for the three-dimensional Ricci scalar

$${}^{(3)}R = R + 2R^{\mu\nu}n_\nu n_\mu + K^{\mu\nu}K_{\mu\nu} - K^2\,. \tag{8.112}$$

The quantities on the right hand side of the equation already have known transformations. The Ricci scalar R transforms into itself

$$R \rightarrow R\,, \tag{8.113}$$

as it is a scalar quantity. The second terms transformation at first order is given by

$$\begin{aligned}2R^{\mu\nu}n_\nu n_\mu \rightarrow 2R^{\mu\nu}&\left[n_\nu(1-\dot{\pi}) - \partial_\nu\pi\right]\left[n_\mu(1-\dot{\pi}) - \partial_\mu\pi\right] =\\ &= 2R^{\mu\nu}n_\mu n_\nu\left(1-2\dot{\pi}\right) - 2R^{\mu\nu}n_\mu\partial_\nu\pi - 2R^{\mu\nu}n_\nu\partial_\mu\pi =\\ &= 2R^{\mu\nu}n_\mu n_\nu - 4R^{00}n_0 n_0\dot{\pi} - 4R^{00}n_0\dot{\pi} =\\ &= 2R^{\mu\nu}n_\mu n_\nu\,. \end{aligned} \tag{8.114}$$

Therefore this term does not change under the transformation at first order. The third and fourth terms of equation (8.112) transform with (8.105) and (8.106). In particular, the third term have the following transformation

$$\begin{aligned}K^{\mu\nu}K_{\mu\nu} = K^{ij}K_{ij} = g^{ir}g^{js}K_{rs}K_{ij} &\rightarrow g^{ir}g^{js}\left(K_{rs} - \partial_r\partial_s\pi\right)\left(K_{ij} - \partial_i\partial_j\pi\right) =\\ &= K^{ij}K_{ij} - 2g^{ir}g^{js}K^{rs}\partial_i\partial_j\pi\\ &= K^{ij}K_{ij} - 2\delta^{ir}\delta^{js}a^{-4}\left(-Hh_{rs}\right)\partial_i\partial_j\pi\\ &= K^{ij}K_{ij} + 2\frac{H}{a^2}\partial^2\pi\,, \end{aligned} \tag{8.115}$$

where we recall the definition $\partial^2 \equiv \partial_i\partial^i$. The fourth term transformation is

$$K^2 \to \left(K - \frac{1}{a^2}\partial^2\pi\right)\left(K - \frac{1}{a^2}\partial^2\pi\right) = K^2 - 2\frac{K}{a^2}\partial^2\pi = K^2 + 2\frac{H}{a^2}\partial^2\pi\,. \tag{8.116}$$

Using all the results above, we obtain the final transformation

$${}^{(3)}R \to {}^{(3)}R + 4\frac{H}{a^2}\partial^2\pi\,. \tag{8.117}$$

8.5.2 Summary of the transformations.

Using the Stueckelberg trick transformation

$$x^\mu \to \bar{x}^\mu = x^\mu + \delta_0^\mu\pi(x)\,, \tag{8.118}$$

we can restore the time diffeomorphism in the action, i.e., we go from the unitary gauge, where no Goldstone boson appears, to a gauge where this appears explicitly. The Goldstone boson is the π appearing in the transformation, which is different from the scalar field ϕ of the covariant action (see note below).

The important quantities transform under this transformation (at first order) as follows

$$f \to f + \dot{f}\pi \tag{8.119}$$
$$g^{00} \to g^{00} + 2g^{\alpha 0}\partial_\alpha\pi \tag{8.120}$$
$$\delta R \to \delta R - \pi\dot{R}^{(0)} \tag{8.121}$$
$$\delta K_{ij} \to \delta K_{ij} + \dot{H}\pi h_{ij} - \partial_i\partial_j\pi \tag{8.122}$$
$$\delta K \to \delta K - \frac{1}{a^2}\partial^2\pi + 3\pi\dot{H} \tag{8.123}$$
$${}^{(3)}R \to {}^{(3)}R + 4\frac{H}{a^2}\partial^2\pi \tag{8.124}$$
$${}^{(3)}R_{ij} \to {}^{(3)}R_{ij} + H(\partial_i\partial_j\pi + \delta_{ij}\partial^2\pi)\,, \tag{8.125}$$

where $\partial^2 \equiv \partial_i\partial^i$. The last transformation has not been derived, and is added for completeness even if is not strictly necessary, as this terms does not appear in the EFT action (8.81). Starting again from a convenient form of the Gauss-Codazzi equation, its derivation is similar to the previous ones.

The functional inequality in the scheme in Figure 8.3 is given by the fact that going from the covariant action to the unitary gauge Lagrangian we are neglecting higher order terms in the fluctuations δT of the quantities we consider. This means that, even if we restore the symmetry by abandoning the unitary gauge, we are only transforming the low order parts of the action. In principle, the covariant action and the non-unitary gauge effective Lagrangian would be the same if we consider all the higher order terms (up to the infinite order), but this is unnecessary if we aim to build an effective theory. This is similar to what happens for standard Effective Field Theories in Chapter 7, where the effective action only capture the small energy regime of the UV complete theory (rule **R3**), and in principle, the equivalence can be restored only considering the infinite terms in the expansion.

8.6 Perturbation equations

Once we have all the Stueckelberg transformations, we can find the perturbation equations for a general effective Lagrangian. Since the computation is lengthy but straightforward, we omit the computations and show only the results. We will follow the procedure of [70].[§] Before stating the procedure, we define

[§] A complete derivation of the perturbation equations for the other matter components (standard matter, radiation, neutrinos) can instead be found in [74].

the perturbed line element. If we consider four scalar fields Φ, Ψ, B and E we can write the most general perturbed line element at first order as

$$ds^2 = -(1+2\Phi)dt^2 - 2\partial_i B\, dt dx^i + a^2(t)\left[(1-2\Psi)\delta_{ij} + 2\chi_{ij}\right] dx^i dx^j \,. \tag{8.126}$$

Here χ_{ij} is traceless quantity which can be rewritten in terms of the scalar field E as $\chi_{ij} \equiv (\partial_i\partial_j - \frac{1}{3}\delta_{ij}\partial^2)E$. We can also write the extrinsic curvature and the three-dimensional Ricci tensor on this equal-time hypersurfaces as

$$\bar{K}_{ij} = e^{-\Phi}(H - \dot{\Psi})h_{ij} + \dot{\chi}_{ij} - \partial_i\partial_j B \,, \tag{8.127}$$

$${}^{(3)}\bar{R}_{ij} = \partial_i\partial_j\Psi + \delta_{ij}\partial^2\Psi + 2\partial_k\partial_{(i}\chi_{j)}^k - \partial^2\chi_{ij} \,. \tag{8.128}$$

These quantities are two geometrical objects different from the K_{ij} and ${}^{(3)}R_{ij}$ defined in unitary gauge since when we abandon the unitary gauge with the Stueckelberg trick we are restoring the time diffeomorphism invariance of the action, obtaining new equal-time hypersurfaces.

Another definition we need is the one related to the perturbation of the stress-energy tensor. We define

$$T^0_{\ 0} \equiv -(\rho_m + \delta\rho_m) \,, \tag{8.129}$$

$$T^0_{\ i} \equiv (\rho_m + p_m)\partial_i v = -a^2 T^i_{\ 0} \,, \tag{8.130}$$

$$T^i_{\ j} \equiv (p_m + \delta p_m)\delta^i_j + \left(\partial^i\partial_j - \frac{1}{3}\delta^i_j\partial^2\right)\sigma \,. \tag{8.131}$$

Remember that ρ_m and p_m are the background energy density and pressure of the standard matter components. In these definitions we also introduce $\delta\rho_m$ and δp_m as their perturbations, v as the (three dimensional) velocity and σ as the scalar anisotropic stress.

The procedure that leads to the perturbation equations consists in rewriting the effective action (8.81) using the Stueckelberg transformed quantities (8.119)-(8.125). Then we vary the resultant action with respect to the scalar fields available (π, Ψ, Φ, B and E). We write the result for the simple case $\bar{\lambda} = \bar{m}_5 = \bar{m}_4^2 = m_2^2 = 0$, that are the terms which make appear derivatives with order higher than two (see discussion near equation (8.81) about its third line). This case is interesting when we consider the Horndeski Lagrangian as the covariant action. In Newtonian gauge (i.e. with $B = E = 0$), we obtain the following equations (named as the correspondent Einstein equations components):

(i) 00-component

$$\begin{aligned} &M_*^2\Big[-2f\left(\frac{k^2}{a^2}\Psi + 3H\dot{\Psi} + 3H^2\Phi\right) + \dot{f}\left(\frac{k^2}{a^2}\pi + 3H^2\pi - 3H(\Phi - \dot{\pi}) - 3(\dot{\Psi} + H\Phi)\right) + 3H\dot{f}\pi\Big] \\ &- (\dot{c} + \dot{\Lambda})\pi + (2c + 4M_2^4 + 3Hm_3^3)(\Phi - \dot{\pi}) + (m_3^3 - 4Hm_4^2)\left[-\frac{k^2}{a^2}\pi + 3(H\Phi + \pi\dot{H} + \dot{\Psi})\right] \\ &- 4\frac{k^2}{a^2}\tilde{m}_4^2(\Psi + H\pi) = \delta\rho_m \,. \end{aligned} \tag{8.132}$$

(ii) 0i-component:

$$\begin{aligned} &M_*^2\left[(H\dot{f} - \ddot{f})\pi + \dot{f}(\Phi - \dot{\pi}) + 2f(H\Phi + \dot{\Psi})\right] - 2c\pi - m_3^3(\Phi - \dot{\pi}) + 4m_4^2(H\Phi + \dot{\Psi} + \dot{H}\pi) \\ &= -(p_m + \rho_m)v \,. \end{aligned} \tag{8.133}$$

(iii) ij-trace component:

$$
\begin{aligned}
& M_*^2\Big\{2f\left[-\frac{1}{3}\frac{k^2}{a^2}(\Phi-\Psi)+(3H^2+2\dot{H})\Phi+H(\dot{\Phi}+3\dot{\Psi})+\ddot{\Psi}\right] \\
& +\dot{f}\left[-\frac{2}{3}\frac{k^2}{a^2}\pi+2H\Phi+2H(\Phi-\dot{\pi})-(3H^2+2\dot{H})\pi+2\dot{\Psi}+\dot{\Phi}-\ddot{\pi}\right] \\
& +\ddot{f}\left[-2H\pi+2(\Phi-\dot{\pi})\right]-f^{(3)}\pi\Big\}+(\dot{\Lambda}-\dot{c})\pi+2c(\Phi-\dot{\pi}) \\
& -\frac{4}{3}\frac{k^2}{a^2}\left[\tilde{m}_4^2(\Phi-\dot{\pi})+\left(Hm_4^2+(m_4^2)^{\cdot}\right)\pi+m_4^2\dot{\pi}\right] \\
& +4(\dot{H}m_4^2)^{\cdot}\pi+4m_4^2\dot{H}\dot{\pi}-\left[(m_3^3)^{\cdot}+3Hm_3^3\right](\Phi-\dot{\pi})-m_3^3(\dot{\Phi}-\ddot{\pi}) \\
& +4\left[H(m_4^2)^{\cdot}+3H^2m_4^2+\dot{H}m_4^2\right]\Phi+4(m_4^2)^{\cdot}\dot{\Psi}+4m_4^2H(3\dot{H}\pi+\dot{\Phi}+3\dot{\Psi})+4m_4^2\ddot{\Psi}=\delta p_m\,. \qquad (8.134)
\end{aligned}
$$

(iv) ij-traceless component:

$$
M_*^2\left[f(\Phi-\Psi)+\dot{f}\pi\right]+2\left[m_4^2\dot{\pi}+m_4^2H\pi+(m_4^2)^{\cdot}\pi\right]+2\tilde{m}_4^2(\Phi-\dot{\pi})=\sigma\,. \qquad (8.135)
$$

(v) Generalized Poisson equation:

$$
\begin{aligned}
& -\frac{k^2}{a^2}\left[(2fM_*^2+4\tilde{m}_4^2)\Psi-(\dot{f}M_*^2-m_3^3+4Hm_4^2-4H\tilde{m}_4^2)\pi\right]+(6M_*^2H^2\dot{f}-6Hc-\dot{c}-\dot{\Lambda}+3m_3^3\dot{H})\pi \\
& -(2c+4M_2^4)\dot{\pi}-(3M_*^2H\dot{f}-2c-4M_2^4)\Phi-3M_*^2\dot{f}\dot{\Psi}+3m_3^3(\dot{\Psi}+H\Phi)=\rho_m\delta_m\,. \qquad (8.136)
\end{aligned}
$$

The general version (without considering any EFT functions null) of the first-order perturbation equations can be found in [70].

8.7 Conclusion

In this Chapter, we derived some general results of the non-covariant EFT of Gravity. The most important feature of this EFT is its model-independence, namely the fact that, once we apply the "top-down" procedure on any covariant theory (with one additional degree of freedom with respect to General Relativity) and we have the EFT functions appearing in the action (8.81), we can immediately write the background equations of motion among with the perturbation equations in a model-independent formalism, ready to be solved with a Boltzmann solver software.

The resulting theory is an Effective theory, in the sense of Chapter 7. To obtain the action, we expanded the action with all the terms which respect the (unbroken) symmetries (rule **R1**) and considered the lower energy terms (i.e. lower order in the perturbation) as dominant (rule **R3**). The higher order perturbations are non-negligible in the small scales regime (higher energies). Moreover, with the "top-down" approach, the coefficients of this expansion come from the underlying UV theory, the covariant UV complete theory (rule **R2**). But, again, the EFT of Gravity has an underlying UV complete theory given by the covariant theory, while the standard EFT for gravity as seen in Chapter 7 is considered a low energy effective theory of an unknown UV complete theory of gravity (as Maxwell theory is a low energy regime of Quantum Electrodynamics). In a sense, the EFT of Gravity introduced in this Chapter should be interpreted as an *expansion in perturbations* because, as we have seen, it is a useful tool to extract the perturbations from a covariant theory in a model-independent formalism.

There are indeed some questions left to be answered: how can we be sure that the perturbations are stable? How can we obtain the EFT functions starting from a covariant action in practice? In the next Chapters, we will answer the first question through the study of the second-order action using the ADM formulation. Then we will partially answer the second question with an example in the framework of the Horndeski theory.

Chapter 9

Arnowitt–Deser–Misner formulation of the EFT of Gravity

In this Chapter, we exploit the Hamiltonian (ADM) formulation to obtain the velocity of scalar and tensor waves in unitary gauge, with the stability conditions for the first order perturbations. The analysis of the stability is performed following the discussion in section 4.2. The derivation is a more detailed version of [71].

9.1 Scalar waves velocity - Background action

In this section we want to analyse the background action (8.44) using the ADM formalism and, in particular, the Hamiltonian formulation of this theory. The metric is the usual ADM metric (3.10)

$$ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt)\,, \tag{9.1}$$

where $h_{ij} = g_{ij}$. We also consider the following form of h_{ij}

$$h_{ij} = a^2(t) e^{2\zeta} \delta_{ij}\,, \tag{9.2}$$

that is, we consider $\zeta = \zeta(x^\mu)$ as the field that parametrize h_{ij} scalar perturbations. Our aim is to find the second order action for this field, in order to study the stability of the models given their action functions $f(t)$, ... We stress that we should raise and lower indices with h_{ij} and not with δ_{ij}, since they are metric related to two different manifolds.

In the following sections, we follow a derivation similar to the Hamiltonian ADM formulation Section 3.7. We start from the background action and firstly derive the Hamiltonian of this theory, and use it to find some constraints equations. We use these equations to obtain the value of the velocity of the scalar perturbations of ζ. Once the procedure has been discussed, we cite the results for the non-background action (with higher order terms in the effective Lagrangian).

9.1.1 Background action

Consider the background action (8.44) without matter

$$S^{(0)} = \int d^4x \sqrt{-g} \left[\frac{M_*^2}{2} f(t) R - \Lambda(t) - c(t) g^{00} \right] . \tag{9.3}$$

We start from the equation (3.112)

$$R = {}^{(3)}R + K_{\mu\nu}K^{\mu\nu} - K^\mu_\mu K^\nu_\nu - 2\nabla_\mu \left(K n^\mu + n^\nu \nabla_\nu n^\mu \right) , \tag{9.4}$$

and insert it into the action (9.3). The last term of equation (9.4) can be integrated by parts

$$
\begin{aligned}
-2\int d^4x\sqrt{-g}\,\frac{M_*^2}{2}f(t)\nabla_\mu\left[Kn^\mu+n^\nu\nabla_\nu n^\mu\right] &= 2\int d^4x\nabla_\mu\left[\sqrt{-g}\,\frac{M_*^2}{2}f(t)\right]\left[Kn^\mu+n^\nu\nabla_\nu n^\mu\right]= \\
&= 2\int d^4x\sqrt{-g}\,\frac{M_*^2}{2}\left[\partial_\mu f(t)\right]\left[Kn^\mu+n^\nu\nabla_\nu n^\mu\right]= \\
&= 2\int d^4x\sqrt{-g}\,\frac{M_*^2}{2}\dot{f}(t)\left[Kn^0+n^\nu\nabla_\nu n^0\right]= \\
&= 2\int d^4x\sqrt{h}\,N\frac{M_*^2}{2}\dot{f}(t)K\frac{1}{N}= \\
&= 2\int d^4x\sqrt{h}\,\frac{M_*^2}{2}\dot{f}(t)K\,, \qquad (9.5)
\end{aligned}
$$

where in the first line we perform an integration by parts; in the second equation we use the fact that the covariant derivative of the metric is null; in the fourth line we consider $n^0=1/N$ and the normal vector property (3.25), i.e., $n_\mu n^\nu\nabla_\nu n^\mu=0$, from which we obtain that $n^\nu\nabla_\nu n^\mu$ can not have a time component, i.e. $n^\nu\nabla_\nu n^0=0$.

Using this result we can rewrite (9.3) as

$$
S^{(0)}=\int d^4x\sqrt{h}N\left\{\frac{M_*^2}{2}f\left[{}^{(3)}R+K_{\mu\nu}K^{\mu\nu}-K^2+2\frac{\dot{f}}{f}\frac{K}{N}\right]-\Lambda(t)+c(t)\frac{1}{N^2}\right\}\,, \qquad (9.6)
$$

where we use $g^{00}=-1/N^2$. This action can be rewritten as a pure spatial action using $K_{\mu\nu}K^{\mu\nu}=K_{ij}K^{ij}$ because $K^{0\mu}=0$ for all μ. Moreover, the extrinsic curvature is defined in equation (3.51), and can be rewritten as (3.62)

$$
K_{ij}=\frac{1}{2N}\left(D_iN_j+D_jN_i-\dot{h}_{ij}\right)\,, \qquad (9.7)
$$

where D_i is the three-dimensional derivative defined in (3.30), and N and N^j are defined respectively in (3.5) and (3.8). The action using the ADM formalism becomes

$$
\begin{aligned}
S^{(0)} &= \int d^4x\sqrt{h}N\left\{\frac{M_*^2}{2}f\left[{}^{(3)}R+K_{ij}K^{ij}-K^2+2\frac{\dot{f}}{f}\frac{K}{N}\right]-\Lambda(t)+c(t)\frac{1}{N^2}\right\}\equiv \\
&\equiv \int d^4x\sqrt{-g}\mathcal{L}_{\mathrm{ADM}}\,. \qquad (9.8)
\end{aligned}
$$

In this action, we have that h_{ij} appears also with time derivatives through the presence of the extrinsic curvature (9.7), while time derivatives of N and N^i are not present.

9.1.2 Legendre transformation

The canonical momenta of h_{ij} is defined as (3.146)

$$
p^{ij}\equiv\frac{\partial}{\partial\dot{h}_{ij}}\left[\sqrt{-g}\mathcal{L}_{\mathrm{ADM}}\right]\,. \qquad (9.9)
$$

Again, the time derivative of h_{ij} comes only from the extrinsic curvature, and therefore we can write (3.147)

$$
p^{ij}=\frac{\partial K_{rs}}{\partial\dot{h}_{ij}}\frac{\partial}{\partial K_{rs}}\left[\sqrt{-g}\mathcal{L}_{\mathrm{ADM}}\right]\,. \qquad (9.10)
$$

If we rewrite the $\mathcal{L}_{\rm ADM}$ as

$$\begin{aligned}
\sqrt{-g}\mathcal{L}_{\rm ADM} &= \sqrt{h}N\left\{\frac{M_*^2}{2}f\left[{}^{(3)}R + K_{ij}K^{ij} - K^2 + 2\frac{\dot f}{f}\frac{K}{N}\right] - \Lambda(t) + c(t)\frac{1}{N^2}\right\} = \\
&= \sqrt{h}N\left\{\frac{M_*^2}{2}f\left[{}^{(3)}R + h^{is}h^{jr}\left(K_{ij}K_{sr} - K_{is}K_{sr}\right) + 2\frac{\dot f}{f}\frac{h^{ij}K_{ij}}{N}\right] - \Lambda(t) + c(t)\frac{1}{N^2}\right\} = \\
&= \sqrt{h}N\left\{\frac{M_*^2}{2}f\left[{}^{(3)}R + \left(h^{is}h^{jr} - h^{ij}h^{sr}\right)K_{ij}K_{sr} + 2\frac{\dot f}{f}\frac{h^{ij}K_{ij}}{N}\right] - \Lambda(t) + c(t)\frac{1}{N^2}\right\}, \quad (9.11)
\end{aligned}$$

we can easily compute the canonical momenta as

$$\begin{aligned}
p^{ij} &= \frac{\partial K_{mn}}{\partial \dot h_{ij}}\sqrt{h}N\frac{\partial}{\partial K_{mn}}\left\{\frac{M_*^2}{2}f\left[\left(h^{is}h^{jr} - h^{ij}h^{sr}\right)K_{ij}K_{sr} + 2\frac{\dot f}{f}\frac{h^{ij}K_{ij}}{N}\right]\right\} = \\
&= \left(-\frac{1}{2N}\right)\frac{\sqrt{h}NfM_*^2}{2}\left[2\left(h^{is}h^{jr} - h^{ij}h^{sr}\right)K_{sr} + 2\frac{\dot f}{f}\frac{h^{ij}}{N}\right] = \\
&= -\frac{\sqrt{h}\,fM_*^2}{2}\left[\left(K^{ij} - h^{ij}K\right) + \frac{\dot f}{f}\frac{h^{ij}}{N}\right], \quad (9.12)
\end{aligned}$$

where we computed $\partial K_{rs}/\partial \dot h_{ij}$ using the extrinsic curvature equation (9.7). The factors 2 in the second line comes from the redefinition of dummy indices in the summations.

9.1.3 Hamiltonian action

We now derive the explicit form of the Hamiltonian action, and use the variational principle to derive the equations of motion. From the definition (3.152), the Hamiltonian is

$$\begin{aligned}
\mathcal{H}_{\rm ADM} &= p^{ij}\dot h_{ij} - \sqrt{-g}\mathcal{L}_{\rm ADM} = \\
&= \frac{\sqrt{h}\,fM_*^2}{2}\left[\left(K^{ij} - h^{ij}K\right) + \frac{\dot f}{f}\frac{h^{ij}}{N}\right]\left(2NK_{ij} - D_iN_j - D_jN_i\right) + \\
&\quad - \sqrt{h}N\left\{\frac{M_*^2}{2}f\left[{}^{(3)}R + K_{ij}K^{ij} - K^2 + 2\frac{\dot f}{f}\frac{K}{N}\right] - \Lambda + c\frac{1}{N^2}\right\} = \\
&= \frac{\sqrt{h}\,fM_*^2}{2}\left(2NK^{ij}K_{ij} - 2NK^2 - 2K^{ij}D_iN_j + 2Kh^{ij}D_iN_j\right) + \\
&\quad + \frac{\sqrt{h}\,\dot fM_*^2}{2}\frac{h^{ij}}{N}\left(2NK_{ij} - D_iN_j - D_jN_i\right) + \sqrt{h}N\left(\Lambda - \frac{c}{N^2}\right) + \\
&\quad - \frac{\sqrt{h}\,NfM_*^2}{2}\left[{}^{(3)}R + K_{ij}K^{ij} - K^2 + 2\frac{\dot f}{f}\frac{K}{N}\right] = \\
&= \frac{\sqrt{h}\,NfM_*^2}{2}\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) + \sqrt{h}N\left(\Lambda - \frac{c}{N^2}\right) - \frac{\sqrt{h}\,M_*^2}{N}\dot fh^{ij}D_iN_j + \\
&\quad - \frac{\sqrt{h}\,fM_*^2}{2}\left[2K^{ij} - 2h^{ij}K\right]D_iN_j = \\
&= \frac{\sqrt{h}\,NfM_*^2}{2}\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) + \sqrt{h}N\left(\Lambda - \frac{c}{N^2}\right) - \frac{\sqrt{h}\,M_*^2}{N}\dot fh^{ij}D_iN_j + \\
&\quad - \sqrt{h}D_i\left[\frac{fM_*^2}{2}\left(2K^{ij} - 2h^{ij}K\right)N_j\right] + \sqrt{h}D_i\left[\frac{fM_*^2}{2}\left(2K^{ij} - 2h^{ij}K\right)\right]N_j\,, \quad (9.13)
\end{aligned}$$

where we have used several times the symmetry of the extrinsic curvature $K_{ij} = K_{ji}$. We can neglect the total derivative term (is a total derivative in the three-dimensional hypersurface), and write the Hamiltonian as

$$H_{\rm ADM} \equiv \int_\Sigma d^3y\,\mathcal{H}_{\rm ADM} = \int_\Sigma d^3y\,\sqrt{h}\left\{\frac{NfM_*^2}{2}\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) + N\left(\Lambda - \frac{c}{N^2}\right) + \right.$$
$$\left. + D_i\left[\frac{fM_*^2}{2}\left(2K^{ij} - 2h^{ij}K\right)\right]N_j - \frac{M_*^2}{N}\dot{f}h^{ij}D_iN_j\right\}\,. \tag{9.14}$$

The extrinsic curvature K_{ij} implicitly contains the dependence on the canonical variables (and N) through

$$\frac{\sqrt{h}fM_*^2}{2}K^{ij} = -\left[p^{ij} - \frac{1}{2}ph^{ij} - \frac{\sqrt{h}M_*^2}{4N}\dot{f}h^{ij}\right]\,, \tag{9.15}$$

as can be easily proved by inserting this into the RHS of the p^{ij} definition (9.12), and find that is indeed equal to p^{ij}.

From the Hamiltonian theory, we know that we can write the action as

$$S_H = \int_{t_1}^{t_2} dt\left\{\int_\Sigma d^3y\,p^{ij}\dot{h}_{ij} - H_{\rm ADM}\right\}\,, \tag{9.16}$$

which is called Hamiltonian action. Our canonical coordinates are h_{ij} and p_{ij}, among with the coordinates N and N^i.

Varying the action (9.16) with respect to these four coordinates, we find the Hamilton equations (3.163)-(3.166)

$$\frac{dh_{ij}}{dt} = \frac{\delta H_{\rm ADM}}{\delta p^{ij}} \equiv Q_{ij}\,, \qquad \frac{dp^{ij}}{dt} = -\frac{\delta H_{\rm ADM}}{\delta h_{ij}} \equiv P^{ij}\,, \tag{9.17}$$
$$C \equiv \frac{\delta H_{\rm ADM}}{\delta N} = 0\,, \qquad C_i \equiv \frac{\delta H_{\rm ADM}}{\delta N^i} = 0\,. \tag{9.18}$$

The first constraint equation is given by

$$C = \frac{\delta H_{\rm ADM}}{\delta N} = \frac{fM_*^2}{2}\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) + \left(\Lambda + \frac{c}{N^2}\right) + \frac{fNM_*^2}{2}\frac{\delta}{\delta N}\left(K_{ij}K^{ij} - K^2\right) +$$
$$-\sqrt{h}\,M_*^2\frac{\delta}{\delta N}\left[\frac{1}{N}\dot{f}h^{ij}D_iN_j + f\left[K^{ij} - h^{ij}K\right]D_iN_j\right]\,. \tag{9.19}$$

But

$$\frac{\delta K_{ij}}{\delta N} = -h^{ij}\frac{\dot{f}}{2fN^2}\,, \tag{9.20}$$
$$\frac{\delta K}{\delta N} = \frac{\delta}{\delta N}\left(\frac{3\dot{f}}{2Nf}\right) = -\frac{3\dot{f}}{2N^2f}\,, \tag{9.21}$$
$$\frac{\delta}{\delta N}(K_{ij}K^{ij}) = K^{ij}\frac{\delta K_{ij}}{\delta N} + K_{ij}\frac{\delta K^{ij}}{\delta N} = -K\frac{\dot{f}}{N^2f}\,, \tag{9.22}$$
$$\frac{\delta(K^2)}{\delta N} = 2K\frac{\delta K}{\delta N} = -K\frac{3\dot{f}}{N^2f}\,, \tag{9.23}$$

and therefore

$$\frac{fNM_*^2}{2}\frac{\delta}{\delta N}\left(K_{ij}K^{ij} - K^2\right) = K\frac{\dot{f}M_*^2}{N}\,, \tag{9.24}$$
$$-\sqrt{h}\,M_*^2\frac{\delta}{\delta N}\left[\frac{1}{N}\dot{f}h^{ij}D_iN_j + f\left[K^{ij} - h^{ij}K\right]D_iN_j\right] = 0\,. \tag{9.25}$$

Thus, the result for the variation of N is

$$C = \frac{\delta H_{\rm ADM}}{\delta N} = \frac{f M_*^2}{2}\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) + \left(\Lambda + \frac{c}{N^2}\right) + \frac{\dot{f} M_*^2}{N} K\,. \tag{9.26}$$

The variation with respect to N^j only requires an additional step

$$-\frac{\sqrt{h}\,M_*^2}{N}\dot{f} h^{ij} D_i N_j = -\sqrt{h} D_i\left[\frac{M_*^2}{N}\dot{f} h^{ij} N_j\right] + \sqrt{h} D_i\left[\frac{M_*^2}{N}\dot{f} h^{ij}\right] N_j\,, \tag{9.27}$$

and therefore, neglecting the total derivative term and lowering the index j, we obtain

$$C_j = D_i\left[\frac{f M_*^2}{2}\left(2K^i_j - 2\delta^i_j K\right) + \frac{M_*^2}{N}\dot{f}\delta^i_j\right]\,. \tag{9.28}$$

Again, we stress that even if K_{ij} depends on N^i by definition (9.7), in the Hamiltonian formulation K_{ij} must be considered as a function of the Hamiltonian variables as in equation (9.15). Therefore, we do not need to derive K_{ij} with respect to N^i.

The final constraint equations are

$$C = \frac{f M_*^2}{2}\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right) + \left(\Lambda + \frac{c}{N^2}\right) + \frac{\dot{f} M_*^2}{N} K = 0\,, \tag{9.29}$$

$$C_j = D_i\left[f M_*^2\left(K^i_j - \delta^i_j K\right) + \frac{M_*^2}{N}\dot{f}\delta^i_j\right] = 0\,. \tag{9.30}$$

Again, these equations are considered as constraints. In fact, they do not add any evolution information to N and N^i since they do not depend on the time derivatives of these two quantities. They only act as constraints on the values of h^{ij} and p^{ij}, in particular for their initial conditions.

The form of P^{ij} and Q^{ij} is more complex and can be computed using the same procedure as for the computation of C, i.e. it is necessary to explicitly write p^{ij} and h^{ij} dependences of K_{ij} as in equation (9.15). Since these results are not required for future discussions, we omit their equations.

Finally, you can recover the General Relativity results of Section 3.7 setting $f(t) = 1$ and $\Lambda(t) = c(t) = 0$.

9.1.4 Quadratic action of ζ

We can also derive the quadratic action for the scalar perturbations introduced with the function ζ as $h_{ij} = a^2(t)e^{2\zeta}\delta_{ij}$. We expand N and N^i at first order as

$$N = 1 + \delta N\,, \qquad N_i = \partial_i\psi + N_{T,i} \quad \text{where} \quad D_i N^i_T = 0\,. \tag{9.31}$$

The first definition is natural, since in the case of a $t =$ constant hypersurface, $N = 1/\sqrt{-g^{00}}$, that is 1 at first order. The second definition is an expansion of N^i into two quantities at first order, a scalar ψ part and a transverse part N^i_T, which means that $D_i N^i_T = 0$. Note that N_i is a purely spatial vector, and therefore we want $N_0 = 0$, and this means that $n^\mu\partial_\mu\psi \propto \partial_0\psi = 0$.

