UNIVERSITAT DE BARCELONA

Towards a non-perturbative description of cosmological inflation

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Tesi Doctoral

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Universitat de Barcelona

Setembre, 2023

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Towards a non-perturbative description of cosmological inflation

Memòria presentada per optar al grau de doctor per la Universitat de Barcelona.

Programa de doctorat en Física.

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Barcelona, Setembre de 2023

ABSTRACT

From the observation of the cosmic microwave background radiation (CMBR) we know that the universe have the same temperature for all direction in the sky, up to tiny fluctuations of order 10^{-5}. This tell us that the universe is isotropic on scales larger than $\sim$ 75 Megaparsec to at least one part in 100000. The leading paradigm for explaining this observational data is that the universe underwent a period of accelerated expansion in its earliest stages, called cosmological inflation (or simply inflation from now on).

Inflation does not only give a convincing explanation for the homogeneity and isotropy of the universe, but also provides a causal mechanism for generating anisotropies on cosmological scales. These anisotropies result from the amplification of the unavoidable vacuum quantum excitations of the gravitational and matter fields due to the accelerated expansion. In particular, it is possible to explain the almost scale invariant power spectrum of the CMBR temperature map with a very simple inflationary regime called Slow Roll (SR) inflation, in which the acceleration of the universe is driven by a scalar field which is slowly rolling down a potential at almost constant speed.

Quantum fluctuations are usually assumed to be small enough such that they are well described as perturbations over an homogeneous and isotropic space-time background. This approach is commonly known as cosmological perturbation theory. However rare large quantum fluctuations can also be randomly generated during inflation. These large inhomogeneities are of great interest because they can lead to the formation of Primordial Black Holes (PBH) and the probability of its generation is related with the amplitude of the power spectrum.

Both the amplitude of the power spectrum and the non-gaussianities measured at the CMBR are too small to generate a relevant amount of large fluctuations. In order to form enough PBH that could represent for example a significant fraction of the dark matter, we need to exponentially enhance the amplitude of the power spectrum on scales which are not probed by the CMBR, for which a violation of SR is needed.

Although the growth of the power spectrum can be described at leading order in perturbation theory, the description of the tail of the Probability Distribution Function (PDF), where the large inhomogeneities are located, must be done beyond linear per-

turbation theory, hopefully in a non-perturbative way. To do that we study two main approaches that aim to describe inflation in a non-perturbative way, the δN formalism and the stochastic approach.

Both approaches are based on gradient expansion, which assumes that the effect of quantum fluctuations whose characteristic wavelength is much larger than the Hubble radius is well described by an ensemble of locally homogeneous and isotropic patches, where spatial gradients are negligible. Contrary to cosmological perturbation theory, the gradient expansion is valid for any amplitude of local over-densities. In this thesis we show that spatial gradients and the momentum constraint of general relativity play an essential role when we use global coordinates, which are necessary to describe the statistical properties of the inhomogeneities by comparing different patches. As a byproduct we find a symmetry of the perturbative Einstein equations in the long-wavelength limit and in Newtonian gauge related to a time-dependent solution for the curvature perturbation, which becomes important beyond SR. This extends an earlier result of Weinberg, where only a constant solution was recovered.

The δN formalism and the stochastic inflation represent consistent ways of providing initial conditions to gradient expansion. In the δN formalism, initial conditions on the field fluctuations are perturbatively given. On the other hand, the idea of stochastic inflation is fully non-perturbative. In this approach, the long-wavelength part of the field follows the evolution dictated by gradient expansion and the short-wavelength part act as a random noise continuously changing local trajectories. Although the amplitude of the noise is computed using linear perturbation theory and it is small by definition, its cumulative behaviour can induce non-perturbative effects in the local patch.

During this thesis we formulate for the first time a stochastic approach to inflation which includes spatial gradients and the momentum constraint and hence it is in principle able to describe the correct long-wavelength dynamics of inflationary inhomogeneities in a non-perturbative way and at all order in the slow-roll parameters. To test our results, we show that for any inflationary regime, the stochastic inflation so formulated, precisely reproduces the results of perturbative correlators in all regimes in which perturbation theory is supposed to work. This is the first step towards the computation of the tail of the PDF of inflationary density perturbations, where large non-perturbative fluctuations important for PBHs are located.

We also elucidate that, in order to take into account the whole non-perturbative dynamics of the local patches via stochastic inflation, the noises must be computed over the stochastically corrected local background rather than over the fiducial deterministic global background, as it is typically done in the literature.

RESUMEN

A partir de la observación de la radiación cósmica de fondo de microondas (CMBR) sabemos que el universo tiene la misma temperatura para todas las direcciones en el cielo, hasta pequeñas fluctuaciones del orden de 10^{-5}. Esto nos dice que el universo es isótropo en escalas mayores que ~ 75 Megaparsec hasta al menos una parte en 100000. La teoría más popular para explicar estos datos observacionales es que el universo sufrió un periodo de expansión acelerada en sus primeras etapas, llamado inflación cosmológica (inflación a partir de ahora).

La inflación no sólo ofrece una explicación convincente de la homogeneidad e isotropía del universo, sino que también proporciona un mecanismo causal para generar anisotropías a escalas cosmológicas. Estas anisotropías resultan de la amplificación de las inevitables excitaciones cuánticas en el vacío de los campos gravitatorio y de materia debidas a dicha expansión acelerada. En particular, es posible explicar el espectro de potencia casi invariante de escala en el mapa de temperatura del CMBR con un régimen inflacionario muy simple denominado inflación Slow-Roll (SR), en el que la aceleración del universo está impulsada por un campo escalar que se mueve lentamente en un potencial a velocidad casi constante.

Se suele suponer que las fluctuaciones cuánticas son lo suficientemente pequeñas como para que se describan bien como perturbaciones sobre un fondo espacio-temporal homogéneo e isótropo. Este enfoque se conoce comúnmente como teoría cosmológica de perturbaciones. Sin embargo, durante la inflación también pueden generarse aleatoriamente grandes fluctuaciones cuánticas poco frecuentes. Estas grandes inhomogeneidades son de gran interés porque pueden conducir a la formación de Agujeros Negros Primordiales (PBH) y la probabilidad de su generación está relacionada con la amplitud del espectro de potencia.

Tanto la amplitud del espectro de potencia como las no gaussianidades medidas en el CMBR son demasiado pequeñas para generar una cantidad relevante de grandes fluctuaciones. Para formar suficientes PBH que pudieran representar, por ejemplo, una fracción significativa de la materia oscura, necesitamos aumentar exponencialmente la amplitud del espectro de potencia en escalas que no son sondeadas por el CMBR, para

lo cual se necesita una violación de la inflación SR.

Aunque el crecimiento del espectro de potencia puede describirse en orden lineal en teoría de perturbaciones, la descripción de la cola de la función de distribución de probabilidad (PDF), donde se localizan las grandes inhomogeneidades, debe hacerse más allá de la teoría de perturbaciones lineales, idealmente de forma no perturbativa. Para ello estudiamos dos enfoques que pretenden describir la inflación de forma no perturbativa, el formalismo δN y el enfoque estocástico.

Ambos enfoques se basan en la expansión de gradientes, que supone que el efecto de las fluctuaciones cuánticas cuya longitud de onda característica es mucho mayor que el radio de Hubble está bien descrito por un conjunto de parches localmente homogéneos e isótropos, donde los gradientes espaciales son despreciables. Contrariamente a la teoría cosmológica de perturbaciones, la expansión de gradientes es válida para cualquier amplitud de inhomogeneidades locales. En esta tesis mostramos que los gradientes espaciales y la ecuación para el momento de la relatividad general juegan un papel esencial cuando usamos coordenadas globales, las cuales son necesarias para describir las propiedades estadísticas de las inhomogeneidades comparando diferentes parches. Además, encontramos una simetría de las ecuaciones perturbativas de Einstein en el límite de longitud de onda larga y en el gauge Newtoniano relacionada con una solución dependiente del tiempo para la perturbación de la curvatura, que adquiere importancia más allá de SR. Esto amplía un resultado anterior de Weinberg, en el que sólo se recuperaba una solución constante.

El formalismo δN y la inflación estocástica representan formas coherentes de proporcionar condiciones iniciales a la expansión de gradientes. En el formalismo δN, las condiciones iniciales sobre las fluctuaciones del campo se dan perturbativamente. Por otro lado, la idea de inflación estocástica es totalmente no perturbativa. En este enfoque, la parte de longitud de onda larga del campo sigue la evolución dictada por la expansión de gradiente y la parte de longitud de onda corta actúa como un ruido aleatorio que cambia continuamente las trayectorias locales. Aunque la amplitud del ruido se calcula utilizando la teoría de perturbaciones lineales y es pequeña por definición, su comportamiento acumulativo puede inducir efectos no perturbativos en el parche local.

En esta tesis formulamos por primera vez una inflación estocástica que incluye gradientes espaciales y la ecuación para el momento y, por tanto, es en principio capaz de describir la dinámica correcta de las inhomogeneidades inflacionarias (en el límite longitud de onda larga) de forma no-perturbativa y a todos los órdenes en los parámetros SR. Para comprobar nuestros resultados, mostramos que, para cualquier régimen inflacionario, la inflación estocástica así formulada reproduce con precisión los resultados de los momentos perturbativos en todos los regímenes en los que se supone que funciona la teoría de perturbaciones. Este es el primer paso hacia el cálculo de la cola de la PDF de las perturbaciones de la densidad, donde se localizan las grandes fluctuaciones no perturbativas importantes para los PBHs.

También elucidamos que, para tener en cuenta toda la dinámica no-perturbativa de los parches locales a través de la inflación estocástica, los ruidos deben calcularse sobre el fondo local corregido estocásticamente en lugar de sobre el fondo global determinista y ficticio, como se suele hacer en la literatura.

ACKNOWLEDGEMENT

This thesis would not have been possible without the help and support of many people and institutions. Therefore, it is my duty to acknowledge all those who have helped me during these years.

First of all, I would like to acknowledge financial support, during this thesis, I have been supported by the Spanish MECD (Ministerio de Educación, Cultura y Deporte) fellowship PRE2018-086135. Apart from my fellowship, I have also received financial support from the Unidad de Excelencia Maria de Maeztu Grant No. CEX2019-000918-M, and the Spanish national grants PID2019-105614GB-C22 and PID2019-106515GB-I00.

I would like to thank my supervisor Cristiano Germani. I met him during my master studies when he gave me the opportunity to start a very exciting project about stochastic inflation, after I got the master's degree we fought together to get a fellowship and continue with the project during my PhD. After we got the fellowship he has been supporting and guiding me along these years.