We can rewrite the extrinsic curvature tensor and the three-dimensional Ricci tensor using these definitions. The fist can be computed starting from the equation of the extrinsic curvature (9.7)

$$K_{ij} = \frac{1}{2N}\left(D_i N_j + D_j N_i - \dot{h}_{ij}\right)\,, \tag{9.32}$$

and evaluate the term in the square brackets. We substitute the three-dimensional metric (9.2),

$$h_{ij} = a^2(t)e^{2\zeta}\delta_{ij}\,, \tag{9.33}$$

and the last term of the extrinsic curvature becomes

$$-\dot{h}_{ij} = -\left(2a\dot{a} + 2a^2\dot{\zeta}\right) e^{2\zeta}\delta_{ij} = -\left(2H + 2\dot{\zeta}\right) h_{ij} \,. \tag{9.34}$$

The first two terms can be rewritten using the definitions of N and N^i in equation (9.31), and we obtain

$$D_iN_j + D_jN_i = D_i\partial_j\psi + D_j\partial_i\psi + D_iN_{T,j} + D_jN_{T,i} \,. \tag{9.35}$$

Using the definition of the three-dimensional covariant derivative (8.32)

$$D_i\partial_j\psi = \partial_i\partial_j\psi - {}^{(3)}\Gamma^{\,s}_{ij}\,\partial_s\psi \,, \tag{9.36}$$

where we used the fact that $\partial_\mu\psi$ is purely spatial. The three-dimensional Christoffel symbols are given by

$$\begin{aligned}
{}^{(3)}\Gamma^k_{ij} &= \frac{1}{2}h^{ks}\left(\partial_i h_{sj} + \partial_j h_{is} - \partial_s h_{ij}\right) = \\
&= \frac{1}{2}h^{ks}a^2e^{2\zeta}\left(2\delta_{is}\partial_j\zeta + 2\delta_{js}\partial_i\zeta - 2\delta_{ij}\partial_s\zeta\right) = \\
&= \frac{1}{2}h^{ks}\left(2h_{is}\partial_j\zeta + 2h_{js}\partial_i\zeta - 2h_{ij}\partial_s\zeta\right) = \\
&= \delta^k_i\partial_j\zeta + \delta^k_j\partial_i\zeta - h_{ij}\partial^k\zeta \,.
\end{aligned} \tag{9.37}$$

By substituting this result into (9.36), we obtain

$$D_i\partial_j\psi = \partial_i\partial_j\psi - \partial_i\psi\partial_j\zeta - \partial_j\psi\partial_i\zeta + h_{ij}\partial_s\psi\partial^s\zeta = D_j\partial_i\psi \,, \tag{9.38}$$

and therefore

$$\begin{aligned}
K_{ij} &= \frac{1}{2N}\left(D_iN_j + D_jN_i - \dot{h}_{ij}\right) \\
&= \frac{1}{N}\left[-\left(H + \dot{\zeta}\right)h_{ij} + \left(\partial_i\partial_j\psi - \partial_i\psi\partial_j\zeta - \partial_j\psi\partial_i\zeta + h_{ij}\partial_s\psi\partial^s\zeta\right) + \frac{1}{2}\left(D_iN_{T,j} + D_jN_{T,i}\right)\right] .
\end{aligned} \tag{9.39}$$

Moreover, we have

$$\begin{aligned}
NK^j_i &= Nh^{js}K_{is} = \\
&= -h^{js}\left(H + \dot{\zeta}\right)h_{is} + \frac{1}{2}\left(D_iN^j_T + D^jN_{T,i}\right) + \\
&\quad + h^{js}\left(\partial_i\partial_s\psi - \partial_i\psi\partial_s\zeta - \partial_s\psi\partial_i\zeta + h_{is}\partial_r\psi\partial^r\zeta\right) = \\
&= -\delta^j_i\left(H + \dot{\zeta} - \partial_r\psi\partial^r\zeta\right) + \frac{1}{2}\left(D_iN^j_T + D^jN_{T,i}\right) - \\
&\quad - \left(\partial^j\psi\partial_i\zeta + \partial_i\psi\partial^j\zeta\right) + \partial_i\partial^j\psi \,,
\end{aligned} \tag{9.40}$$

where we have used the fact that $D_ih_{jk} = 0$, and therefore

$$NK = NK^i_i = -3(H + \dot{\zeta}) + \partial_i\psi\partial^i\zeta + D_iN^i_T + \partial_i\partial^i\psi \,. \tag{9.41}$$

In principle the same method can be used to compute the three-dimensional Ricci tensor ${}^{(3)}R_{ij}$ in terms of ζ. Instead, we want to use an alternative method based on the conformal transformations, using equation (D.8) of [75]

$$\begin{aligned}
\tilde{R}_{\mu\nu} &= R_{\mu\nu} - (n-2)\nabla_\mu\nabla_\nu\ln\Omega - g_{\mu\nu}g^{\rho\sigma}\nabla_\rho\nabla_\sigma\ln\Omega + \\
&\quad + (n-2)(\nabla_\mu\ln\Omega)(\nabla_\nu\ln\Omega) - (n-2)g_{\mu\nu}g^{\rho\sigma}(\nabla_\rho\ln\Omega)(\nabla_\sigma\ln\Omega) \,.
\end{aligned} \tag{9.42}$$

This formula provides the conformal transformed $\tilde{R}_{\mu\nu}$, i.e. the Ricci tensor built with the conformal transformed metric $\tilde{g}_{\mu\nu} = \Omega(x^\rho)^2 g_{\mu\nu}$, where $\Omega(x^\mu)$ is the conformal factor; and n is the dimension of the manifold. Note that the covariant derivatives are built with the connections of the manifold paired with the metric $g_{\mu\nu}$. In our case, the induced metric form (9.33) can be seen as a conformal transformation in the three-dimensional hypersurface ($n = 3$) of the form $h_{ij} = \Omega(x^k)^2 \eta_{ij}$, where the metric $\eta_{ij} = \delta_{ij}$ (restriction of the Minkowski metric) and the conformal factor is $\Omega(x^k) = a(t)e^{\zeta(x^k)}$. Since we consider hypersurfaces with $t =$ constant, $a(t)$ is also a constant in the considerations that follow. Therefore, using the intermediate results

$$\nabla_i \ln \Omega = \nabla_i \ln \left[a(t)e^{\zeta(x^k)}\right] = \nabla_i \left[\ln a(t) + \zeta\right] = \nabla_i \zeta = \partial_i \zeta \,, \tag{9.43}$$

$$\nabla_j \nabla_i \ln \Omega = \nabla_j \partial_i \zeta = \partial_j \partial_i \zeta \,, \tag{9.44}$$

where we use the fact that the Christoffel symbols evaluated with $\eta_{ij} = \delta_{ij}$ are null. Since the Ricci scalar built with a metric $\eta_{ij} = \delta_{ij}$ is null, we obtain the result

$${}^{(3)}R_{ij} = -\partial_i \partial_j \zeta - \delta_{ij} \partial^k \partial_k \zeta + \partial_i \zeta \partial_j \zeta - \delta_{ij} \partial^k \zeta \partial_k \zeta \,, \tag{9.45}$$

and thus

$${}^{(3)}R = {}^{(3)}R_{ij} h^{ij} = -2a^{-2} e^{-2\zeta} \delta^{ij} \left(\partial_i \zeta \partial_j \zeta + 2\partial_i \partial_j \zeta\right) = -2\left(\partial_i \zeta \partial^i \zeta + 2\partial^i \partial_i \zeta\right) \,. \tag{9.46}$$

Both the results for the extrinsic curvature (9.39) and the three-dimensional Ricci tensor (9.45) are exact results.

The next step is to find the relation between δN, N_T^i and ζ. To obtain these relations, we start from the constraints of the Hamiltonian formulations (9.29) and (9.30). From the second equation, by substituting the results above (we also use the fact that $N = 1 + \delta N$, or $1/(1 + \delta N) \cong 1 - \delta N$), we obtain the first order expression

$$\begin{aligned}
C_j &= D_i \left[f M_*^2 \left(K_j^i - \delta_j^i K\right) + \frac{M_*^2}{N} \dot{f} \delta_j^i\right] = \\
&= D_i \Bigg[M_*^2 \left(2f\dot{\zeta} - 2fH\delta N - \dot{f}\delta N\right) \delta_j^i + \frac{f M_*^2}{2} \left(D_j N_T^i + D^i N_{T,j} - 2\delta_j^i D_s N_T^s\right) + \\
&\quad + f M_*^2 \left(\partial_j \partial^i \psi - \delta_j^i \partial_k \partial^k \psi\right)\Bigg] = 0 \,.
\end{aligned} \tag{9.47}$$

Consider the last term. The three-dimensional covariant derivative acts with the three-dimensional Christoffel symbols (9.37), which are first-order quantities since they are proportional to ζ. Therefore, when we compute the three-dimensional covariant derivatives of quantities that are at first order, if we want a result at first order, we can simply substitute D_i with the partial derivative ∂_i. Thus, the last term is

$$D_i \left[\partial_j \partial^i \psi - \delta_j^i \partial_k \partial^k \psi\right] = \partial_i \left(\partial_j \partial^i \psi - \delta_j^i \partial_k \partial^k \psi\right) = 0 \,, \tag{9.48}$$

where we have used the commutative property of the partial derivatives. Therefore we are left with the first line of C_j, i.e. the second line of equation (9.47), which satisfies the constraint if we consider

$$\delta N = \frac{\dot{\zeta}}{H + \frac{\dot{f}}{2f}} \equiv \frac{\dot{\zeta}}{A_0} \qquad \text{and} \qquad N_T^i = 0 \,. \tag{9.49}$$

These conditions are derived considering the fact that we want independent conditions for our (small valued) variables δN, N_T^i and ψ, in terms of ζ. Note again that these conditions are valid only at first order.

Substituting the results for the three-dimensional Ricci scalar (9.46), the extrinsic curvature (9.39)-(9.41) (some terms in the $K^{ij}K_{ij} - K^2$ cancel), and using the conditions just derived, we can rewrite the action (9.8) at second order in ζ. The action becomes

$$S^{(0)} = \int d^4x \sqrt{h} \left\{ \left(1 + \frac{\dot{\zeta}}{A_0}\right) \left[-M_*^2 f a^{-2} e^{-2\zeta} \delta^{ij} \left(2\partial_i\partial_j\zeta + \partial_i\zeta\partial_j\zeta\right) - \Lambda\right] + \right.$$
$$\left. + \left(1 + \frac{\dot{\zeta}}{A_0}\right)^{-1} \left[-3M_*^2 f \left(H + \dot{\zeta}\right)^2 - 3M_*^2 \dot{f} \left(H + \dot{\zeta}\right) + c\right] \right\}, \tag{9.50}$$

where we substituted $N = 1 + \delta N = 1 + \dot{\zeta}/A_0$. We want to obtain a quadratic action, and therefore we should expand the term $(1 + \dot{\zeta}/A_0)^{-1}$ in powers of $\dot{\zeta}/A_0$, which is a small quantity, up to the second order. We obtain

$$\left(1 + \dot{\zeta}/A_0\right)^{-1} \cong 1 - \frac{\dot{\zeta}}{A_0} + \left(\frac{\dot{\zeta}}{A_0}\right)^2 . \tag{9.51}$$

We rewrite the action collecting the terms with $\frac{\dot{\zeta}}{A_0}$, obtaining

$$S_0 = \int d^4x \, a^3 e^{3\zeta} \left\{ -M_*^2 f a^{-2} e^{-2\zeta} \delta^{ij} \left(2\partial_i\partial_j\zeta + \partial_i\zeta\partial_j\zeta\right) \left(1 + \frac{\dot{\zeta}}{A_0}\right) + \right.$$
$$+ \left(-\Lambda - 3M_*^2 f H^2 - 3M_*^2 \dot{f} H + c\right) +$$
$$+ \left(-\Lambda - c + 3M_*^2 f H^2 + 3M_*^2 \dot{f} H - 6M_*^2 f H A_0 - 3M_*^2 \dot{f} A_0\right) \frac{\dot{\zeta}}{A_0} +$$
$$\left. + \left(-3M_*^2 f A_0^2 + 6M_*^2 f H A_0 + 3M_*^2 \dot{f} A_0 - 3M_*^2 f H^2 - 3M_*^2 \dot{f} H + c\right) \left(\frac{\dot{\zeta}}{A_0}\right)^2 \right\} . \tag{9.52}$$

The term proportional to $(\dot{\zeta}/A_0)^2$ is

$$-3M_*^2 f A_0^2 + 6M_*^2 f H A_0 + 3M_*^2 \dot{f} A_0 - 3M_*^2 f H^2 - 3M_*^2 \dot{f} H + c =$$
$$= -3M_*^2 f \left(H + \frac{\dot{f}}{2f}\right)^2 + 3M_*^2 \left(2fH + \dot{f}\right) \left(H + \frac{\dot{f}}{2f}\right) - 3M_*^2 f H^2 - 3M_*^2 \dot{f} H + c =$$
$$= \frac{3}{4} M_*^2 \frac{\dot{f}^2}{f} + c \, . \tag{9.53}$$

The other terms can be simplified using the background equations (8.58) and (8.59) (without matter, since we are using the background action without the matter content), rewritten in the form

$$3M_*^2 \left[H^2 f + H\dot{f}\right] M_*^2 - c - \Lambda = 0 \, , \tag{9.54}$$
$$M_*^2 \left[\ddot{f} - H^2 f + 2\dot{f} H\right] = -2c \, , \tag{9.55}$$

where the second equation can be easily obtained substituting Λ from (8.58) into (8.59). Thus, the term proportional to $(\dot{\zeta}/A_0)^1$ is, using equation (9.54),

$$-\Lambda - c + 3M_*^2 f H^2 + 3M_*^2 \dot{f} H - 6M_*^2 f H A_0 - 3M_*^2 \dot{f} A_0 = -6M_*^2 f H A_0 - 3M_*^2 \dot{f} A_0 \, . \tag{9.56}$$

We can integrate by parts the last two terms of equation (9.56)

$$
\begin{aligned}
-\int d^4x\, a^3 \left(3\dot{\zeta}e^{3\zeta}\right) M_*^2 \left(2fH+\dot{f}\right) &= -\int d^4x\, a^3 \frac{d}{dt}\left(e^{3\zeta}\right) M_*^2 \left(2fH+\dot{f}\right) = \\
&= \int d^4x\, e^{3\zeta} M_*^2 \frac{d}{dt}\left[a^3\left(2fH+\dot{f}\right)\right] + \text{b.t.} = \\
&= \int d^4x\, e^{3\zeta} a^3 M_*^2 \left(6fH^2+5H\dot{f}+2\dot{H}f+\ddot{f}\right) + \text{b.t.} = \\
&= \int d^4x\, e^{3\zeta} a^3 \left(6M_*^2 fH^2+6M_*^2 H\dot{f}-2c\right) + \text{b.t.}\,, \qquad (9.57)
\end{aligned}
$$

where b.t. is a negligible boundary term in the action, and in the last equality we use the background equation (9.55). We are left with the term proportional to $(\dot{\zeta}/A_0)^0$, i.e., the second line of equation (9.52) plus the new terms coming from the integration by parts that are now terms at zero order in $\dot{\zeta}/A_0$

$$
-\Lambda - 3M_*^2 fH^2 - 3M_*^2 \dot{f}H + c + 6M_*^2 fH^2 + 6M_*^2 H\dot{f} - 2c = 0\,, \qquad (9.58)
$$

where the equality comes from the use of the background equation (9.54). After these simplifications, the action (9.52) becomes

$$
S_0 = \int d^4x\, a^3 e^{3\zeta} \left\{ -M_*^2 f a^{-2} e^{-2\zeta} \delta^{ij} \left(2\partial_i\partial_j\zeta + \partial_i\zeta\partial_j\zeta\right)\left(1+\frac{\dot{\zeta}}{A_0}\right) + \left(\frac{3}{4}M_*^2\frac{\dot{f}^2}{f}+c\right)\left(\frac{\dot{\zeta}}{A_0}\right)^2 \right\}\,. \qquad (9.59)
$$

We analyse the first term

$$
\begin{aligned}
Y \equiv -\int d^4x\, a^3 e^{3\zeta} M_*^2 f a^{-2} e^{-2\zeta} \delta^{ij} \left(2\partial_i\partial_j\zeta + \partial_i\zeta\partial_j\zeta\right)\left(1+\frac{\dot{\zeta}}{A_0}\right) &= \\
= -\int d^4x\, a\left(1+\zeta\right) M_*^2 f \delta^{ij} \left(2\partial_i\partial_j\zeta + \partial_i\zeta\partial_j\zeta\right)\left(1+\frac{\dot{\zeta}}{A_0}\right) &= \\
\cong -\int d^4x\, a M_*^2 f \delta^{ij} \left[2\partial_i\partial_j\zeta + 2\zeta\partial_i\partial_j\zeta + \partial_i\zeta\partial_j\zeta + 2\frac{\dot{\zeta}}{A_0}\partial_i\partial_j\zeta\right] &= \\
= -\int d^4x\, a M_*^2 f \delta^{ij} \left[2\partial_i\partial_j\zeta - \partial_i\zeta\partial_j\zeta + 2\frac{\dot{\zeta}}{A_0}\partial_i\partial_j\zeta\right]\,, \qquad (9.60)
\end{aligned}
$$

where were we neglect higher order terms. In the last equality we integrate by parts the second term and obtain $2\zeta\partial_i\partial_j\zeta \to -2\partial_i\zeta\partial_j\zeta$ (f and a do not depend on space coordinates). For a similar reason, the first term $2\partial_i\partial_j\zeta$ is a negligible spatial total derivative term in the action. Moreover, we can evaluate the last term integrating by parts, in the following way

$$
\begin{aligned}
2M_*^2 \int d^4x\, a f \frac{\dot{\zeta}}{A_0} \delta^{ij}\partial_i\partial_j\zeta = -2M_*^2 \int d^4x\, a f \delta^{ij}\partial_i\left(\frac{\dot{\zeta}}{A_0}\right)\partial_j\zeta &= \\
= 2M_*^2 \int d^4x\, \delta^{ij}\partial_i\zeta \frac{d}{dt}\left(\frac{af\partial_j\zeta}{A_0}\right) &= \\
= 2M_*^2 \int d^4x\, \delta^{ij}\frac{\partial_i\zeta}{A_0}\left(aH f\partial_j\zeta + a\dot{f}\partial_j\zeta + af\partial_j\dot{\zeta} - \frac{\dot{A}_0}{A_0}af\partial_j\zeta\right)&\,. \qquad (9.61)
\end{aligned}
$$

Since δ^{ij} is symmetric, this implies that

$$-2M_*^2\int d^4x\,af\frac{\dot\zeta}{A_0}\delta^{ij}\partial_i\partial_j\zeta = 2M_*^2\int d^4x\,af\delta^{ij}\partial_i\left(\frac{\dot\zeta}{A_0}\right)\partial_j\zeta =$$
$$= -M_*^2\int d^4x\,\delta^{ij}\frac{\partial_i\zeta}{A_0}\left(aH\dot f\partial_j\zeta + a\dot f\partial_j\zeta - \frac{\dot A_0}{A_0}af\partial_j\zeta\right). \tag{9.62}$$

Therefore we have

$$Y = -\int d^4x\,a^3M_*^2f\frac{\delta^{ij}\partial_i\zeta\partial_j\zeta}{a^2A_0^2}\left(HA_0 - A_0^2 + \frac{\dot f}{f}A_0 - \dot A_0\right) =$$
$$= -\int d^4x\,a^3M_*^2f\frac{\delta^{ij}\partial_i\zeta\partial_j\zeta}{a^2A_0^2}\left(\frac{3\dot f^2}{4f^2} + \frac{H\dot f}{2f} - \frac{\ddot f}{2f} - \dot H\right) =$$
$$= -\int d^4x\,a^3\frac{\delta^{ij}\partial_i\zeta\partial_j\zeta}{a^2A_0^2}\left(\frac{3}{4}M_*^2\frac{\dot f^2}{f} + c\right), \tag{9.63}$$

where in the last equality we used the background equation (9.55).

Finally, using the results (9.59) and (9.63) above, we can rewrite the background action, quadratic in the scalar metric perturbation ζ, as

$$S_0 = \int d^4x\,a^3\frac{1}{A_0^2}\left(\frac{3}{4}M_*^2\frac{\dot f^2}{f} + c\right)\left[\dot\zeta^2 - \frac{1}{a^2}\delta^{ij}\partial_i\zeta\partial_j\zeta\right]. \tag{9.64}$$

The form of the action is similar to the one in section 4.2 where we discuss the stability conditions for the perturbations. The scalar perturbation speed $c_s^2 = 1$, which is the standard General Relativity result for scalar perturbations in the empty space. This is the reason why, even if the action $S^{(0)}$ in equation (9.3) is not at first order in the corrections (it also contains a term proportional to g^{00}), we call it background equation.

9.2 Scalar waves velocity - Quadratic action

We can now analyse the contribution to c_s^2 from higher order terms in the action (8.81). In addition to the background action, we firstly consider the following terms of the action

$$S = S^{(0)} + \int d^4x\sqrt{-g}\left[\frac{M_2^4(t)}{2}(\delta g^{00})^2 - \frac{m_3^3(t)}{2}\delta K\delta g^{00} - \right.$$
$$\left. -m_4^2(t)(\delta K^2 - \delta K^\mu{}_\nu\delta K^\nu{}_\mu) + \frac{\tilde m_4^2(t)}{2}\,{}^{(3)}R\delta g^{00}\right], \tag{9.65}$$

where $S^{(0)}$ is the background action. We will see that these terms do not generate spatial derivatives with orders higher than two. This means that these terms do not introduce corrections with k^n, where $n > 2$, to the quadratic action of ζ.

In principle, to find the value of the c_s^2, we should make the same computation carried above: find the Hamiltonian action, derive the constraints and the conditions, and in the end, write the action in terms of ζ. In practice, we can evaluate only the new terms, since the background terms do not change their contribution, and find the analogue of the C_j constraint (the derivative of the Hamiltonian with respect to N^i), as the sum of a background part and the new part from the new quadratic operators. After this, we can find the action in the same way as we did for the background action.

To find the Hamiltonian action we have to compute the canonical momentum p^{ij} for the action (9.65). We can rewrite the action, using the background values of the operators shown in Table 8.2, as

$$S = S^{(0)} + \int d^4x\sqrt{-g}\left[\frac{M_2^4(t)}{2}(\delta g^{00})^2 + \frac{3}{2}m_3^3(t)H\delta g^{00} - 6m_4^2(t)H^2 + \frac{\tilde{m}_4^2(t)}{2}\,{}^{(3)}R\delta g^{00} - \right.$$
$$\left. -\frac{1}{2}m_3^3(t)K_{ij}h^{ij}\delta g^{00} + m_4^2(t)(h^{is}h^{jr} - h^{ij}h^{sr})K_{ij}K_{sr} - 4m_4^2(t)HK_{ij}h^{ij}\right] . \tag{9.66}$$

The second line contains the terms that contribute to the canonical momentum. Indeed, using the definition of p^{ij} available in equation (9.9), we obtain

$$p^{ij} = p^{(0)\,ij} + \frac{\partial K_{mn}}{\partial \dot{h}_{ij}}\sqrt{h}N\frac{\partial}{\partial K_{mn}}\left\{-\frac{1}{2}m_3^3(t)K_{pq}h^{pq}\delta g^{00} + m_4^2(t)(h^{ps}h^{qr} - h^{pq}h^{sr})K_{pq}K_{sr} - 4m_4^2(t)HK_{pq}h^{pq}\right\}$$
$$= p^{(0)\,ij} - \frac{\sqrt{h}}{2}\left[-\left(\frac{m_3^3}{2}\delta g^{00} - 4m_4^2H\right)h^{ij} + 2m_4^2\left(K^{ij} - h^{ij}K\right)\right] . \tag{9.67}$$

Therefore the action can be computed using the Hamiltonian definition (3.152), as

$$\mathcal{H}_{\rm ADM} = \mathcal{H}_{\rm ADM}^{(0)} -$$
$$-\frac{\sqrt{h}}{2}\left\{\left[-\left(\frac{m_3^3}{2}\delta g^{00} - 4m_4^2H\right)h^{ij} + 2m_4^2\left(K^{ij} - h^{ij}K\right)\right](2NK_{ij} - D_iN_j - D_jN_i) + \right.$$
$$+\frac{M_2^4(t)}{2}(\delta g^{00})^2 + \frac{3}{2}m_3^3(t)H\delta g^{00} - 6m_4^2(t)H^2 + \frac{\tilde{m}_4^2(t)}{2}\,{}^{(3)}R\delta g^{00} -$$
$$\left. -\frac{1}{2}m_3^3(t)K_{ij}h^{ij}\delta g^{00} + m_4^2(t)(h^{is}h^{jr} - h^{ij}h^{sr})K_{ij}K_{sr} - 4m_4^2(t)HK_{ij}h^{ij}\right\} . \tag{9.68}$$

Considering that K_{ij} is a function of the Hamiltonian variables p^{ij}, h^{ij} and N, but not N^i, we can write the constraint

$$C_j \equiv \frac{\partial \mathcal{H}_{\rm ADM}}{\partial N^j} = C_j^{(0)} + D_i\left[\left(\frac{m_3^3}{2}\delta g^{00} + 4m_4^2H\right)\delta^i_j + 2m_4^2\left(K^i_j - \delta^i_jK\right)\right] = 0 . \tag{9.69}$$

We can also rewrite the fluctuation of the 00 component of the metric in terms of N using

$$g^{00} = -\frac{1}{N^2} = -\frac{1}{(1+\delta N)^2} \cong -1 + 2\delta N, \qquad \text{from which we have} \qquad \delta g^{00} = 2\delta N . \tag{9.70}$$

Therefore

$$C_j = C_j^{(0)} + D_i\left[\left(m_3^3\delta N + 4m_4^2H\right)\delta^i_j + 2m_4^2\left(K^i_j - \delta^i_jK\right)\right]$$
$$= C_j^{(0)} + D_i\left[m_3^3\delta N\delta^i_j + 2m_4^2\left(\delta K^i_j - \delta^i_j\delta K\right)\right] . \tag{9.71}$$

From the first line we see that the term $4m_4^2H\delta^i_j$ is a background term that does not contribute to the first order conditions analogous of equations (9.49). The first term and the last term are only additions to the already evaluated terms in equation (9.47), e.g. the term proportional to δN becomes $-(2fH + \dot{f})\delta N \to -(2fH + \dot{f} - m_3^3)\delta N$ and similarly for the term proportional to $K^i_j - \delta^i_jK$. Therefore we obtain the condition

$$\delta N = \frac{\dot{\zeta}}{A} \qquad \text{where} \qquad A = H + \frac{\dot{f}M_*^2 - m_3^3}{2\left(fM_*^2 + 2m_4^2\right)} . \tag{9.72}$$

After this derivation, we can rewrite the total action in terms of ζ in the previous section after equation (9.50). We omit the computation since is the same as above, with the addition of new terms in the action. Note that A_0 must be replaced with A, and therefore some steps for $S^{(0)}$ are not the same as above, in particular when we substitute for the explicit form of A. We obtain

$$S = \int d^4x a^3 \left[\alpha\dot{\zeta}^2 - \frac{1}{a^2}\beta\,\delta^{ij}\partial_i\zeta\partial_j\zeta\right], \tag{9.73}$$

where

$$\alpha = \frac{1}{A^2}\left[c + 2M_2^4 + \frac{3}{4}\frac{\left(M_*^2\dot{f} - m_3^3\right)^2}{M_*^2 f + 2m_4^2}\right], \tag{9.74}$$

$$\beta = -M_*^2 f + \frac{1}{2a}\frac{d}{dt}\left[\frac{2\left(M_*^2 f + 2\tilde{m}_4^2\right)a}{A}\right]. \tag{9.75}$$

We can see from the quadratic action that there are no terms with spatial derivatives with order higher than 2, leaving the dispersion relation in the form $\omega^2 = c_s^2 k^2$, where $c_s^2 = \beta/\alpha$. A simplified expression can be obtained using the background equations in addition to the condition $m_4^2 = 0 = \tilde{m}_4^2$, that is

$$c_s^2 = \frac{\beta}{\alpha} = \frac{c + \frac{3}{4}M_*^2\dot{f}^2/f - \frac{1}{4}m_3^6/(M_*^2 f) + \frac{1}{2}\left(\dot{m}_3^3 + Hm_3^3\right)}{c + 2M_2^4 + \frac{3}{4}M_*^2\dot{f}^2/f - \frac{3}{2}m_3^3\dot{f}/f + \frac{3}{4}m_3^6/(M_*^2 f)}. \tag{9.76}$$

As a final note, as expected the c_s^2 does not depend on the scale, i.e. is independent of k. Adding terms in the third line of the action (8.81) we can add dependence on the scale since these terms contain higher order space derivatives.

9.2.1 Redundant operator

In writing the action (9.65), we omitted a possible operator that does not contains spatial derivatives with order higher than 2, which is

$$\lambda(t)\left({}^{(3)}R_{\mu\nu}\delta K^{\mu\nu} - \frac{1}{2}\,{}^{(3)}R\delta K\right). \tag{9.77}$$

This omission does not change the result for the action (9.73), since it can be rewritten at quadratic order as the operator $\dot{\lambda}\,{}^{(3)}R\delta g^{00}$ up to a proportionality factor and some boundary terms.

In order to show this, we will start proving that

$$\int d^4x\sqrt{-g}\left[\lambda R_{\mu\nu}K^{\mu\nu} - \frac{\lambda}{2}\,{}^{(3)}RK + \frac{\dot{\lambda}}{2N}\,{}^{(3)}R\right] = 0\,. \tag{9.78}$$

The last two terms can be rewritten using the fact that $K = -\nabla_\mu n^\mu$, as

$$\begin{aligned}
-\int d^4x\sqrt{-g}\left[\frac{\lambda}{2}\,{}^{(3)}RK - \frac{\dot{\lambda}}{2N}\,{}^{(3)}R\right] &= \int d^4x\sqrt{-g}\left[\frac{\lambda}{2}\,{}^{(3)}R\,\nabla_\mu n^\mu + \frac{\dot{\lambda}}{2N}\,{}^{(3)}R\right] \\
&= \int d^4x\sqrt{-g}\left[-\nabla_\mu\left(\frac{\lambda}{2}\,{}^{(3)}R\right)n^\mu + \frac{\dot{\lambda}}{2N}\,{}^{(3)}R\right] + \text{b.t.} \\
&= \int d^4x\sqrt{-g}\left[-\frac{n^\mu\nabla_\mu\lambda}{2}\,{}^{(3)}R - \frac{\lambda}{2}n^\mu\nabla_\mu\,{}^{(3)}R + \frac{\dot{\lambda}}{2N}\,{}^{(3)}R\right] + \text{b.t.} \\
&= \int d^4x\sqrt{-g}\left[-\frac{\dot{\lambda}}{2N}\,{}^{(3)}R - \frac{\lambda}{2}n^\mu\nabla_\mu\,{}^{(3)}R + \frac{\dot{\lambda}}{2N}\,{}^{(3)}R\right] + \text{b.t.} \\
&= -\int d^4x\sqrt{-g}\left[\frac{\lambda}{2}n^\mu\nabla_\mu\,{}^{(3)}R\right] + \text{b.t.}\,,
\end{aligned} \tag{9.79}$$

where in the fourth equality we have considered $n^\mu \nabla_\mu \lambda = -N g^{0\mu} \partial_\mu \lambda = -N g^{00} \partial_0 \lambda = \partial_0 \lambda / N$, where $n^\mu = -N g^{0\mu}$. Therefore equation (9.78) becomes

$$\int d^4x \sqrt{-g} \left[\lambda R_{\mu\nu} K^{\mu\nu} - \frac{\lambda}{2} {}^{(3)}RK + \frac{\dot{\lambda}}{2N} {}^{(3)}R \right] = \int d^4x \sqrt{-g} \lambda \left[R_{\mu\nu} K^{\mu\nu} - \frac{1}{2} n^\mu \nabla_\mu {}^{(3)}R \right] . \tag{9.80}$$

Since (again) $K^{\mu 0} = 0$, we can replace $K^{\mu\nu}$ in the action with K^{ij} defined in equation (9.7). Equation (9.80) becomes

$$\begin{aligned} \int d^4x \sqrt{-g} \lambda \left[R_{\mu\nu} K^{\mu\nu} - \frac{1}{2} n^\mu \nabla_\mu {}^{(3)}R \right] = \\ = \int d^4x \sqrt{h} \lambda \left[{}^{(3)}R_{ij} \left(D^i N^j - \frac{1}{2} \dot{h}_{rs} h^{rj} h^{si} \right) + \frac{N^2}{2} g^{0\mu} \nabla_\mu {}^{(3)}R \right] . \end{aligned} \tag{9.81}$$

The last term is

$$\begin{aligned} \frac{N^2}{2} g^{0\mu} \nabla_\mu {}^{(3)}R &= \frac{N^2}{2} g^{00} \partial_0 {}^{(3)}R + \frac{N^2}{2} g^{0i} \partial_i {}^{(3)}R \\ &= -\frac{1}{2} {}^{(3)}\dot{R} + \frac{N^i}{2} D_i {}^{(3)}R , \end{aligned} \tag{9.82}$$

where we have used the fact that $D_i {}^{(3)}R = \partial_i {}^{(3)}R$. Using this, we can rewrite (9.81) as

$$\int d^4x \sqrt{h} \lambda \left[{}^{(3)}R_{ij} \left(D^i N^j - \frac{1}{2} \dot{h}_{rs} h^{rj} h^{si} \right) - \frac{1}{2} {}^{(3)}\dot{R} + \frac{N^i}{2} D_i {}^{(3)}R \right] . \tag{9.83}$$

But

$$\begin{aligned} \int d^4x \sqrt{h} \lambda \left[{}^{(3)}R_{ij} D^i N^j + \frac{N^i}{2} D_i {}^{(3)}R \right] = \\ = - \int d^4x \sqrt{h} \lambda N^j D^i \left[{}^{(3)}R_{ij} - \frac{1}{2} h_{ij} {}^{(3)}R \right] + \text{b.t} = \text{b.t} , \end{aligned} \tag{9.84}$$

since the continuity equation for the Einstein tensor must be valid also on the three-dimensional hypersurfaces. The only two terms left from (9.83) are

$$- \int d^4x \sqrt{h} \frac{\lambda}{2} \left[{}^{(3)}R_{ij} \dot{h}_{rs} h^{rj} h^{si} + {}^{(3)}\dot{R} \right] . \tag{9.85}$$

The terms in the square brackets are

$${}^{(3)}R_{ij} \dot{h}_{rs} h^{rj} h^{si} + {}^{(3)}\dot{R} = {}^{(3)}R_{ij} \dot{h}_{rs} h^{rj} h^{si} + {}^{(3)}\dot{R}_{ij} h^{ij} + {}^{(3)}R_{ij} \dot{h}^{ij} = {}^{(3)}\dot{R}_{ij} h^{ij} , \tag{9.86}$$

where the last step comes from $0 = d/dt(\delta_i^j) = d/dt(h^{is} h_{sj}) = \dot{h}^{is} h_{sj} + h^{is} \dot{h}_{sj}$, that gives $\dot{h}^{ij} = -\dot{h}_{sr} h^{si} h^{rj}$. Finally we can write the last remaining term

$$- \int d^4x \sqrt{h} \frac{\lambda}{2} \dot{R}_{ij} h^{ij} = 0 , \tag{9.87}$$

which is null (up to a boundary term) since $\dot{R}_{ij} h^{ij}$ can be written as a covariant derivative of a three-vector J^i, i.e. $\dot{R}_{ij} h^{ij} = D_i J^i$.

With this proof we have shown that

$$\lambda(t) \left({}^{(3)}R_{\mu\nu} \delta K^{\mu\nu} - \frac{1}{2} {}^{(3)}R \delta K \right) = \frac{\dot{\lambda}}{4} {}^{(3)}R \delta g^{00} , \tag{9.88}$$

where the conversion from the equation (9.78) (where we had K and K_{ij}) to this equation (where we have δK and δK_{ij}) can be obtained using the definition of δK and considering only the quadratic order.