Apart from my supervisor, there has been many professors who have given me the opportunity to work and learn from them. For that, I wish to thank Tomislav Prokopec, with who I had the pleasure to collaborate in my first paper, Vincent Vennin, for all the discussions about stochastic inflation that we have had along these years, Shi Pi, who has offered me the postdoctoral position for the next years and with who I have already started some projects, and Misao Sasaki, who gave me the opportunity to visit the Kavli Institute for the Physics and Mathematics of the Universe (IPMU) in Tokyo and learn from all the people working there, specially from him.

I would like to acknowledge all the people who has been part of this journey: First, I thank my colleagues from the university of Barcelona Ivan, Cristian, Íñigo, Paula, Miguel, Mikel, Aniol, Carlos and Marc for making my daily life in Barcelona much easier, comfortable and enjoyable. I would also like to thank my childhood friends, both from my hometown (Teruel) and my village (Villastar) for making me forget for a while about all the problems that arise when pursuing a PhD or living in a big city when I come back to Teruel. It is amazing how, despite the distance and the lack of daily contact, the connection between true friends is never lost. Thank you peña la unión of

Villastar and la bodegueta of Teruel.

I want to thank my family for their constant support and love, if I can pursuit my dream of becoming a great physicist is because of them. Thank you mom for teaching me that time puts everyone in its right place and that effort does not always have an immediate reward, I have though about that countless times since the beginning of the thesis. Thank you dad for caring and worrying so much about me even when you do not understand why many times I act as I do. Thank you Belén for being so proud of me, even if I do not express it, you have always made me feel a special big brother. I also thank all the people from my family like my "Tata" that, although they do not fully understand what I am doing, they try to understand and care about it.

Finally, I would like to thank my girlfriend (soon wife) Aida. Who would have thought that my first roommate when I arrived in Barcelona would become such an important person in my life?. Thank you for always being there for me and believing in me, even when I could not do it. The completion of this thesis would not have been possible without your laughter, your jokes and your love, even in difficult times. "*Si nunca pensé que el mundo pudiera ser tan cruel es porque tú me sacabas de él*". Our journey together has just started, I love you.

LIST OF PUBLICATIONS

This thesis is based on the following papers

1. D. Cruces, C. Germani and T. Prokopec, "Failure of the stochastic approach to inflation beyond slow-roll," JCAP **03** (2019), 048
2. D. Cruces and C. Germani, "Stochastic inflation at all order in slow-roll parameters: Foundations," Phys. Rev. D **105** (2022) no.2, 023533
3. D. Cruces, C. Germani and A. Palomares, "An update on adiabatic modes in cosmology and δN formalism," JCAP **06** (2023), 002

Also, some of the results of the articles above were recapitulated in the following single-authored review:

1. D. Cruces, "Review on Stochastic Approach to Inflation," Universe **8** (2022) no.6, 334

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CHAPTER 1

Introduction

We can define cosmology as the science concerned with the dynamics of the universe as a whole. Of course this is a very broad definition which depends on what we understand by universe, or in other words, what we consider to be all of space and time and their contents. For example, Anaximander, a pre-Socratic greek philosopher who is widely referred to as the "father of cosmology", believed that everything we could observe was inside a huge spherical shell surrounded by a rim of fire, the earth had a cylindrical shape and was at the center of this sphere and all the stars (including the Sun) were represented by holes in the shell that allowed us to see the bright rim of fire behind it. For him, and for many other phylosophers after him, the universe was that spherical shell and everything inside it. Hence cosmology at that time could be defined as the description of the dynamics of that shell and of the relative positions of the earth, sun and moon. All of this was described by the use of the geometry and mathematics that he learned form his mentor Thales.

Twenty six centuries have now passed since the cosmological model of Anaximander and the understanding of our universe has greatly improved: we will argue why a period of accelerated expansion of the universe called "cosmological inflation" is a plausible way to explain the available observational data. But before that, and in the same way that the cosmological model of Anaximander could not be formulated without the mathematical tools of Thales, we will introduce the mathematical framework of our cosmological model: the General theory of Relativity (GR).

Firstly published by Einstein in 1915 [1], general relativity is the theory that describes gravitation in modern physics. It provides a unified description of gravity as a geometric property of space and time. As we will see, general relativity tell us that space-time and matter are tightly connected. Matter dictates the geometry of the space-time and the geometry of the space-time dictates how matter should move. There are many books and reviews focused on the theory of general relativity [2, 3, 4] so we will not review here how this theory arises, on the other hand, we will pay more attention on how the Einstein's field equation of general relativity can be derived from an action, which will be more useful in the context of this thesis.

1.1 The Einstein-Hilbert action

Although the original derivation of Einstein's field equations of general relativity is different, in this section we will use a modern approach based on the concept of an action, named the Einstein-Hilbert action [5].

The dynamics of a generic 4-dimensional space-time metric $g_{\mu\nu}$, related to a line element $ds^2 = g_{\mu\nu}dx^\mu dx^\nu$ can be described by the Einstein-Hilbert action

$$S_G^{EH} = \frac{M_{PL}^2}{2}\int d^4x\sqrt{-g}R\,, \tag{1.1}$$

where we are using the metric signature $(-,+,+,+)$. In the action (1.1), $M_{PL} = 1/\sqrt{8\pi G} \simeq 2.44 \cdot 10^{18}GeV$ in natural units of $c = \hbar = 1$, is the reduced Planck mass, $d^4x\sqrt{-g}$ is the 4-dimensional volume element, and R is the Ricci scalar (defined as the contraction of the Ricci tensor i.e. $R = R^\mu_\mu$). Note that we can defined the Lagrangian density corresponding to the action (1.1) as $S_G = \int d^4x\mathcal{L}_G$, reason why this formulation of general relativity is sometimes referred as Lagrangian formulation [4].

The stationary-action principle tells us that to recover a physical law, we must demand that variation of this action with respect to the inverse metric to be zero, yielding:

$$0 = \delta S_G^{EH} = \frac{M_{PL}^2}{2}\int\left[\frac{\delta\left(\sqrt{-g}R\right)}{\delta g^{\mu\nu}}\right]\delta g^{\mu\nu}d^4x\,, \tag{1.2}$$

which gives rise to the following equation of motion for the metric field in vacuum:

$$\frac{\delta R}{\delta g^{\mu\nu}} + \frac{R}{\sqrt{-g}}\frac{\delta\sqrt{-g}}{\delta g^{\mu\nu}} = 0\,. \tag{1.3}$$

The computation of the variation of the Ricci scalar and the determinant is a well-known academic exercise that we will not repeat here, for the interested reader we refer to [6]. The result are the Einstein field equations in vacuum

$$R_{\mu\nu} = 0\,. \tag{1.4}$$

Note that, because we are in 4 dimensions and hence μ and ν run from 0 to 3, equation (1.4) is actually a system of 16 second-order partial differential equations for the metric tensor field $g_{\mu\nu}$. However, because $R_{\mu\nu}$ is actually a symmetric two-index tensor, 6 out of these 16 are redundant. Furthermore, the Bianchi identities, which are a result of the redundancy in any given representation of the metric due to the freedom to choose different coordinates, represents 4 constraints on $R_{\mu\nu}$. Thus, the number of degrees of freedom (and hence of independent dynamical equations) reduce to $16-6-4=6$. We will however see in a more clear way in the next section that there are 4 more constraints on the initial data of the system, leaving the final number of degrees of freedom of general relativity in vacuum to be equal to 2.

1.2 Arnowitt-Deser-Misner decomposition

Although the Lagrangian formulation of general relativity presented above already gives a straightforward understanding about how Einstein's field equations can be derived from an action, it is sometimes hard to understand what is the dynamical content of these equations.

An alternative but equivalent approach is the Hamiltonian formulation of general relativity or ADM formalism, in honor of Arnowitt, Deser and Misner, the first authors who introduced this formulation [7]. We will not give here a formal development of the ADM formalism which can be found for example in [8] but we will rather give a conceptual idea, which in enough for our purposes.

The ADM formulation is a Hamiltonian rather than a Lagrangian formulation of general relativity. As any Hamiltonian formulation of a field theory, the ADM formalism requires the definition of canonically conjugate momenta for the dynamic variables (i.e. for the dynamic components of the metric tensor). To introduce these variables we want to give some privilege direction in time.

One way of doing so is to consider space-time as formed by a collection of non-intersecting 3-dimensional hypersurfaces Σ_t labeled by a number t, we can then think of the dynamical evolution as the change of these hypersurfaces in the parameter t. By providing each hypersurface with a three-dimensional metric γ_{ij}, determined by the way the space-time is cut, it is possible to consider the metric $\gamma_{ij}(t)$ as the dynamic variable.[1]

Note that γ_{ij} has 6 independent components (it is symmetric), in order to reach the 10 independent components of the original metric metric we still need 4 more functions, which are those responsible to describe the foliation of the hypersurfaces in the space time. These variables are:

- The lapse function α, which measures the rate of flow of proper time with respect to t as one moves normally to Σ_t and hence it is related to the separation between each hypersurface.

- The shift vector β^i, which measures how much the local spatial coordinate system shifts tangential to Σ_t, when moving from Σ_t to $\Sigma_{t+\delta t}$ along the normal direction to Σ_t.

[1] We will see later on that the variables that define the foliation of Σ_t are actually constraints and hence the only dynamical variable is γ_{ij}.

A schematic picture of what each one of the variables defined above represent can be found in Fig. 1.1[2].

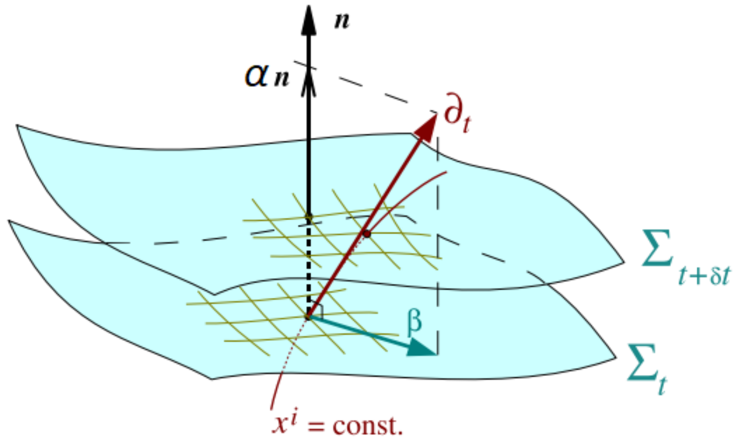

Fig. 1.1 Schematic representation of the 3+1 decomposition of the space-time used in the ADM formalism.

Once we have identified the variables of interest, we can write a generic line element accordingly with these new variables:

$$ds^2 = -\alpha^2(t,\mathbf{x})dt^2 + \gamma_{ij}(t,\mathbf{x})\left[dx^i + \beta^i(t,\mathbf{x})dt\right]\left[dx^j + \beta^j(t,\mathbf{x})\right] . \tag{1.5}$$

The last step is to write the Ricci scalar R and the volume element $dx^4\sqrt{-g}$ appearing in (1.1) in terms of these variables. In this step, the extrinsic curvature K_{ij} plays a very important role and it is defined as

$$K_{ij} \equiv -\nabla_i n_j = -\frac{1}{2\alpha}\left(\dot{\gamma}_{ij} - D_i\beta_j - D_j\beta_i\right) , \tag{1.6}$$

where $n_i \equiv (-\alpha, 0, 0, 0)$ is the unit vector normal to the spatial hypersurfaces, a dot represent a derivative with respect to t and ∇_μ and D_i are the covariant derivatives with respect to $g_{\mu\nu}$ and γ_{ij}, respectively. Finally, the Einstein-Hilbert action is re-expressed with these new variables in the form:

$$S_G^{ADM} = \frac{M_{PL}^2}{2}\int dt \int d^3x\sqrt{\gamma}\alpha\left(R^{(3)} + K_{ij}K^{ij} - K^2\right) , \tag{1.7}$$

where $\sqrt{\gamma}\alpha$ is the decomposed 4-dimensional invariant volume element, $R^{(3)}$ is the Ricci scalar of γ_{ij} and $K = \gamma^{ij}K_{ij}$.

Note that the action (1.7) does not depend on $\partial_t\alpha$ nor $\partial_t\beta_i$, which allow us to consider them as non-dynamical variables, or in other words, the lapse function α and the

[2] We thank Prof. Eric Gourgoulhon for letting us use the image of Fig. 1.1, which originally comes from his nice book on the 3+1 decomposition of general relativity [8].

shift vector β_i act as Lagrange multipliers and hence the variation of the action with respect to these variables will give us 4 constraint equations. Together with the 6 independent degrees of freedom of the 3-dimensional metric γ_{ij}, leave only the 2 degrees of freedom of general relativity in vacuum.

To construct the Hamiltonian density we define the canonically conjugated momenta of γ_{ij} as

$$\pi^{ij} \equiv \frac{\partial \mathcal{L}_G^{ADM}}{\partial \dot{\gamma_{ij}}} = \sqrt{\gamma}\left(K\gamma^{ij} - K^{ij}\right) . \tag{1.8}$$

Then, the Hamiltonian density is defined as follows

$$\mathcal{H}_G^{ADM} = \pi^{ij}\dot{\gamma}_{ij} - \mathcal{L}_G^{ADM} . \tag{1.9}$$

The minimization of the ADM action of (1.7) is equivalent to the Hamilton equations

$$\frac{\delta \mathcal{H}_G^{ADM}}{\delta \alpha} = 0 , \tag{1.10}$$

$$\frac{\delta \mathcal{H}_G^{ADM}}{\delta \beta^i} = 0 , \tag{1.11}$$

$$\frac{\delta \mathcal{H}_G^{ADM}}{\delta \pi^{ij}} = \dot{\gamma}_{ij} , \tag{1.12}$$

$$\frac{\delta \mathcal{H}_G^{ADM}}{\delta \gamma_{ij}} = -\dot{\pi}^{ij} . \tag{1.13}$$

Note that (1.10) and (1.11) are just constraint equations and confirm the fact that α and β^i are non-dynamical variables. Equation (1.10) is the so-called Hamiltonian constraint and it can be written as

$$R^{(3)} - K_{ij}K^{ij} + K^2 = 0 . \tag{1.14}$$

Equation (1.11) represents the momentum constraint:

$$D_j K_i^j - D_i K = 0 . \tag{1.15}$$

Equations (1.12) and (1.13) represent instead dynamical equations for the metric and its canonical momenta. Since for the rest of the thesis we are not really interested in the canonical momenta π_{ij} but rather in the extrinsic curvature K_{ij}, we will write (1.13) in terms of K_{ij} rather than in terms of π_{ij}. Note that this is not what it was done in the original paper of the ADM formalism [7]. After a tedious but straightforward computation we obtain, from (1.12), the equation of motion for the metric

$$\left(\partial_t - \beta^k \partial_k\right) \gamma_{ij} = -2\alpha K_{ij} + \gamma_{kj}\partial_i \beta^k + \gamma_{ik}\partial_j \beta^k \,, \tag{1.16}$$

and, from (1.13), the equation of motion for the extrinsic curvature

$$\left(\partial_t - \beta^k \partial_k\right) K_{ij} = -D_i D_j \alpha + \alpha \left[R^{(3)}_{ij} + K K_{ij} - 2K_{ik}K^k_j\right] + K_{kj}\partial_i \beta^k + K_{ik}\partial_j \beta^k \,. \tag{1.17}$$

Although the ADM system of equations (1.10)-(1.13) are exactly equivalent to the vacuum Einstein field equations of (1.4), they can be understood in a more intuitive way thanks to its relation with the classical Hamiltonian formulation of any field theory. This is one of the reasons why the ADM equations are the ones most widely used for numerical simulations [9].

1.3 Beyond pure gravity

Both the Einstein-Hilbert and the ADM actions presented above are very useful to understand the nature of gravity in vacuum. However, for cosmological purposes, we need to introduce gravitating matter and a cosmological constant Λ. The Einstein-Hilbert action in this case is:

$$S^{EH} = \frac{M_{PL}^2}{2} \int d^4x \sqrt{-g} \left(R - 2\Lambda\right) + \int d^4x \sqrt{-g} \mathcal{L}_m \tag{1.18}$$

where $\mathcal{L}_m$ is the Lagrangian density of the gravitating matter. Varying the full action S^{EH} with respect to the inverse metric in a similar way as in section 1.2 we can write the Einstein field equations in presence of matter and a gravitational constant

$$R_{\mu\nu} + \frac{1}{2} R g_{\mu\nu} + \lambda g_{\mu\nu} = \frac{1}{M_{PL}^2} T_{\mu\nu} \,, \tag{1.19}$$

where we have introduced the stress-energy tensor $T_{\mu\nu}$, defined as

$$T_{\mu\nu} = \mathcal{L}_m g_{\mu\nu} - 2\frac{\delta \mathcal{L}_m}{\delta g^{\mu\nu}} \,. \tag{1.20}$$

Following the same procedure of section 1.2, we can write the ADM system of equations (1.10)-(1.13) including a cosmological constant and matter. The result is:

- Hamiltonian constraint

$$R^{(3)} - K_{ij}K^{ij} + K^2 - 2\Lambda = \frac{2}{M_{PL}^2} E \,, \tag{1.21}$$

where we define $E \equiv T_{\mu\nu} n^\mu n^\nu$.

- Momentum constraint
$$D_j K_i^j - D_i K = \frac{1}{M_{PL}^2} J_i \tag{1.22}$$
where we defined $J_i =\equiv -T_{\mu\nu} n^\mu \gamma_i^\nu$.

- Equation of motion for the spatial metric
$$\left(\partial_t - \beta^k \partial_k\right) \gamma_{ij} = -2\alpha K_{ij} + \gamma_{kj}\partial_i \beta^k + \gamma_{ik}\partial_j \beta^k \,. \tag{1.23}$$

- Equation of motion for the extrinsic curvature
$$\begin{aligned}\left(\partial_t - \beta^k \partial_k\right) K_{ij} = &- D_i D_j \alpha + \alpha \left[R_{ij}^{(3)} - \Lambda \gamma_{ij} + K K_{ij} - 2K_{ik}K_j^k\right] \\ &+ K_{kj}\partial_i \beta^k + K_{ik}\partial_j \beta^k + \frac{\alpha}{2M_{PL}^2}\left[(S-E)\,\gamma_{ij} - 2S_{ij}\right] \,,\end{aligned} \tag{1.24}$$
where we define $S_{ij} = T_{ij}$ and hence $S = \gamma^{ij} S_{ij}$.

Again, the system of equations (1.21)-(1.24) is exactly equivalent to the Einstein field equations (1.19).

1.4 The cosmological principle and the model of our universe.

Although there are many textbooks devoted to this topic [10, 11, 12, 13, 14], it is worthy for the rest of the thesis to give a brief overview of our standard cosmological model, which is based on the cosmological principle.

The cosmological principle is the guiding principle in all of cosmology and it states that the universe must look the same for all observers, which requires that it must be homogeneous and isotropic everywhere. In other words, the cosmological principle requires the universe to look the same at every location and in every direction. Although this principle does not apply at small scales (for example in the solar system), at cosmological distances (typically about 1 Gly or greater) it seems to be fairly accurate as far as observations are concerned [15, 16, 17, 18, 19, 20].

In order to obey the cosmological principle, the 3-dimensional hypersurface of Fig. 1.1 must be a maximally symmetric manifold. We can then choose appropriate coordinates to write the 4-dimensional space-time metric as
$$ds^2 = -dt^2 + a^2(t) d\bar{\sigma}^2 \,, \tag{1.25}$$
where $d\bar{\sigma}^2$ is the line element of the maximally symmetric 3-dimensional metric and $a(t)$ is the scale factor. Note that $a(t)$ cannot depend on x^i because otherwise it would

violate homogeneity. One now has to impose the Riemann curvature tensor to be the one of a maximally symmetric 3-dimensional metric γ_{ij}^{MS}, i. e.

$$R^{(3)}_{ijkl} = \kappa \left(\gamma_{ij}^{MS}\gamma_{jl}^{MS} - \gamma_{il}^{MS}\gamma_{jk}^{MS}\right) , \tag{1.26}$$

where κ is the Gaussian (or intrinsic) curvature of 3-space. The Ricci tensor is then straightforwardly computed as

$$R^{(3)}_{ij} = 2\kappa\gamma_{ij}^{MS} . \tag{1.27}$$

The next step is to choose the following ansatz for the a spherically-symmetric 3-dimensional space

$$d\bar{\sigma}^2 = \gamma_{ij}^{MS} dx^i dx^j = e^{2\zeta(\bar{r})} dr^2 + \bar{r}^2 d\theta^2 + \bar{r}^2 \sin^2\theta d\phi^2 . \tag{1.28}$$

One can now compute the Ricci tensor of the metric (1.29) and use (1.27) to compute $\zeta(\bar{r})$. The result is [6]:

$$d\bar{\sigma}^2 = \frac{d\bar{r}^2}{1-\kappa\bar{r}^2} + \bar{r}^2 d\theta^2 + \bar{r}^2 \sin^2\theta d\phi^2 . \tag{1.29}$$

Note that (1.29) depends on the exact intrinsic curvature κ, however, it can be actually reparametrized such that any curvature κ can be normalized to $+1$ or -1. In this case we have $\kappa = \omega k$, with $k \in (-1, 0, +1)$. If we also reparametrize the radial coordinate such that $r = \omega\bar{r}$ we have that the most general 4-dimensional metric consistent with the cosmological principle is

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -dt^2 + a^2(t)\left(\frac{dr^2}{1-kr^2} + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2\right) , \qquad k \in (-1, 0, +1) . \tag{1.30}$$

The metric (1.30) is the so called Friedmann-Lemaître-Robertson-Walker (FLRW) metric [21, 22, 23, 24] and it is the metric that describes an homogeneous and isotropic universe, which at the same time can be expanding or contracting. From (1.30) we can see that the comoving distance d_{com} between two points in the constant time hypersurface Σ_t, is related with the physical distance d_{phys} as

$$d_{phys} = a(t) d_{com} , \tag{1.31}$$

from where it is clear the physical meaning of the scale factor $a(t)$: it sets the physical expansion of the 3-dimensional homogeneous and isotropic hypersurfaces Σ_t.