9.3 Tensor wave velocity

To compute the tensor wave velocity, we use the TT-gauge for the tensor part (1.58)

$$ds^2 = -dt^2 + a(t)^2 e^{2\zeta}\left[(1+E_+)dx^2 + 2E_\times dxdy + (1-E_+)dy^2 + dz^2\right] . \tag{9.89}$$

The two functions E_+ and $E_\times$ satisfy the usual conditions for gravitational (tensor) waves: they are components of the traceless, divergenceless and symmetric tensor E_{ij}

$$h_{ij} = a(t)^2 e^{2\zeta}\left(\delta_{ij} + E_{ij}\right) = a(t)^2 e^{2\zeta}\begin{pmatrix} 1+E_+ & E_\times & 0 \\ E_\times & 1-E_+ & 0 \\ 0 & 0 & 1\end{pmatrix} , \tag{9.90}$$

which means $E_{ii} = 0$ and $\partial_i E_{ij} = 0$. Since we are interested in the second order action, we must add a second order term to following matrix and write

$$\begin{aligned} h_{ij} &= a(t)^2 e^{2\zeta}\left(\delta_{ij} + E_{ij} + \frac{1}{2}E_{ik}E_{kj}\right) \\ &= a(t)^2 e^{2\zeta}\begin{pmatrix} 1+E_+ + \frac{1}{2}\left(E_+^2 + E_\times^2\right) & E_\times & 0 \\ E_\times & 1-E_+ + \frac{1}{2}\left(E_+^2 + E_\times^2\right) & 0 \\ 0 & 0 & 1\end{pmatrix} . \end{aligned} \tag{9.91}$$

Moreover, the decomposition theorem ensures that the scalar and the tensor perturbations decouple in the action, and therefore we can set $\zeta = 0$ and work only with the E_α (with $\alpha = +, \times$) functions.

We proceed computing the quantities in the second order action without higher order spatial derivatives, i.e., the background action (9.8) (in the ADM formulation) plus the terms written in (9.65). The metric component g^{00} is not modified by tensor waves (see the line element above), and therefore we can set $\delta g^{00} = 0$ (and $N = 1$) for this computation. The remaining terms are the following

$$S = \int d^4x \sqrt{h}\left\{\frac{M_*^2}{2} f\left[{}^{(3)}R + K_{ij}K^{ij} - K^2 + 2\frac{\dot{f}}{f}K\right] - \Lambda + c - m_4^2(\delta K^2 - \delta K^\mu{}_\nu \delta K^\nu{}_\mu)\right\} . \tag{9.92}$$

Note that if $g^{00} = -1$, $n_\mu = -\delta^0_\mu$. We can compute the terms of the action above using their definitions. At second order in small quantities (h_α) we find

$$K_{\mu\nu} = -\nabla_\mu n_\nu - n^\rho n_\mu \nabla_\rho n_\mu , \tag{9.93}$$

$$K = g^{\mu\nu} K_{\mu\nu} = -3H , \tag{9.94}$$

$${}^{(3)}R = g^{\mu\nu}\, {}^{(3)}R_{\mu\nu} = h^\rho_\mu h^\sigma_\nu h^{\alpha\beta} R_{\rho\beta\sigma\alpha} - K_{\mu\nu}K - K^\rho_\mu K_{\rho\nu} = -\frac{1}{2a^2}\left[(\partial_z E_+)^2 + (\partial_z E_\times)^2\right] , \tag{9.95}$$

$$K_{\mu\nu}K^{\mu\nu} - K^2 = -6H^2 + \frac{1}{2}\left[\dot{E}_+^2 + \dot{E}_\times^2\right] . \tag{9.96}$$

Inserting these results in the action we obtain, up to some irrelevant background terms, the following second-order action

$$S_T = \int d^4x \sqrt{h}\frac{M_*^2 f}{4}\left\{\left(1 + \frac{2m_4^2}{M_*^2 f}\right)\left(\dot{E}_+^2 + \dot{E}_\times^2\right) - \frac{1}{a^2}\left[(\partial_z E_+)^2 + (\partial_z E_\times)^2\right]\right\} . \tag{9.97}$$

Therefore, the speed of tensor waves is given by

$$c_T^2 = \frac{1}{1 + \frac{2m_4^2}{M_*^2 f}} . \tag{9.98}$$

This result shows that the only contribution to the tensor waves linear dispersion relation is given by the terms m_4^2.

This result has a great physical meaning. As it should be clear from the derivation, the c_T^2 is the velocity (squared) of the tensor waves, which include the gravitational waves. We know that they must travel at the speed of light in General Relativity, and this is consistent since m_4^2 is always null for the standard Einstein–Hilbert action. Therefore if the model admits a m_4^2 term different from 0 at some times, the velocity of gravitational waves will be affected and different from the speed of light.

9.4 Stability

A brief comment about stability is necessary. In this Chapter, we derived the second-order action for both scalar and tensor waves. From (9.73) and (9.97) we can also derive the stability conditions that the functions of time in the action must satisfy to have a theory that is ghost and gradient instabilities free. Following the discussion in section 4.2, the stability conditions are

$$Q_s = \frac{1}{A^2}\left[c + 2M_2^4 + \frac{3}{4}\frac{\left(M_*^2\dot{f} - m_3^3\right)^2}{M_*^2 f + 2m_4^2}\right] > 0\,, \tag{9.99}$$

$$c_s^2 = \frac{1}{Q_s}\left\{-M_*^2 f + \frac{1}{2a}\frac{d}{dt}\left[\frac{2\,(M_*^2 f + 2\tilde{m}_4^2)\,a}{A}\right]\right\} > 0\,, \tag{9.100}$$

$$Q_T = \frac{M_*^2 f}{4}\left(1 + \frac{2m_4^2}{M_*^2 f}\right) > 0\,, \tag{9.101}$$

$$c_T^2 = \left(1 + \frac{2m_4^2}{M_*^2 f}\right)^{-1} > 0\,, \tag{9.102}$$

where

$$A = H + \frac{\dot{f}M_*^2 - m_3^3}{2\,(fM_*^2 + 2m_4^2)}\,. \tag{9.103}$$

We stress that the previous derivation has been performed neglecting the matter contribution, as you can see from the initial action (9.3). In particular, as it happens in Horndeski theory, the c_s^2 of the scalar field might be affected by the standard matter, in the form of its energy density and pressure ρ_m and P_m. In the Horndeski gravity case $\bar{m}_4^2(t) = \bar{m}_5(t) = \bar{\lambda}(t) = m_2^2 = 0$, and $m_4^2(t) = \tilde{m}_4^2(t)$ at every time, we obtain the following equation for the c_s^2

$$c_s^2 = \frac{1}{Q_s}\left\{-M_*^2 f + \frac{1}{2a}\frac{d}{dt}\left[\frac{2\,(M_*^2 f + 2\tilde{m}_4^2)\,a}{A}\right]\right\} - \frac{(\rho_m + P_m)(M_*^2 f + 2m_4^2)}{(2c + 4M_2^4)(M_*^2 f + 2m_4^2) + \frac{3}{2}(m_3^3 - M_*^2\dot{f})^2}\,, \tag{9.104}$$

while the other three stability conditions do not change. This equation has been computed using the equation for the c_s^2 in Horndeski theory (5.27), and exploiting the map between the Horndeski theory functions and the EFT functions. For more details about the derivation, see Chapter 10, and the discussion around equation (10.31).

Finally, as already noted in section 4.2, we should always distinguish the instabilities that might arise from the eventual negativity of the functions above and the ones coming from the presence of higher order derivatives in the Lagrangian. The former is related to the first-order perturbation functions and might arise even if the Lagrangian is at second order in the derivatives, while the latter instabilities affect also the background evolution and appear accordingly to the Ostrogradski theorem [23, 24].

Chapter 10

Horndeski theory with the EFT of Gravity

In the previous Chapters we have explored the left-hand side of the scheme in Figure 8.3 (the parts related to the effective Lagrangians), and briefly mentioned the top-down procedure to go from the covariant Lagrangian to the effective one (see section 8.4). In this Chapter we present a practical example, considering the Horndeski theory action as our covariant action.

We start showing the main general mapping result between the Horndeski covariant theory functions and the EFT of gravity functions. Then we discuss an original example, providing results both in the covariant and the effective theory and comparing them: we expect the results to be the same up to the difference based on the different numerical approaches used to solve the equations in the two cases. Finally we study the instabilities of the model following the original work discussion in [10].

10.1 Horndeski gravity

We briefly recall the main equations from Chapter 5. The Horndeski gravity action is

$$S[g_{\mu\nu},\phi] = \frac{1}{8\pi G}\int d^4x\sqrt{-g}\sum_{i=2}^{5}\mathcal{L}_i[g_{\mu\nu},\phi] + S_M[g_{\mu\nu}]\,, \tag{10.1}$$

where the four Lagrangian $\mathcal{L}_i$ are defined as

$$\mathcal{L}_2 = G_2[\phi, X]\,, \tag{10.2}$$

$$\mathcal{L}_3 = -G_3[\phi, X]\Box\phi\,, \tag{10.3}$$

$$\mathcal{L}_4 = G_4[\phi, X]R + G_{4X}[\phi, X]\left[(\Box\phi)^2 - \phi_{;\mu\nu}\phi^{;\mu\nu}\right]\,, \tag{10.4}$$

$$\mathcal{L}_5 = G_5[\phi, X]G_{\mu\nu}\phi^{;\mu\nu} - \frac{1}{6}G_{5X}[\phi, X]\left[(\Box\phi)^3 - 3(\Box\phi)\phi_{;\mu\nu}\phi^{;\mu\nu} + 2\phi_{;\mu}{}^{\nu}\phi_{;\nu}{}^{\alpha}\phi_{;\alpha}{}^{\mu}\right]\,, \tag{10.5}$$

where $G_i[\phi, X]$ are four arbitrary functions of a scalar field ϕ and $X = \partial_\mu\phi\partial^\mu\phi$*.

By varying the action (10.1) and imposing the flat FLRW metric, we obtain the energy density and pressure of the scalar field (we define it with the ϕ subscript in order to distinguish it from the one defined in a general EFT, with the subscript d)

$$\begin{aligned}\frac{8\pi G}{3}\rho_\phi = &-\frac{1}{3}G_2 + \frac{2}{3}X\left(G_{2X} - G_{3\phi}\right) - \frac{2H^3\dot{\phi}X}{3}\left(7G_{5X} + 4XG_{5XX}\right)\\ &+ H^2\left[1 - M_\bullet^2\left(1-\alpha_B\right) - 4X\left(G_{4X} - G_{5\phi}\right) - 4X^2\left(2G_{4XX} - G_{5\phi X}\right)\right]\,,\end{aligned} \tag{10.6}$$

* We should be careful about the definition of X. In many articles, X is differently defined, i.e. with a minus sign and/or a 1/2 factor. Moreover, some differences might come from the convention on the signs of the metric, the definition of the time variable (cosmological t/conformal η), since these choices change the explicit expression of $\partial_\mu\phi\partial^\mu\phi = g^{00}\dot{\phi}^2$ (when $\phi = \phi(t/\eta)$ is a function of time only), and the definition of the extrinsic curvature (8.28). Our convention is to use the cosmological time t, $g^{00} < 0$ and a minus sign in the definition of the extrinsic curvature.

$$\frac{8\pi G}{3}P_\phi = \frac{1}{3}G_2 - \frac{2}{3}X\left(G_{3\phi} - 2G_{4\phi\phi}\right) + \frac{4H\dot{\phi}}{3}\left(G_{4\phi} - 2XG_{4\phi X} + XG_{5\phi\phi}\right) - \frac{\ddot{\phi}}{3\dot{\phi}}HM_\bullet^2\alpha_B - \frac{4}{3}H^2X^2G_{5\phi X} - \left(H^2 + \frac{2\dot{H}}{3}\right)\left(1 - M_\bullet^2\right) + \frac{2H^3\dot{\phi}}{3}XG_{5X}\,. \tag{10.7}$$

We recall the α-functions

(i) the *cosmological strength of gravity*

$$M_\bullet^2 \equiv 2\left[G_4 - 2XG_{4X} + XG_{5\phi} - H\dot{\phi}XG_{5X}\right]. \tag{10.8}$$

and its derivative

$$\alpha_M \equiv \frac{d\,\ln\,M_\bullet^2}{d\,\ln\,a} = \frac{1}{H}\frac{d\,\ln\,M_\bullet^2}{dt}\,; \tag{10.9}$$

(ii) the *kineticity*

$$H^2M_\bullet^2\alpha_K \equiv 2X\left[G_{2X} + 2XG_{2XX} - 2G_{3\phi} - 2XG_{3\phi X}\right] + 12H\dot{\phi}X\left[G_{3X} + XG_{3XX} - 3G_{4\phi X} - 2XG_{4\phi XX}\right] + 12H^2X\left[G_{4X} - G_{5\phi} + X\left(8G_{4XX} - 5G_{5\phi X}\right) + 2X^2\left(2G_{4XXX} - G_{5\phi XX}\right)\right] + 4H^3\dot{\phi}X\left[3G_{5X} + 7XG_{5XX} + 2X^2G_{5XXX}\right]\,; \tag{10.10}$$

(iii) the *braiding*

$$HM_\bullet^2\alpha_B \equiv 2\dot{\phi}\left[XG_{3X} - 2G_{4\phi} - 2XG_{4\phi X}\right] + 8HX\left[G_{4X} + 2XG_{4XX} - G_{5\phi} - XG_{5\phi X}\right] + 2H^2\dot{\phi}X\left[3G_{5X} + 2XG_{5XX}\right]\,; \tag{10.11}$$

(iv) the *tensor excess*

$$M_\bullet^2\alpha_T \equiv 4X\left[G_{4X} - G_{5\phi}\right] - 2\left[\ddot{\phi} - H\dot{\phi}\right]XG_{5X}\,. \tag{10.12}$$

We can also define the state parameter ω_ϕ for the scalar field with the usual definition

$$\omega_\phi = \frac{\rho_\phi}{P_\phi}\,. \tag{10.13}$$

10.1.1 Stability

The stability conditions are

$$Q_s \equiv \frac{2M_\bullet^2D}{(2-\alpha_B)^2} > 0\,, \tag{10.14}$$

$$c_s^2 \equiv \frac{1}{D}\left[(2-\alpha_B)\left(-\frac{\dot{H}}{H^2} + \frac{1}{2}\alpha_B\left(1+\alpha_T\right) + \alpha_M - \alpha_T\right) - \frac{(\rho_m + P_m)}{H^2M_*^2} + \frac{\dot{\alpha_B}}{H}\right] > 0\,, \tag{10.15}$$

$$Q_T \equiv \frac{M_\bullet^2}{8} > 0\,, \tag{10.16}$$

$$c_T^2 \equiv 1 + \alpha_T > 0\,, \tag{10.17}$$

where ρ_m and P_m are respectively the energy density and the pressure of all matter (radiation, baryons, etc) without the scalar field contribution, and $D \equiv \alpha_K + 3\alpha_B^2/2$.

10.2 Top-down construction

In the previous section, we defined the Horndeski theory covariant action, in the sense of the scheme in Figure 8.3. In this section, we show the top-down approach to find the expression of the EFT functions appearing in the action (8.81) in terms of the functions appearing in the covariant action (10.1), i.e. the G_i and the α functions. After defining the mapping, we are able to write the effective Lagrangian.

Mapping with G_i functions

The derivation of the mapping is a standard exercise that can be found in several articles [70, 76], thus we only show the main results. The EFT functions are given by

$$
\begin{aligned}
M_*^2 f &= 2G_4 - G_{5\phi}\dot{\phi}^2 + 2G_{5X}\dot{\phi}^2\ddot{\phi}\,, && (10.18)\\
\Lambda &= XG_{2X} - G_2 + \dot{\phi}^2(\ddot{\phi} + 3H\dot{\phi})G_{3X} + \dot{\mathcal{F}}_4/2 + 3H\dot{X}G_{4X} - 18H^2G_{4X}\dot{\phi}^2\\
&\quad +6HG_{4\phi X}\dot{\phi}^3 + 12H^2G_{4XX}\dot{\phi}^4 + \dot{\mathcal{F}}_5/2 + 3M_*^2H^2 f_5 + 3M_*^2H\dot{f}_5/2\\
&\quad -6H^2G_{5\phi}\dot{\phi}^2 - 7H^3G_{5X}\dot{\phi}^3 + 3H^2G_{5\phi X}\dot{\phi}^4 + 2H^3G_{5XX}\dot{\phi}^5\,, && (10.19)\\
c &= XG_{2X} + \dot{\phi}^2(-\ddot{\phi} + 3H\dot{\phi})G_{3X} + \dot{\phi}^2G_{3\phi} - \dot{\mathcal{F}}_4/2 + 3H\dot{X}G_{4X}\\
&\quad -6H^2G_{4X}\dot{\phi}^2 + 6HG_{4\phi X}\dot{\phi}^3 + 12H^2G_{4XX}\dot{\phi}^4 - \dot{\mathcal{F}}_5/2 + 3M_*^2H\dot{f}_5/2\\
&\quad -3H^2G_{5\phi}\dot{\phi}^2 - 3H^3G_{5X}\dot{\phi}^3 + 3H^2G_{5\phi X}\dot{\phi}^4 + 2H^3G_{5XX}\dot{\phi}^5\,, && (10.20)\\
M_2^4 &= X^2G_{2XX} + (\ddot{\phi} + 3H\dot{\phi})G_{3X}\dot{\phi}^2/2 - 3HG_{3XX}\dot{\phi}^5 - G_{3\phi X}\dot{\phi}^4/2\\
&\quad +\dot{\mathcal{F}}_4/4 - 3H\dot{X}G_{4X}/2 + 6HG_{4\phi X}\dot{\phi}^3 + 18H^2G_{4XX}\dot{\phi}^4 - 6HG_{4\phi XX}\dot{\phi}^5\\
&\quad -12H^2G_{4XXX}\dot{\phi}^6 + \dot{\mathcal{F}}_5/4 - 3M_*^2H\dot{f}_5/4 - 3H^3G_{5X}\dot{\phi}^3/2\\
&\quad +6H^2G_{5\phi X}\dot{\phi}^4 + 6H^3G_{5XX}\dot{\phi}^5 - 3H^2G_{5\phi XX}\dot{\phi}^6 - 2H^3G_{5XXX}\dot{\phi}^7, && (10.21)\\
m_3^3 &= 2G_{3X}\dot{\phi}^3 + 2\dot{X}G_{4X} - 8HG_{4X}\dot{\phi}^2 + 4G_{4\phi X}\dot{\phi}^3 + 16HG_{4XX}\dot{\phi}^4\\
&\quad +M_*^2\dot{f}_5 - 4HG_{5\phi}\dot{\phi}^2 - 6H^2G_{5X}\dot{\phi}^3 + 4HG_{5\phi X}\dot{\phi}^4 + 4H^2G_{5XX}\dot{\phi}^5, && (10.22)\\
m_4^2 = \tilde{m}_4^2 &= 2G_{4X}\dot{\phi}^2 + G_{5\phi}\dot{\phi}^2 + HG_{5X}\dot{\phi}^3 - G_{5X}\dot{\phi}^2\ddot{\phi}\,, && (10.23)
\end{aligned}
$$

where

$$
\begin{aligned}
\mathcal{F}_4 &= 2\dot{X}G_{4X} - 8HG_{4X}\dot{\phi}^2\,, && (10.24)\\
\mathcal{F}_5 &= 2M_*^2Hf_5 + M_*^2\dot{f}_5 - 2HG_{5\phi}\dot{\phi}^2 - 2H^2G_{5X}\dot{\phi}^3\,, && (10.25)\\
M_*^2 f_5 &= -G_{5\phi}\dot{\phi}^2 + 2G_{5X}\dot{\phi}^2\ddot{\phi}\,. && (10.26)
\end{aligned}
$$

All the other functions are null. Once we solve the Klein-Gordon equation for the field $\phi(t) = \phi_0(t)$ (in unitary gauge $\delta\phi(t,\vec{x}) = 0$), we have all the ingredient we need to write all the EFT functions. Since the link between the EFT Lagrangians with and without the Goldstone boson π is known and functionally independent of the form of the covariant action (see Figure 8.3), we also have the expression of the perturbation equations for the scalar degree of freedom. The perturbation equations are shown in section 8.6.

Mapping with the α-functions

The (inverse) mapping with the α functions is given by the following prescriptions [77, 38]

$$M_\bullet^2 = M_*^2 f + 2m_4^2\,, \tag{10.27}$$

$$\alpha_M = \frac{M_*^2\dot{f} + 2\dot{m}_4^2}{H(M_*^2 f + 2m_4^2)}\,, \tag{10.28}$$

$$\alpha_B = \frac{m_3^3 - M_*^2\dot{f}}{H(M_*^2 f + 2m_4^2)}\,, \tag{10.29}$$

$$\alpha_K = \frac{2c + 4M_2^4}{H^2(M_*^2 f + 2m_4^2)}, \tag{10.30}$$

$$\alpha_T = -\frac{2m_4^2}{M_*^2 f + 2m_4^2}. \tag{10.31}$$

Using this mapping, we can rewrite the term of the c_s^2 equation in Horndeski theory (10.15) that contains matter (the one proportional to $\rho_m + P_m$) in terms of the EFT functions. Adding this result to the EFT c_s^2 without matter in equation (9.100), we obtain the c_s^2 written with the EFT functions containing the matter contribution, equation (9.104).

10.3 An example with dark matter

In this part, we consider a specific sector of Horndeski gravity as an example. The model was studied for its useful properties in modeling neutron stars [78, 79]. Recently an analysis on the background level was carried on by M. Rinaldi [13], showing the possibility in this theory for the scalar field ϕ to mimic the dark matter. Unfortunately, we will show that the model is unavoidably unstable in the first-order perturbations sector [10]. However, we can still use this model as a simple example (as we will see, an analytical solution for the evolution of the scalar field is available) for the background compatibility of the effective Lagrangian and the covariant one. Moreover, since this model mimics dark matter instead of dark energy, we can appreciate the versatility of the effective field theory for describing different phenomena. We will compare the EFT results with the covariant results, computed with the Boltzmann solver `hi_class` [80], a modification of `CLASS` [81, 82] which includes also the possibility to solve for the evolution of a Horndeski model.

10.3.1 Action and analytical results

The action of the model considered is

$$S[g_{\mu\nu}, \phi] = \int d^4x\sqrt{-g}\left[\frac{M_{\rm Pl}^2}{2}(R - 2\Lambda) - \frac{1}{2}(\alpha g_{\mu\nu} - \xi G_{\mu\nu})\nabla^\mu\phi\nabla^\nu\phi\right] + S_m[g_{\mu\nu}], \tag{10.32}$$

where α and ξ are the two parameters of the theory, and the reduced Planck mass is $M_{\rm Pl}^2 = 1/8\pi G$. In the article [13], the ξ is defined as η. We consider ϕ as the field which mimics dark matter. The dark energy is therefore a term independent of the scalar field ϕ, and we include it in the S_M part of the action in the form of the cosmological constant Λ. Note that the Lagrangian is independent from the scalar field $\phi(t)$, but not on its derivative. Therefore the model is shift-symmetric, i.e., it is invariant under any transformation $\phi(x^\mu) \to \phi(x^\mu)+$ constant. Numerically this means that the value of the initial condition for ϕ does not influence the evolution.

The equations of motion obtained varying this action are

$$G_{\mu\nu} + \Lambda g_{\mu\nu} + H_{\mu\nu} = \frac{1}{M_{\rm Pl}^2}T_{\mu\nu}, \tag{10.33}$$

which are the Einstein equations of the General Relativity with an additional term $H_{\mu\nu}$. Without going into the details of the form of $H_{\mu\nu}$, which is explicited in [13], we note that $H_{\mu\nu}$ must depend only on the derivatives of ϕ since the model is shift-symmetric.

From the equations of motion (10.33) we find an analytical result for the evolution of the field

$$\dot{\phi} \equiv \psi = \frac{q}{a^3(\alpha + 3\xi H^2)}, \tag{10.34}$$

where q is an integration constant. We can neglect the value of ϕ, since the model is shift symmetric. We can also find the equation for the fractional density

$$\Omega_\phi = \frac{1}{6M_{\rm Pl}^2}\frac{q^2(\alpha+9\xi H^2)}{H^2a^6(\alpha+3\xi H^2)^2}\,. \tag{10.35}$$

Finally, we define a new parameter

$$\beta = \xi\Lambda\,. \tag{10.36}$$

This is the parameter we will consider in the numerical evaluations since is on the order of 1 when we want to model dark matter with the scalar field ϕ.

G_i functions

Some steps are required to find the G_5 function from the action (10.32). In fact, we want the $G_{\mu\nu}$ term in our action in a form similar to the one in the Horndeski action (10.1). This can be done integrating by parts the term as follows

$$\begin{aligned}\int d^4x\sqrt{-g}\frac{1}{2}\xi G_{\mu\nu}\nabla^\mu\phi\nabla^\nu\phi &= -\int d^4x\phi(\nabla^\mu\phi)\frac{1}{2}\xi\nabla^\nu\left[\sqrt{-g}G_{\mu\nu}\right] - \int d^4x\sqrt{-g}\frac{1}{2}\xi\phi G_{\mu\nu}(\nabla^\nu\nabla^\mu\phi)\\ &\quad+\cancel{\int d^4x\nabla^\nu\left[\sqrt{-g}\frac{1}{2}\xi G_{\mu\nu}(\nabla^\mu\phi)\phi\right]}\\ &= -\int d^4x\phi(\nabla^\mu\phi)\frac{1}{2}\xi\sqrt{-g}\cancel{(\nabla^\nu G_{\mu\nu})} - \int d^4x\phi(\nabla^\mu\phi)\frac{1}{2}\xi\cancel{(\nabla^\nu\sqrt{-g})}G_{\mu\nu}\\ &\quad-\int d^4x\sqrt{-g}\frac{1}{2}\xi\phi G_{\mu\nu}(\nabla^\nu\nabla^\mu\phi)\\ &= -\int d^4x\sqrt{-g}\frac{1}{2}\xi\phi G_{\mu\nu}(\nabla^\nu\nabla^\mu\phi)\,.\end{aligned} \tag{10.37}$$

where in the first equality we neglect the border term because the action is defined up to a constant (the equations of motion are obtained varying the action), and in the second equality we consider the fact that the metric and the Einstein tensor are divergence free.

Finally, comparing the definition of the Horndeski gravity action (10.1), our model action (10.32) and the last result (10.37), we can find the G_i functions

$$G_2[\phi,X] = -\Lambda+\frac{\alpha X}{M_{\rm Pl}^2}\,,\qquad G_3[\phi,X] = 0\,,\qquad G_4[\phi,X]=\frac{1}{2}\,,\qquad G_5[\phi,X] = -\frac{\xi\phi}{2M_{\rm Pl}^2}\,. \tag{10.38}$$

α functions

Using the G_i functions (10.38) and the equations for the α functions (10.8)-(10.12), we also show the α functions for our model

$$M_\bullet^2 = 1-\frac{\xi X}{M_{\rm Pl}^2}\,, \tag{10.39}$$

$$\alpha_M = -\frac{2\xi\psi\dot\psi}{H^2\left(M_{\rm Pl}^2-\xi X\right)}\,, \tag{10.40}$$

$$\alpha_K = \frac{2X\left(\alpha+3\xi H^2\right)}{H^2\left(M_{\rm Pl}^2-\xi X\right)}\,, \tag{10.41}$$

$$\alpha_B = \frac{4\xi X}{M_{\rm Pl}^2-\xi X}\,, \tag{10.42}$$

$$\alpha_T = \frac{2\xi X}{M_{\rm Pl}^2-\xi X} = \frac{1}{2}\alpha_B\,. \tag{10.43}$$

10.3.2 Top-down construction

In this section we will derive all the useful quantities we will need, using the mapping procedure. Using equations (10.18)-(10.26), among with the definition of the G_i functions for our model (10.38), we obtain the EFT functions which depends only on the scale factor a, the field ψ and their derivatives

$$M_*^2 f = \frac{\xi\psi^2}{2M_{\rm Pl}^2}\,, \tag{10.44}$$

$$c = \frac{\xi}{2M_{\rm Pl}^2}\left[\left(3H^2 - 2\dot{H}\right)\psi^2 - H\psi\dot{\psi} - \psi\ddot{\psi} - \dot{\psi}^2\right], \tag{10.45}$$

$$\Lambda = \frac{\xi}{2M_{\rm Pl}^2}\left[\left(2\dot{H} + 9H^2\right)\psi^2 + 7H\psi\dot{\psi} + \psi\ddot{\psi} + \dot{\psi}^2\right], \tag{10.46}$$

$$M_2^4 = \frac{\xi}{4M_{\rm Pl}^2}\left[\left(H\dot{\psi} + \ddot{\psi}\right)\psi + 2\psi^2\dot{H} + \dot{\psi}^2\right], \tag{10.47}$$

$$m_3^3 = \frac{\xi}{M_{\rm Pl}^2}\psi\left(2H\psi + \dot{\psi}\right), \tag{10.48}$$

$$m_4^2 = \tilde{m}_4^2 = -\frac{\xi\psi^2}{2M_{\rm Pl}^2}\,. \tag{10.49}$$

It is straightforward to compute the energy density and the pressure of the scalar field using equations (8.72) and (8.73), obtaining

$$\rho_d = \frac{\psi^2\left(\alpha + 9\xi H^2\right)}{2M_{\rm Pl}^2}\,, \tag{10.50}$$

$$P_d = \frac{\left(\alpha - 2\xi\dot{H} - 3\xi H^2\right)\psi^2 - 4\xi H\psi\dot{\psi}}{2M_{\rm Pl}^2}\,, \tag{10.51}$$

$$\omega_d \equiv \frac{P_d}{\rho_d} = \frac{\psi\left(\alpha - 2\xi\dot{H} - 3\xi H^2\right) - 4\xi H\dot{\psi}}{\psi\left(\alpha + 9\xi H^2\right)}\,. \tag{10.52}$$

Moreover, using the EFT functions expressions and the scalar field evolution equation for this model (10.34), we can also write the expression for the stability functions

$$Q_s = \frac{\psi^2\left(2M_{\rm Pl}^2 - \xi\psi^2\right)\left[3\xi H^2\left(2M_{\rm Pl}^2 + 3\xi\psi^2\right) + \alpha\left(2M_{\rm Pl}^2 - \xi\psi^2\right)\right]}{2M_{\rm Pl}^2 H^2\left(2M_{\rm Pl}^2 - 3\xi\psi^2\right)^2}\,, \tag{10.53}$$

$$\begin{aligned} Q_s c_s^2 = &-\frac{1}{2M_{\rm Pl}^2 H^2\left(2M_{\rm Pl}^2 - 3\xi\psi^2\right)^2}\left\{\left(\xi\psi^2 - 2M_{\rm Pl}^2\right)^2\left[\dot{H}\left(2M_{\rm Pl}^2 - 3\xi\psi^2\right) + M_{\rm Pl}^2(\rho_m + P_m)\right] + \right.\\ &\left. -2\xi H\psi\dot{\psi}\left(4M_{\rm Pl}^4 + 4M_{\rm Pl}^2\xi\psi^2 - 3\xi^2\psi^4\right) + 4\xi^2 H^2\psi^4\left(3\xi\psi^2 - 2M_{\rm Pl}^2\right)\right\}, \end{aligned} \tag{10.54}$$

$$Q_T = \frac{1}{4} - \frac{\xi\psi^2}{8M_{\rm Pl}^2}\,, \tag{10.55}$$

$$c_T^2 = 1 + \frac{2\xi q^2}{2M_{\rm Pl}^2 a^6\left(\alpha + 3\xi H^2\right)^2 - \xi q^2}\,, \tag{10.56}$$

and the form of the fractional density of the scalar field

$$\Omega_d \equiv \frac{\rho_d}{\rho_d + \rho_m} = \frac{\rho_d}{3H^2 M_{\rm Pl}^2} = \frac{q^2\left(\alpha + 9\xi H^2\right)}{6M_{\rm Pl}^2 a^6 H^2\left(\alpha + 3\xi H^2\right)^2}\,. \tag{10.57}$$

10.3.3 Time evolution

Before computing the background evolution, we must solve two problems. The first is related to the Hubble parameter evolution, while the second concerns the value of the integration constant q which appears in the analytical solution of the (background) scalar field (10.34).

Hubble parameter evolution

To obtain the time evolution of the functions above (ρ_d, P_d, c_s^2, ...), i.e. to write these quantities as functions of the scale factor only, we need the value of the Hubble parameter and its derivative as functions of the scale factor. In principle, also the evolution of the background field (from a Klein–Gordon-like equation) is needed. In this case, we have an analytical form for the scalar field, which depends on the Hubble parameter. Therefore, once we find the Hubble parameter evolution, we also obtain the evolution of the scalar field as a function of the scale factor only.