Note also that, depending on the value of k, the FLRW metric describes different 3-dimensional spaces. For $k = -1$ it describes a 3-dimensional hyperbolic space, for

$k = 0$ it describes a 3-dimensional flat (Euclidean) space and for $k = 1$ it describes a 3-dimensional sphere.

In order to obtain the FLRW metric (1.30), we have assumed, based on the cosmological principle, that our universe is homogeneous and isotropic. To solve the Einstein field equations we need a stress-energy tensor which is also homogeneous and isotropic, the most general form of the stress-energy tensor which is compatible with homogeneity and isotropy is the one of a perfect fluid [25]

$$T_{\mu\nu} = (\rho + p)u_\mu u_\nu + p g_{\mu\nu} \, , \tag{1.32}$$

where ρ is the energy density of the fluid and p its pressure. Homogeneity implies that the pressure and density should be independent on the location in the 3-dimensional hypersurface Σ_t and hence they can only depend on time in the coordinates (1.25). Finally, u_μ is the relative four-velocity between the fluid and the observer and it must only have a time component in order to be compatible with our assumption of spatial isotropy, in other words, the fluid flow is orthogonal to the 3-dimensional hypersurfaces Σ_t, with this in mind, we have that the stress-energy tensor must be diagonal in the coordinates (1.30) i.e.

$$T_{\mu\nu} = \text{diag}\,(\rho, p, p, p) \; . \tag{1.33}$$

Knowing the form of the metric (1.30) and of the stress-energy tensor (1.33) we can write specifically the Einstein field equations that describe a generic homogeneous and isotropic universe. We will use the ADM formalism (2.19)-(2.24), the reason is that this is precisely the formalism we are going to use along the thesis so it is worthy to introduce it here. In order to use the ADM formalism it is better to write the FLRW metric in cartesian coordinates i.e.

$$ds^2 = -dt^2 + a^2(t)\frac{dx^2 + dy^2 + dz^2}{\left(1 + \frac{1}{4}k\left(x^2 + y^2 + z^2\right)\right)^2} \, . \tag{1.34}$$

Comparing (1.34) with the general ADM metric of (1.5), it is clear that the lapse function and the shift vector in a homogeneous and isotropic universe with coordinates (1.30) are simply $\alpha = 1$ and $\beta_i = 0$, respectively. Furthermore using the decomposition of the spatial metric $\gamma_{ij} = a^2(t)e^{2\zeta}\tilde{\gamma}_{ij}$, we have $\tilde{\gamma}_{ij} = \delta_{ij}$, where δ_{ij} is the Kronecker delta and

$$\zeta = \log\left[\frac{1}{1 + \frac{1}{4}k\left(x^2 + y^2 + z^2\right)}\right] \, . \tag{1.35}$$

The extrinsic curvature is simply

$$K_{ij} = -\frac{1}{2}\partial_t \left(\frac{a^2(t)}{\left(1+\frac{1}{4}k\left(x^2+y^2+z^2\right)\right)^2} \right) \delta_{ij} \,, \tag{1.36}$$

from which we can easily identify $K = -3\frac{\dot{a}}{a}$. Finally, the Ricci scalar of the 3-dimensional metric can be computed to be $R^{(3)} = \frac{6k}{a^2(t)}$. The relevant ADM equations (the only ones which are not trivially satisfied) are then the Hamiltonian constraint (1.21) and the equation of motion for the trace of the extrinsic curvature (1.24), which are respectively

$$\frac{k}{a^2} + \left(\frac{\dot{a}}{a}\right)^2 - \frac{\Lambda}{3} = \frac{1}{3M_{PL}^2}\rho \,, \tag{1.37}$$

$$3\frac{\ddot{a}}{a} = \Lambda - \frac{1}{2M_{PL}^2}\left(\rho + 3p\right) \,, \tag{1.38}$$

also known as Friedmann equations [21].

Taking the time derivative of (1.37) and inserting it into (1.38) we get the continuity equation,

$$\dot{\rho} = -3\frac{\dot{a}}{a}\left(\rho + p\right) \,, \tag{1.39}$$

which can also be derived by derived by imposing the covariant conservation of the stress-energy tensor i.e. $\nabla_\mu T^\mu_\nu = 0$.

The continuity equation has a very simple solution if we assume a equation of state of the form $p = \omega\rho$, where ω is a constant

$$\rho(a) = \rho^{in}\left(\frac{a}{a^{in}}\right)^{-3(1+\omega)} \,. \tag{1.40}$$

In (1.40), ρ^{in} is the value of the energy density at initial time when $a = a^{in}$. For example, for non-relativistic $\omega_{mat} = 0$, $\rho_{mat} \propto a^{-3}$. As one would expect, the density of non-relativistic matter decays with the volume, on the other hand, for relativistic matter (or radiation) where $\omega_{rad} = 1/3$, $\rho_{rad} \propto a^{-4}$. The extra $1/a$ that appears in the time evolution of the energy density of radiation is due to the fact that the wavelengths of radiation are redshifted.

Before further proceeding, let us go back to the Hamiltonian constraint of an homogeneous and isotropic universe of equation (1.37) and note that it can be written as

$$H^2 = \frac{\rho_T}{3M_{PL}^2} \,, \tag{1.41}$$

where we have defined the Hubble rate as $H \equiv \frac{\dot{a}}{a}$ and ρ_T as the total energy density.

Component	$\rho(a)$	ω	Ω^0
Non-relativistic matter	$\rho_{mat} \propto a^{-3}$	$\omega_{mat} = 0$	$\Omega^0_{mat} \simeq 0.311$
Radiation	$\rho_{rad} \propto a^{-4}$	$\omega_{rad} = \frac{1}{3}$	$\Omega^0_{rad} \simeq 9.23 \cdot 10^{-5}$
Cosmological constant	$\rho_\Lambda \propto$ constant	$\omega_\Lambda = -1$	$\Omega^0_\Lambda \simeq 0.689$
Curvature	$\rho_k \propto a^{-2}$	$\omega_k = -\frac{1}{3}$	$\lvert\Omega^0_K\rvert < 0.01$

Table 1.1 Different components of the universe and the evolution of the energy density associated to each component.

Note that ρ_T does not only include the energy density that appears in the stress-energy tensor of (1.33), but also includes two other components that, although strictly speaking do not represent any kind of matter, they participate in the Hamiltonian constraint in the similar way as matter does. These components are the cosmological constant and the curvature. Their associated densities are $\rho_\Lambda = M_{PL}^2 \Lambda$ and $\rho_k = -\frac{3M_{PL}^2 k}{a^2}$. The behavior of each component of the universe are summarized in Table 1.1.

Note also that, if we assume the different components to be non interacting, we can write the total energy density as

$$\rho_T(a) = \rho^{in}_{mat} \left(\frac{a}{a^{in}}\right)^{-3} + \rho^{in}_{rad} \left(\frac{a}{a^{in}}\right)^{-4} + \rho^{in}_\Lambda + \rho^{in}_k \left(\frac{a}{a^{in}}\right)^{-2} . \tag{1.42}$$

or, using the Hamiltonian constraint (1.41), as

$$\left(\frac{H}{H_0}\right)^2 = \frac{\Omega^0_{mat}}{a^3} + \frac{\Omega^0_{rad}}{a^4} + \Omega_\Lambda + \frac{\Omega^0_k}{a^2} . \tag{1.43}$$

Ee have defined the dimensionless quantity $\Omega^0_i \equiv \frac{\rho^0_i}{3M_{PL}H_0^2}$ as the value of the dimensionless energy density of each component at current time $a^0 = 1$ and H_0 is today's Hubble rate. This simple formula tell us that, under two simple assumptions, namely that 1) each component of the universe has a constant equation of state and 2) they do not interact with each other, we can estimate the energy density of each constituent of the universe at any given time by knowing their current values. In Table 1.1 we give the values of Ω^0 for each known constituent of the universe measured by the Planck collaboration [19][3].

As a side note, it is important to remark that, although we are considering in Table 1.1 all the non-relativistic matter today to be the same, it contains two main elements: a) the baryonic matter (atoms, nuclei, etc), for which $\Omega_{bary} \simeq 0.049$ and b) the dark matter, whose precise nature is still unknown and for which $\Omega_{DM} \simeq 0.262$.

From (1.42) and (1.43) we can clearly see that the term dominating the energy density of the universe depends on the value of the scale factor. As it can be seen in Table

[3]Because this thesis is not really devoted to any observational measurement, we will only write the approximated values of Ω^0, for the reader interested in how each measurement is made and the corresponding error bars, we refer to [19]

1.1, the cosmological constant is the component that dominates today, however, this is not true earlier because of a smaller value of the scale factor. If we consider $\Omega_k = 0$, we can distinguish 2 important events in the history of the universe:

1. Matter radiation equality:

   This is the moment in which the energy density of matter and of radiation contribute equally to the total budget of energy density in the universe, this happens when

$$\frac{\Omega^0_{mat}}{a^3} = \frac{\Omega^0_{rad}}{a^4}\,, \tag{1.44}$$

   which corresponds to a value of the scale factor of $a(t_{eq}) \simeq 3 \cdot 10^{-4}$.

2. Matter-Λ equality:

   In the same way, we can obtain the value of the scale factor in the moment in which the energy density of matter and of the cosmological constant contribute equally to the total budget of energy density in the universe

$$\frac{\Omega^0_{mat}}{a^3} = \Omega^0_\Lambda\,, \tag{1.45}$$

   which corresponds to a value of the scale factor of $a(t_{eq}^{mat\to\Lambda}) \simeq 0.767$.

These 2 main events allow us to distinguish 3 different epochs in the universe:

1. The first one would be the radiation dominated era, which corresponds to the blue region in Fig 1.2. In this era, radiation was the most important contribution to the total energy density of the universe. If we approximate $\rho_T \simeq \rho_{rad}$ during this era we get from (1.41) that the evolution of the scale factor with cosmic time t is $a(t) \propto t^{1/2}$.

2. The second epoch is the so-called matter dominated era, which corresponds to the orange region in Fig. 1.2. In this case, matter dominates the total energy density of the universe so $\rho_T \simeq \rho_{mat}$ and hence $a(t) \propto t^{2/3}$.

3. Finally, the third era is the one towards we are evolving in right now in which the cosmological constant will eventually dominates the total energy density of the universe. In this case $\rho_T \simeq \rho_\Lambda$ and hence $a(t) \propto e^{Ht}$, where H is constant.

Of course the 3 epochs presented above are limiting cases of the true dynamics of the universe, the reason is that there is almost always more than one component whose contribution to the energy density is important as it happens for example in our current universe, where we are in a transition between the second and the third epochs and around 70% of the total energy density comes from the cosmological constant while the spare 30% corresponds to non-relativistic matter.

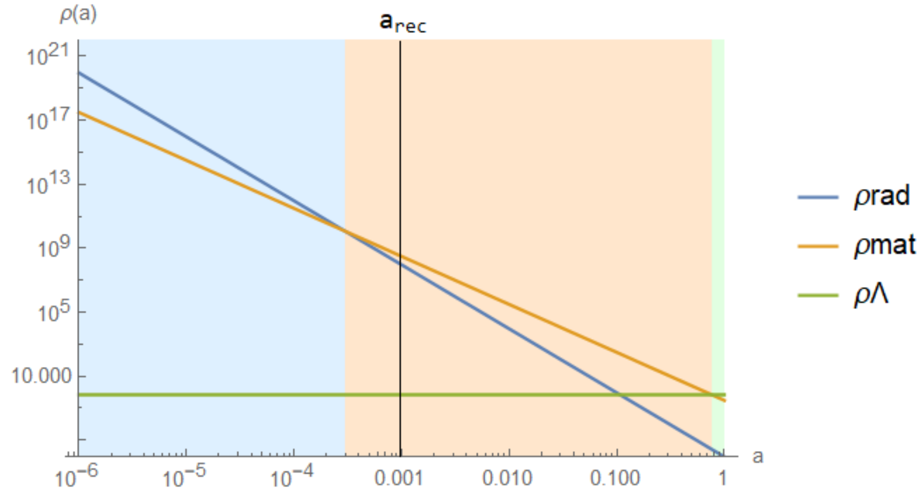

Fig. 1.2 Evolution of the energy density of each component of the universe with the scale factor.

The extremely simple model presented here is the most accepted model of the universe nowadays and it is sometimes referred to as ΛCDM model (or Hot Big Bang model), where Λ states the necessity of a cosmological constant (and therefore a ρ_Λ) in order to explain the accelerated expansion observed in our universe nowadays and CDM states by Cold Dark Matter, meaning that the unknown component of matter (dark matter) act as non-relativistic matter and not as radiation. Of course among the 3 epochs presented above, many other key moments in the evolution of the universe took place.

In this thesis we are not interested in almost any of them but we will just enumerate them here with corresponding references for the interested reader:

1. During the radiation dominated epoch:
   - Electroweak phase transition [26, 27, 28, 29, 30, 31, 32][4]
   - Quark-hadron transition [33, 34, 35, 36, 37, 38]
   - Nucleosynthesis [39, 40, 41, 42]
2. During the matter dominated epoch:
   - **Recombination** [43, 44, 45, 46]
   - First galaxies are formed. [47, 48, 49]
   - Reionization [50, 51, 52]

[4]Some references place this phase transition earlier than the radiation dominated epoch, however this is still a question under debate, see references in the main text for more details.

3. After matter-Λ equality.

    - First stellar systems are formed [53].

The reason why recombination is in bold in is because we will pay slightly more attention to this particular event, as it will become clear in the following. The ΛCDM model of the universe assumes that the universe starts with a hot plasma that contains all the fundamental particles of the Standard Model, after that, the universe starts to cool down and the different particles start binding together and forming increasingly complex structures. At $a \sim 0.001$ (see Fig. 1.2), the universe has cooled enough that charged electrons can bind with protons to form the first neutral hydrogen atom, this is the so-called recombination epoch. At this point, photons decouple from matter and travel freely through the universe, constituting what it is observed today as the Cosmic Microwave Background Radiation (CMBR). This ”Oldest light of the universe” was accidentally discovered by Arno Penzias and Robert Wilson in 1965 [54] and since then more and more precise measurements have been done, being the latest image released by the Plank satellite the one in Fig 1.3 [55]. The CMBR is consistent with homogeneity and isotropy of the universe, with small deviations from homogeneity up to one part in 10^5. As we will see later on, both the almost perfect agreement with homogeneity of the CMBR and the existence of small inhomogeneities motivate the existence of a period of accelerated expansion in the very early universe called cosmological inflation, which is the main topic of this thesis.

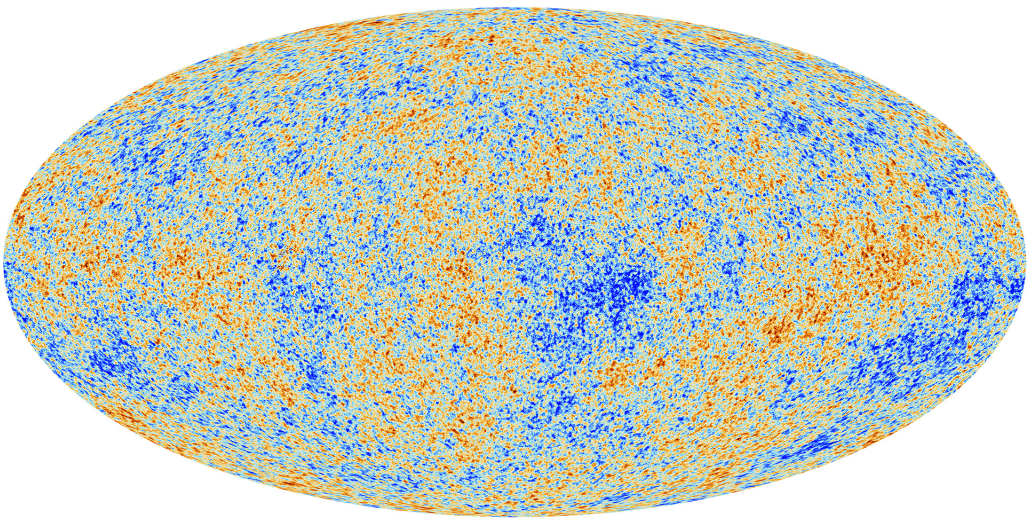

Fig. 1.3 Cosmic microwave background radiation temperature map from Planck 2018. The temperature of the CMB today is $2.725\ K$ with fluctuations of just 0.01%

1.5 Initial conditions in the ΛCDM model.

The ΛCDM model is very compelling, in fact, despite being a rather simple model based on the cosmological principle and the theory of general relativity, it is able to give a reasonable explanation of the universe we observe nowadays.

However, there exists a series of puzzles in the ΛCDM model related with the extreme fine-tuning of some initial conditions necessary to describe our universe. These fine-tuning issues can be solved with a simple extension of the ΛCDM model in which we include a short period of accelerated expansion in the very early universe called cosmological inflation. Because this thesis is mainly devoted to cosmological inflation, we will present these fine tuning issues in detail and show how inflation take care of them.

1.5.1 Flatness problem

As already commented around Table 1.1, our universe shows no sign of spatial curvature. ($|\Omega_k^0| < 0.01$). Because the curvature energy density scales as $1/a^2$ and hence much slower than the energy density of matter ($1/a^3$) or radiation ($1/a^4$), any small amount of curvature at the very early universe should have relatively grown over time, leading to a initial fine-tuning problem.

In order to quantify the magnitude of it let us put some numbers. In our computations we will the cosmological constant contribution to the total energy density because, although it currently dominates, it has been irrelevant for most of the universe's history as it can be seen in Fig. 1.2. As we saw in section 1.4, from $a \simeq 3 \cdot 10^{-4}$ until recently, the universe was matter dominated. In this case

$$\frac{\rho_k(a)}{\rho_{mat}(a)} = \frac{\rho_k^0}{\rho_{mat}^0} a\,, \quad \Rightarrow \quad \Omega_k(a) = \frac{\Omega_k^0}{\Omega_{mat}^0} \Omega_{mat}(a) a\,. \tag{1.46}$$

Formula (1.46) approximately holds all the way back to matter-radiation equality at $a = a_{eq} = 3 \cdot 10^{-4}$, where $\Omega_{mat}(a_{eq}) \simeq 1/2$. Using the present day value of $\frac{\Omega_k^0}{\Omega_{mat}^0} \lesssim 0.01$, we must have

$$|\Omega_k(a_{eq})| \leq 10^{-6}\,, \tag{1.47}$$

which already represents a huge fine-tuning problem, the situation is even worse if we study Ω_k at earlier times. In this case the universe is radiation dominated and hence the relevant formula is

$$\frac{\rho_k(a)}{\rho_{rad}(a)} = \frac{\rho_k^0}{\rho_{rad}^0} a^2\,, \quad \Rightarrow \quad \Omega_k(a) = \frac{\Omega_k(a_{eq})}{\Omega_{rad}(a_{eq})} \frac{a^2}{a_{eq}^2} \Omega_{rad}(a)\,, \tag{1.48}$$

where $\Omega_{rad}(a_{eq}) = 1/2$ and $\Omega_k(a_{eq})$ is given by (1.49). We can now use (1.48) to compute $\Omega_k(a)$ at some time in the radiation dominated universe, for example at $a = a_{rad} = 10^{-15}$ and $\Omega_{rad}(a_{rad}) = 1$. In this case the constraint on the energy density of the curvature is

$$|\Omega_k(a_{rad})| \leq 10^{-29}\,, \tag{1.49}$$

Why should the early universe be flat to such precision?, there is no reason a priori to think so, this is known as the flatness problem.