To find the value of the Hubble parameter we can proceed without the need to solve any differential equation. We consider the Friedmann equation (8.74)

$$H^2 = \frac{1}{3}\frac{1}{M_{\rm Pl}^2}\left[\rho_m(a) + \rho_d(a,H)\right] , \tag{10.58}$$

where ρ_d is in equation (10.50), we write explicitly the dependencies of the functions to the scale factor and the Hubble parameter, and we fix the value of the constant $M_*^2 = M_{\rm Pl}^2$. From this point, we consider standard matter (baryionic matter and radiation), among with the contribution coming from the dark energy. The energy density and the pressure of the standard matter are

$$\rho_m = 3M_{\rm Pl}^2 H_0^2\left(\frac{\Omega_b^0}{a^3} + \frac{\Omega_r^0}{a^4} + \Omega_\Lambda^0\right) , \tag{10.59}$$

$$P_m = 3M_{\rm Pl}^2 H_0^2\left(\frac{1}{3}\frac{\Omega_r^0}{a^4} - \Omega_\Lambda^0\right) . \tag{10.60}$$

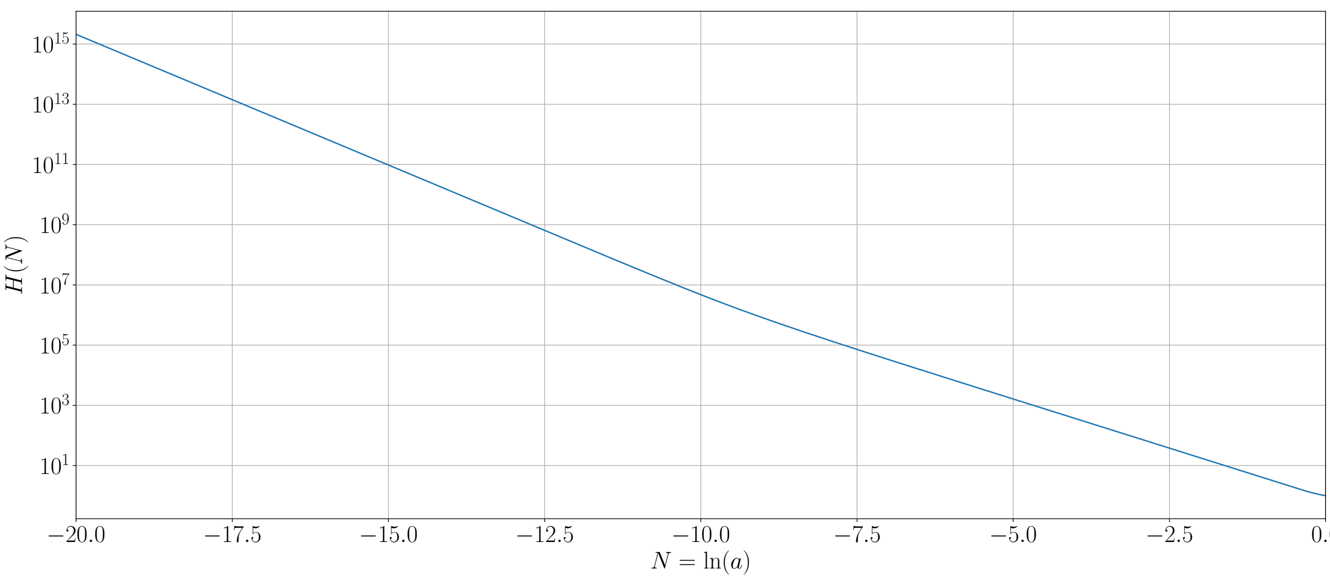


Figure 10.1: Plot of the Hubble parameter H as a function of $N = \ln(a)$, for $\alpha = 1$ and $\beta = 1$. The units are set with $H_0 = 1$ and $M_{\rm Pl}^2 = 1$. The value of q is computed following the prescription explained in the next section.

For numerical computations, we consider $\Omega_r^0 = 8 \times 10^{-5}$, $\Omega_b^0 = 0.2589$ and $\Omega_\Lambda^0 = 0.6911$. Therefore, substituting every occurrence of ψ with equation (10.34), the equation can be solved analytically. We find a very complex expression (that we do not write explicitly) which depends only on the scale factor and the constants of the theory. We plot the result for $\alpha = 1$ and $\beta = 1$ in Figure 10.1.

Moreover, once we have an analytical form of the Hubble parameter, we can also obtain its derivative simply differentiating the $H(a)$ result with respect to the time coordinate t, and substituting every occurrence of $\dot{a}$ with the H result previously found. Another possibility is to use the procedure above again, considering the second Friedmann equation

$$\dot{H} = -\frac{1}{2}\frac{1}{M_{\rm Pl}^2}\left[\rho_m(a) + P_m(a) + \rho_d(a,H) + P_d(a,H,\dot{H})\right] , \tag{10.61}$$

and solving it in order to find $\dot{H} = \dot{H}(a)$. The plot of the (absolute value of the) result found with the latter procedure is in Figure 10.2.

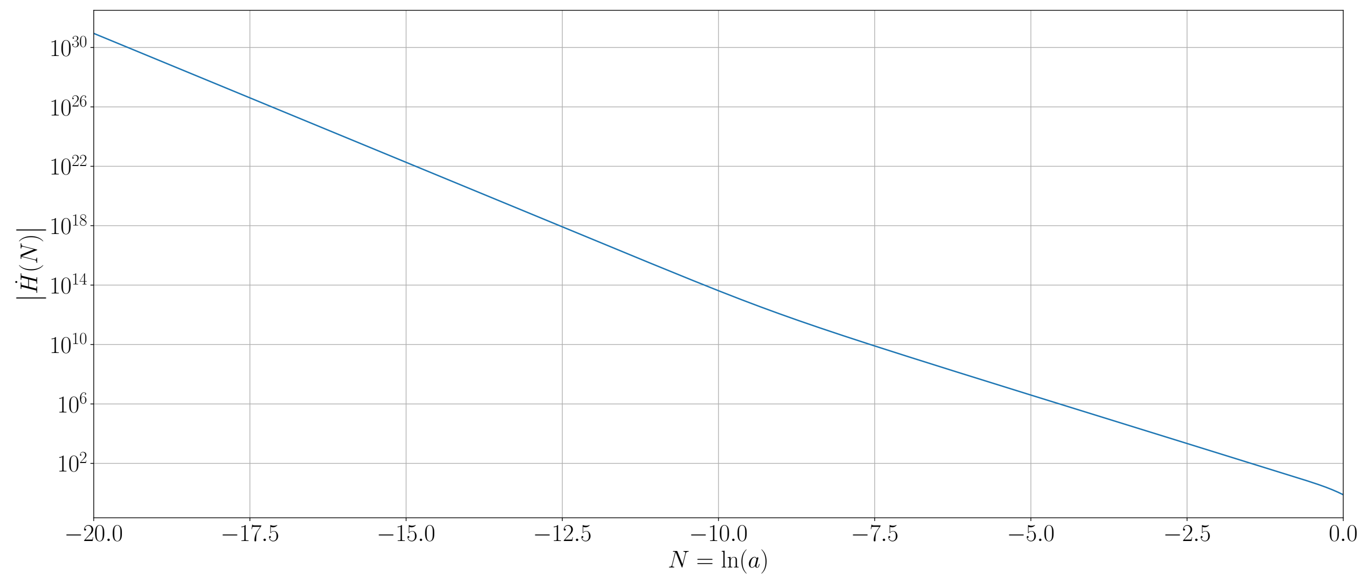


Figure 10.2: Plot of the absolute value of the derivative of the Hubble parameter $\dot{H}$ ($\dot{H} < 0\ \forall N$ in the range considered) as a function of $N =\ln(a)$, for $\alpha = 1$ and $\beta = 1$. The units are set with $H_0 = 1$ and $M_{\rm Pl}^2 = 1$. The value of q is computed following the prescription explained in the next section.

Integration constant value

The analytical result for the scalar field (10.34) contains an integration constant. This comes from solving the Klein–Gordon equation without fixing the initial condition, i.e. the value of the field at some time. We can exploit this freedom on the choice of q, i.e. the freedom to choose the initial condition of a Cauchy problem, to find the initial value of the field which gives the density today predicted by the ΛCDM model.

This procedure can be implemented numerically solving the equation (as a function of the unknown variable q)

$$\Omega_d(a = a_0 = 1) \equiv \Omega_d^0 = \Omega_{\rm cdm}^0(\Lambda{\rm CDM}) , \tag{10.62}$$

where the numerical value we will use for our numerical analysis is $\Omega^0_{\rm cdm} = 1 - \Omega^0_{\rm r} - \Omega^0_{\rm b} - \Omega^0_{\Lambda} \cong 0.2589$. Note that, in principle an analytical solution of the equation above in order to find q might be computable. In practice, the high order of q appearing in the equation make the computation of a solution a very complex procedure.

In Figure 10.3 we show the plot of equation (10.62) as a function of the integration constant q. The values of q we are searching are the ones that makes $\Omega_d^0 = \Omega^0_{\rm cdm}$, i.e. the zeros of the function plotted.

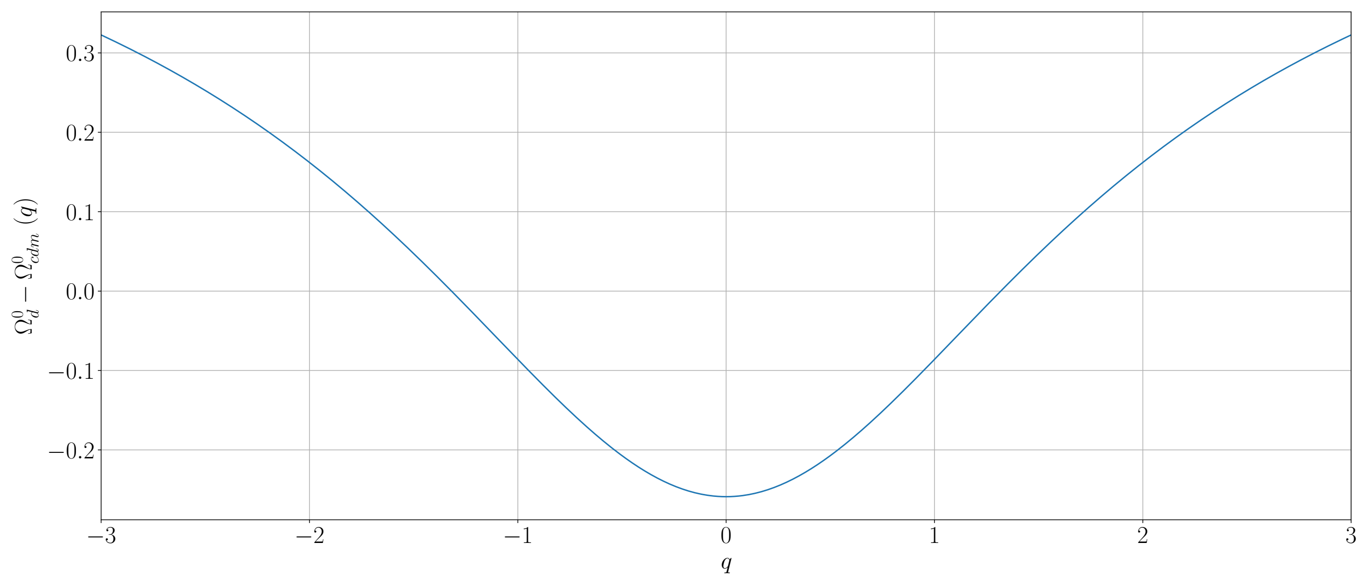


Figure 10.3: Plot of $\Omega_d^0 - \Omega_{\rm cdm}^0$ as a function of the integration constant q, for $\alpha = 1$ and $\beta = 1$. The zeros of this function give the desired q in order to mimic dark matter with the Horndeski model considered.

10.3.4 Results

We can finally compute the evolution (in terms of the scale factor) of the interesting quantities shown above. We compare them with the results found solving numerically the Horndeski theory in its covariant form using the `hi_class` software.

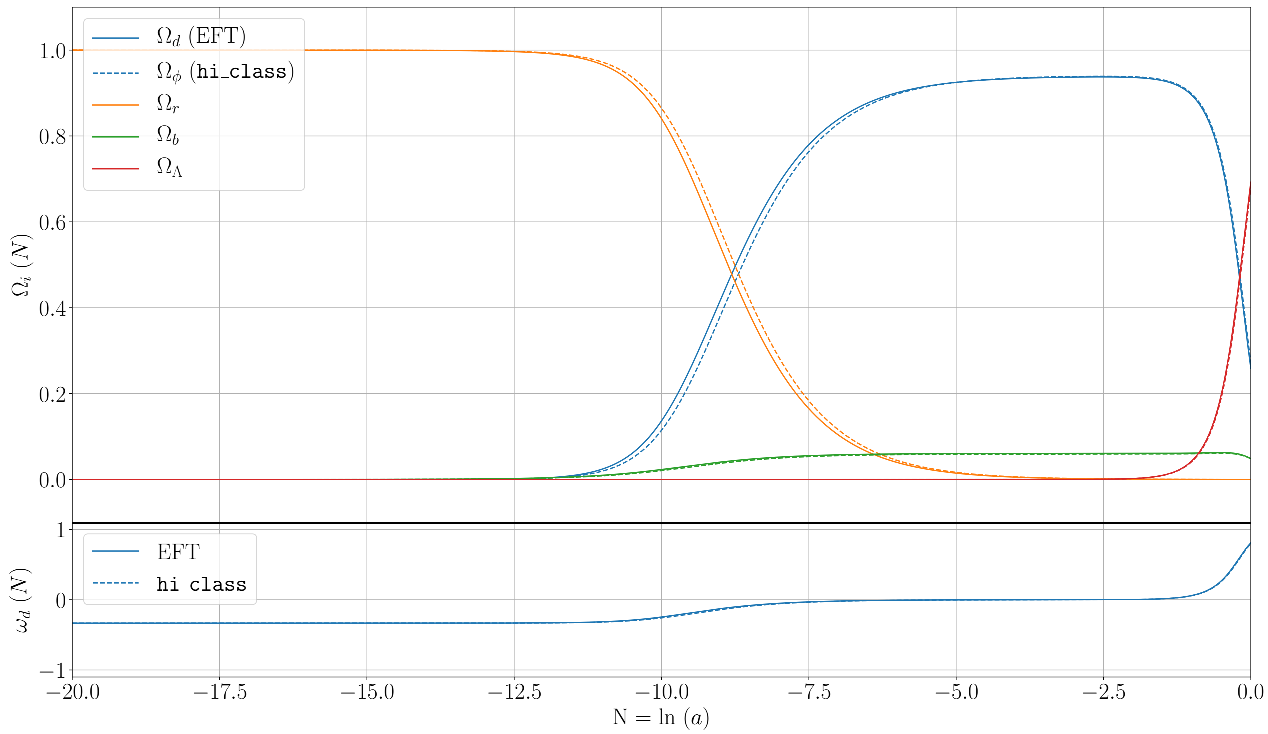


Figure 10.4: Plot of fractional densities Ω of the main components of the matter and the equation of state parameter for the scalar field, in the case $\alpha = \beta = 1$. The continuous lines are the results from the EFT, while the dashed lines come from the equations of motion of the covariant theory. The latter results have been computed using `hi_class`.

The first results are the energy densities evolutions, which we plot in the form of fractional densities

$\Omega_i \equiv \rho_i/\rho_{\rm tot} = \rho_i/3H^2M_{\rm Pl}^2$. We plot both the result from EFT (continuous lines) and the result from the equations of motion in the covariant theory (dashed lines). In Figure 10.4 we show the results for $\alpha = 1$ and $\beta = 1$.

Especially at the matter-radiation equality epoch, there is a discrepancy between the two approaches. This is not unexpected if we consider that our analytical model only considers radiation, baryonic matter, and dark energy (in addition to the scalar field contribution we are computing), while `hi_class` is a full Boltzmann solver which for instance also considers the presence of neutrinos, increasing the radiation energy density. Despite these differences, we obtain a very close match between the results computed with the two different approaches.

We can also plot the stability conditions, which, as already mentioned, determine the stability of a model in the perturbation sector. In Figure 10.5 we plot the functions Q_s, Q_T and c_T^2. They are all always positive, which means at least the tensor sector is stable (free from ghost and gradient instabilities) at first order in the perturbations. The scalar sector, from the fact that $Q_s > 0$, is free from ghost instabilities.

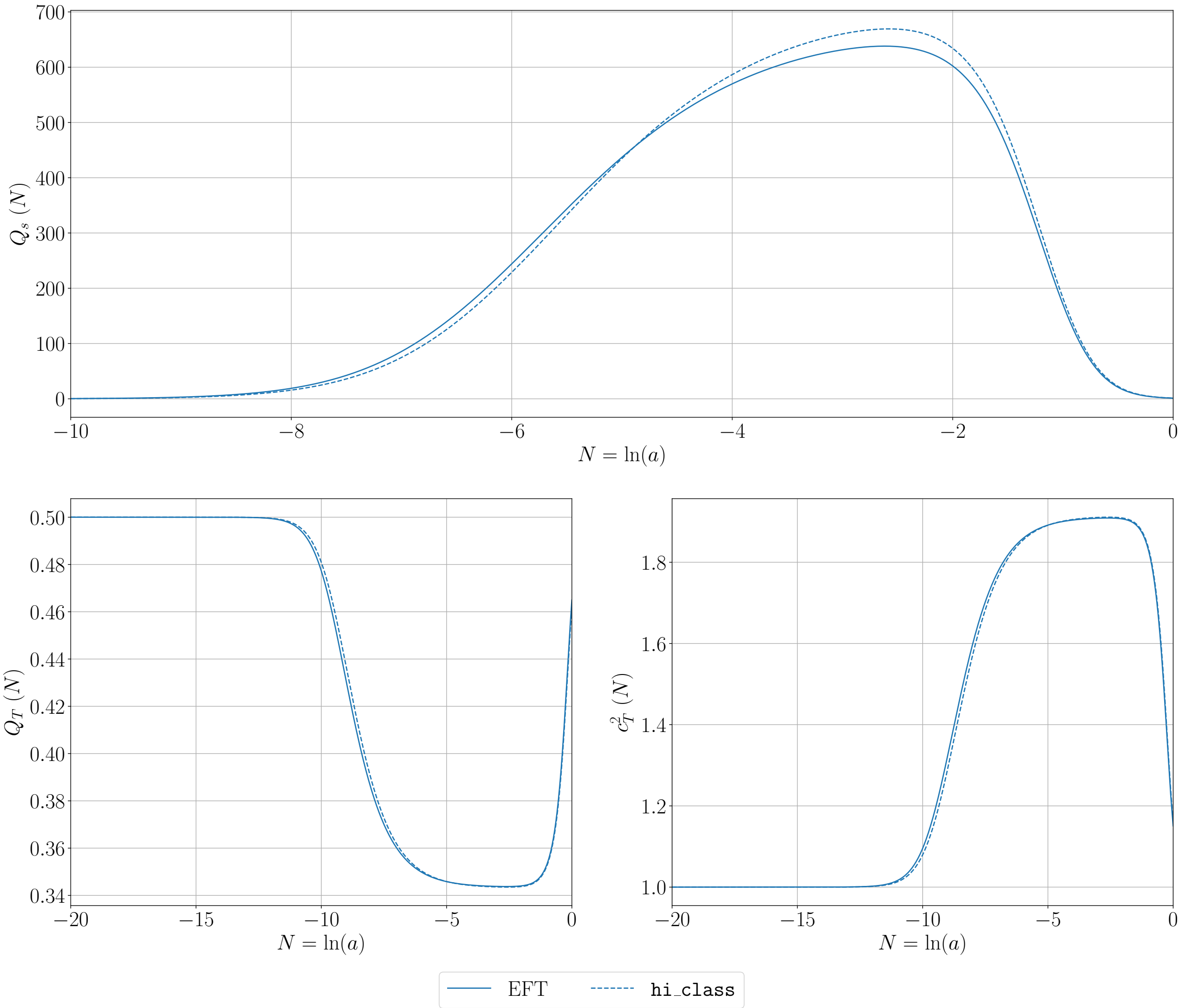


Figure 10.5: Plot of the Q_s, Q_T and c_T^2 stability functions. We can see the concordance between the EFT and the covariant approach, with the exception of some discrepancy that might arise from the fact that we used two different numerical methods (in the EFT case we have solved almost all analytically, with the exception of the value of q).

However, the plot in Figure 10.6 shows a negative c_s^2 at some times. As discussed in 4.2, this might be a source of gradient instabilities. A complete study of the instabilities that might arise from the negative c_s^2 is performed in the next section.

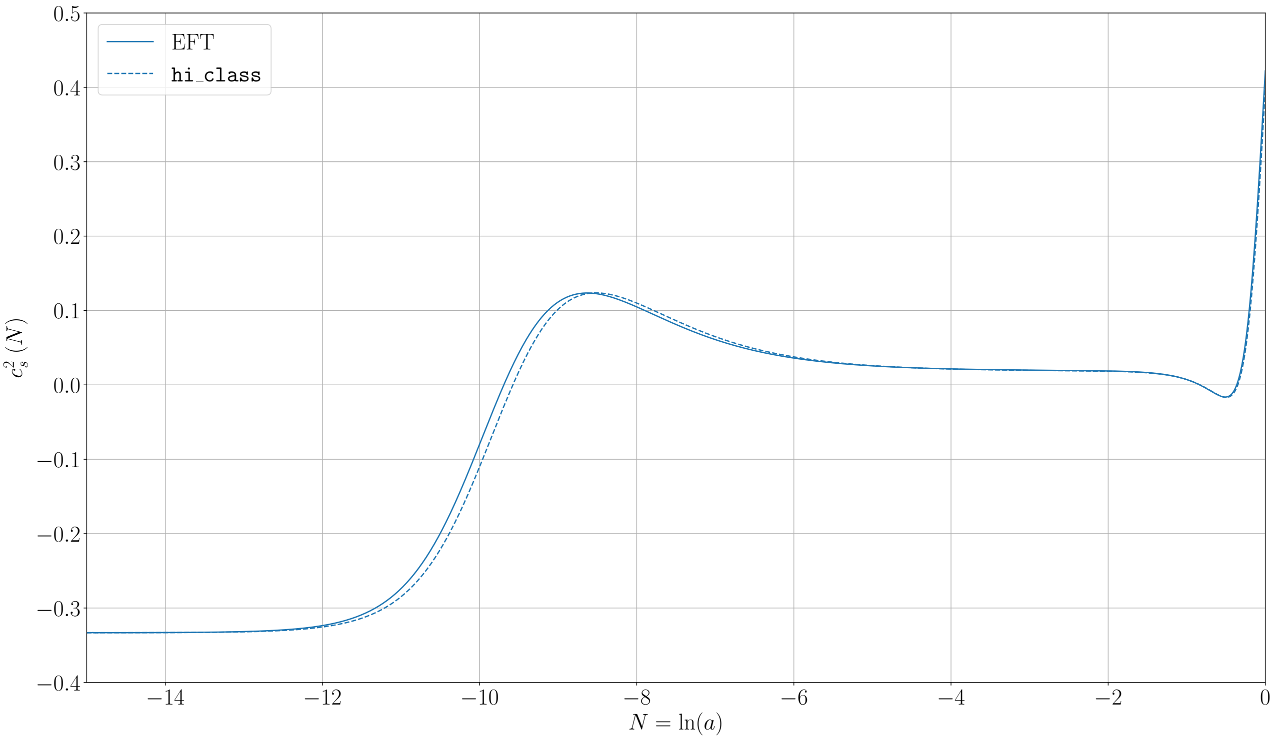


Figure 10.6: Plot of the c_s^2 stability function. Since the c_s^2 depends on $\rho_m + P_m$ in both the EFT and the covariant approaches, the reason for the discrepancy is the same as for the previous plots (see discussion around Figure 10.4).

10.3.5 Instabilities

In this section, we study the scalar gradient instabilities appearing in the model, following the discussion in [10]. In the following, we will consider not only the case when the scalar field simulates the cosmological dark matter fluid but also the case when it is sub-dominant at the background level. All the numerical evaluations are performed with the Boltzmann solver `hi_class`, and the results are checked against another Boltzmann solver `EFTCAMB` [83] (a modified version of `CAMB` [84] which includes EFT equations of motion) to confirm the equivalence of the results also the linear perturbations level.

c_s^2 analysis. From Figure 10.6, we note that the c_s^2 in negative at very early times and near $N \cong 0$. We firstly analyse the more problematic instability at early times. By expanding c_s near $a = 0$ (or $N \to -\infty$) we find

$$c_s^2 = -\frac{1}{3} + \frac{4\Omega_\phi(3\beta + \alpha\Omega_\Lambda^0)^2}{9\beta(\Omega_r^0)^2(9\beta + \alpha\Omega_\Lambda^0)}a^2 - \frac{5\alpha\Omega_\Lambda^0}{6\beta\Omega_r^0}a^4 + \mathcal{O}\left(a^5\right) =$$
$$= -\frac{1}{3} + \frac{2\Omega_\Lambda^0 q^2}{27H_0^2(\Omega_r^0)^2\beta}a^2 - \frac{5\alpha\Omega_\Lambda^0}{6\beta\Omega_r^0}a^4 + \mathcal{O}\left(a^5\right) \,, \tag{10.63}$$

where for simplicity we consider only radiation as matter content, i.e., $H = H_0\sqrt{\Omega_r}/a^2$. The second equality is computed substituting Ω_ϕ with the fractional density equation (10.35). We readily see that c_s^2 is negative at $a = 0$, and therefore it does not satisfy the Horndeski stability condition (10.15) at all times.

In principle, carefully choosing the parameters of (10.63), we can push the negative c_s^2 values in time, until the model is no longer valid as the Universe is in the inflationary phase. As we can see in (10.63), to make the sound speed positive at the beginning of our post-inflationary computation (numerically, we set $a_{\text{start}} = 10^{-14}$) we need the condition $a_{\text{start}}^2 q^2 / H_0^2 \beta \gtrsim 1$, that is

$$\beta \lesssim q^2 10^{-20} \,. \tag{10.64}$$

The integration constant q^2 is usually small because it is directly related to the value of the scalar field at a_{start}, which cannot be too large (otherwise ψ becomes dominant at a_{start}). Therefore we would need a very small β to have a positive c_s^2 and cancel the instability. But β small means that the action (10.32) becomes a Quintessence action with a null potential. This is potentially a problem because the state parameter in a Quintessence model with null potential leads to a ω_ϕ equal to 1 from the beginning of the evolution. This means that the scalar field would be either dominant or, if q is small enough, the scalar field would be not dominant but still have a non-physical value of ω_ϕ if we want to mimic dark matter.

We will further investigate the implications of these results in the next sections. Finally, there is a second instability at recent times (near $N \cong 1$). As we will see below, this instability can also cause instabilities in the perturbations.

Note that the violation of condition (5.27) does not automatically means that the model will be affected by instabilities since the perturbation differential equations stability conditions depend also on other terms, as we will see in equation (10.65).

CMD and matter power spectrum analysis. In the following we show the results of the numerical evaluation. Consider the following situations:

(i) the scalar field accounts for dark matter energy density entirely, i.e. $\alpha \cong \beta \cong 1$. From Figure 10.7, we note that the instability in the matter power spectrum of the matter at almost every scale k of interest.

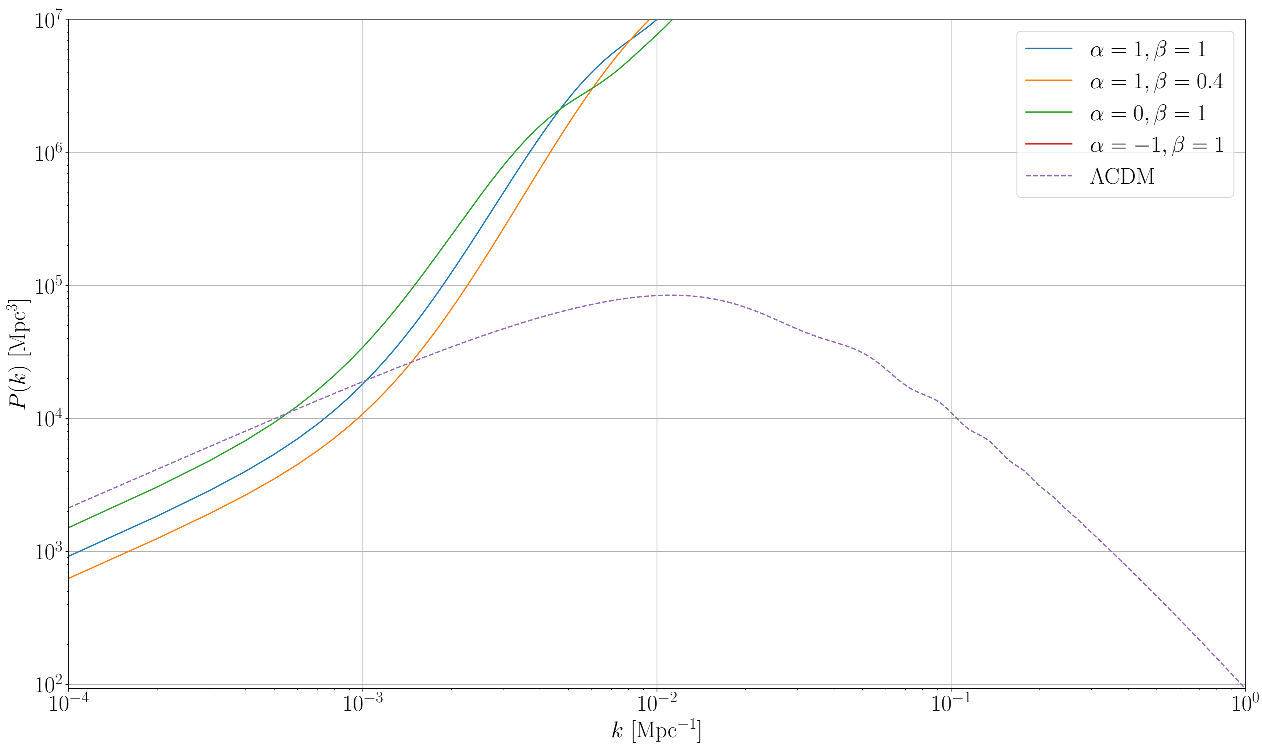


Figure 10.7: Plot of the matter power spectrum in the case (i). The parameters are on the order of the unity, i.e. values for which the scalar field mimics dark matter at the background level.

(ii) $\alpha = 1$, $\beta = 10^{-10}$, and ΛCDM dark matter with $\Omega_{cdm}h^2 = 0.1197$. In this case, the effects of the scalar field should be negligible at the perturbation level. As previously mentioned in the analysis of c_s^2, when β is small, also $\psi \cong 10^{-10}$ should be on the same order of magnitude, otherwise the scalar field will dominate the other components from the beginning. Nevertheless, although the scalar field is sub-dominant, it is enough to cause divergences in the perturbations, as one can see in Figure 10.8 and, to a lesser extent, in Figure 10.9.

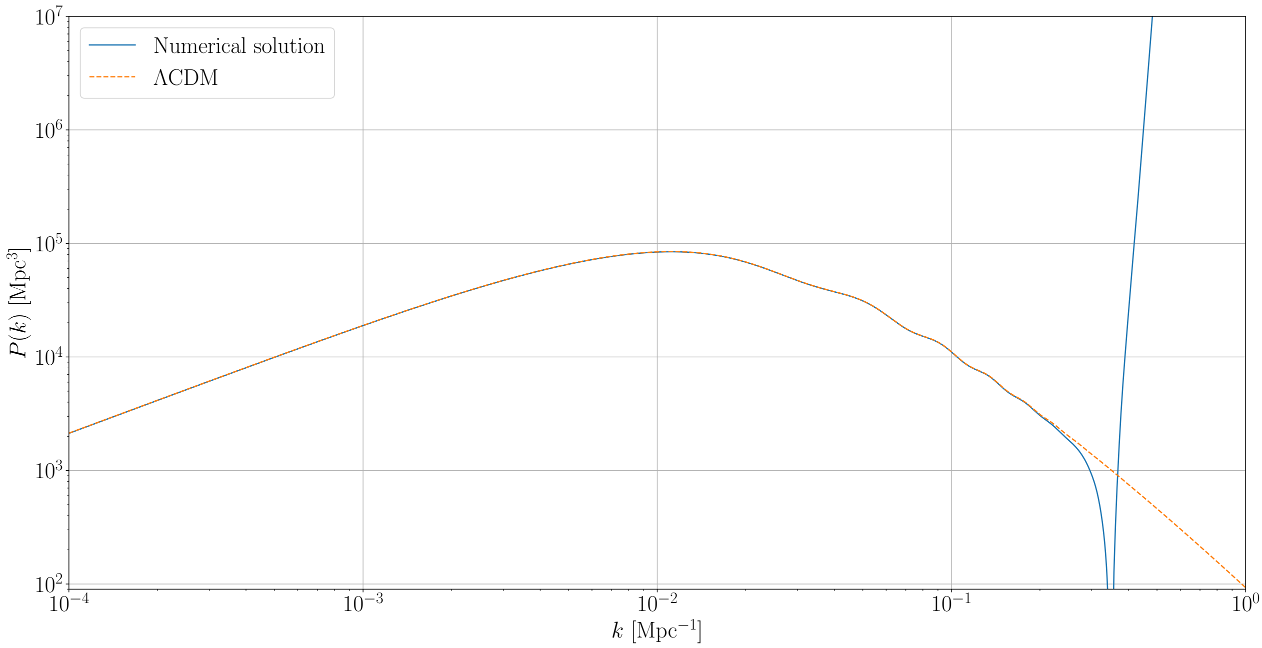


Figure 10.8: Plot of the matter power spectrum in the case (ii) where $\alpha = 1$, $\beta = 10^{-10}$, $\Omega_{cdm}h^2 = 0.1197$ and ϕ modelling dark energy. In this plot the divergence at small scales (large k) is clearly evident.

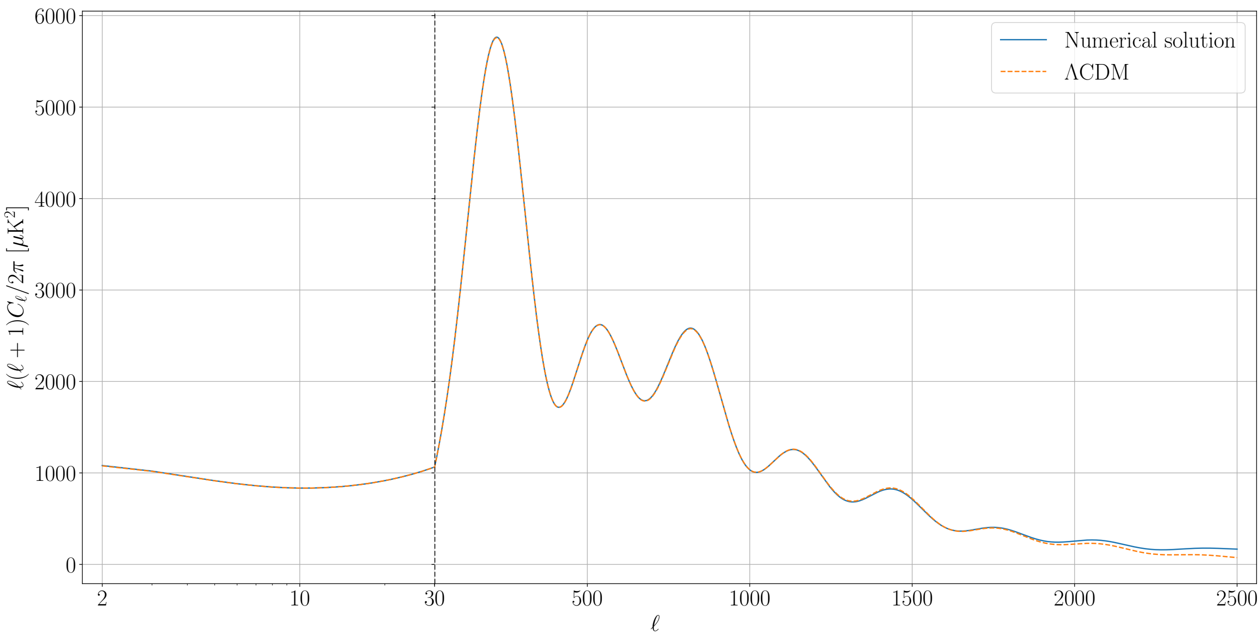


Figure 10.9: Plot of the CMB in the case (ii) where $\alpha = 1$, $\beta = 10^{-10}$, $\Omega_{cdm}h^2 = 0.1197$ and ψ is modelling dark energy. We plot the non-lensed C_ℓ. In this plot the divergence is not evident, but you can see the slightly difference of the model with respect to ΛCDM at small scales (large ℓ).