1.5.2 Horizon problem.

For the horizon problem it is needed to introduce the concept of horizon itself, which will be determined by the propagation of light in an expanding spacetime. Because we assume a spacetime flat and isotropic, we can describe the evolution of light using a 2-dimensional line element as

$$ds^2 = a^2(\tau)\left[d\tau^2 - dr^2\right]\,, \tag{1.50}$$

where we have defined the conformal time τ as $a(\tau)d\tau = dt$. Since light travels along null geodesics ($ds^2 = 0$), their path is simply given by

$$\Delta r = \pm\delta\tau\,, \tag{1.51}$$

where the plus and minus corresponds to outgoing and ingoing photons, respectively. For the horizon problem we are interested in the events in the past that can affect a future observer, this is called the comoving particle horizon.

$$d_{ch}(\tau) = \tau - \tau_{in} = \int_0^t \frac{dt}{a(t)}\,. \tag{1.52}$$

As it is clear form (1.52), a comoving particle can only affect an observer at P if the particle's worldline intersect the past lightcone of P. In other words, if we consider two observers with a comoving separation $L(\tau) > d_{ch}(\tau)$, the two observers could never have communicated before the time τ.

The horizon problem arises when we realize the almost perfect homogeneity and isotropy of the CMBR (see Fig. 1.3). As we will show in the following, according to the ΛCDM model presented before, many different parts of the sky are outside each others particle horizons at the time the CMBR is formed.

For a purely matter dominated universe[5], where $a(t) = (t/t_0)^{2/3}$, the comoving particle horizon of (1.52) at recombination time t_{rec} is $d_{ch} = 3t_{rec}$, which can be written

[5]Of course, this is an oversimplification because we had a period of radiation domination in the early universe, however, including this period would complicate the computation and obscure the main result, which can be already seen in a purely matter dominated universe.

as

$$d_{ch}(a_{rec}) = \frac{2a_{rec}^{2/3}}{H_0}\,, \tag{1.53}$$

where we have used $H(t) = \frac{2}{3t} = \frac{H_0}{a^{3/2}}$. The comoving particle horizon at recombination time $d_{ch}(a_{rec})$ has been stretched by the expansion of the universe until the value of $\frac{d_{ch}(a_{rec})}{a_{rec}}$ today, where the comoving particle horizon is $d_{ch}(a_0) = \frac{2}{H_0}$. Thus, the sizes of the region in the sky that were in causal contact before the emission of the CMBR are within an observable angle of

$$\theta \simeq \frac{d_{ch}(a_{rec})}{a_{rec} d_{ch}(a_0)} \simeq 0.03\text{rad}\,. \tag{1.54}$$

This means that, within the ΛCDM model, patches of the sky separated by more than ~ 0.03 rad had no casual contact at the time CMBR was emitted. We would then expect a CMBR full of circles of ~ 0.03 rad, each one with different temperature. How different parts of the universe have reached thermal equilibrium without ever being in causal contact? This is the so called horizon problem, Fig.1.4 shows a schematic plot of the different comoving particle horizons that we have used in the computation above that clarifies the problem in a very intuitive way.

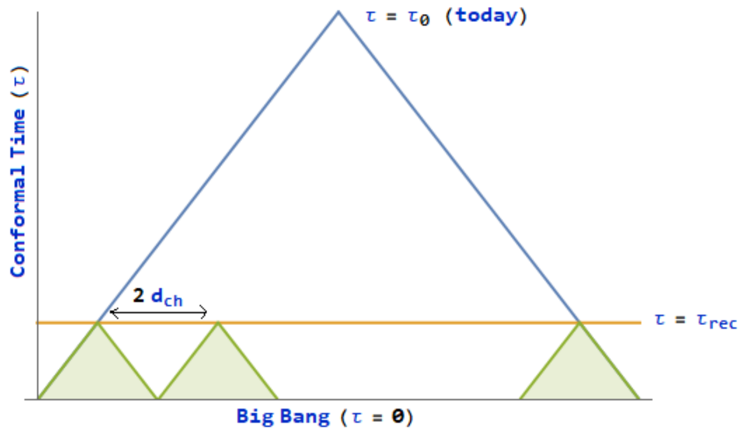

Fig. 1.4 Schematic plot of the horizon problem. Although the CMBR (orange surface) is almost perfect homogeneous and isotropic, it can be seen that different patches in that surface were never in causal contact in the ΛCDM model

1.6 An early acceleration phase as a solution for the fine-tuning problems.

As anticipated before, there exists a neat solution to the problems that have to do with fine-tuning issues, namely the flatness and horizon problems. The solution consists of a period of accelerating expansion in the very early universe called cosmological inflation (inflation from now on) and it is the leading paradigm for the very beginning of the universe. As we will see later on, the success of inflation does not only resides in the way that it solves the fine-tuning problems of the ΛCDM model. Possibly a more important consequence of inflation is that quantum fluctuations of the gravitational and matter fields generated during that phase can provide the seed of the large-scale structure of our universe. In this section we will nevertheless only talk about inflation as a solution of the fine-tuning problems.

An accelerating phase means $a(t) \sim t^n$ with $n > 1$ or a de Sitter-type phase with $a(t) \sim e^{\Lambda t}$ with constant Λ. Note that a phase of this form would naturally solve the flatness problem, in fact, the background energy density of such an accelerating phase scales as

$$\begin{aligned} H_{acc} &\sim \frac{1}{a^{2/n}}\,, \quad \text{for} \quad a(t) \sim t^n \quad \text{with} \quad n > 1 \\ H_{acc} &\sim \text{constant}\,, \quad \text{for} \quad a(t) \sim e^{Ht} \end{aligned} \tag{1.55}$$

which obviously dilutes away slower than the curvature ρ_k ($\sim 1/a^2$). This means that if we wait a sufficiently long period, the accelerating phase will make the spatial curvature as relatively small as we like. One can think intuitively as a smooth and curved manifold that gets enlarged because of inflation, then any small region of this manifold looks increasingly flat.

In the same way, one can easily argue that the particle comoving horizon defined in (1.52) actually diverges for $a(t) \sim t^n$ when $n > 1$ and for $a(t) \sim e^{Ht}$. This means that an early accelerating phase push τ_{in} towards $-\infty$, contrary to what happens in Fig. 1.4, and allows more and more separated regions to be in causal contact, a schematic picture of how the horizon problem is solved when we push $\tau \to -\infty$ is shown in Fig 1.5.

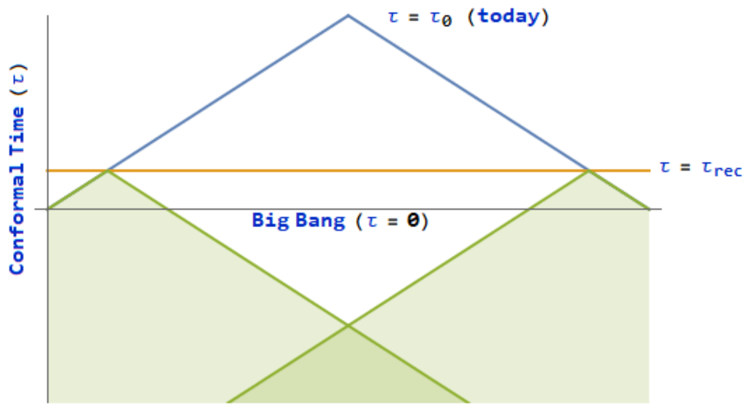

Fig. 1.5 Schematic plot of the solution of the horizon problem. Farther patches of the orange line are now in causal contact due to the inclusion of an accelerating phase in the early universe that pushes $\tau \to -\infty$

An accelerating phase in an universe filled with a perfect fluid can only be achieved for some specific values of ω, in fact, one can check from (1.41) that

$$\begin{aligned} a(t) \sim t^n \quad \text{with} \quad n > 1 \quad &\rightarrow \quad -1 < \omega < -\frac{1}{3}\,, \\ a(t) \sim e^{Ht} \quad &\rightarrow \quad \omega = -1\,, \end{aligned} \tag{1.56}$$

which also means that $\rho + 3p < 0$.

Using the second Friedmann equation (1.38) in absence of cosmological constant we have

$$\frac{da^2}{dt^2} > 0 \quad \rightarrow \quad \frac{d}{dt}\left(\frac{1}{aH}\right) < 0\,. \tag{1.57}$$

The conditions in (1.57) motivate us to define another quantity, the Hubble radius $d_H \equiv (aH)^{-1}$, which must decrease during inflation. Note that, contrary to what happens to the comoving particle horizon in (1.52), the fact that two particles are separated by a distance $L(\tau) > r_H$, does not mean that these particles never have communicated with each other before but rather that they cannot communicate to each other now. In this sense, we might have regions of the universe separated by a $L(\tau_0) > (a_0 H_0)^{-1}$ today that were in causal contact during inflation, the reason is that, during inflation the Hubble radius decreased: there was a moment in the very early universe in which $L(\tau_0) < (a(\tau_{inf})H(\tau_{inf}))^{-1}$.

The definition of Hubble radius will be of crucial importance when exploring how quantum fluctuations produced during inflation can provide the seed of the large-scale structure of the late-time universe.

CHAPTER 2

Cosmological inflation

Although the first ideas of inflationary-type models in the universe were introduced by Starobinsky [56, 57], it was not until 1981 when Guth proposed an inflationary model that was physically motivated by the fine-tuning problems of the ΛCDM model [58]. According to his model, the exponential expansion of the universe happens because, as the universe cools down, it gets trapped in a false vacuum with a high energy density, which is much like a cosmological constant. Then the false vacuum decays, the bubbles of the new phase collide, and our universe becomes hot. Unfortunately, despite it success to solve the fine tuning problems of the ΛCDM model, Guth's original formulation was problematic. The reason is that if inflation lasted long enough to solve the fine tuning problems, collision between bubbles became exponentially rare and hence there is no way to bring an end to inflation and end up with a radiation dominated universe, this was known as the graceful exit problem [59, 60].

The graceful exit problem was solved by Linde [61] and independently by Albrecht and Steinhardt [62] in a model named new inflation or slow-roll inflation (Guth's model then became known as old inflation). In this model, instead of tunneling out of a false vacuum state, inflation occurred by a scalar field rolling down a potential energy hill. When the field rolls very slowly compared to the expansion of the Universe, inflation occurs. However, when the hill becomes steeper, inflation ends and reheating can occur.

It is important to remark that new inflation also suffers from severe fine tuning problems, in fact, this scenario requires the universe to have a scalar field with an especially flat potential and special initial conditions. These fine tuning problems of the potential can be justified for example in the Starobinsky model, in which inflation occurs because the Einstein-Hilbert action of (1.1) also contains a $\propto R^2$ term, this quadratic term acts effectively as a scalar field with a rather flat potential [63]. Another option is to consider that Inflation will occur in virtually any universe that begins in a chaotic, high energy state that has a scalar field with unbounded potential energy, reason why this scenario is called chaotic inflation [64]. Although the problem of fine tuning in the potential is very interesting we will not further develop it in this thesis.