(iii) the case $\alpha = 1$ and $\beta = 1$, but with the addition of some cold dark matter. For instance, we consider $\Omega^0_{cdm} = 0.1$. In other words, we assume that the scalar field contributes only partially to the dark matter content of the Universe. The background evolution is shown in Fig. 10.10. Also in this case divergences appear at small scales, see Fig. 10.11.

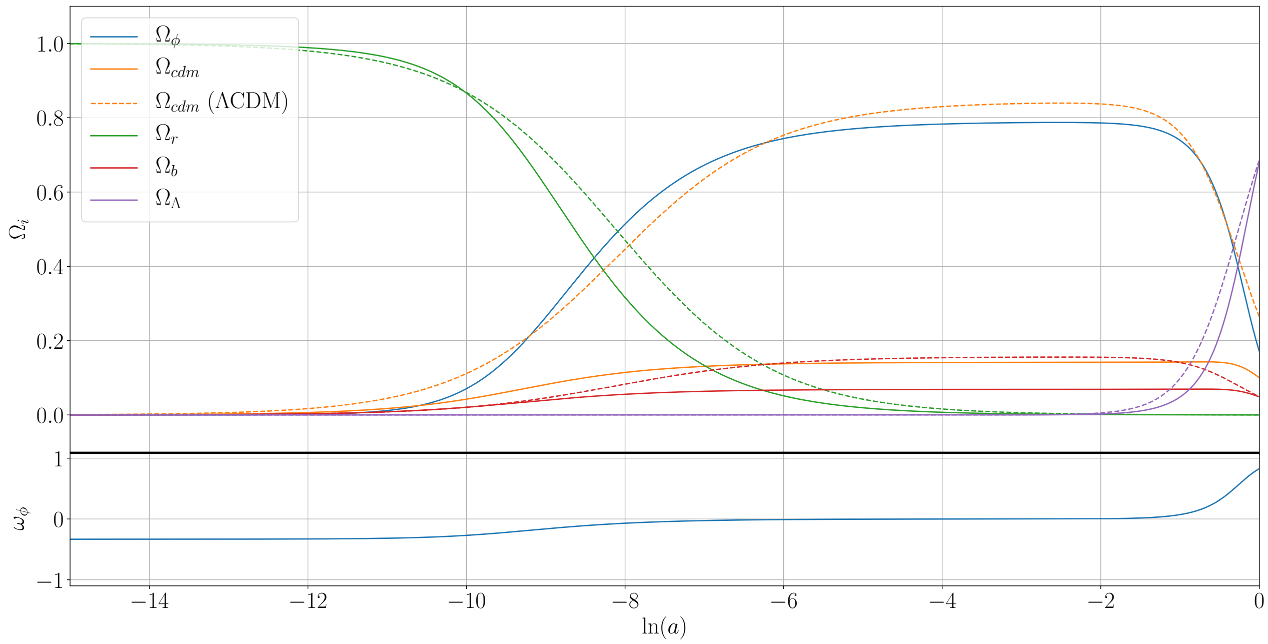


Figure 10.10: Plot of the background in the case (iii) where $\Omega^0_{cdm} = 0.1$. The dashed lines are the ΛCDM densities. Since the state parameter $\omega_\phi = 0$, the scalar field behaves like the dark matter in the matter domination period, but has smaller fractional densities values with respect to the $\Omega^0_{cdm} = 0$ case, Figure 10.4, due to the presence of a cold dark matter fraction $\Omega^0_{cdm} = 0.1$.

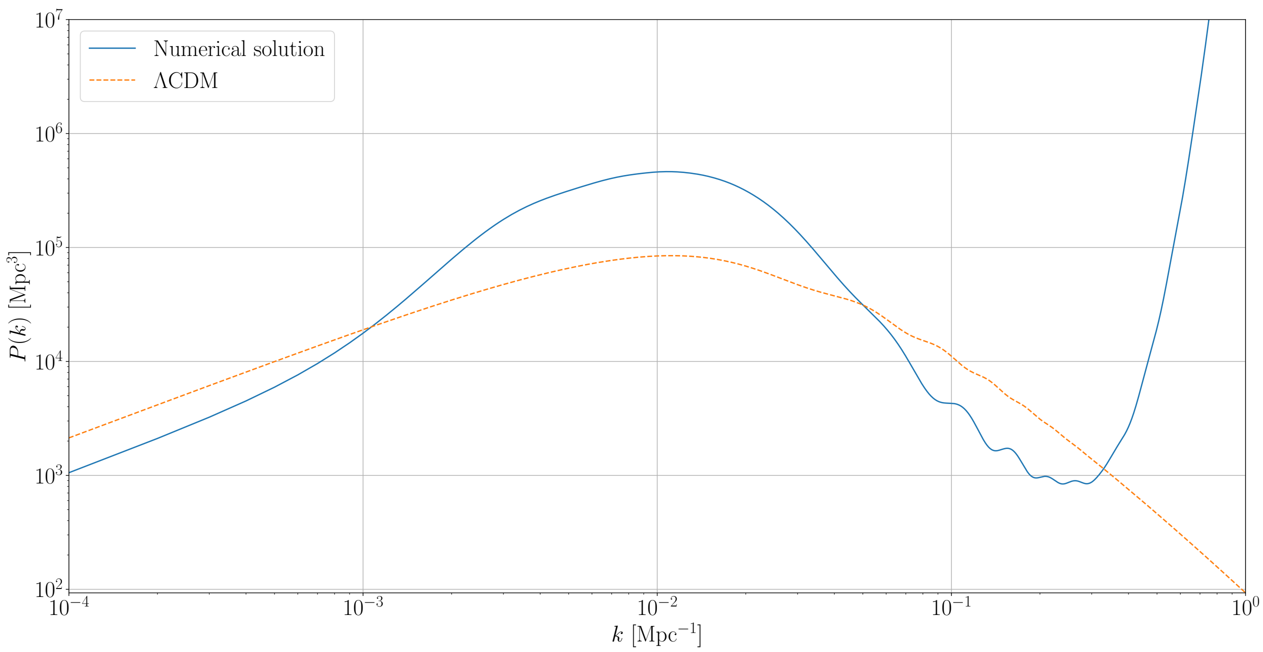


Figure 10.11: Plot of matter power spectrum in the case (iii) where $\Omega^0_{cdm} = 0.1$.

Analysis of divergences. The instabilities can be partly explained by the fact that the sound speed c_s^2 is negative at early times. Consider the differential equation for the scalar field perturbations (A.18) of [80]. In synchronous gauge, it reads

$$\ddot{v}_X + A\dot{v}_X + \frac{2a^2H^2}{2-\alpha_B}\left(\frac{c_s^2k^2}{a^2H^2} - 4\frac{\lambda_8}{D}\right)v_X = F, \tag{10.65}$$

where the α functions of the models are (10.39)–(10.43), the c_s^2 is defined in equation (10.15), k is the perturbation mode wavenumber, $D \equiv \alpha_K + 3\alpha_B^2/2$, and $v_X = \delta\phi/\phi$. The functions A and F depend on the α functions, but the exact form is irrelevant for our purposes. The function λ_8 is given by (A.27) of [80], namely

$$\begin{aligned}\lambda_8 = &-\frac{\lambda_2}{8}\left(D - 3\lambda_2 + \frac{3\dot{\alpha}_B}{aH}\right) + \frac{1}{8}(2-\alpha_B)\left[(3\lambda_2 - D)\frac{\dot{H}}{aH^2} - \frac{9\alpha_B\dot{P}_m}{2aH^3M_*^2}\right] - \\ &-\frac{D}{8}(2-\alpha_B)\left[4 + \alpha_M + \frac{2\dot{H}}{aH^2} + \frac{\dot{D}}{aHD}\right].\end{aligned} \tag{10.66}$$

The differential equation (10.65) has harmonic oscillator solutions if the coefficient of the v_X term is positive. Conversely, if the coefficient is negative, we obtain an exponential behaviour. Therefore, the condition $c_s^2 > 0$ is not sufficient to obtain oscillatory solutions. Rather, we must require the whole coefficient of v_X to be positive. We define the coefficient as

$$C_{v_X} = \frac{1}{2-\alpha_B}\left(\frac{c_s^2k^2}{a^2H^2} - 4\frac{\lambda_8}{D}\right), \tag{10.67}$$

and rewrite the condition as $C_{v_X} > 0$. Analogously to the sound speed, we can expand C_{v_X} near $a = 0$, assuming again a radiation dominated Universe. We find

$$\begin{aligned}C_{v_X} &= -1 + \frac{\left(\frac{15\Omega_\phi(3\beta+\alpha\Omega_\Lambda^0)^2}{\beta(9\beta+\alpha\Omega_\Lambda^0)} - \frac{2\Omega_r^0k^2}{H_0^2}\right)}{12\left(\Omega_r^0\right)^2}a^2 + \mathcal{O}\left(a^4\right) \\ &= -1 + \frac{5\Omega_\Lambda^0q^2 - 4\beta\Omega_r^0k^2}{24\beta H_0^2(\Omega_r^0)^2}a^2 + \mathcal{O}\left(a^4\right).\end{aligned} \tag{10.68}$$

For small a, C_{v_X} is negative and this leads to an exponential growth of v_X. To confirm the analysis we plot C_{v_X} in Figure 10.12. Note that the series truncated at the second order (dashed lines) in a is not enough to approximate C_{v_X} (continuous lines) after $a \cong 10^{-5}$.

We can try to fix the instability choosing q and β such that the term proportional to a^2 in the expansion (10.68) is equal or bigger than 1, i.e.

$$\frac{5\Omega_\Lambda^0q^2 - 4\beta\Omega_r^0k^2}{24\beta H_0^2(\Omega_r^0)^2}a^2 \geq 1\,. \tag{10.69}$$

We can translate this into a condition on β

$$\beta \lesssim \frac{5q^2\Omega_\Lambda^0}{24a^{-2}H_0^2(\Omega_r^0)^2 + 4k^2\Omega_r^0}\,. \tag{10.70}$$

Consider again the first case (i) where the scalar field mimics the dark matter (a similar analysis can be carried on in the other two cases (ii) and (iii)). Computing the initial value of the scalar field with `hi_class`, we can compute the maximum value of β allowed in order to avoid instabilities from the condition (10.70). Since the condition explicitly depends on the wavenumbers and on time, in Figure 10.13 we show the results for different k, as a function of the scale factor a.

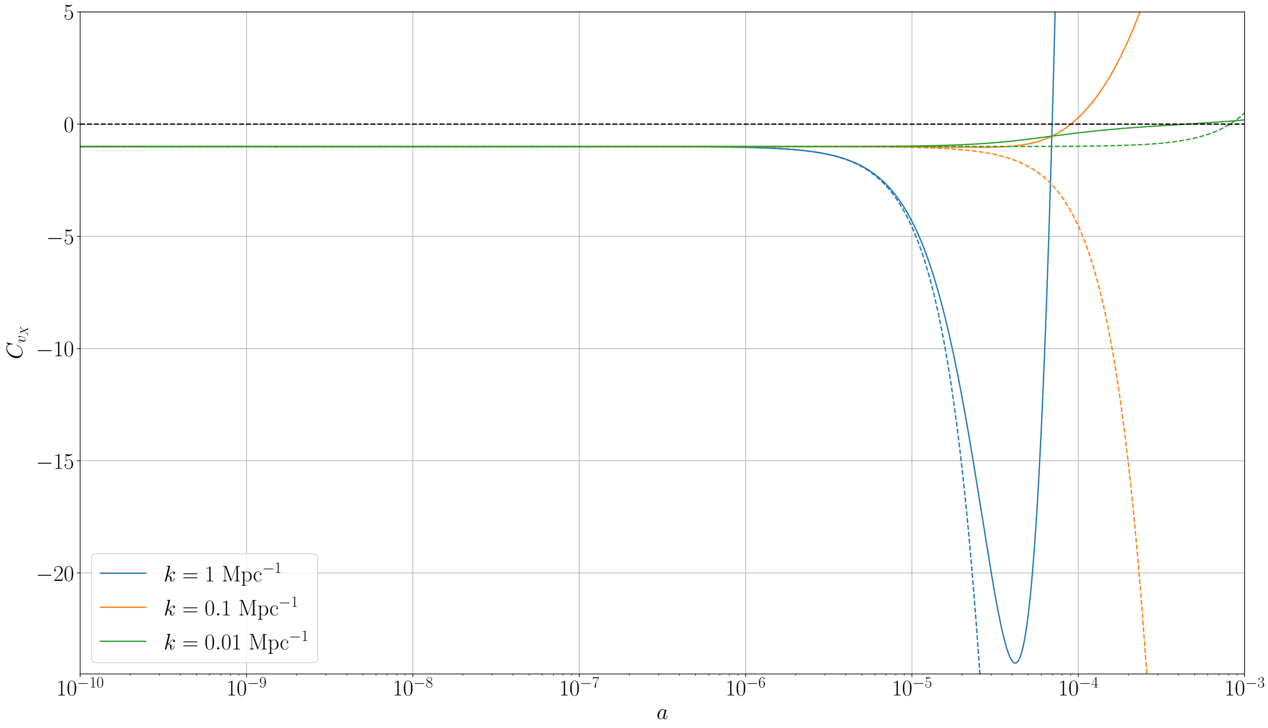


Figure 10.12: Plot of C_{v_X} in the $\alpha = 1$ and $\beta = 1$ case. The continuous lines are the numerical result for C_{v_X}, and the dashed lines are the series truncated at the second order in a^2. We can see that the truncated analytical series is good only for $a < 10^{-5}$. Above the black dashed line, $C_{v_X} > 0$ and the scalar field perturbations differential equation (10.65) has an oscillatory behaviour.

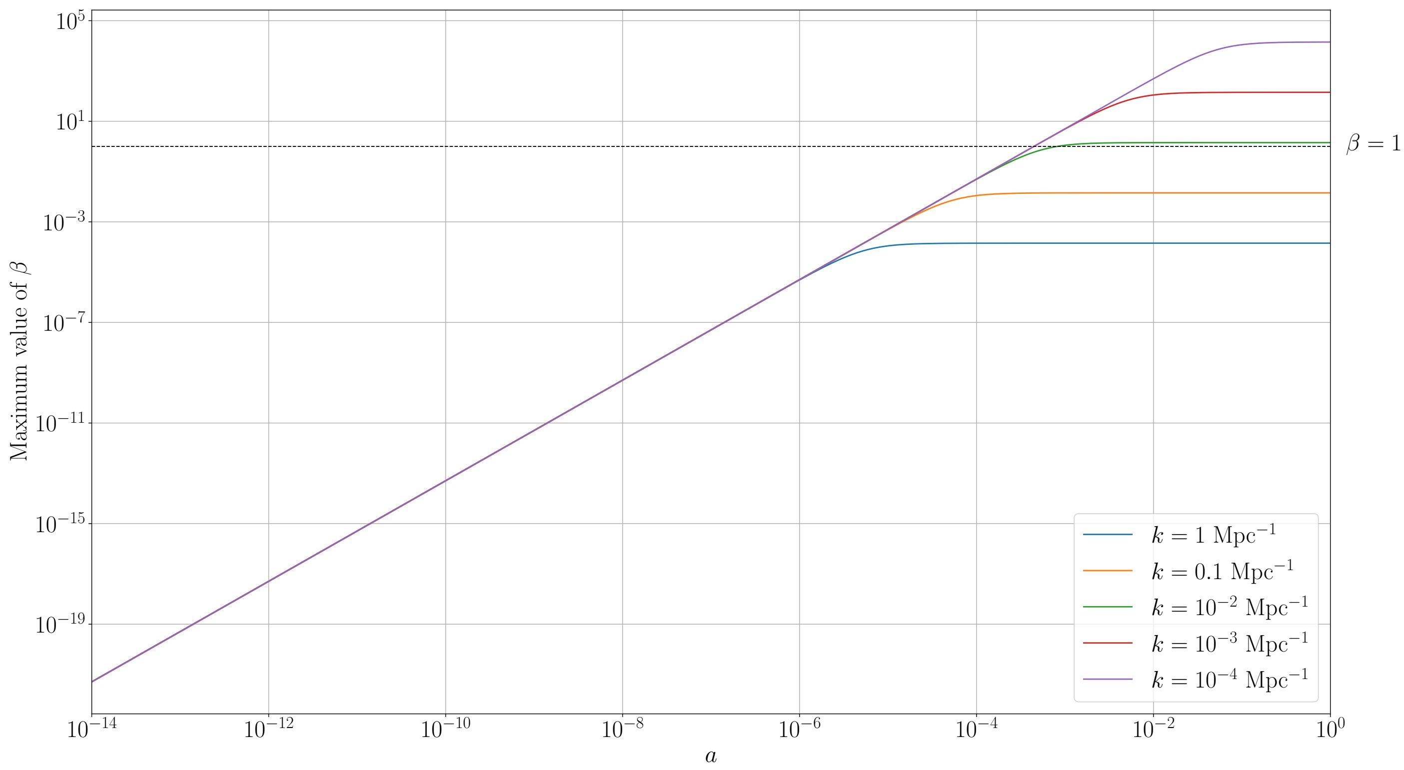


Figure 10.13: Plot of the maximum value of β allowed to avoid large deviations in the CMB and in the matter power spectrum, with $\alpha = 1$ and $\beta = 1$.

To better understand Figure 10.13, we should consider the computation scheme of `CLASS`. The time at which the computation of the perturbations starts depends on the wavenumber k. For large scales (typically $k \lesssim 10^{-2}$ Mpc^{-1}), the computation starts at a conformal time $\eta \cong 5 \times 10^2$ Mpc, that is $a \cong 10^{-5}$. For smaller scales, the computation starts earlier with the earlier time being $\eta \cong 10^2$ Mpc, that is $a \cong 10^{-7}$.

Therefore, for large scales, the β condition (10.70) is not met for a short interval of time. Later on, these scales will inevitably fall in the regime where the condition is satisfied. On the contrary, small scales never satisfy the condition and therefore show exponential growth during the epoch where the scalar field dominates, causing the large deviations that we see in the matter power spectrum in Figure 10.7. Further confirmation of this analysis is the divergence of the matter power spectrum at $k > 10^{-3}$ Mpc^{-1}.

Note that the condition (10.70), and therefore our previous considerations, is only an approximation of the real condition after equality. We computed the condition on β assuming H dominated only by radiation, and this is not true at late times. Moreover, the value of a is not small at late times and therefore higher orders in the series might become non-negligible. This can also be seen in Figure 10.12, where we plotted the truncated analytical series at second order in a from which we have computed the condition on β. In fact, after $a = 10^{-5}$ the truncated analytical series (dashed lines) is not a good approximation of C_{v_X} (continuous lines).

Finally, if we plot the entire numerical evolution of C_{v_X} up to today, where the condition for β (10.70) is not valid any more, we see that modes fall again in the exponential regime (where $C_{v_X} < 0$). If the period where $C_{v_X} < 0$ is long enough, this might introduce additional instabilities even at large scales (small k), and produce divergences at all scales. The period where $C_{v_X} < 0$ depends on the parameter β chosen. This is explicitly shown in Figure 10.14 for two wave-numbers.

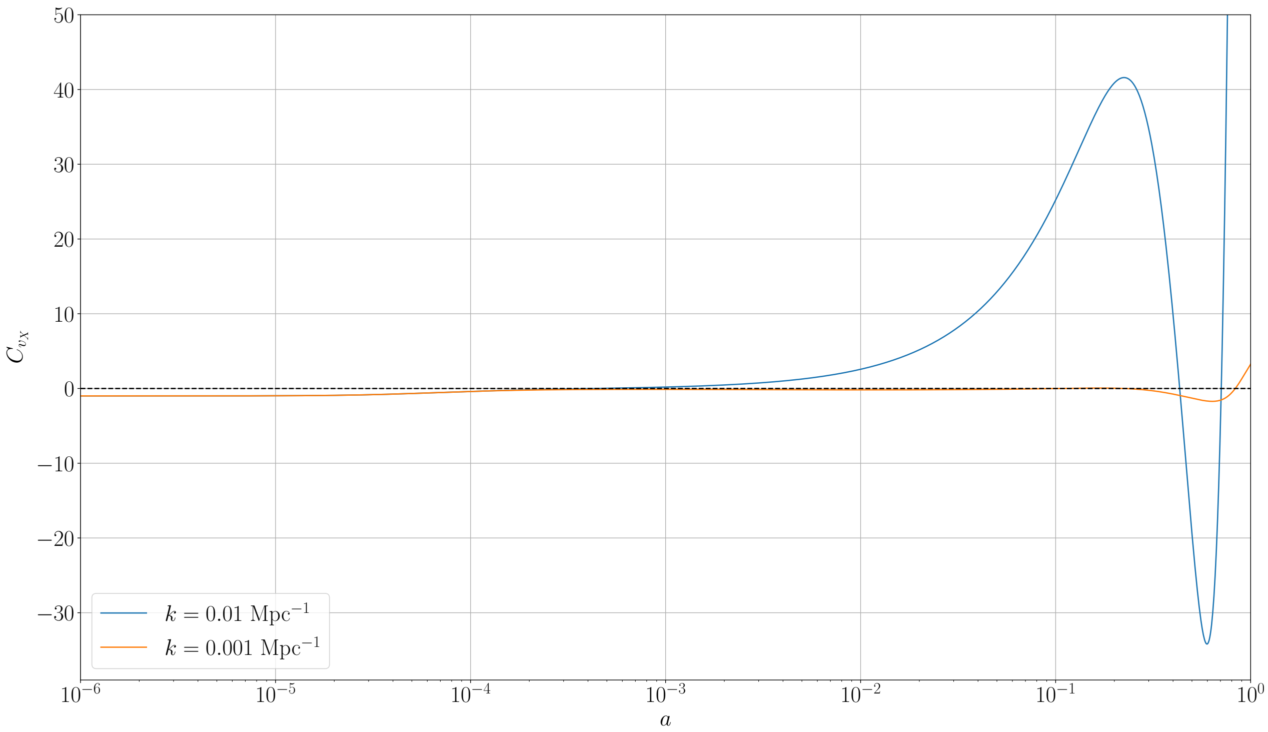


Figure 10.14: Plot of C_{v_X} in the $\alpha = 1$ and $\beta = 1$ case, for two modes. Above the black dashed line, $C_{v_X} > 0$ and the scalar field perturbations differential equation (10.65) solutions have an oscillatory behaviour. The two modes have a second period where $C_{v_X} < 0$ near today. Since this instabilities are well inside the period where `hi_class` evaluates the perturbations, they can be source of instabilities in the perturbation functions.

Finally, note that all the computations performed with `hi_class` have been checked against `EFTCAMB` results, confirming once again the equivalence between the covariant and EFT approaches.

10.3.6 Conclusion

In this section, we studied a Horndeski model that mimics dark matter at the background level. In particular, we show the match between the EFT and the covariant approaches. They describe equivalently the evolution of a single scalar degree of freedom, being it dark matter or dark energy (or both if described by a single scalar field).

Moreover, we analyse the stability of the model. The negative c_s^2 creates gradient instabilities that are confirmed with the computation of the CMB and matter power spectra for different values of the action parameters.

Conclusion

In the thesis, we studied some theoretical and numerical methods in the context of General Relativity and alternative models. Some unknown phenomena, namely dark energy and dark matter, are still under investigation, and additional models might be needed to describe them. Moreover, the increasing amount of data and computational power in the last decades open a new realm of possibilities in the field, from statistical analysis to large numerical simulations.

In the first Part, we briefly introduced some aspects of cosmology and the open questions in General Relativity. A Chapter is dedicated to the Hamiltonian formulation (Arnowitt–Deser–Misner formulation) of General Relativity, which is explained from the basic concepts to the derivation of the equations of motion. The ADM formulation is especially relevant for numerical applications since it effectively split the time contribution from the Einstein equation from the dynamically relevant spatial coordinates. Therefore we can consider time as a label for evolution, similar to the classical Newtonian gravity. This feature can also be exploited in some spacetimes such as FLRW to create an Effective Field Theory for early and late times cosmology, which is the topic of the fourth Part of the thesis.

The second Part is dedicated to the Modified Gravity (MG) models. In the first Chapter we argue that alternative models of gravity might be a solution to dark energy and dark matter effects, and provide some mathematical conditions that should be respected when we propose MG models to avoid solutions' instabilities. In the second Chapter, we consider one of the most famous MG models: Horndeski gravity. Its second-order differential equations are necessary to avoid the mathematical instabilities mentioned above, and it provides an additional degree of freedom that can be used to model dark energy and dark matter. We discuss the constraints on this model coming from the recent observation of the speed of gravitational waves; its possible de Sitter solutions; and an extension of Horndeski which possesses higher order differential equations without creating Ostrogradski instabilities. The last Chapter of this Part is a discussion of a particular mimetic gravity model. We build it from a broken Horndeski gravity action adding a mimetic field, which effectively acts as a Lagrange multiplier on the first Horndeski scalar field. This model perfectly mimics the standard model dark matter effects. We also perform a Bayesian parameter estimation on the action parameters, showing that the model can also be compatible with the gravitational waves speed constraint.

The third Part is about a recently proposed Effective Field Theory (EFT) for cosmological applications. After listing the main EFT rules in the first Chapter, we build the effective Lagrangian in the second Chapter through a time diffeomorphism symmetry breaking, and the main equations. This theory allows for the treatment of perturbations in a model-independent way, since its form is the most general way to write a theory with one additional degree of freedom. Once we analyse and constraint the EFT parameters, we can link any *covariant* model (such as Horndeski gravity) into the EFT. Therefore, we can efficiently constraint any model with one additional degree of freedom without performing a new computation of the perturbation equations. We also provide the ADM formulation version of this EFT, which is used to compute the stability functions mentioned in the third Part. Finally, we provide an example with Horndeski gravity to show the accordance between the results from EFT and the standard covariant approach.

Finally, in the Appendix we present two numerical methods that are used throughout the thesis. The first is a tensor computer algebra software, `xAct`. Especially in the context of Modified Gravity, where the theoretical models might be complicated, this Mathematica add-on is essential to quickly compute not only the full equations of motions written in abstract index notation but also to re-write them in any coordinate system. Moreover, it computes the perturbation equations at any order with a few lines of code. The second Chapter is about Bayesian probability, an alternative to the frequentist approach to statistics. In cosmology, we usually deal with a small amount of data (and we can make experiments only on one possible random realization of the Universe from the predicted power spectrum of the inflationary epoch), and therefore a frequentist approach is not suited for experimental data statistical analysis. On the contrary, the Bayes theorem allows for a careful estimation of theoretical model parameters even with just one data, as we explain in the mimetic gravity example in the second part. This does not mean we obtained the final result, but that we were able to compute a meaningful parameter value estimation while we wait for additional observational data.

Appendix

Appendix A

Tensor Computer Algebra: xAct

In this chapter we introduce the tensor computer algebra Mathematica add-on `xAct` [85], which is freely available on the official website [86] (where the instruction for its installation are also available).

We will show the power of this add-on with an example of great importance in cosmology, the derivation of the equations for linear perturbations in General Relativity, creating an original notebook [87]. In particular, we will use `xPand` [88], an add-on of `xAct`, to find the perturbation equations with standard cosmological metrics. We will confront the results obtained in the Dodelson book [16], and in the Ma–Bertschinger review [74]. Finally, we will sketch the introduction of an additional degree of freedom, with quintessence (scalar field kinetic term and potential) as an example.

Note that the number of available commands of `xAct` is far more vast than the limited subset we will use in this section. In fact, it is possible to show a list of all available commands of an addon with the following Mathematica command. For instance, consider the list of `xTensor` commands.

```
?xAct‘xTensor‘*
```

A.1 Preliminary definitions

Firstly we need to run the add-on in Mathematica. We will start running `xPand`, an add-on of `xAct` to find the perturbation equations with standard cosmological metrics.

```
In[3]:= <<xAct‘xPand‘
```

We can now define the main quantities we need for running `xPand`. Firstly we define the manifold `M` with `DefManifold`. It requires the name of the manifold, the number of dimensions of the manifold (although it is possible to use an unfixed number of dimensions), and the name of the covariant indices.

```
In[4]:= DefManifold[M,4,{a,b,c,d,e}];
```

Then we can define a generic metric with `DefMetric`. The first input is the time-time metric component convention, -1 for negative time. We also need to specify the name of the metric, with the correct indices which have been defined in `DefManifold`. Note the convention on the indices, writing a $-$ we are considering covariant (lower indices), the contrary if we do not write the $-$ (it is not necessary to write $+$ to specify contravariant indices). The other inputs are: the name of the covariant derivative and, within curly brackets, how we want it to be printed in the output. The last optional `PrintAs` can be used to choose how to print the defined object in the output and can be added to almost every defined object in `xAct`.

```
In[5]:= DefMetric[-1,g[-a,-b],CD,{";",∇̄},PrintAs→ḡ];
```

Since xPand is based on ADM decomposition, we should set the slicing based on the metric g we previously defined. This will internally generate all the ADM quantities needed for the computation, in particular the normal vector n (3.5) and the induced metric on the hypersurfaces h (3.15). From Chapter 3 we know that this is sufficient to determine the foliation of spacetime. We should also define a covariant derivative cd on the hypersurfaces, i.e., (3.30) for a vector. Finally we should specify the metric we want to use. For instance, FLFlat for flat FLWR (FLRW metric (1.15) with null spatial curvature k)

$$ds^2 = -dt^2 + a(t)^2 \delta_{ij} dx^i dx^j \, . \tag{A.1}$$

Other options available in xPand are Anisotropic, BianchiB, BianchiA, BianchiI, FLCurved and Minkowski. Note also that, since this add-on is based on ADM formulation, only spacetimes that admit a space-like hypersurfaces foliation can be used. For other metrics, the more general package xPert can be used.

```
In[6]:= SetSlicing[g,n,h,cd,{"|",D̄},"FLFlat"];
```

We also need to specify the metric g perturbed field dg based on the foliation given by h. Similarly, if we also consider matter, we can define its 4-velocity u and perturbation du. The latter function will also create the matter energy density ρ and pressure P, and its perturbations, which can be used to specify the matter content.

```
In[7]:= DefMetricFields[g,dg,h];
        DefMatterFields[u,du,h];
```

Some functions are also usually defined to simplify the call of xPand functions and obtain more readable outputs. For instance

```
In[8]:= MakeBoxes[ϵ,StandardForm]:=
        StyleBox[ToString[$PerturbationParameter],FontColor→RGBColor[0.0, 0.0, 1]]
        MyToxPand[expr_,gauge_,order_]:=ToxPand[expr, dg, u, du, h, gauge, order]
        org[expr_]:=NoScalar@Collect[ContractMetric[expr],
        PerturbationParameter, ToCanonical]
```

A.2 Metric and Gauge Definitions

We now want to set up the perturbations we want to consider. By default, all perturbations (scalar, vector, tensor) are computed. With the following flags, exploiting the perturbation decomposition theorem, we can reduce to the single sectors. We might also want to use cosmological time t instead of conformal time τ. With $ConformalTime = True all the quantities will be written in terms of conformal time quantities. For instance, if we choose the conformal time the Hubble factor will be $\mathcal{H} = a^{-1}\, da/d\tau$ instead of $H = a^{-1}\, da/dt$.

```
In[9]:= $FirstOrderVectorPerturbations=False;
        $FirstOrderTensorPerturbations=False;
        $ConformalTime=False;
```

Note that we can convert the time of already computed equations with the two xPand functions ToCosmicTime and ToConformalTime.

Up to now, we have not specified the gauge we would like to use for computing the perturbations. There are several options, which can be listed with the following function.

```
In[10]:= ?$ListOfGauges
```

The complete list of gauges is `AnyGauge`, `FluidComovingGauge`, `ScalarFieldComovingGauge`, `FlatGauge`, `IsoDensityGauge`, `NewtonGauge` and `SynchronousGauge`. In our derivation we will use the Newtonian Gauge, given by (1.55)

$$ds^2 = -\left[1 + 2\Psi(t, \vec{x})\right] dt^2 + a^2(t) \left[1 + 2\Phi(t, \vec{x})\right] \delta_{ij} dx^i dx^j \,. \tag{A.2}$$

This is the standard convention for writing the gravitational potential Φ and Ψ in the Newtonian gauge, the Dodelson convention [16] (while in the Ma–Bertschinger review [74] there is a minus sign in front of Φ). However, if we check how the metric is used in `xPand` we find a different convention. To show this, we can use a function we defined at the end of the previous section, `MyToxPand`. To call this function, we should specify the tensor we want to expand, in our example the metric `g`, the gauge, and the expansion order of perturbation.

```
In[11]:= MyToxPand[g[-b,-c],"NewtonGauge",1]
```

The output will be written in terms of ADM quantities. In our coordinate system, the normal vector is exactly (3.28) $n^\mu = \delta^\mu_0$, and therefore the $n_b n_c$ parts identify the time-time component of the metric `g + dg` (the metric with its perturbation at first order). Moreover $h_{ij} = g_{ij}$ from (3.16), and therefore the h_{bc} are the space-space components of the metric. The order of perturbations is given by powers of ϵ, e.g., all quantities multiplied by ϵ^1 will be at linear order.

Out[∘]= $a^2\, \bar{h}_{bc} - a^2\, \bar{n}_b\, \bar{n}_c + \epsilon \left(-2\, a^2\, \bar{n}_b\, \bar{n}_c \left({}^{(1)}\phi \right) - 2\, a^2\, \bar{h}_{bc} \left({}^{(1)}\psi \right) \right)$

But we can also use `VisualizeTensor` to write it in a more readable form, where the induced metric `h` is a necessary input to specify in which coordinates the tensor should be written. Note that the `%` in Mathematica corresponds to a reference to the previous output (not necessarily on the same cell).

```
In[12]:= MyToxPand[g[-b,-c],"NewtonGauge",1]
         VisualizeTensor[%,h]
```

The output is more readable, and the block of the matrix is easily comparable with the perturbed FLRW metric (A.2). We see that ϕ and ψ are inverted in `xPand`, and there is an additional minus in the definition of the gravitational potential in the spatial part.

Out[∘]=

	n	h
n	$-1 - 2\epsilon \left({}^{(1)}\phi \right)$	0
h	0	$a^2\, \bar{h}_{bc} - 2\epsilon\, a^2\, \bar{h}_{bc} \left({}^{(1)}\psi \right)$

To avoid any confusion, we provide Table A.1 to transform from `xPand` results, our convention in [16] as in (A.2), and the Ma–Bertschinger review [74] one. The Mathematica output will use the `xPand` convention, while the results will be written with (A.2) convention.

`xPand`	Dodelson [16]	Ma–Bertschinger [74]
ψ	- Φ	ϕ
ϕ	Ψ	ψ

Table A.1: Table for comparison of gravitational potential conventions in `xPand`, [16] and [74].

A.3 Matter Definitions

The last definitions we need before we can compute the perturbations equations are the stress-energy tensor ones. Although we previously defined the energy density ρ, the matter pressure P and the 4-velocity u, using DefMatterFields, we should specify how matter is introduced in our theory. We start defining a standard generic xAct tensor which we call Tmunu, using the DefTensor function. Since we are defining a generic covariant tensor, a xAct tensor rather than a xPand tensor, it only needs its name (with its indices) and the manifold on which it is defined.

```
In[13]:= DefTensor[Tmunu[-b,-c], M]
```

Unfortunately the default xPand definition does not contain contributions from the anisotropic stress Σ_{ij}, i.e. the traceless part of the spatial part of the stress-energy tensor. Therefore we define, with DefTensor, another tensor Tstress which contains the anisotropic stress contribution. Moreover, as we do with xPert, we should define the perturbation of the second tensor with the xAct function DefTensorPerturbation. In the second function, we need to specify the name of the perturbation tensor Tstressu, which will be the perturbation of Tstress. In defining Tstressu we also need to add a LI[order], which will be filled by xAct with the correct perturbation order when we make computations with this tensor.

```
In[14]:= DefTensor[Tstress[-b,-c],M,PrintAs→"Σ"]
         DefTensorPerturbation[Tstressu[LI[order],-b,-c], Tstress[-b,-c], M,
         PrintAs→"Σ"]
```

But we also know that the second tensor does not make any contribution to the background. Therefore we define, with DefProjectedTensor, a xPand spatial tensor which can be decomposed with the xPand convention. In other words, we need a tensor written in coordinates to associate the covariant tensor component with. We know that it's symmetric and traceless, so we can include that in the definition instead of correcting the final results.

```
In[15]:= DefProjectedTensor[Tstressuij[-b,-c],h,
         TensorProperties→{"SymmetricTensor","Traceless"},PrintAs→"Σ"]
```

Then we have to define a set of Mathematica rules which tells xPand how to split the Tstress perturbations. The background order is set to 0, while the first order (denoted by LI[1]) is a purely spatial tensor, which was defined with DefProjectedTensor.

```
In[16]:= FieldGauge={Tstress[b_,c_]:→0,
         Tstressu[LI[1],a_,b_]:→Tstressuij[LI[1],a,b]}

Out[•]= {Σbc :→ 0, Σ¹ab :→ Σ¹ab}
```

Note that this procedure (DefTensor → DefProjectedTensor → definition of splitting rules) can be used to define any new tensor you want to add to the theory. For instance, you can use this procedure to add a scalar or tensor field.

Finally, we define the stress-energy tensor of a perfect fluid stress-energy tensor using IndexSet. This function tells xPand how to replace occurrences of the stress-energy tensor with functions already defined. We also added a $Dust parameter to consider dust (pressure-less matter) if it is set to True. In our case we want to consider it general, so we will set it False. The final command prints the Tmunu tensor, which is written in the standard perfect fluid form with an eventual perturbation anisotropic stress part.

In[17]:=
```
$Dust=False;
IndexSet[Tmunu[b_,c_],(ρ[u][]+If[$Dust,0,P[u][]])*u[b]*u[c]
+If[$Dust,0,P[u][]]*g[b,c]+Tstress[b,c]];
Tmunu[-b,-c]
```

Out[•]= $\bar{g}_{bc}\,\mathrm{Pu} + \Sigma_{bc} + u_b\,u_c\,(\mathrm{Pu} + \rho\mathrm{u})$

A.4 Einstein equations

We can now define the Einstein equations we can perturb to get the perturbation equations. If we want to keep track of the units, we can define the Newton constant as a constant symbol. It is important to define all objects that are going to be used in the Einstein equations, to tell `xAct` how to treat them.

In[18]:=
```
DefConstantSymbol[G]
```

The Einstein equations can now be defined. When we defined the metric with `DefMetric`, `xAct` already defined the curvature tensors and the Einstein tensor. To distinguish curvature tensors defined with different covariant derivatives, `xAct` appends the name of the covariant derivative to the tensor name. In our case, we need the full four-dimensional Einstein tensor, and therefore we need to add `EinsteinCD`. Similarly we can add to any expression the Ricci tensor and scalar respectively as `RicciCD` and `RicciScalarCD`, and the Riemann tensor as `RiemannCD`.

In[19]:=
```
EinsteinEquation=8*Pi*G*Tmunu[-a,-b]-EinsteinCD[-a,-b]
```

Note in the output that `xAct` substituted the stress-energy tensor with the definition we gave with `IndexSet`.

Out[•]= $-G[\overline{\nabla}]_{ab} + 8\,G\,\pi\,\left(\bar{g}_{ab}\,\mathrm{Pu} + \Sigma_{ab} + u_a\,u_b\,(\mathrm{Pu} + \rho\mathrm{u})\right)$

A.5 Scalar perturbations

We can perturb the Einstein equations with the function `MyToxPand` at first order. The `org` function collects all the terms with the same power of ϵ.If for instance we requested the second order, a new term with ϵ^2 would be collected. Note that also the background equations is computed.

In[20]:=
```
pertEinstein=MyToxPand[EinsteinEquation,"NewtonGauge",1]//org
```

The superscript (1) on the perturbation quantities, which denotes the perturbation of the quantity. This does not substitute the role of ϵ, and it is useful when we consider higher order perturbations.

Out[•]=
$$3a^2\,\bar{h}_{ab}\,H^2 + 2a^2\,\bar{h}_{ab}\,\dot{H} - 3a^2H^2\,\bar{n}_a\,\bar{n}_b + 8G\pi a^2\,\bar{h}_{ab}\,\mathrm{Pu} + 8G\pi a^2\,\Sigma_{ab} + 8G\pi a^2\,\bar{n}_a\,\bar{n}_b\,\rho\mathrm{u} +$$
$$\epsilon\Big(8G\pi a^2\,\bar{h}_{ab}\,\big(\overset{(1)}{\mathrm{Pu}}\big) + 8G\pi a^2\,\Sigma^1{}_{ab} + 8G\pi a^2\,\bar{n}_a\,\bar{n}_b\,\big(\overset{(1)}{\rho\mathrm{u}}\big) - 6a^2\,\bar{h}_{ab}\,H^2\,\big(\overset{(1)}{\phi}\big) - 4a^2\,\bar{h}_{ab}\,\dot{H}\,\big(\overset{(1)}{\phi}\big) +$$
$$16G\pi a^2\,\bar{n}_a\,\bar{n}_b\,\rho\mathrm{u}\,\big(\overset{(1)}{\phi}\big) - 2a^2\,\bar{h}_{ab}\,H\,\big(\overset{(1)}{\dot{\phi}}\big) - 6a^2\,\bar{h}_{ab}\,H^2\,\big(\overset{(1)}{\psi}\big) - 4a^2\,\bar{h}_{ab}\,\dot{H}\,\big(\overset{(1)}{\psi}\big) - 16G\pi a^2\,\bar{h}_{ab}\,\mathrm{Pu}\,\big(\overset{(1)}{\psi}\big) -$$
$$6a^2\,\bar{h}_{ab}\,H\,\big(\overset{(1)}{\dot{\psi}}\big) + 6a^2H\,\bar{n}_a\,\bar{n}_b\,\big(\overset{(1)}{\dot{\psi}}\big) - 2a^2\,\bar{h}_{ab}\,\big(\overset{(1)}{\ddot{\psi}}\big) + 8G\pi a^2\,\bar{n}_b\,\mathrm{Pu}\,\big(\bar{D}_a\overset{(1)}{\mathrm{Vu}}\big) + 8G\pi a^2\,\bar{n}_b\,\rho\mathrm{u}\,\big(\bar{D}_a\overset{(1)}{\mathrm{Vu}}\big) +$$
$$2aH\,\bar{n}_b\,\big(\bar{D}_a\overset{(1)}{\phi}\big) + 2a\,\bar{n}_b\,\big(\bar{D}_a\overset{(1)}{\dot{\psi}}\big) + 8G\pi a^2\,\bar{n}_a\,\mathrm{Pu}\,\big(\bar{D}_b\overset{(1)}{\mathrm{Vu}}\big) + 8G\pi a^2\,\bar{n}_a\,\rho\mathrm{u}\,\big(\bar{D}_b\overset{(1)}{\mathrm{Vu}}\big) + 2aH\,\bar{n}_a\,\big(\bar{D}_b\overset{(1)}{\phi}\big) +$$
$$2a\,\bar{n}_a\,\big(\bar{D}_b\overset{(1)}{\dot{\psi}}\big) + \bar{D}_b\bar{D}_a\overset{(1)}{\phi} - \bar{D}_b\bar{D}_a\overset{(1)}{\psi} - \bar{h}_{ab}\,\big(\bar{D}_c\bar{D}^c\overset{(1)}{\phi}\big) + \bar{h}_{ab}\,\big(\bar{D}_c\bar{D}^c\overset{(1)}{\psi}\big) - 2\,\bar{n}_a\,\bar{n}_b\,\big(\bar{D}_c\bar{D}^c\overset{(1)}{\psi}\big)\Big)$$

In the output above, Σ is a term of the background equation, i.e. there is a term Σ not multiplied by ϵ. To avoid this, we should tell `xPand` to enforce our perturbation splitting rules (given by the previously defined `FieldGauge`) using the `SplitPerturbation` function. This function needs as input the equations to apply the rules to, a set of rules and the metric `h` which is used for the split.

In[21]:=
```
pertEinstein=SplitPerturbations[pertEinstein,FieldGauge,h]
```

The output is now correct, and the Σ background contribution is deleted.

Out[•]=
$$3\,a^2\,\bar{h}_{ab}\,H^2 + 2\,a^2\,\bar{h}_{ab}\,\dot{H} - 3\,a^2\,H^2\,\bar{n}_a\,\bar{n}_b + 8\,G\,\pi\,a^2\,\bar{h}_{ab}\,Pu + 8\,G\,\pi\,a^2\,\bar{n}_a\,\bar{n}_b\,\rho u + \epsilon\Big(8\,G\,\pi\,a^2\,\bar{h}_{ab}\left({}^{(1)}Pu\right) + 8\,G\,\pi\,a^2\left({}^{(1)}\Sigma_{ab}\right) + 8\,G\,\pi\,a^2\,\bar{n}_a\,\bar{n}_b\left({}^{(1)}\rho u\right) - 6\,a^2\,\bar{h}_{ab}\,H^2\left({}^{(1)}\phi\right) - 4\,a^2\,\bar{h}_{ab}\,\dot{H}\left({}^{(1)}\phi\right) +$$
$$16\,G\,\pi\,a^2\,\bar{n}_a\,\bar{n}_b\,\rho u\left({}^{(1)}\phi\right) - 2\,a^2\,\bar{h}_{ab}\,H\left({}^{(1)}\dot{\phi}\right) - 6\,a^2\,\bar{h}_{ab}\,H^2\left({}^{(1)}\psi\right) - 4\,a^2\,\bar{h}_{ab}\,\dot{H}\left({}^{(1)}\psi\right) - 16\,G\,\pi\,a^2\,\bar{h}_{ab}\,Pu\left({}^{(1)}\psi\right) -$$
$$6\,a^2\,\bar{h}_{ab}\,H\left({}^{(1)}\dot{\psi}\right) + 6\,a^2\,H\,\bar{n}_a\,\bar{n}_b\left({}^{(1)}\dot{\psi}\right) - 2\,a^2\,\bar{h}_{ab}\left({}^{(1)}\ddot{\psi}\right) + 8\,G\,\pi\,a^2\,\bar{n}_b\,Pu\left(\bar{D}_a\,{}^{(1)}Vu\right) + 8\,G\,\pi\,a^2\,\bar{n}_b\,\rho u\left(\bar{D}_a\,{}^{(1)}Vu\right) +$$
$$2\,a\,H\,\bar{n}_b\left(\bar{D}_a\,{}^{(1)}\phi\right) + 2\,a\,\bar{n}_b\left(\bar{D}_a\,{}^{(1)}\dot{\psi}\right) + 8\,G\,\pi\,a^2\,\bar{n}_a\,Pu\left(\bar{D}_b\,{}^{(1)}Vu\right) + 8\,G\,\pi\,a^2\,\bar{n}_a\,\rho u\left(\bar{D}_b\,{}^{(1)}Vu\right) + 2\,a\,H\,\bar{n}_a\left(\bar{D}_b\,{}^{(1)}\phi\right) +$$
$$2\,a\,\bar{n}_a\left(\bar{D}_b\,{}^{(1)}\dot{\psi}\right) + \bar{D}_b\,\bar{D}_a\,{}^{(1)}\phi - \bar{D}_b\,\bar{D}_a\,{}^{(1)}\psi - \bar{h}_{ab}\left(\bar{D}_c\,\bar{D}^c\,{}^{(1)}\phi\right) + \bar{h}_{ab}\left(\bar{D}_c\,\bar{D}^c\,{}^{(1)}\psi\right) - 2\,\bar{n}_a\,\bar{n}_b\left(\bar{D}_c\,\bar{D}^c\,{}^{(1)}\psi\right)\Big)$$

This first step was necessary to compute all the components of the perturbed Einstein equations. We can then extract the single components with `ExtractComponents`. We start with the time-time equation.

In[22]:=
```
pertEinsteinEquationTT=ExtractComponents[pertEinstein,h,{"Time","Time"}]
```

Out[•]=
$$-3\,H^2 + 8\,G\,\pi\,\rho u + \epsilon\left(8\,G\,\pi\left({}^{(1)}\rho u\right) + 16\,G\,\pi\,\rho u\left({}^{(1)}\phi\right) + 6\,H\left({}^{(1)}\dot{\psi}\right) - \frac{2\left(\bar{D}_c\,\bar{D}^c\,{}^{(1)}\psi\right)}{a^2}\right)$$

From which we can also immediately obtain the background equation (the term not multiplied by the perturbation factor ϵ)

$$H^2 = \frac{8\pi G}{3}\rho\,, \tag{A.3}$$

which is indeed the first Friedmann equation (1.16). But we can also extract the first order only with `ExtractOrder`.

In[23]:=
```
ExtractOrder[pertEinsteinEquationTT,1]
```

Out[•]=
$$8\,G\,\pi\left({}^{(1)}\rho u\right) + 16\,G\,\pi\,\rho u\left({}^{(1)}\phi\right) + 6\,H\left({}^{(1)}\dot{\psi}\right) - \frac{2\left(\bar{D}_c\,\bar{D}^c\,{}^{(1)}\psi\right)}{a^2}$$

This equation is compatible: with (5.26) of [16] up to a substitution of ρ`u` with the background equation (A.3), and the convention in Table A.1; and with [74] up to a conversion to conformal time. In fact, using the definition of the ADM spatial covariant derivative, it can be proved that the D_cD^c term we have in the `xAct` equation is exactly the $\partial_i\partial^i$. Therefore, going into Fourier space, we obtain the usual equation

$$\frac{k^2}{a^2}\Phi + 3H\left(\dot{\Phi} - H\Psi\right) = 4\pi G\,\delta\rho\,, \tag{A.4}$$

where $\delta\rho$ is the perturbation of the energy density defined with the stress-energy tensor, i.e., the total energy density $\rho(t) + \delta\rho(t,\vec{x})$ is given by two contributions from the background and the perturbations, the latter given by ρ`u` with a superscript (1) in `xPand` notation. Similarly we can define the pressure perturbation as δP. A similar procedure can be applied to compute the time-space and space-space components. For instance, the space-space component can be computed as follows.

```
In[24]:= pertEinsteinEquationSS=ExtractComponents[pertEinstein,h,{"Space","Space"}]
```

Out[∘]= $3 a^2 \bar{h}_{ab} H^2 + 2 a^2 \bar{h}_{ab} \dot{H} + 8 G \pi a^2 \bar{h}_{ab} Pu + \epsilon \Big(8 G \pi a^2 \bar{h}_{ab} \big(\overset{(1)}{Pu}\big) + 8 G \pi a^2 \big(\overset{(1)}{\Sigma}_{ab}\big) - 6 a^2 \bar{h}_{ab} H^2 \big(\overset{(1)}{\phi}\big) - 4 a^2 \bar{h}_{ab} \dot{H} \big(\overset{(1)}{\phi}\big) - 2 a^2 \bar{h}_{ab} H \big(\overset{(1)}{\dot{\phi}}\big) - 6 a^2 \bar{h}_{ab} H^2 \big(\overset{(1)}{\psi}\big) - 4 a^2 \bar{h}_{ab} \dot{H} \big(\overset{(1)}{\psi}\big) - 16 G \pi a^2 \bar{h}_{ab} Pu \big(\overset{(1)}{\psi}\big) - 6 a^2 \bar{h}_{ab} H \big(\overset{(1)}{\dot{\psi}}\big) - 2 a^2 \bar{h}_{ab} \big(\overset{(1)}{\ddot{\psi}}\big) + \bar{D}_b \bar{D}_a \overset{(1)}{\phi} - \bar{D}_b \bar{D}_a \overset{(1)}{\psi} - \bar{h}_{ab} \big(\bar{D}_c \bar{D}^c \overset{(1)}{\phi}\big) + \bar{h}_{ab} \big(\bar{D}_c \bar{D}^c \overset{(1)}{\psi}\big)\Big)$

From which we can immediately identify the background and the perturbation equation, and eventually extract them with `ExtractOrder`.

Another equation that is usually computed is the traceless part of the space-space component. This can be achieved by a combination of two commands. The first is `Projectorh` (similarly to the covariant derivative, every time a slicing is defined with `DefSlicing`, a `Projector` operator is defined with the name of the induced metric appended to the projector name), which project the result into the hypersurface. With `STFPart`, which requires to specify the induced metric, we obtain the traceless part. It is easy to see that the trace of the output is null.

```
In[25]:= pertTracelessScalar=STFPart[Projectorh[MyToxPand[EinsteinEquation,
         "NewtonGauge",1]],h]//org;
         SplitPerturbations[%,FieldGauge,h];
         ExtractOrder[%,1]
```

Out[∘]= $8 G \pi a^2 \big(\overset{(1)}{\Sigma}_{ab}\big) + \bar{D}_b \bar{D}_a \overset{(1)}{\phi} - \bar{D}_b \bar{D}_a \overset{(1)}{\psi} - \frac{1}{3} \bar{h}_{ab} \big(\bar{D}_c \bar{D}^c \overset{(1)}{\phi}\big) + \frac{1}{3} \bar{h}_{ab} \big(\bar{D}_c \bar{D}^c \overset{(1)}{\psi}\big)$

Since all terms giving the trace has been removed from the space-space Einstein equation in the previous step, we can apply to the last output a projection operator to also obtain the longitudinal trace-less equation

$$\left(\hat{k}^i\hat{k}^j - \frac{1}{3}\delta^{ij}\right)\left[8\pi G a^2 \Sigma_{ij} - k_i k_j(\Psi+\Phi)\right] = 8\pi G a^2 \Sigma - \frac{2}{3}k^2(\Psi+\Phi)\,, \tag{A.5}$$

where

$$\Sigma \equiv \left(\hat{k}^i\hat{k}^j - \frac{1}{3}\delta^{ij}\right)\Sigma_{ij}\,. \tag{A.6}$$

Therefore the final equation is

$$k^2\left(\Phi+\Psi\right) = 12\pi G a^2 \Sigma\,, \tag{A.7}$$

which is compatible with both [16] and [74].

A.6 Tensor perturbations

The tensor perturbations can be computed using the same procedure as for scalar perturbations. Unfortunately, there is no way to cancel scalar perturbations setting one flat as we did for tensor and vector perturbations in the previous section. However, we can enable tensor perturbations with the following commands, and using the decomposition theorem we can simply subtract the scalar perturbations result. A fully equivalent treatment would be to eliminate terms of the scalar perturbation quantities (the gravitational potential Φ and Ψ) but, since we already have the scalar perturbation results, it requires fewer commands to subtract them from the tensor perturbation results.

In[26]:=
```
$FirstOrderTensorPerturbations=True;
```

We can also visualize the tensor as we did for the scalar perturbations.

In[27]:=
```
MyToxPand[g[-b,-c],"NewtonGauge",1];
VisualizeTensor[%,h]
```

The output corresponds to the metric

$$ds^2 = -dt^2 + (\delta_{ij} + 2E_{ij})\, dx^i dx^j \,, \tag{A.8}$$

where E_{ij} is the tensor perturbation metric.

Out[∘]=

	n	h
n	$-1 - 2\,\epsilon\,\left(\overset{(1)}{\phi}\right)$	0
h	0	$a^2\,\bar{h}_{bc} + \epsilon\left(2\,a^2\left(\overset{(1)}{E}_{bc}\right) - 2\,a^2\,\bar{h}_{bc}\left(\overset{(1)}{\psi}\right)\right)$

Using the same procedure carried on for scalar perturbations, we can find the tensor perturbation longitudinal trace-less equation. Note that in the first command we also subtracted the scalar perturbations result.

In[28]:=
```
pertTracelessScalarTensor=STFPart[Projectorh[MyToxPand[EinsteinEquation,
"NewtonGauge",1]],h]-pertTracelessScalar//org;
SplitPerturbations[%,FieldGauge,h];
pertTracelessScalarTensor1=ExtractOrder[%,1]
```

Out[∘]= $-a^2\left(\overset{(1)}{\ddot{E}}_{ab}\right) - 3\,a^2\left(\overset{(1)}{\dot{E}}_{ab}\right) H + 6\,a^2\left(\overset{(1)}{E}_{ab}\right) H^2 + 4\,a^2\left(\overset{(1)}{E}_{ab}\right)\dot{H} + 16\,G\,\pi\,a^2\left(\overset{(1)}{E}_{ab}\right) Pu + \bar{D}_c\,\bar{D}^c\,\overset{(1)}{E}_{ab}$

This result can be simplified using the space-space background Einstein equation. We already computed it in the previous section, and we can access it with `ExtractOrder`.

In[29]:= `bkgEinsteinSS=ExtractOrder[pertEinsteinEquationSS,0]/.`$\bar{h}_{ab}$ `:→1`

Out[∘]= $3\,a^2\,H^2 + 2\,a^2\,\dot{H} + 8\,G\,\pi\,a^2\,Pu$

Finally, solving the background equation for P using the Mathematica function `Solve`, substituting the result in the perturbation equation and dividing by a^2 we obtain the usual result for tensor perturbations. Note that we divided by `ah[]` and not `a`, because as other aforementioned quantities, the scale factor is defined for each slicing, and therefore the name of the induced metric is appended to `a`. Moreover, `a` was defined as an index with `DefManifold`, and trying to divide by it would produce meaningless results.

In[30]:=
```
Solve[bkgEinsteinSS==0, Pu][[1,1]]
-pertTracelessScalarTensor1/ah[]^2/.%//org//Simplify
```

Out[∘]= $Pu \rightarrow \frac{-3H^2 - 2\dot{H}}{8G\pi}$

Out[∘]= $\overset{(1)}{\ddot{E}}_{ab} + 3\left(\overset{(1)}{\dot{E}}_{ab}\right)H - \frac{\bar{D}_c\bar{D}^c\overset{(1)}{E}_{ab}}{a^2}$

Therefore, in Fourier space, we obtain the tensor perturbations equation

$$\ddot{E}_{ij} + 3H\dot{E}_{ij} + \frac{k^2}{a^2}E_{ij} = 0\,, \tag{A.9}$$

which is compatible with [16] and [74] results. Note that there is an additional factor 2 in `xPand` definition of E_{ij}. Our result is obviously not affected by this factor, but it is important to keep track of these conventions when we compute higher order perturbations equations, where scalar and tensor perturbations are usually mixed.

A.7 Time derivative

We might want to derive one of the perturbation equations with respect to the time, to find the second order in time differential equations. This cannot be achieved with a simple Derivative of the results with respect to t. The correct way is to exploit once again the fact that `xPand` uses the ADM formulation. In fact, the Lie derivative with respect to the normal vector n^μ, at least in FLWR metrics where the shift vector N^μ has null components, always coincides with the derivative with respect to time, as in (3.43).

Consider the following example. We want to obtain the derivative of the time perturbed Einstein equation. Consider only scalar perturbations for simplicity.

In[31]:=
```
$FirstOrderTensorPerturbations=False;
```

In[32]:=
```
pertEinsteinEquationTT
LieD[n[a]]@%//org
```

Out[∘]= $-3H^2 + 8G\pi\rho u + \epsilon\left(8G\pi\left(\overset{(1)}{\rho u}\right) + 16G\pi\rho u\left(\overset{(1)}{\phi}\right) + 6H\left(\overset{(1)}{\dot{\psi}}\right) - \frac{2\left(\bar{D}_c\bar{D}^c\overset{(1)}{\psi}\right)}{a^2}\right)$

Out[∘]= $-6aH\dot{H} + 8G\pi a\dot{\rho u} + \epsilon\left(8G\pi a\left(\overset{(1)}{\dot{\rho u}}\right) + 16G\pi a\dot{\rho u}\left(\overset{(1)}{\phi}\right) + 16G\pi a\rho u\left(\overset{(1)}{\dot{\phi}}\right) + 6a\dot{H}\left(\overset{(1)}{\dot{\psi}}\right) + 6aH\left(\overset{(1)}{\ddot{\psi}}\right) + \frac{4H\left(\bar{D}_c\bar{D}^c\overset{(1)}{\psi}\right)}{a} - \frac{2\left(\bar{D}_c\bar{D}^c\overset{(1)}{\dot{\psi}}\right)}{a}\right) +$
$8G\pi\left(\overset{(1)}{\rho u}\right)\left(\mathcal{L}_{\bar{n}}\epsilon\right) + 16G\pi\rho u\left(\overset{(1)}{\phi}\right)\left(\mathcal{L}_{\bar{n}}\epsilon\right) + 6H\left(\overset{(1)}{\dot{\psi}}\right)\left(\mathcal{L}_{\bar{n}}\epsilon\right) - \frac{2\left(\bar{D}_c\bar{D}^c\overset{(1)}{\psi}\right)\left(\mathcal{L}_{\bar{n}}\epsilon\right)}{a^2}$

As you can see also Lie derivatives of the perturbation parameter ϵ appear. You can solve it by substituting it with zero, or work on each order as follows.

In[33]:=
```
LieD[n[a]]@ExtractOrder[pertEinsteinEquationTT,0]//org
LieD[n[a]]@ExtractOrder[pertEinsteinEquationTT,1]//org
```

Out[ ]= $-6\,a\,H\,\dot{H} + 8\,G\,\pi\,a\,\dot{\rho u}$

Out[ ]= $8\,G\,\pi\,a\left(\overset{(1)}{\dot{\rho u}}\right) + 16\,G\,\pi\,a\,\dot{\rho u}\left(\overset{(1)}{\phi}\right) + 16\,G\,\pi\,a\,\rho u\left(\overset{(1)}{\dot{\phi}}\right) + 6\,a\,\dot{H}\left(\overset{(1)}{\dot{\psi}}\right) + 6\,a\,H\left(\overset{(1)}{\ddot{\psi}}\right) + \frac{4\,H\left(\overline{D}_c\,\overline{D}^c\,\overset{(1)}{\psi}\right)}{a} - \frac{2\left(\overline{D}_c\,\overline{D}^c\,\overset{(1)}{\dot{\psi}}\right)}{a}$

Note that it is not necessary to apply the Lie derivative if we want to consider a single object. In fact, all the quantities defined by `xPand` carry several indices. For instance consider the gravitational potential

```
ϕh[LI[1],LI[1]]
```

The first `LI[1]` denotes the order of the perturbation (the superscript (1) we can see for instance in the previous output), while the second is the order of the time derivative. For instance, this is the first time derivative of the gravitational potential. To obtain the second time derivative of the gravitational potential we can simply write

```
ϕh[LI[1],LI[2]]
```

Finally note that, since the gravitational potentials are defined for each slicing we introduce, we should append the name of the induced metric to the gravitational potential similarly to what we did for the `Projector` function.

A.8 Additional degrees of freedom

If we want to add additional degrees of freedom, the first equations we usually want to compute are the modified Einstein equations. This can be performed with `xPert` package of `xAct`. We will find the equations of motion in a covariant form, without specifying any coordinate system. The FLRW coordinates will be introduced when we will use the equations of motion in `xPand`.

A.8.1 Equations of motion

Firstly, before switching to another `xAct` package, it is always important to quit the Mathematica kernel to avoid any definition clashing. This can be done in the Mathematica Kernel settings or using the following Mathematica command.

```
In[34]:= Quit[]
```

As in the `xPand` case, we should call the add-on and define the manifold and the metric.

```
In[3]:= <<xAct`xPert`
```

```
In[4]:= DefManifold[M,4,{a,b,c,d,e,f,h,i,j,k,l}]
        DefMetric[-1,g[-a,-b],CD]
```

When we use `xPert`, we can define a general metric perturbation, which is used for the action variation, with the `DefMetricPerturbation` function. It needs the name of the metric we want to perturb, the name of the perturbation we want to create, and the name of the perturbation parameter (similarly to ϵ in `xPand`). With the second line, we show an alternative method to call `PrintAs` on the already defined `gpert`.

```
In[5]:= DefMetricPerturbation[g,gpert,ϵ];
        PrintAs[gpert]^= "h";
```

To obtain a more readable result, where the perturbation index is shown in the output with a different color (blue in the command below), we can do the following. Note that `IndexForm` is a function protected from changes in `xAct`, and it should be unprotected before we can modify it. If you use `Unprotect`, remember to protect it after the changes to avoid unwanted changes to core functions.

```
In[6]:= Unprotect[IndexForm];
        IndexForm[LI[x_]]:=ColorString[ToString[x],RGBColor[0,0,1]];
        Protect[IndexForm];
```

In this example we want to add a new degree of freedom to the action. Consider the addition of a scalar field (the same procedure can be extended to higher order tensors). Since the scalar field we are considering is a scalar function, i.e. a $(0,0)$-rank tensor, we define it with `DefTensor`, which requires the name of the tensor we want to define and the manifold where to define it. In general, every degree of freedom, i.e. every quantity we want to perform the action variation with, should be defined as tensors. Moreover, similarly to the metric, we should define the perturbation of this new tensor, similarly to what we did for `Tmunu`.

```
In[7]:= DefTensor[Phi[],M,PrintAs→"φ"]
        DefTensorPerturbation[PertPhi[LI[order]],Phi[],M,PrintAs→"δφ"]
```

We consider the simplest scalar field dynamic addition to the action, called quintessence. Its action part is given by

$$S_\varphi = -\frac{1}{2}\varphi_{;\rho}\varphi^{;\rho} - V(\varphi)\,, \tag{A.10}$$

where the first part is the kinetic energy of the scalar field, and the second a generic potential. We can define a generic function of any tensor with

```
In[8]:= DefScalarFunction[V]
```

Note that if we need coupling constants, we can define them with `DefConstantSymbol` as we did for the Newton constant. For instance consider the following command for defining a constant `alpha` which will be printed as α in the outputs.

```
In[9]:= DefConstantSymbol[alpha, PrintAs→"α"]
```

In the quintessence case, we do not need to define a coupling constant, therefore we will not use this definition.

We can finally define the Lagrangian, which should contain the determinant. The determinant `Det` is another object which is defined every time we define a metric, and the name of the metric is appended to it.

```
In[10]:= L=Sqrt[-Detg[]](1/(16*Pi*G)RicciScalarCD[]-1/2*CD[-b][Phi[]]*CD[b][Phi[]]
         -V[Phi[]])
```

Out[•]= $\sqrt{-\tilde{\tilde{g}}}\left(\frac{R[\nabla]}{16\,G\,\pi} - V[\varphi] - \frac{1}{2}\,(\nabla_b\,\varphi)\,(\nabla^b\,\varphi)\right)$

To obtain the perturbation of the Lagrangian we can use a sequence of commands: `Perturbation` compute the perturbation at linear order (as a second input we can specify the order of the expansion in the perturbation); `ExpandPerturbation` gives the equation where all the quantities are expanded in terms of the metric perturbations; `ContractMetric` contracts all possible indices with the metric; `ToCanonical` is one of the most useful functions of `xAct`, which simplifies and canonically reorganizes all the tensors, according to the tensors symmetries and the position of dummy indices.