Furthermore, in an attempt to motivate the inflationary potential from the point of view of quantum gravity theories such as supergravity or string theory, inflationary models with more than one scalar field have also been proposed, an example is hybrid inflation [65]. Nowadays the number of inflationary models that are motivated for different reasons are very large [66]. In this thesis we will discuss the simplest, but yet very predictive, case of single field inflation with canonical kinetic term.

In section 1.6 we saw that the background dynamics of a phase of inflation that solves the horizon and flatness problem must be dominated by a fluid that satisfies $\rho + 3p = \rho(1 + 3\omega) < 0$. i.e. a negative pressure fluid (since we always have $\rho > 0$). A universe dominated by the gravitational constant ($\omega = -1$) might then seem like the natural choice for inflation, however, as we discussed before, in this case there is no standard mechanism to end inflation. The most simple alternative to the cosmological constant is to consider the energy density of the early universe to be dominated by a single quantum scalar field $\phi(\mathbf{x}, t)$ (called the inflaton) evolving in a potential $V(\phi)$. The first realization that the energy density of a scalar field can play the role of the cosmological constant was proposed even before the theory of inflation [67]. A quantum scalar field has the following properties to play the role of inflaton:

1. It is compatible with the flatness, homogeneity and isotropy of the very early universe. As a counterexample, an universe whose background energy density is dominated by a vector field would introduce some preferred direction and hence it would violate isotropy.

2. It provides a natural way of ending inflation. The reason is that, as the inflaton rolls down the potential, Ω will eventually becomes larger than $-1/3$ so the accelerated expansion of the universe will stop. Furthermore, there exists a more or less well know procedure, called reheating [68, 69, 70, 71, 72], in which the potential energy of the inflaton decays into standard model particles, and hence starting the radiation dominated phase of the universe.

3. The inflaton, contrary to what would happen if the cosmological constant would drive inflation, produces quantum vacuum fluctuations. As we will see later on, these fluctuations, when combined with inflation, provide a convincing mechanism for the origin of the CMBR anisotropies. In fact, we will see in this section that, if certain conditions are satisfied, inflation driven by a single scalar field predicts that the spectrum of the cosmological fluctuations should be almost scale invariant, which is fully consistent with observations [55].

2.1 Background evolution during inflation

Having motivated the choice of the a scalar field as the responsible of the background energy density during inflation, we can write the ADM action (1.7) with the inclusion of the Lagrangian for a single scalar field with canonical kinetic term:

$$S = \frac{1}{2}\int \sqrt{\gamma}\left[M_{PL}^2\left(\alpha R^{(3)} + \alpha\left(K_{ij}K^{ij} - K^2\right)\right)\right.$$
$$\left. -2\alpha V(\phi) + \alpha^{-1}\left(\dot{\phi} - \beta^i\partial_i\phi - \alpha\gamma^{ij}\partial_i\phi\partial_j\phi\right)\right] \,, \tag{2.1}$$

which has the following associated stress energy tensor

$$T_{\mu\nu} = \partial_\mu\phi\partial_\nu\phi - \frac{1}{2}g_{\mu\nu}\left(g^{\alpha\beta}\partial_\alpha\phi\partial_\beta\phi + 2V(\phi)\right) \,. \tag{2.2}$$

We can now easily compute the energy density and the pressure of the scalar field in the homogeneous and isotropic background (from now on the background) given by the flat FLRW metric:

$$\bar{\rho} = \frac{\dot{\bar{\phi}}^2}{2} + V\left(\bar{\phi}\right) \,, \qquad \bar{p} = \frac{\dot{\bar{\phi}}^2}{2} - V\left(\bar{\phi}\right) \,, \tag{2.3}$$

where we are introducing the notation with a bar to denote that they are background quantities. Note also that, because these quantities are evolving in a perfectly homogeneous and isotropic universe, they are only time dependent.

Finally, we can obtain the relevant ADM equations (the Hamiltonian constraint (1.21) and the equation of motion for the the extrinsic curvature (1.24)) for this system

$$\bar{H}^2 = \frac{1}{3M_{PL}^2}\left(\frac{\dot{\bar{\phi}}^2}{2} + V\left(\bar{\phi}\right)\right) \,, \tag{2.4}$$

$$\dot{\bar{H}} + \bar{H}^2 = -\frac{1}{3M_{PL}^2}\left(\dot{\bar{\phi}}^2 - V\left(\bar{\phi}\right)\right) \,. \tag{2.5}$$

Although equations (2.4) and (2.5) are the equations that we get by the direct application of the ADM formalism, (2.5) is usually combined with the time derivative of (2.4) to get an equation of motion for the scalar field

$$\bar{H}^2 = \frac{1}{3M_{PL}^2}\left(\frac{\dot{\bar{\phi}}^2}{2} + V\left(\bar{\phi}\right)\right) \,, \tag{2.6}$$

$$\ddot{\bar{\phi}} + 3\bar{H}\dot{\bar{\phi}} + V_{\bar{\phi}}\left(\bar{\phi}\right) = 0 \,. \tag{2.7}$$

Note that (2.7) is the usual Klein-Gordon equation for a scalar field in a flat FLRW universe, where $V_{\bar{\phi}}\left(\bar{\phi}\right) = \frac{dV\left(\bar{\phi}\right)}{d\bar{\phi}}$.

Before proceeding further, it is very useful to define a dimensionless parameter which tell us when we are in an accelerating universe and when we are not. From (1.57) we know that, in order to have an accelerating expanding universe we need $\frac{\ddot{a}}{a} > 0$, this condition can be rewritten as

$$\frac{\ddot{a}}{a} = \dot{\bar{H}} + \bar{H}^2 = \bar{H}^2 \left(1 + \frac{\dot{\bar{H}}}{\bar{H}^2}\right) > 0 \,. \tag{2.8}$$

Motivated by (2.8), we can define the first slow roll parameter ϵ_1 as

$$\epsilon_1 \equiv -\frac{\dot{\bar{H}}}{\bar{H}^2} \,. \tag{2.9}$$

It is then clear that, in order to have an accelerating expansion of the universe we need $0 < \epsilon_1 < 1$. If $\epsilon_1 \ll 1$, then $\bar{H}$ is almost constant and hence the expansion is almost exponential i.e. the geometry is almost de-Sitter. In other words, the smaller the value for ϵ_1, the closer we are to a FLRW universe whose background energy is dominated by a cosmological constant. The parameter ϵ_1 can also be written in terms of the velocity of the field using (2.5), the result is

$$\epsilon_1 = \frac{\dot{\bar{\phi}}^2}{2M_{PL}^2 \bar{H}^2} \,. \tag{2.10}$$

With the definition of ϵ_1 in terms of the velocity of the field (2.10), we can also very conveniently write the equation of state of the scalar field as

$$p = \omega \rho \,, \qquad \text{where} \qquad \omega = -1 + \frac{2}{3}\epsilon_1 \,. \tag{2.11}$$

Finally, we will define higher slow roll parameters as follows

$$\epsilon_i \equiv \frac{1}{\bar{H}\epsilon_{i-1}} \frac{d\epsilon_{i-1}}{dt} \,. \tag{2.12}$$

Note that, although in order to have an accelerated expansion of the universe we need to impose a condition on ϵ_1, this is in principle not true for higher slow roll parameters. For example ϵ_2 can be of the same order of ϵ_1, but it can also be much larger or even negative. The different behaviour of the higher order slow roll parameters allow us to define different inflationary regimes.

1. **Slow Roll inflation (SR):** Perhaps the most known inflationary regime because, as we will see in the next section, is the one responsible to describe the almost scale invariant power spectrum of density fuctuations observed in the CMBR. In this case the field is slowly rolling down a potential with an almost constant velocity which makes the acceleration negligible. The equation of motion (2.7) is approximately

$$3\bar{H}\dot{\bar{\phi}} + V_{\bar{\phi}}\left(\bar{\phi}\right) \simeq 0\,. \tag{2.13}$$

All the SR parameters are much smaller than one ($\epsilon_i \ll 1$). The first and the second one can be written in terms of the potential as

$$\epsilon_1^{SR} \simeq \frac{M_{PL}^2}{2}\left(\frac{V_{\phi^b}}{V}\right)^2 \;; \qquad \epsilon_2^{SR} \simeq -2M_{PL}^2\left(\frac{V_{\phi^b\phi^b}}{V}\right) + 4\epsilon_1^{SR}\,. \tag{2.14}$$

Note that the approximations done in (2.13) and (2.14) are valid up to $\mathcal{O}\left(\epsilon_i^{SR}\right)$ (they fail at $\mathcal{O}\left(\left(\epsilon_i^{SR}\right)^2\right)$). In the same way, the time derivative of ϵ_1 is $\bar{H}\epsilon_1\epsilon_2$ and since both ϵ_1 and ϵ_2 are much smaller than 1, we can conclude that ϵ_1 (and consequently ω in (2.11)[1]) is constant up to $\mathcal{O}\left(\epsilon_i^{SR}\right)$.

2. **Ultra Slow Roll inflation (USR) [73, 74, 75, 76, 77]:** The field is moving along an exactly flat potential ($V_\phi = 0$), which makes the acceleration relevant. In this case the equation of motion (2.7) is

$$\ddot{\phi}^b + 3H^b\dot{\phi}^b = 0\,. \tag{2.15}$$

From (2.15) one can infer that the velocity of the field (and hence ϵ_1) exponentially decreases, which makes some $\epsilon_i \sim \mathcal{O}(1)$. More precisely:

$$\begin{aligned} \epsilon_i^{USR} &= -6 + 2\epsilon_1^{USR} \qquad \text{when} \quad i \quad \text{even.} \\ \epsilon_i^{USR} &= 2\epsilon_1^{USR} \qquad \text{when} \quad i > 1 \quad \text{and odd.} \end{aligned} \tag{2.16}$$

In the case of USR, both ϵ_1 and ω in (2.11) are constant only if we do not consider any ϵ_1 term, we will call this leading order in ϵ_1. Note that, in this specific regime, a time dependent ω does not imply $\bar{p} \neq \bar{p}(\bar{\rho})$ as one would think, in fact, because $V(\bar{\phi}) = V_0$ is a constant, we can exactly write $\bar{p} = \bar{\rho} - 2V_0$ and hence $\bar{p} = \bar{p}(\bar{\rho})$ in USR.

Because $\bar{p} = \bar{p}(\bar{\rho})$ holds up to $\mathcal{O}\left(\epsilon_i^{SR}\right)$ in SR and exactly in USR, we will say that SR is approximately adiabatic and USR is exactly adiabatic [78].