In[11]:=
```
Lpert=ToCanonical@ContractMetric@ExpandPerturbation@Perturbation@L
```

Out[∘]=
$$-\frac{\sqrt{-\tilde{\tilde{g}}}\; h^{1ba}\, R[\nabla]_{ba}}{16\,G\,\pi}+\frac{\sqrt{-\tilde{\tilde{g}}}\; h^{1b}{}_{b}\, R[\nabla]}{32\,G\,\pi}-\frac{1}{2}\sqrt{-\tilde{\tilde{g}}}\; h^{1b}{}_{b}\, V[\varphi]-\frac{\sqrt{-\tilde{\tilde{g}}}\; h^{1b}{}_{b}{}^{;a}{}_{;a}}{16\,G\,\pi}+\frac{\sqrt{-\tilde{\tilde{g}}}\; h^{1ba}{}_{;b;a}}{16\,G\,\pi}-$$
$$\sqrt{-\tilde{\tilde{g}}}\,(\nabla_b\varphi)\;\delta\varphi^{1;b}+\frac{1}{2}\sqrt{-\tilde{\tilde{g}}}\; h^{1}{}_{ba}\,(\nabla^a\varphi)\,(\nabla^b\varphi)-\frac{1}{4}\sqrt{-\tilde{\tilde{g}}}\; h^{1a}{}_{a}\,(\nabla_b\varphi)\,(\nabla^b\varphi)-\sqrt{-\tilde{\tilde{g}}}\;\delta\varphi^{1}\, V'[\varphi]$$

The final step is the variation with VarD. The syntax requires the perturbation quantity with respect to which we are making the variation, the covariant derivative, and as another input the quantity to perform the variation on. For instance the variation of Lpert with respect to the metric g is given by

```
VarD[gpert[LI[1],a,b],CD][Lpert]
```

In practice, we can simplify the result deleting the determinant and a spurious perturbation indices delta, and transforming the Ricci tensors to Einstein tensor with the following commands.

In[12]:=
```
0==-2*(VarD[gpert[LI[1],a,b],CD][Lpert]/Sqrt[-Detg[]]
/.delta[-LI[1],LI[1]]→1//Simplify//RicciToEinstein)//Expand//ContractMetric
//ToCanonical
```

Out[∘]=
$$0 == \frac{G[\nabla]_{ab}}{8\,G\,\pi}+g_{ab}\,V[\varphi]-(\nabla_a\varphi)\,(\nabla_b\varphi)+\frac{1}{2}\,g_{ab}\,(\nabla_c\varphi)\,(\nabla^c\varphi)$$

A similar procedure can be applied for the Klein–Gordon equation, i.e. the equation computed from the variation of the Lagrangian with respect to the scalar field.

In[13]:=
```
0==(VarD[PertPhi[LI[1]],CD][Lpert]/Sqrt[-Detg[]]
/.delta[-LI[1],LI[1]]→1//Simplify)
```

Out[∘]=
$$0 == \nabla_a\nabla^a\varphi - V'[\varphi]$$

A.8.2 Perturbations

We can use again xPand to compute the perturbation equations. The generalization of the General Relativity procedure for a theory with an additional degree of freedom is straightforward. In fact, xPand automatically create a scalar field φ[] that can be added directly in the Einstein equations. For instance, consider again the quintessence example.

The modified Einstein equations of quintessence found with xPert

$$G_{\mu\nu}-\varphi_{;\mu}\varphi_{;\nu}+\frac{1}{2}g_{\mu\nu}\,\varphi_{;\rho}\varphi^{;\rho}+g_{\mu\nu}V(\varphi)=8\pi G T_{\mu\nu}\,, \tag{A.11}$$

can be implemented in xPand following the same procedure we used for standard General Relativity. As first step, remember to quit the kernel. Then include the new definitions: for instance V in the case of quintessence. Again, for quintessence is not necessary to add a new scalar field definition because one, called φ[], is already automatically defined by xPand. Then we can replace the EinsteinEquation, copying the xPert result above, substituting the field definition Phi[] with φ[] and adding the stress-energy tensor.

```
EinsteinEquation=Tmunu[-a,-b]-EinsteinCD[-a, -b]/(8*Pi*G)
-g[-a,-b] V[φ[]] +(CD[-a][φ[]])(CD[-b][φ[]])
-1/2 g[-a,-b] (CD[-c][φ[]])(CD[c][φ[]])//SeparateMetric[g]
```

Then following the General Relativity procedure we can obtain the perturbations equations for quintessence. The same can be applied to the Klein–Gordon equation to find the perturbed Klein–Gordon equation.

If there are additional tensor degrees of freedom, we can proceed in defining them with the procedure used to define the anisotropic stress.

A.9 Conclusion

In this section, we showed a simple example of the application of `xAct` on a very well-known cosmology problem. In particular, we used `xPand` to compute the linear perturbations with matter described by a perfect fluid stress-energy tensor with the addition of anisotropic stress. We also introduced the possibility of adding a new degree of freedom.

Note that in this derivation we neglected the nature of matter included in the stress-energy tensor, using a generic perfect fluid description. In practice, we should consider not only the matter terms coming from the single matter components (baryons, radiation, dark matter, dark energy, ultra-relativistic particles, etc..) but also their eventual interaction. For instance, standard baryonic matter and radiation can exchange momenta, at least before recombination, due to Compton scattering. We neglect the full discussion about these collisional terms: the complete details about the matter part of the perturbation equations can be found for instance in [16, 74].

Finally, it is important to note that the perturbations in General Relativity are known to be mathematically stable. However, when we compute the perturbations in the presence of additional degrees of freedom (for instance a scalar field as we did in section A.8), it is also important to check the mathematical stability of the perturbation quantities. We defer the discussion of this problem to Chapter 4 dedicated to modified gravity theories.

Appendix B

Bayesian probability

In this Chapter, we introduce the Bayesian probability, and then describe the process of parameter estimation to obtain constraints using observational data, which is applied in Chapter 6. The first introduction section is based on [89]. The discussion is based on several courses notes, e.g., [90, 91].

B.1 Why Bayesian probability?

The Bayesian probability is an alternative way to study statistics. It is usually compared with the *frequentist* probability, which has the following definition for the probability of an event.

> *The probability of an event is the quotient of the number of times the event occurs and the total number of trials, in the limit of a large set of repetitions with the same probability.*

The first evident problem with this definition is its *circularity*. The definition of an event relies on the definition of equiprobability, which is based on the notion of probability itself, which is the entity we are trying to define. Besides this technical issue, we can also see two practical limitations of this approach.

(i) The number of repetitions required by the definition should be *large*. In practice, it is very common, also in cosmology, to deal with a small number of experimental data. Moreover, there is no prescription on how large the set should be to comply with the definition.

(ii) Unique propositions can not be handled. A question like *What was the probability of rain in Rome yesterday?* can not be formulated, as the answer would require infinite (> 1) repetitions. The same issue can be translated into cosmology. When we estimate an observable, we can make an experiment on only one possible realization of the Universe.

The Bayesian approach is based on a different probability (of an event) definition.

> *The probability of an event is the measurement of the degree of belief about a proposition.*

In addition to the obvious advantage of being able to assign a probability to unique events, the Bayesian probability can be preferred for other reasons:

(i) it deals with *nuisance parameters* with easily and with small (also numerical) efforts. These parameters are all the quantities that influence the data but are not interesting in describing the physical process we are studying. For instance, the noise affecting some data. There might be some parameters that describe the noise, which we do not need to estimate. In Bayesian analysis, we can simply integrate the probability over all possible values of these parameters to *marginalize* over it. On the contrary, the frequentist approach does not have a simple prescription to deal with nuisance parameters;

(ii) it can integrate *prior informations*. For instance, we can enforce the constraint of a mass to be positive, while in the frequentist approach the best-fit value might be a meaningless negative one;

(iii) while in the frequentist approach we usually deal with the probability distribution of data that are not obtained, the Bayesian probability can be considered only with available data;

(iv) it can recover the classical statistics in the cases when the proposition in the frequentist approach can be formulated. This limit can be achieved when the number of available data is *large enough*. Therefore the Bayesian probability can account for frequentist results, plus all the additional cases we mentioned above.

We should note that, even though these motivations seem to prefer the Bayesian approach in all applications, the debate between statisticians is still open. However, as physicists, we should prefer the approach which can be used for more applications and provides more efficient prescriptions to deal with data. We will see in the next Chapters that the Bayesian approach, in some cosmological applications, is the only possible way to infer physical properties from data.

B.2 Definition

The formal definition of the probability of an event in Bayesian statistics is the following.

> *The probability* $\mathrm{P}(A|B)$ *is the degree of which the truth of a logical proposition* B *implies that a logical proposition* A *is also true.*

This definition should be accompanied by an explanation of the term *degree*, which should *calibrate* the probability scale in order to define the value of true and false events, and order the probabilities based on their likeliness to be true. In fact, we can clarify the meaning of *degree* using the conventional probabilities

(i) $0 \leq \mathrm{P}(A|B) \leq 1$ for all A and B;

(ii) if $\mathrm{P}(A|B) = 0$ and B is true, then A is false;

(iii) if $\mathrm{P}(A|B) = 1$ and B is true, then A is true;

(iv) if $0 < \mathrm{P}(A|B) < 1$ and B is true, then A *might* be true;

(v) if B is true, then the probability that A is not true is $1-\mathrm{P}(A|B)$;

(vi) if $\mathrm{P}(A|B) > \mathrm{P}(C|B)$ and B is true, then it is more likely that A will be true than C. In particular, the ratio $\mathrm{P}(A|B)/\mathrm{P}(C|B)$ is the factor of which A is more likely to be true than C, provided that $\mathrm{P}(C|B) > 0$. If $\mathrm{P}(C|B) = 0$, then A is infinitely more likely to be true.

Another feature of this definition is that any probabilistic statement is conditioned to other information. Therefore, in the context of Bayesian analysis, it is meaningless to write $\mathrm{P}(A)$ if it is not conditioned to other statements. Moreover, it is important to stress that $\mathrm{P}(A|B)$ is defined only if the statements A and B are *related*. For instance, we can not define $\mathrm{P}(A|B)$ where A is *The dice result is* 2 and B is *It rained in Rome yesterday*. However, it might be possible to obtain $\mathrm{P}(A|B, C_i)$, the probability of A conditioned to B and to additional statements C_i which provide a possible model connecting the dice result and the weather (if any).

B.3 Bayesian inference

After the definition of $\mathrm{P}(A|B)$, we want to find the relation between $\mathrm{P}(A|B)$ and $\mathrm{P}(B|A)$, i.e. establish an *inference method*. We can obtain the link between these two probabilities by taking a step back. We introduce some self-consistency relations, called *Cox's axioms*.

(i) **Comparability**: the probability of any two propositions must be representable mathematically in such a way they can be ordered (and therefore compared).

(ii) **Negation**: the probability that a proposition is true must have some deterministic relationship to the probability that it is not true.

(iii) **Consistency**: if the probability that a proposition is true can be derived in different ways, their results must be numerically the same.

The *Cox's theorem* states that the introduction of these axioms leads to the definition of a mathematically founded probability theory. We already introduced the implications of the first two axioms in the previous section. In particular, comparability implies we can write (i), where we assign a real number to any probability; negation implies that we can write the probability of A not true starting from (ii) and (iii) (where we assigned the probability of a true statement to 1, and 0 if false), obtaining $\mathrm{P}(\bar{A}|B) = 1-\mathrm{P}(A|B)$.

The last axiom has less obvious implications. Consider three propositions A, B and C, not necessarily related, and a set of background information I that is informative enough to specify $P(A|I)$, $P(B|I)$ and $P(C|I)$, without the need for each of these probabilities to reference to the other two.

Consider the *joint* probability that both A and B are true conditioned to I, $\mathrm{P}(A, B|I)$. It must depend on both the probability of A being true, $\mathrm{P}(A|I)$ and B being true given A is true, $\mathrm{P}(B|A, I)$. Therefore, there should exist a function $f(x, y)$ such that

$$\mathrm{P}(A, B|I) = f\left[\mathrm{P}(A|I), \mathrm{P}(B|A, I)\right] . \tag{B.1}$$

But the same reasoning can be applied to obtain a similar result

$$\mathrm{P}(A, B|I) = f\left[\mathrm{P}(B|I), \mathrm{P}(A|B, I)\right] . \tag{B.2}$$

The LHS should be false if one of the propositions A or B is false, i.e. $f(0, y) = 0$; but it should be false also if the probability of A given B (or the contrary) is false. i.e. $f(x, 0) = 0$. Moreover, if A or B are true, we expect the probability of both A and B being true to only depend on $\mathrm{P}(B|A, I)$ (or the contrary), i.e. $f(1, y) = y$, and similarly, $f(x, 1) = x$. Obviously, this does not uniquely define the function f.

We can extend the joint probability with three statements A, B and C. With a similar argument we can obtain

$$\begin{aligned}\mathrm{P}(A, B, C|I) &= f\left[\mathrm{P}(A, B|I), \mathrm{P}(C|A, B, I)\right] = \\ &= f\left\{f\left[\mathrm{P}(A|I), \mathrm{P}(B|A, I)\right], \mathrm{P}(C|A, B, I)\right\} ,\end{aligned} \tag{B.3}$$

but also

$$\begin{aligned}\mathrm{P}(A, B, C|I) &= f\left[\mathrm{P}(A|I), \mathrm{P}(B, C|A, I)\right] = \\ &= f\left\{\mathrm{P}(A|I), f\left[\mathrm{P}(B|A, I), \mathrm{P}(C|A, B, I)\right]\right\} .\end{aligned} \tag{B.4}$$

Enforcing the consistency axiom, since the two quantities in both previous equations are the same, we obtain

$$f\left\{f\left[\mathrm{P}(A|I), \mathrm{P}(B|A, I)\right], \mathrm{P}(C|A, B, I)\right\} = f\left\{\mathrm{P}(A|I), f\left[\mathrm{P}(B|A, I), \mathrm{P}(C|A, B, I)\right]\right\} . \tag{B.5}$$

In other words, we want to find the function $f(x,y)$ which satisfies the border conditions $f(x,0) = f(0,y) = 0$, $f(x,1) = x$ and $f(1,y) = y$, and the equation

$$f\left[f(x,y),z\right] = f\left[x,f(y,z)\right] , \tag{B.6}$$

with $0 \leq x,y,z \leq 1$. It can be proved (Cox, 1946) that there is no unique choice of f; however, they are all equivalent to define

$$f(x,y) = xy , \tag{B.7}$$

up to the definition of a new scale, e.g., the square of the probabilities x and y.

Therefore, the consistency axiom leads to the inference result

$$\mathrm{P}(A,B|I) = \mathrm{P}(A|I)\mathrm{P}(B|A,I) = \mathrm{P}(B|I)\mathrm{P}(A|B,I) . \tag{B.8}$$

Although this is a standard result in probability, we proved it using probabilistic implications, without the need for countability arguments or the notion of frequencies.

B.4 Bayes theorem

From the previous result (B.8), we can derive the fundamental tool of Bayesian probability, the *Bayes theorem*

$$\mathrm{P}(A|B,I) = \frac{\mathrm{P}(A|I)\mathrm{P}(B|A,I)}{\mathrm{P}(B|I)} . \tag{B.9}$$

The key feature of this theorem is that we can *invert* the probabilities $\mathrm{P}(A|B,I)$ and $\mathrm{P}(B|A,I)$. However, the probability $\mathrm{P}(A|B,I)$ does not depend only on $\mathrm{P}(B|A,I)$, but also on $\mathrm{P}(A|I)$ and on the background informations I. The latter dependence is crucial because it permits a correct definition of all the probabilities in the Bayes theorem, even in the case when A and B are not related and $\mathrm{P}(A|B)$ can not be defined.

Note that the theorem can also be formulated in the case of probabilities for continuous random variables, in terms of probability density functions. In that case, if x and y are two continuous random variables, we obtain the relation

$$\mathrm{P}(x|y,I) = \frac{\mathrm{P}(x|I)\mathrm{P}(y|x,I)}{\mathrm{P}(y|I)} . \tag{B.10}$$

B.4.1 Normalization

It is implicit in the definition of any discrete and continuous variable that the sum/integral of the probability over all possible values should be unity. Consider a set of N *exhaustive* propositions $\{S_i\} = \{S_1, \ldots, S_N\}$, i.e. one of them should be true and they are mutually exclusive. Therefore, when we sum all the probabilities of the statements from this set conditioned to a proposition B and the background informations I, we have the requirement

$$\sum_{i=1}^{N} \mathrm{P}(S_i|B,I) = 1 . \tag{B.11}$$

Applying the Bayes theorem (B.9), we obtain

$$\sum_{i=1}^{N} \mathrm{P}(S_i|I)\mathrm{P}(B|S_i,I) = \mathrm{P}(B|I) . \tag{B.12}$$

Therefore the Bayes theorem can be rewritten as

$$\mathrm{P}(S_i|B,I) = \frac{\mathrm{P}(S_i|I)\mathrm{P}(B|A,I)}{\sum_{j=1}^{N} \mathrm{P}(S_j|I)\mathrm{P}(B|S_j,I)} . \tag{B.13}$$

In the case of continuous variables, it can be proved that the sum should be replaced by an integral. For instance, if the continuous random variable x can have any real value, its probability density function conditioned to B is

$$\mathrm{P}(x|B,I) = \frac{\mathrm{P}(x|I)\mathrm{P}(B|x,I)}{\int_{-\infty}^{\infty} dx'\, \mathrm{P}(x'|I)\mathrm{P}(B|x',I)} \,. \tag{B.14}$$

B.4.2 Change of variables

We might be interested in the change of variables transformation of a *known* continuous probability density distribution $\mathrm{P}(x,I)$ from the random variable x to a (related) deterministic quantity $y = y(x)$. We do not restrict the discussion to the case where $y(x)$ is bijective (and therefore invertible), but we allow the existence of more x_i for which $y(x_i)$ has the same value. The joint probability is

$$\begin{aligned} \mathrm{P}(x,y|I) &= \mathrm{P}(x|I)\mathrm{P}(y|x,I) = \\ &= P(x|I)\delta[y - y(x)] \,, \end{aligned} \tag{B.15}$$

where δ is the Dirac delta distribution. A useful property of this distribution is

$$\delta[g(x)] = \sum_{i=1}^{N} \frac{\delta(x - x_i)}{|dg/dx|_{x=x_i}|} \,, \tag{B.16}$$

where x_i are all values of x such that $g(x) = 0$.

Therefore, the probability distribution of y can be rewritten as the marginalization of the x random variable, as

$$\begin{aligned} \mathrm{P}(y|I) &= \int_{-\infty}^{\infty} dx\, \mathrm{P}(x,y|I) = \\ &= \int_{-\infty}^{\infty} dx\, \mathrm{P}(x|I)\mathrm{P}(y|x,I) = \\ &= \int_{-\infty}^{\infty} dx\, \mathrm{P}(x|I)\delta[y - y(x)] = \\ &= \int_{-\infty}^{\infty} dx\, \mathrm{P}(x|I) \sum_{i=1}^{N} \frac{\delta(x - x_i(y))}{|dy/dx|_{x=x_i(y)}|} = \\ &= \sum_{i=1}^{N} \int_{-\infty}^{\infty} dx\, \mathrm{P}(x|I) \frac{\delta(x - x_i(y))}{|dy/dx|_{x=x_i(y)}|} = \\ &= \sum_{i=1}^{N} \frac{\mathrm{P}(x_i(y)|I)}{|dy/dx|_{x=x_i(y)}|} \,, \end{aligned} \tag{B.17}$$

where $\{x_i(y)\}$ are all the values of x such that $y(x) = y$. In the case $y(x)$ is a bijective function of x, we should have only one $x(y)$ such that $y(x) = y$, and therefore the equation simplifies to

$$\mathrm{P}(y|I) = \frac{\mathrm{P}(x(y)|I)}{|dy/dx|_{x=x(y)}|} \,. \tag{B.18}$$

Finally, if there is no x_i, i.e. no x such that $y(x) = y$, the result is $\mathrm{P}(y|I) = 0$.

B.4.3 Data analysis

The most common application of Bayes's theorem in physics is the use of informations gathered about the world, the *data*, to obtain a picture of reality, the *model*, using pre-existing knowledge, the *prior*, and an overall paradigm, the *context*. With this picture, we can re-cast the Bayes's theorem (B.9) as

$$\mathrm{P(model|data,context)} = \frac{\mathrm{P(model|context)\,P(data|model,context)}}{\mathrm{P(data|context)}}\,, \tag{B.19}$$

where

(i) P(model|data,context) is the *posterior* probability, for the model considered and using the *data*;

(ii) P(model|context) is the *prior* probability. It includes the informations about the *model* and does not depend on *data*;

(iii) P(data|model,context) is the *likelihood*. It is also denoted as $\mathcal{L}$(data), implicitly containing the model and context informations;

(iv) P(data|context) is the *prior probability of the data*. It can also be seen as a normalization factor, as discussed near equation (B.9). In fact, it can be interpreted as the prior probability of the *data* averaged over all considered *models*. It is also called *marginal likelihood* or *Bayesian evidence*.

We can rewrite the Bayes's theorem (B.19) in a formal way.

$$\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d}, I) = \frac{\mathrm{P}(\boldsymbol{\theta}|I)\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta}, I)}{\mathrm{P}(\boldsymbol{d}|I)}\,, \tag{B.20}$$

where $\boldsymbol{d} = d_1, d_2, \ldots, d_N$ is the set of *data*, with N the number of available informations gathered about the world; $\boldsymbol{\theta} = \theta_1, \theta_2, \ldots, \theta_{N_p}$ is the set of model parameters, with N_p the number of parameters in the model considered; I is the *context*, a set of assumptions on which the inference problem is conditional.

We can interpret the quantities on the RHS as the input of the inference problem, while the LHS represents the output. We are using Bayes's theorem to incorporate new *data* and update the picture of the world given by the *posterior*. In this sense, the Bayesian analysis process is a *learning algorithm*.

It is important to note that in the Bayes's theorem (B.20), the *data* are available only on the *likelihood* and the *marginal likelihood*. However, as we previously discussed, the second is only a factor that ensures the normalization of the *posterior* probability. Therefore, *data* can affect the *posterior* probability only through the *likelihood*. On the contrary, the posterior must be independent from any *data*. This constraint on the *data* dependence in the Bayes's theorem is usually called **likelihood principle**, although it is just a consequence of the application of Cox's axioms to obtain the theorem.

B.4.4 Subjectivity?

When we consider Bayes's theorem (B.20), the choice of the prior probability might seem arbitrary. However, one key feature of Bayes's theorem is that we can use it repeatedly as new data are available. With the following example we want to show that in the limit of a large number of data, the posterior becomes independent of the prior.

Consider a Gaussian (normal) probability density distribution of a random variable θ*

$$\mathcal{N}(\theta;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}\frac{(\theta-\mu)^2}{\sigma^2}\right]\,, \tag{B.21}$$

where μ is the *mean value* of the normal distribution and σ^2 is the *variance* of the normal distribution. In this example we choose to draw some data from a normal distribution, as in Figure B.1.

* The probability density distribution is related to the probability of obtaining a quantity X with a value between x and $\theta + d\theta$, drawing X from a normal distribution with mean value of the distribution μ and variance σ^2, through the relation

$$\mathrm{P}(\theta \le X \le \theta + d\theta|\mathrm{mean} = \mu, \mathrm{variance} = \sigma^2, \mathrm{normal}) = \mathcal{N}(\theta;\mu,\sigma^2)\, d\theta\,.$$

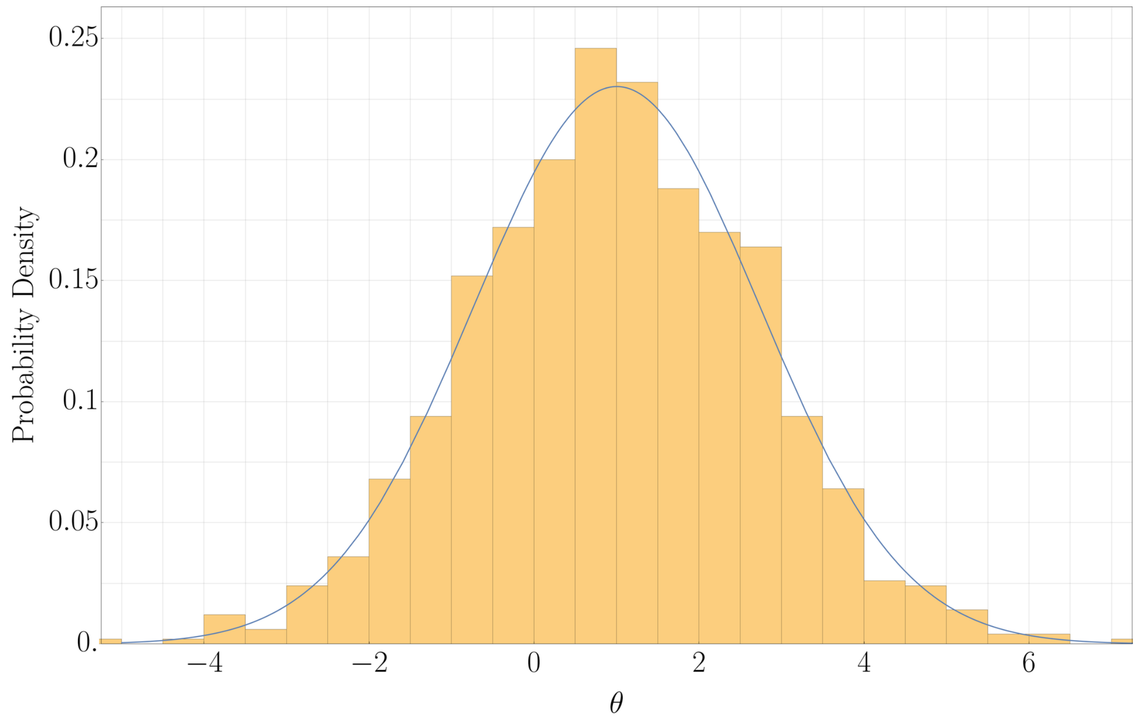


Figure B.1: Plot of the probability density distribution with $\mu_0 = 1$ and $\sigma_0 = \sqrt{3}$ from which we draw the data shown in the (normalized) histogram.

Moreover, consider two different priors, e.g., the case where two scientists have two different context information I_1 and I_2 which lead them to two different prior probabilities $\mathrm{P}(\boldsymbol{\theta}|I_1)$ and $\mathrm{P}(\boldsymbol{\theta}|I_2)$. We plot the two priors considered in Figure B.2.

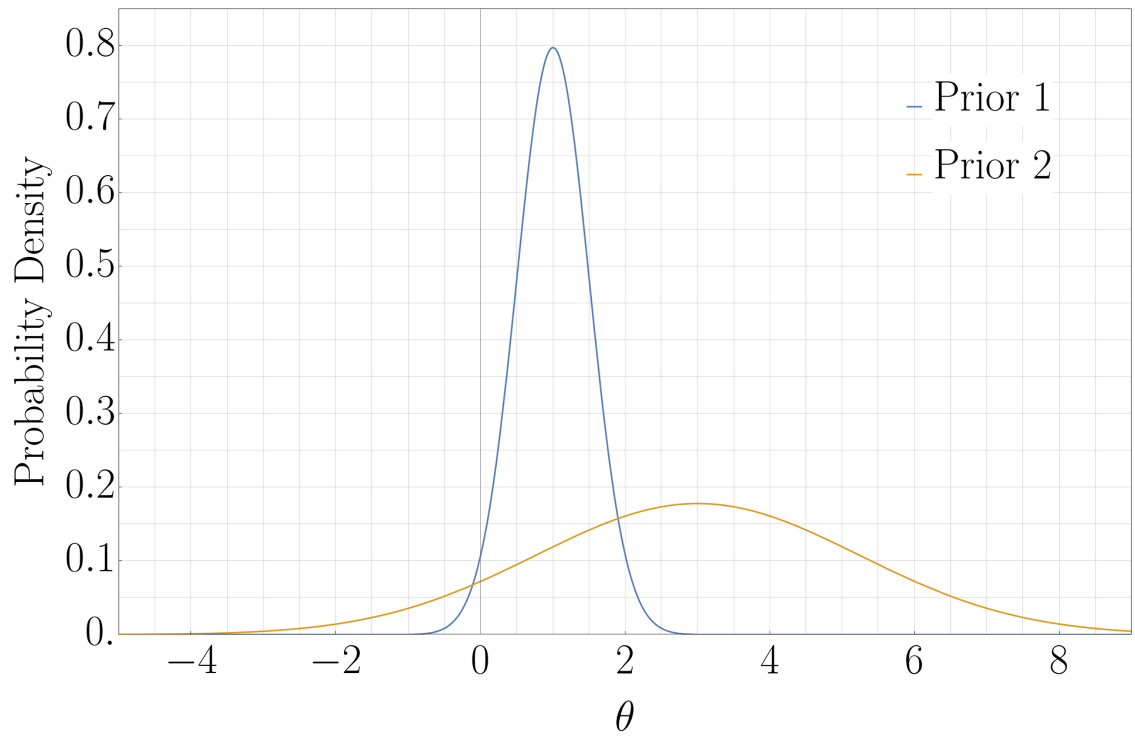
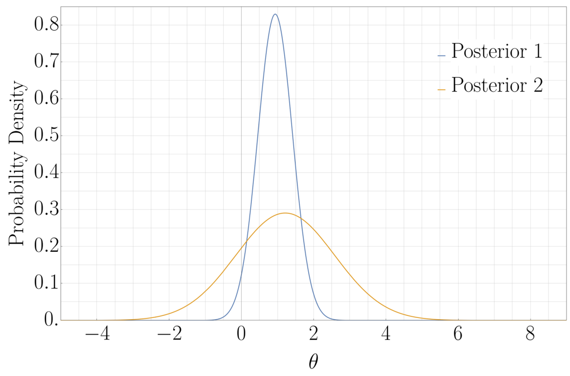
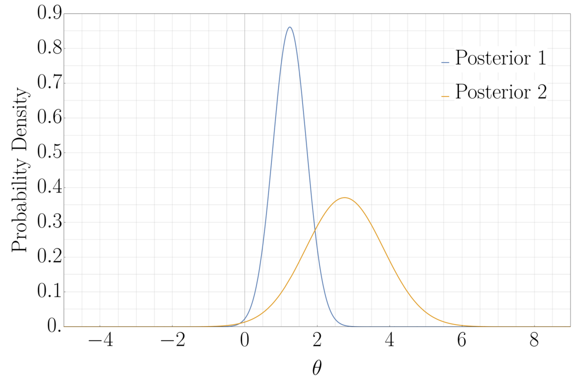


Figure B.2: Plot of the prior probabilities. In this example, we set them to be normal probabilities, respectively with $\mu_1 = 0.5$ and $\sigma_1 = 0.5$ and $\mu_2 = 3$ and $\sigma_2 = \sqrt{5}$.

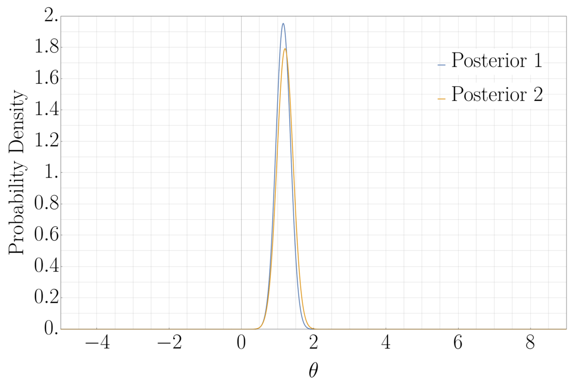
We can use Bayes's theorem (B.20) to compute the two posteriors for the different priors. We consider the first data drawn from the normal distribution in Figure B.1 and compute the likelihood, which is also a normal distribution centered on this data with variance given by σ_0. The posterior probabilities 1 and 2, respectively computed with the priors 1 and 2 in Figure B.2, are available in Figure B.3a. The same procedure can be applied several times, eventually leading to the same posterior distribution independently of the choice of the prior, as we can see in Figure B.3d after the application of Bayes's theorem 180 times.



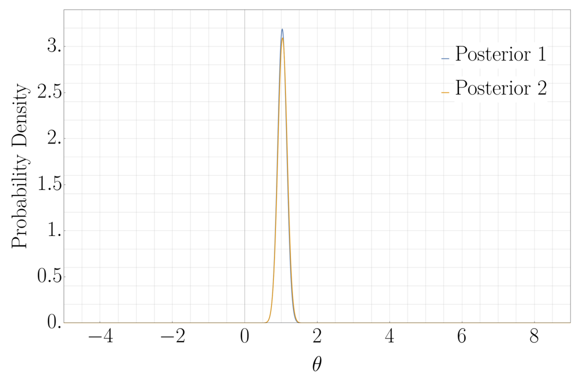
(a) 1 data



(b) 2 data



(c) 60 data



(d) 180 data

Figure B.3: Plot of the posterior probabilities 1 and 2, respectively computed with the priors 1 and 2, in Figure B.2. The number of data refers to the number of applications of the Bayes's theorem.

Therefore, although two scientists might have different context information I, and therefore consider two different priors, in the limit of a large number of data they will eventually agree on the same value of the parameter.

B.5 Parameter estimation

One of the interesting application of the Bayes's theorem in physics is the estimation of the parameters $\boldsymbol{\theta}$ of a theoretical model $\mathcal{M}$, using the experimental data $\boldsymbol{d}$. The picture is the same of the data analysis case (B.20)

$$\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d},\mathcal{M}) = \frac{\mathrm{P}(\boldsymbol{\theta}|\mathcal{M})\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta},\mathcal{M})}{\int d\boldsymbol{\theta}'\,\mathrm{P}(\boldsymbol{\theta}'|\mathcal{M})\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta}',\mathcal{M})}\,, \tag{B.22}$$

where the context I is replaced by the model $\mathcal{M}$, and we explicitly write the denominator $\mathrm{P}(\boldsymbol{d}|M)$ as the normalization factor. The key result is indeed the posterior $\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d},M)$, which gives the constraint on the parameters conditioned to the experimental data $\boldsymbol{d}$ and the model $\mathcal{M}$. Note that the likelihood is also defined in the literature as $\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta},\mathcal{M}) \equiv \mathcal{L}(\boldsymbol{\theta})$, which contains information on the model parameter $\boldsymbol{\theta}$, and implicitly on the model $\mathcal{M}$.

B.5.1 Marginalization

As mentioned in the introduction, one of the key features of Bayesian probability is that we can isolate the conditional probability distribution of only some interesting variables from a distribution that might have many other *nuisance* parameters. This process is called *marginalization*, and it consists on simply summing/integrating the probability over all possible values of the nuisance parameters. A common example in physics might be the presence of an uninteresting noise governed by some nuisance parameters, that we want to factor out from the probability distribution of $\boldsymbol{\theta}$.

For instance, consider a model $\mathcal{M}$ with parameters $\boldsymbol{\theta} = \{\theta_1, \theta_2, \theta_3\}$, where θ_2 and θ_3 are nuisance parameters. We can obtain the posterior distribution of the θ_1 parameter only, integrating the total posterior distribution over the other parameters as

$$\mathrm{P}(\theta_1|\boldsymbol{d}, \mathcal{M}) = \int_{-\infty}^{\infty} d\theta_2' \int_{-\infty}^{\infty} d\theta_3' \, \mathrm{P}(\theta_1, \theta_2', \theta_3'|\boldsymbol{d}, \mathcal{M}) \,. \tag{B.23}$$

B.5.2 Posterior sampling

The analytical form of the posterior $\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d}, M)$, both normalized and unnormalized, might be difficult to obtain. And even if we are just interested in the peaks of the posterior, they can be hard to find too.

An alternative solution for computing the posterior is to use the *sampling* method. We generate N samples $\{\boldsymbol{\theta}_i\}$ from the posterior distribution, which can summed to obtain an approximate version of the posterior

$$\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d}, M) \cong \frac{1}{N} \sum_{i=1}^{N} \delta(\boldsymbol{\theta} - \boldsymbol{\theta}_i) \,, \tag{B.24}$$

where δ is the Dirac delta and we assume for simplicity that the samples are equally-weighted. Although the posterior is not usually a series of peaks, but a smooth function of the parameters, this approximated version is useful to estimate derived quantities or binned/smoothed versions of the posterior itself. For instance, the integral of a function $f = f(\boldsymbol{\theta})$ weighted with the posterior, can be computed from the sampling using

$$\int d\boldsymbol{\theta}' \, f(\boldsymbol{\theta}') \, \mathrm{Pr}(\boldsymbol{\theta}'|\boldsymbol{d}, M) \cong \frac{1}{N} \sum_{i=1}^{N} f(\boldsymbol{\theta}_i) \,. \tag{B.25}$$

B.5.3 Incomplete representations of the posterior

The posterior distribution $\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d}, \mathcal{M})$ is the full result of the application of the Bayes's theorem for the parameter estimation, while any reduced form (or *incomplete representation*), such as the marginalized posterior, loses information. But, as already mentioned, the analytical form of the posterior distribution can not always be found.

Another approach is to describe the posterior distribution using just a few numbers, or some plots. The obvious limit of such incomplete representations will be the fact that they can not fully represent an arbitrary density in even one parameter. However, in most cases they can give a good representation of the posterior distribution. In the following, we cite some of the most common incomplete posterior representations.

Maximum a posteriori probability. The *Maximum a Posteriori Probability* (MAP) is the value $\hat{\boldsymbol{\theta}}$ of $\boldsymbol{\theta}$ for which we have the maximum of $\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d}, \mathcal{M})$

$$\hat{\boldsymbol{\theta}}_{\mathrm{MAP}} = \arg\, \max_{\boldsymbol{\theta}} \, \mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d}, \mathcal{M}) \,. \tag{B.26}$$

This value can be useful to obtain the best possible value of the parameters conditioned to the data and the model. However, it might fail if the posterior is flat or it has more maximums, leading to a choice that might be very far from most of the posterior.

Posterior mean. The *posterior mean* is defined as

$$\hat{\boldsymbol{\theta}}_{\text{mean}} = \int d\boldsymbol{\theta}'\, \boldsymbol{\theta}'\, \mathrm{P}(\boldsymbol{\theta}'|\boldsymbol{d}, \mathcal{M})\,. \tag{B.27}$$

From the definition, $\hat{\boldsymbol{\theta}}_{\text{mean}}$ is more global than $\hat{\boldsymbol{\theta}}_{\text{MAP}}$, but it might not exist if the integral is not defined (e.g. if the tails of the posterior distributions are not negligible). Moreover, depending on the posterior distribution form, it might happen that $\mathrm{P}(\boldsymbol{\theta}'_{\text{mean}}|\boldsymbol{d}, \mathcal{M}) \cong 0$

Credible regions. We can complement the single number representations with measurements of the width of the posterior distribution. This approach consists in defining some *credible regions* that include a specific fraction f of the posterior probability, usually multiple of the normal distribution σ (1σ for $f = 68\%$, 2σ for $f = 95\%$, ...). However note that this definition is ambiguous, because there are infinite ways to create regions enclosing the fraction f of the posterior probability.

For instance, in the case of a single parameter posterior distribution (or the marginalized posterior with one parameter left), any interval $\theta_{\text{min}} \leq \theta \leq \theta_{\text{max}}$ that satisfies

$$f = \mathrm{P}(\theta_{\text{min}} \leq \theta \leq \theta_{\text{max}}|\boldsymbol{d}, \mathcal{M}) = \int_{\theta_{\text{min}}}^{\theta_{\text{max}}} d\theta'\, \mathrm{P}(\theta'|\boldsymbol{d}, \mathcal{M})\,, \tag{B.28}$$

is valid.

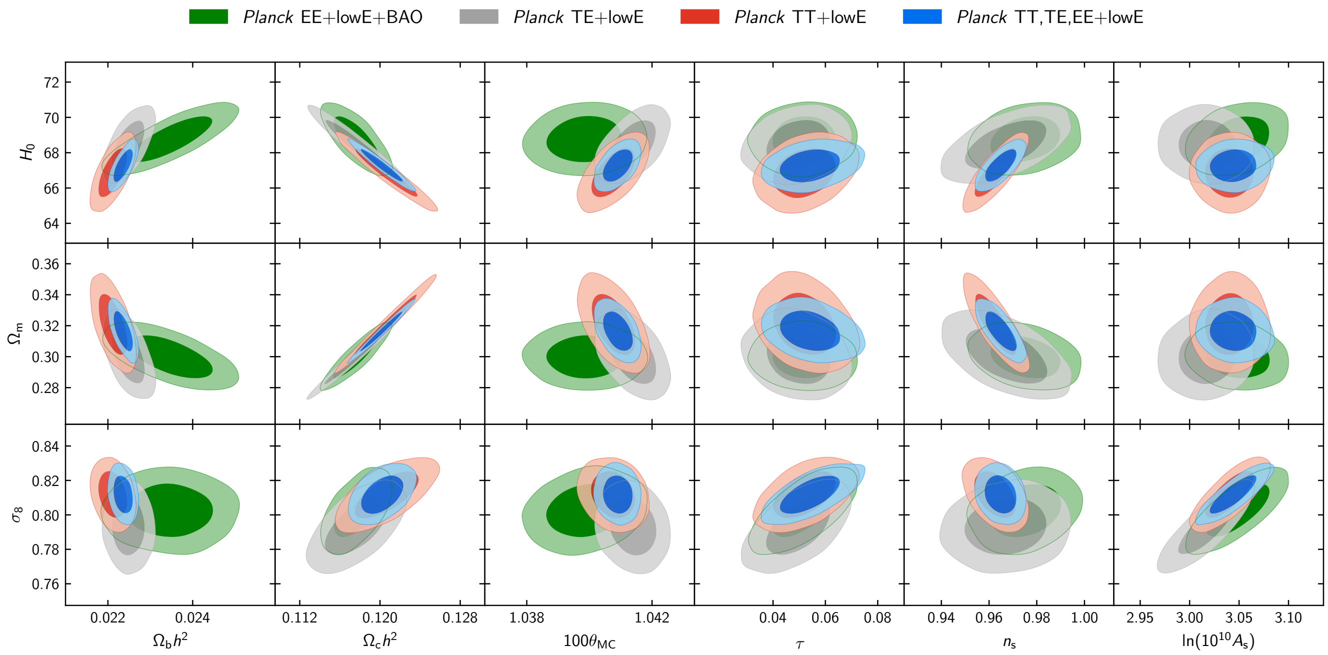


Figure B.4: Plot of the 2018 data analysis results of the Planck experiment (courtesy of [5]). Different colors corresponds to different datasets, and the parameters on the axes are standard model cosmological parameters. The different credible regions are computed from the posterior with the HPD region definition (B.29). The regions of 1σ and 2σ have respectively darker and lighter versions of datasets colors.

The most common region choice is the *Highest Posterior Density* (HPD) region, which is usually uniquely defined. The region is defined as the collection of the parameter values of the posterior which satisfy $\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d}, \mathcal{M}) \geq p$, where p is the value defining the region. In other words, the region is defined by

$$f = \int d\theta'\, \mathrm{P}(\theta'|\boldsymbol{d}, \mathcal{M}) \Theta \left[\mathrm{P}(\theta'|\boldsymbol{d}, \mathcal{M}) - p\right]\,, \tag{B.29}$$

where $\Theta(x)$ is the Heaviside theta step function. Another interesting fact is that all the parameter values on the boundary of the HPD region are equiprobable, and therefore all the models with those parameters are equally probable. Moreover, since all the parameter values inside the HPD region are more probable than points outside the region, the HPD regions are the smallest definable regions with a fraction f. An example from cosmology is shown in Figure B.4.

B.6 Numerical sampling

In the previous sections, we discussed how to use data to update the description of the world we have employing Bayes's theorem. The missing step to obtain a quantitative solution is to find a way to generate the aforementioned sampling of the posterior. In the following, we introduce one possible sampling method based on Markov Chain Monte Carlo (MCMC) and the Metropolis–Hastings (MH) algorithm.

B.6.1 Markov Chains

A Markov Chain is an *ordered* sequence of points $\{\boldsymbol{\theta}_s\} = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_{N_s}\}$ (N_s is the number of sampling points in the chain), where the position of any point $\boldsymbol{\theta}_s$ depends only on $\boldsymbol{\theta}_{s-1}$ and not on other points of the chain. In other words, any point $\boldsymbol{\theta}_s$ (except the first) is drawn from a distribution $\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1})$.

The algorithm is the following:

(i) compute the first sample $\boldsymbol{\theta}_\mathbf{1}$, which in general is chosen randomly. Usually more chains are computed in order to check if the result is *robust* against the change of this initial parameter values;

(ii) for all other $N_s - 1$ points in the chain, starting from $\boldsymbol{\theta}_2$, we draw a trial point $\boldsymbol{\theta}_{\text{trial}}$ from a *proposal* distribution $\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1}, \text{trial})$, which should depend only on the previous samples $\boldsymbol{\theta}_{s-1}$. The trial denotes the proposal algorithm we consider, whose form is usually chosen to increase the efficiency of the algorithm, i.e. to minimize the number of points needed to obtain a reasonably good sampling;

(iii) accept the trial point $\boldsymbol{\theta}_{\text{trial}}$ with an *acceptance* probability $\mathrm{P}(\text{accept}|\boldsymbol{\theta}_{\text{trial}}, \boldsymbol{\theta}_{s-1})$. Also a careful choice of the acceptance probability can boost the efficiency of the algorithm;

(iv) if the trial point is accepted, then we set $\boldsymbol{\theta}_s = \boldsymbol{\theta}_{\text{trial}}$, otherwise $\boldsymbol{\theta}_s = \boldsymbol{\theta}_{s-1}$. It is crucial not to discard the points even if $\boldsymbol{\theta}_s = \boldsymbol{\theta}_{s-1}$, but to *save* them in the Markov chain;

(v) the steps above are repeated for a sufficient amount of iterations until we reach *convergence*, whose definition generally depends on the application.

The choice of the proposal and acceptance probabilities are what define a particular MCMC algorithm. These probabilities can also be condensed into a single probability distribution $\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1})$. We can show this starting from the conditional distribution of $\boldsymbol{\theta}_s$

$$\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{\text{trial}}, \boldsymbol{\theta}_{s-1}) = \mathrm{P}(\text{accept}|\boldsymbol{\theta}_{\text{trial}}, \boldsymbol{\theta}_{s-1})\delta(\boldsymbol{\theta}_s - \boldsymbol{\theta}_{\text{trial}}) + \left[1 - \mathrm{P}(\text{accept}|\boldsymbol{\theta}_{\text{trial}}, \boldsymbol{\theta}_{s-1})\right]\delta(\boldsymbol{\theta}_s - \boldsymbol{\theta}_{s-1})\,. \quad \text{(B.30)}$$

Then, marginalizing over $\boldsymbol{\theta}_{\text{trial}}$, we obtain

$$\begin{aligned} \mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1}) &= \int d\boldsymbol{\theta}'_{\text{trial}}\, \mathrm{P}(\boldsymbol{\theta}'_{\text{trial}}|\boldsymbol{\theta}_{s-1}, \text{trial})\, \mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}'_{\text{trial}}, \boldsymbol{\theta}_{s-1}) = \\ &= \mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1}, \text{trial})\, \mathrm{P}(\text{accept}|\boldsymbol{\theta}_s, \boldsymbol{\theta}_{s-1}) + \\ &\quad + \delta(\boldsymbol{\theta}_s - \boldsymbol{\theta}_{s-1})\left[1 - \int d\boldsymbol{\theta}'\, \mathrm{P}(\boldsymbol{\theta}'|\boldsymbol{\theta}_{s-1}, \text{trial})\, \mathrm{P}(\text{accept}|\boldsymbol{\theta}', \boldsymbol{\theta}_{s-1})\right]. \end{aligned} \quad \text{(B.31)}$$

This form of the probability $\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1})$ does not necessarily produce samples from a target distribution $p(\boldsymbol{\theta})$. In fact, no dependence on any p has been introduced. However, there is a rule we can exploit to find acceptable forms of the proposal and acceptance distributions which generates a MCMC algorithm that samples a given target distribution p. The starting point is that, at least in the limit of large N_s, if $\boldsymbol{\theta}_{s-1}$ has been drawn from p, we want $\mathrm{P}(\boldsymbol{\theta}_s) = p(\boldsymbol{\theta})$. Consider the probability

$$\begin{aligned}
\mathrm{P}(\boldsymbol{\theta}_s) = &\int d\boldsymbol{\theta}'_{s-1}\, p(\boldsymbol{\theta}'_{s-1})\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}'_{s-1}) = \\
= &\int d\boldsymbol{\theta}'_{s-1}\, p(\boldsymbol{\theta}'_{s-1})\left\{\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}'_{s-1},\mathrm{trial})\,\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_s,\boldsymbol{\theta}'_{s-1}) + \right.\\
&\left. + \delta(\boldsymbol{\theta}_s - \boldsymbol{\theta}'_{s-1})\left[1 - \int d\boldsymbol{\theta}'\,\mathrm{P}(\boldsymbol{\theta}'|\boldsymbol{\theta}'_{s-1},\mathrm{trial})\,\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}',\boldsymbol{\theta}'_{s-1})\right]\right\} = \\
= &\, p(\boldsymbol{\theta}_s) + \int d\boldsymbol{\theta}'_{s-1}\, p(\boldsymbol{\theta}'_{s-1})\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}'_{s-1},\mathrm{trial})\,\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_s,\boldsymbol{\theta}'_{s-1}) - \\
&- \int d\boldsymbol{\theta}'\, p(\boldsymbol{\theta}_s)\,\mathrm{P}(\boldsymbol{\theta}'|\boldsymbol{\theta}_s,\mathrm{trial})\,\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}',\boldsymbol{\theta}_s) = \\
= &\, p(\boldsymbol{\theta}_s) + \int d\boldsymbol{\theta}'\,[p(\boldsymbol{\theta}')\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}',\mathrm{trial})\,\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_s,\boldsymbol{\theta}') - \\
&\quad p(\boldsymbol{\theta}_s)\,\mathrm{P}(\boldsymbol{\theta}'|\boldsymbol{\theta}_s,\mathrm{trial})\,\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}',\boldsymbol{\theta}_s)]\ .
\end{aligned} \tag{B.32}$$

Therefore, if we want $\mathrm{P}(\boldsymbol{\theta}_s) = p(\boldsymbol{\theta}_s)$, we should impose that the integral in the equation above is null, i.e. the proposal and acceptance probabilities satisfies

$$\frac{\mathrm{P}(\boldsymbol{\theta}_2|\boldsymbol{\theta}_1,\mathrm{trial})\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_1,\boldsymbol{\theta}_2)}{\mathrm{P}(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2,\mathrm{trial})\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_2,\boldsymbol{\theta}_1)} = \frac{p(\boldsymbol{\theta}_2)}{p(\boldsymbol{\theta}_1)} \qquad \forall \text{ pairs } \boldsymbol{\theta}_1, \boldsymbol{\theta}_1 \tag{B.33}$$

which is known as the *detailed balance* equation.

B.6.2 Metropolis–Hastings algorithm

The Metropolis–Hastings algorithm (MH) is one of most used class of MCMC algorithm. The full algorithm is the following:

(i) compute the first sample $\boldsymbol{\theta}_1$, which in general is chosen randomly;

(ii) for all other $N_s - 1$ points in the chain, starting from $\boldsymbol{\theta}_2$, we draw a trial point $\boldsymbol{\theta}_{\mathrm{trial}}$ from a *proposal* distribution $\mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1},\mathrm{trial})$. The form of the proposal distribution is not fixed in the MH algorithm, and can be chosen case by case in order to obtain the most efficient sampling;

(iii) accept the trial point $\boldsymbol{\theta}_{\mathrm{trial}}$ with an *acceptance* probability

$$\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_{\mathrm{trial}},\boldsymbol{\theta}_{s-1}) = \min\left[\frac{p(\boldsymbol{\theta}_{\mathrm{trial}})}{p(\boldsymbol{\theta}_s)}, 1\right] = \min\left\{e^{\ln[p(\boldsymbol{\theta}_{\mathrm{trial}})]-\ln[p(\boldsymbol{\theta}_s)]}, 1\right\}\ . \tag{B.34}$$

This probability is unity if the trial point is more probable than the previous one, and it is null only if $p(\boldsymbol{\theta}_{\mathrm{trial}})$ is null. The second form might be useful when the numerical precision is not enough to use the first expression. Note also that this probability satisfies the detailed balance equation (B.33), and therefore the MH algorithm correctly samples the target distribution $p(\boldsymbol{\theta})$;

(iv) if the trial point is accepted, then we set $\boldsymbol{\theta}_s = \boldsymbol{\theta}_{\mathrm{trial}}$, otherwise $\boldsymbol{\theta}_s = \boldsymbol{\theta}_{s-1}$;

(v) the steps above are repeated for a sufficient amount of iterations until we reach *convergence*.

In any MH algorithm, we have the freedom to choose the proposal distribution, which can affect the efficiency of the algorithm. For instance, consider the two extreme cases:

(i) if the proposal distribution is very concentrated with respect to the scales of the target density variations, for all $\boldsymbol{\theta}_{\rm trial}$ we have $p(\boldsymbol{\theta}_{\rm trial}) \cong p(\boldsymbol{\theta})$. The acceptance probability is therefore $\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_{\rm trial}, \boldsymbol{\theta}_{s-1}) \cong 1$ for all trial points, and therefore almost all trial points are accepted, slowing down the sampling process. An analogy would be a cosmologist studying the large scale galaxy distribution probing the space with steps of μPc;

(ii) if the proposal distribution is too much broader with respect to the scales of the target density variations, we have the opposite behaviour. For instance, if $p(\boldsymbol{\theta}_{s-1})$ is big, such a proposal distribution will likely propose a $\boldsymbol{\theta}_{\rm trial}$ far away from the high density region of the target distribution, for which $\mathrm{P}(\mathrm{accept}|\boldsymbol{\theta}_{\rm trial}, \boldsymbol{\theta}_{s-1}) \cong 0$. Therefore almost all steps are rejected, leading to a very inefficient sampling and a chain of a huge number of equal points. On the same analogy of the previous case, it would be a cosmologist probing the space with steps of YPc.

Therefore it is good practice to choose a proposal distribution with an intermediate acceptance ratio, in general between 30%-40%. Obviously these figures depend on the problem. The most used proposal distribution is a multi-variate normal distribution

$$\begin{aligned} \mathrm{P}(\boldsymbol{\theta}_s|\boldsymbol{\theta}_{s-1}, \mathrm{trial}) &= \mathcal{N}(\boldsymbol{\theta}_{\rm trial}; \boldsymbol{\theta}_s, \boldsymbol{\Sigma}) = \\ &= \frac{1}{\sqrt{(2\pi)^N \det(\Sigma)}} \exp\left[-\frac{1}{2}(\boldsymbol{\theta}_{\rm trial} - \boldsymbol{\theta}_s)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\theta}_{\rm trial} - \boldsymbol{\theta}_s)\right], \end{aligned} \tag{B.35}$$

where N is the number of parameters $\{\theta_i\}$ and $\boldsymbol{\Sigma}$ is the covariance matrix (the generalization of the uni-variate normal distribution variance σ^2 for the multi-variate normal distribution).

If we do not have any information about the parameters, it is common to start with the assumption of no correlation between the parameters, i.e. with a diagonal covariant matrix $\boldsymbol{\Sigma}$. To increase the efficiency of the algorithm, once we finish a chain, we can start another one *from scratch* using the informations of the first. The mean value over the samples for these additional chains is

$$\hat{\theta}_{p,\rm mean} = \frac{\sum_{s=1}^{N_s} W_s \theta_{p,s}}{\sum_{s=1}^{N_s} W_s}. \tag{B.36}$$

while the covariance matrix is

$$\Sigma_{p,p'} = \frac{\sum_{s=1}^{N_s} W_s \left(\theta_{p,s} - \hat{\theta}_{p,\rm mean}\right)\left(\theta_{p',s} - \hat{\theta}_{p',\rm mean}\right)}{\sum_{s=1}^{N_s} W_s}, \tag{B.37}$$

where W_s are the weights associated to the samples $\{\theta_s\}$, which can be neglected if we choose to weight all samples the same. It is important to start the computation of new chains from scratch, because for the detailed balance equation (B.33) we can not combine different proposal distributions to compute the same chain if we want to probe the same target distribution. Finally note that the equations for the mean value (B.36) and the covariance matrix (B.37) are general, and can be used also in the case of non-normal distributions.

B.6.3 Chain convergence

In the algorithms above, in particular in the steps (v), we did not quantitatively specify what is a *sufficient amount of iterations* we should perform before reaching convergence. There is no defined rule on how to choose the stopping step of an iteration, but there are some heuristic convergence tests that can be applied. The main reason of the heuristic nature of these tests is that they can point out some problems in the sampling, but even if passed they do not guarantee that the the sampling has been effective.

The Gelman and Rubin test [92] is one of the most used. It is based on the idea that different *independent* chains (computed from scratch independently to the others), and the incomplete representation quantities, should converge to the same distribution. If they do not, it might be a symptom that the sampling is not good enough, e.g. different chains are sampling different regions of the parameter space. The test algorithm, performed on N_c chains with equal length N_s with elements $\{\theta_{c,s}\}$, is the following

(i) compute the mean of each chain

$$\bar{\theta}_c \equiv \frac{1}{N_s} \sum_{s=1}^{N_s} \theta_{c,s}\,; \tag{B.38}$$

(ii) compute the variance of each chain

$$\sigma_c^2 \equiv \frac{1}{N_s - 1} \sum_{s=1}^{N_s} \left(\theta_{c,s} - \bar{\theta}_c\right)^2 \tag{B.39}$$

(iii) compute the mean of all chains, which is the best estimate for the mean of the distribution we can obtain from the combined data from all chains

$$\bar{\theta} \equiv \frac{1}{N_c} \sum_{c=1}^{N_c} \frac{1}{N_s} \sum_{s=1}^{N_s} \theta_{c,s} = \frac{1}{N_c} \sum_{c=1}^{N_c} \bar{\theta}_c\,; \tag{B.40}$$

(iv) compute the average of the individual chains variances

$$\sigma_{\text{chain}}^2 \equiv \frac{1}{N_c} \sum_{c=1}^{N_s} \sigma_c^2\,; \tag{B.41}$$

(v) compute the variance of the chains means

$$\sigma_{\text{mean}}^2 \equiv \frac{1}{N_c} \sum_{c=1}^{N_c} \left(\bar{\theta}_c - \bar{\theta}\right)^2\,; \tag{B.42}$$

(vi) compute the Gelman–Rubin ratio

$$\hat{R} = \sqrt{\frac{1}{\sigma_{\text{chain}}^2} \left[\left(1 - \frac{1}{N_c}\right) \sigma_{\text{chain}}^2 + \frac{1}{N_c} \sigma_{\text{mean}}^2\right]}\,; \tag{B.43}$$

(vii) assess the converge with the ratio $\hat{R}$. If the chains are sampling the same regions, we expect the variances computed from the individual chains and from the chains means to be approximately the same, i.e., $\sigma_{\text{mean}}^2 \cong \sigma_{\text{chain}}^2$, and therefore $\hat{R} \cong 1$. On the contrary, if $\sigma_{\text{chain}}^2 < \sigma_{\text{mean}}^2$ (the broadness of each chain is smaller than the combined one, and therefore the individual chains are probing different regions), then $\hat{R} > 1$. The usual choice for convergence is $\hat{R} < 1.2$.

Note that the test should be performed on all different parameters θ of the model $\mathcal{M}$.

B.6.4 Post-processing operations

Once we compute the Markov chain (with any MCMC algorithm), to assess the correctness and the robustness of the results, it might be necessary to perform some operations and checks on the resulting chains.

Acceptance ratio If we save the number of accepted steps during the sampling (or more inefficiently we compute it on the final chain looking at the number of equal sample points), we can compute the acceptance ratio. We expect this value to be nor too small nor close to 1.

For instance, to avoid long runs and/or inefficient samplings using the MH algorithm, we expect the acceptance ratio to be around 40%. If this is not the case, the proposal distribution might be not suited for the problem, e.g., in the case of a normal multi-variate proposal distribution (B.35), the covariance matrix entries might be the culprits.

Burn-in As explained in the first step (i) of the algorithms, the first sample is taken randomly. This might introduce a problem since this point might start a sampling of a region with low density which would have never been probed if the initial point was chosen differently. The most common procedure, called *burn-in*, is to discard the first part of the final chain. Although there is no general rigorous algorithm for choosing how long the discarded chain should be, some heuristic rules have been formulated. A simple rule is based on the fact that any sample which has an appreciable probability (with respect to the peak probability sampled) might have been a plausible first sample if it were possible to draw it from the target distribution. Under the assumption that the chain has eventually reached the region(s) of high probability, the samples that are generated after it has first reached this high region are acceptable.

Correlation Some MCMC algorithms might introduce correlation within samples. This is not necessarily a problem, as the chains can be post-processed. The standard way to quantify the correlation is to compute the *auto-correlation function* defined for *lags* $\Delta = 0, 1, \dots N_s - 1$ (N_s being the number of samples) and for each parameter θ_p

$$\hat{C}_{p,\Delta} \equiv \frac{1}{N_s - \Delta} \sum_{s=1}^{N_s-\Delta} \frac{\left(\theta_{p,s} - \hat{\theta}_{p,\text{mean}}\right)\left(\theta_{p,s+\Delta} - \hat{\theta}_{p,\text{mean}}\right)}{\hat{C}^2_{p,p}}\,, \tag{B.44}$$

where the mean value $\hat{\theta}_{p,\text{mean}}$ is defined in equation (B.36), and the covariance $\hat{C}^2_{p,p}$ in equation (B.37). For $\Delta = 0$ we obtain $C_{p,0} = 1$ since the numerator is exactly $\hat{C}^2_{p,p}$. For bigger values of the lag, if the samples in the chain are uncorrelated we expect $C_{p,\Delta>0} = 0$ for all $\Delta > 0$. Usually this is not the case, and the auto-correlation starts near unity and drops to 0 increasing the lag. The worst case is when $C_{p,\Delta}$ is not null for all lags, which implies a high correlation between the samples. An example of the auto-correlation function behaviour is available in Figure B.5.

To remove the correlation between data, we preserve only one sample every $\tilde{\Delta}$ samples, where $\tilde{\Delta}$ is the lag for which $C_{p,\Delta}$ is less than a certain threshold value. This procedure is called *thinning*. Note that, in the case of more parameters, we should evaluate the auto-correlation function for each of them; then we should apply the thinning procedure using the bigger $\tilde{\Delta}$ among the ones computed for each parameter auto-correlation function. This procedure creates a loss of information because the new chains will be $N_s/\tilde{\Delta}$ long. However, the thinning can greatly simplify the statistical properties of the new chains.

B.6.5 Parameters correlation

Once we obtain a certain sampling of a target distribution, we can perform some operations on the results in order to obtain informations about the parameters of the model $\mathcal{M}$ considered. One test is based on the Person coefficients $\rho_{p,p'}$ between two parameters θ_p and $\theta_{p'}$, is defined as

$$\rho_{p,p'} \equiv \frac{\hat{C}_{p,p'}}{\sqrt{\hat{C}_{p,p}\hat{C}_{p',p'}}}\,. \tag{B.45}$$

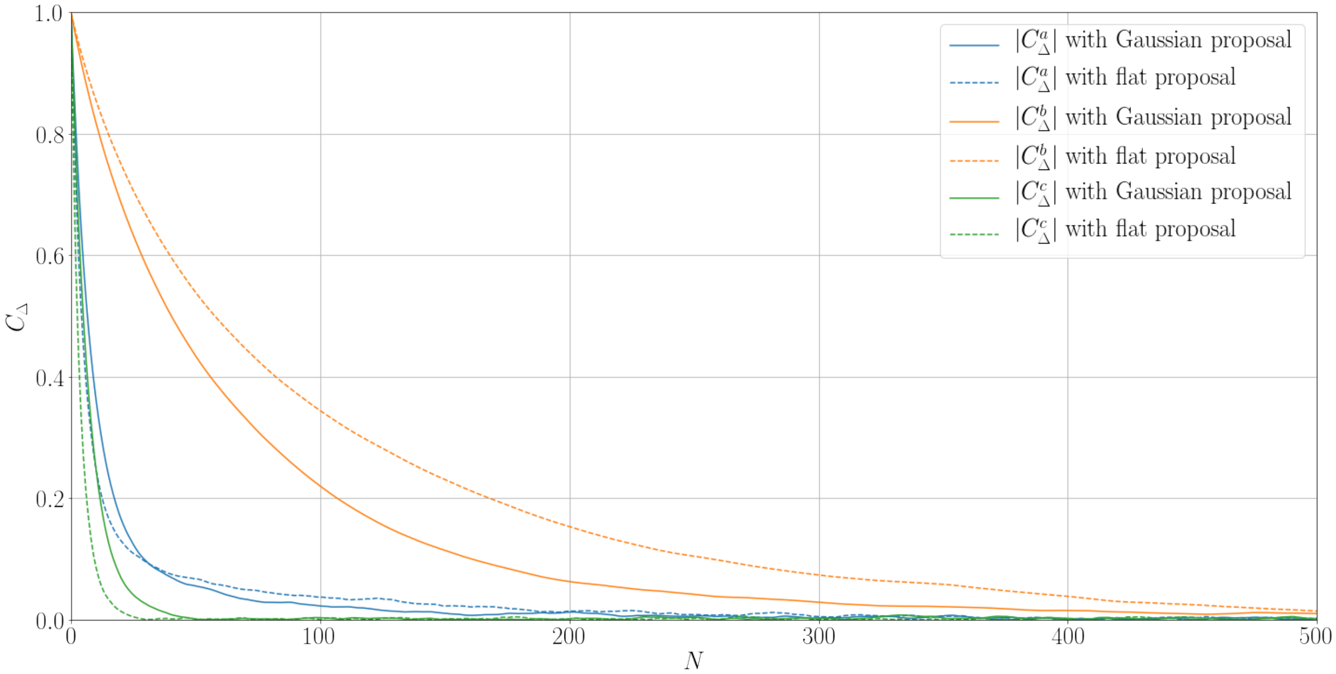


Figure B.5: Plot of the auto-correlation function of a model $\mathcal{M}$ with parameters a, b and c. Two proposal distributions are considered, one is the normal (Gaussian) multi-variate distribution, the other is a flat (constant) distribution. Beside the differences between the two proposal distributions, we can appreciate the strong correlation between the samples for the b parameter. In this case, if we choose the $C_{b,\Delta}$ threshold for thinning to be 0.1, the new approximately uncorrelated chain can be build from the original one taking one point every $\cong 200$.

A value of $|\rho_{p,p'}| < 0.3$ usually denotes a small correlation between the two parameters, while bigger values denote a strong correlation. The value of ρ can be positive, for which we have linear correlation, i.e. $\theta_p = c\,\theta_{p'}$ with $c > 0$); or negative in the case of inverse linear correlation, i.e. $\theta_p = -c\,\theta_{p'}$ with $c > 0$. Therefore the Pearson coefficients can be useful to assess the correlation of the parameters of a model $\mathcal{M}$ that becomes apparent once we add data into the inference problem to compute the posterior.

B.7 Conclusion

In this Chapter we introduce some aspects of the Bayesian probability. Its main tool is the Bayes's theorem (B.9)

$$\mathrm{P}(A|B,I) = \frac{\mathrm{P}(A|I)\mathrm{P}(B|A,I)}{\mathrm{P}(B|I)}\,, \tag{B.46}$$

which links the statistics statements A and B by means of a mathematically well-defined probability (Cox's axioms). A more useful form of the Bayesian theorem in the context of data analysis is given by (B.22)

$$\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d},\mathcal{M}) = \frac{\mathrm{P}(\boldsymbol{\theta}|\mathcal{M})\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta},\mathcal{M})}{\int d\boldsymbol{\theta}'\,\mathrm{P}(\boldsymbol{\theta}'|\mathcal{M})\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta}',\mathcal{M})}\,, \tag{B.47}$$

which updates the values of the parameters $\boldsymbol{\theta}$ of a model $\mathcal{M}$, using the data $\boldsymbol{d}$ coming from the likelihood $\mathrm{P}(\boldsymbol{d}|\boldsymbol{\theta},\mathcal{M})$, to obtain the posterior probability of the parameters conditioned to the data $\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d},\mathcal{M})$.

This Bayes's theorem is especially useful to estimate the parameters of a model $\mathcal{M}$ using the data from experiments. However, although the Bayes's theorem is apparently simple, it might be difficult to obtain an analytical form of the posterior distribution $\mathrm{P}(\boldsymbol{\theta}|\boldsymbol{d},\mathcal{M})$. This justifies the introduction of the Markov Chain Monte Carlo (MCMC) methods, which provides a numerical approximation of the posterior. In particular, in this section, we focused on the Metropolis–Hastings algorithm. Finally, we also defined some diagnostic tests, such as the Gelman–Rubin test, for chain convergence conditions.

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