3. **Constant-Roll (CR) [79, 80]**: Both SR and USR are, at least approximately, subcases of Constant-Roll. Here $\frac{V_{\bar{\phi}}}{\bar{H}\dot{\bar{\phi}}} = \kappa$ where κ is a constant. SR is realized when $\kappa \simeq -3$ while USR when $\kappa = 0$.

In this case, we can write the behaviour of the SR parameters as follows

[1]Note that ω being a constant up to $\mathcal{O}\left(\epsilon_i^{SR}\right)$ means that $p = p(\rho)$ up to the same order.

$$\epsilon_i^{CR} = -6\left(1+\frac{\kappa}{3}\right) + 2\epsilon_1^{CR} \qquad \text{when} \quad i \quad \text{even.}$$
$$\epsilon_i^{CR} = 2\epsilon_1^{CR} \qquad \text{when} \quad i>1 \quad \text{and odd.} \qquad (2.17)$$

Note that, generically, in CR we can only write $p = p(\rho)$ at leading order in ϵ_1. Furthermore, apart from the already explained SR and USR regimes, it is important to distinguish between another three different CR regimes:

- $\boldsymbol{\kappa < -3}$: In this case the field is rolling down the potential with exponentially increasing velocity.
- $\boldsymbol{-3 < \kappa < 0}$: here the field is still rolling down the potential but its velocity is decreasing due to the Hubble friction (the $3H\dot{\bar{\phi}}$ term).
- $\boldsymbol{\kappa > 0}$: In this case the field is climbing up the potential and hence the velocity is exponentially decreasing, this regime is unstable and it cannot be maintained for a long period of time.

It is important to remark that, given a potential, SR, USR or even CR, are only approximated regimes. In order to know the precise dynamics, one should solve the Klein-Gordon equation for the field (2.7) exactly. This is specially important in transition between different regimes, where $\frac{V_{\bar{\phi}}}{\bar{H}\dot{\bar{\phi}}}$ is not a constant, even approximately, we will explore numerical results of these kinds of transitions in section 2.7.

2.2 Cosmological perturbation theory.

The scenario presented in the previous section is of course only a part of the story, the reason is that the inflaton is a quantum field and hence there is unavoidable quantum fluctuations that will backreact on the metric. These fluctuations, which are small (or not so small, as we will see later on) deviations from perfect homogeneity and isotropy, are extremely important during inflation and they are typically studied using linear perturbation theory.

Although cosmological perturbation theory was already a very well-known theory before inflation [81, 82, 83, 84, 85, 86], it was first introduced in the context of inflationary cosmologies in [87, 88, 89] (see [90] for a nice review), where the Einstein equations of (1.19) were perturbed. A more modern approach is to directly perform perturbation theory in the Einstein Hilbert action (1.1) as done for example in [91]. In this thesis we will take a slightly different approach and we will take advantage of the introduction of the ADM formalism in section 1.3 to perturb directly the ADM equations, but first it is convenient to decompose the ADM variables as follows: first, the spatial metric will be written $\gamma_{ij} = a^2(t)e^{2\zeta}\tilde{\gamma}_{ij}$ with $\det\tilde{\gamma}_{ij} = 1$, such that we introduce the space-independent $a(t)$ as the scale factor, second, the extrinsic curvature will be splitted into its trace and traceless part as follows

$$K_{ij} = \frac{\gamma_{ij}}{3}K + a^2e^{2\zeta}\tilde{A}_{ij}\,, \tag{2.18}$$

where $\tilde{\gamma}^{ij}\tilde{A}_{ij} = 0$.

With these new variables, the ADM system (1.21)-(1.24) becomes [8]:

- Hamiltonian constraint

$$R^{(3)} - \tilde{A}_{ij}\tilde{A}^{ij} + \frac{2}{3}K^2 - 2\Lambda = \frac{2}{M_{PL}^2}E\,. \tag{2.19}$$

- Momentum constraint

$$D^j\tilde{A}_{ij} - \frac{2}{3}D_iK = \frac{1}{M_{PL}^2}J_i\,. \tag{2.20}$$

- Equation of motion for the metric:
  - For the trace part:

$$(\partial_t - \beta^k\partial_k)\zeta + \frac{\dot{a}}{a} = -\frac{1}{3}(\alpha K - \partial_k\beta^k)\,. \tag{2.21}$$

  - For the traceless part:

$$(\partial_t - \beta^k\partial_k)\tilde{\gamma}_{ij} = -2\alpha\tilde{A}_{ij} + \tilde{\gamma}_{ik}\partial_j\beta^k + \tilde{\gamma}_{jk}\partial_i\beta^k - \frac{2}{3}\tilde{\gamma}_{ij}\partial_k\beta^k\,. \tag{2.22}$$

- Equation of motion for the extrinsic curvature
  - For the trace part:

$$(\partial_t - \beta^k\partial_k)K = \alpha\left(\tilde{A}_{ij}\tilde{A}^{ij} + \frac{1}{3}K^2 - \Lambda\right) - D_kD^k\alpha + 4\pi G\alpha(E + S^k_k), \tag{2.23}$$

  - For the traceless part:

$$\begin{aligned}(\partial_t - \beta^k\partial_k)\tilde{A}_{ij} = &\frac{e^{-2\zeta}}{a^2}\left[\alpha\left(R^{(3)}_{ij} - \frac{\gamma_{ij}}{3}R^{(3)}\right) - \left(D_iD_j\alpha - \frac{\gamma_{ij}}{3}D_kD^k\alpha\right)\right]\\ &+ \alpha(K\tilde{A}_{ij} - 2\tilde{A}_{ik}\tilde{A}^k_j) + \tilde{A}_{ik}\partial_j\beta^k + \tilde{A}_{jk}\partial_i\beta^k - \frac{2}{3}\tilde{A}_{ij}\partial_k\beta^k\\ &- \frac{8\pi G\alpha e^{-2\zeta}}{a^2}\left(S_{ij} - \frac{\gamma_{ij}}{3}S^k_k\right)\,.\end{aligned} \tag{2.24}$$

Cosmological perturbation theory assumes that the deviations from a perfectly homogeneous and isotropic universe are small and hence we can define a background flat FLRW universe and small fluctuations over it. In the context of the ADM formalism, we already know what are the values that the lapse function, the shift vector and the spatial metric must have if we want to describe a flat FLRW universe (see the discussion below equation (1.34) in section 1.4), so we just have to define small fluctuations over those values as follows:

$$\begin{aligned} \alpha &\simeq 1 + A\,, \\ \beta_j &\simeq 0 + aB_j\,, \\ e^{2\zeta} &\simeq 1 + 2D\,, \\ \tilde{\gamma}_{ij} &\simeq \delta_{ij} - 2E_{ij}\,, \end{aligned} \tag{2.25}$$

where the first term in the left-hand side of (2.25) corresponds to the value of the background metric. E_{ij} must be traceles by definition [2]. Note that the last two linearizations in (2.25) leads to

$$\gamma_{ij} \simeq a^2 \left[(1+2D)\,\delta_{ij} - 2E_{ij} \right] . \tag{2.26}$$

for the spatial metric. The linearized metric is then straightforwardly written down as:

$$ds^2_{\text{lin}} = -(1+2A)dt^2 + 2a(t)B_i dx^i dt + a^2(t) \left[(1+2D)\,\delta_{ij} - 2E_{ij} \right] dx^i dx^j\,. \tag{2.27}$$

Finally, the scalar field responsible for inflation must also be linearized i.e.

$$\phi \simeq \bar{\phi} + \delta\phi\,. \tag{2.28}$$

It can be easily shown that, of the linear variables introduced above, A, D and $\delta\phi$ transform as scalars under rotations in the background space-time coordinates, B_i as a 3-vector and E_{ij} as a 3D-tensor. This does not mean that the only scalar components are A, D and $\delta\phi$, in fact, we know from Euclidean 3D vector calculus that a vector can be decomposed as:

$$B_i = B_i^S + B_i^V \qquad \text{with} \qquad \partial_i B_j^S - \partial_j B_i^S = 0 \qquad \text{and} \qquad \partial^i B_i^V = 0\,, \tag{2.29}$$

[2]The reason why E_{ij} is traceless is because is the perturbation of $\tilde{\gamma}_{ij}$, which has unit determinant. Precisely, any matrix with unit determinant can be written as:

$$\tilde{\gamma}_{ij} = e^{-2M_{ij}}\,,$$

where M_{ij} is traceless.

and hence

$$B_i^S = \partial_i B\,, \tag{2.30}$$

where B is some scalar field.

Similarly, for a tensor field we have

$$E_{ij} = E_{ij}^S + E_{ij}^V + h_{ij}\,, \tag{2.31}$$

where

$$\begin{aligned} E_{ij}^S &= \left(\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2\right)E\,, \\ E_{ij}^V &= \frac{1}{2}\left(\partial_j E_i + \partial_i E_j\right) \qquad \text{with} \qquad \partial^i E_i = 0\,, \\ \partial^i h_{ij} &= 0\,, \\ \delta^{ij} h_{ij} &= 0\,, \end{aligned} \tag{2.32}$$

where E is again a scalar field.

The procedure explained above allows us to decompose the perturbations into a scalar, vector and tensor sector. As we will see in the following, these sectors evolve independently one from each other at linear order in perturbation theory, which make them easier to handle.

2.2.1 Scalar sector

During this thesis we will be mostly focused on scalar perturbations of the metric since they are the ones that couple to the scalar field perturbation $\delta\phi$. The scalar sector of (2.27) is

$$ds^2 = -(1+2A)dt^2 + 2a\partial_i B dx^i dt + a^2\left[(1+2D)\delta_{ij} - 2\left(\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2\right)E\right]dx^i dx^j\,. \tag{2.33}$$

It is worthy to remark that sometimes in the literature the variables proportional to δ_{ij} are written together in such a way that the metric is

$$ds^2 = -(1+2A)dt^2 + 2a\partial_i B dx^i dt + a^2\left[(1+2\psi)\delta_{ij} - 2\partial_i\partial_j E\right]dx^i dx^j\,. \tag{2.34}$$

where $\psi = D + \frac{1}{3}\nabla^2 E$. We will however not use this notation because it is easier to identify the ADM decomposition in trace and traceless parts performed in (2.19)-(2.24) with the linearized metric of (2.33).

Making use of (2.33) and of (2.28) we can easily write the first order in perturbation theory ADM equations as follows (remember that the zeroth order in perturbation theory ADM equations are the ones in (2.4)-(2.5)):

- Hamiltonian constraint

$$2\bar{H}\left(\dot{D}-\bar{H}A-\frac{1}{3}\frac{\nabla^2}{a}B\right)-\frac{2}{3}\frac{\nabla^2}{a^2}\left(D+\frac{1}{3}\nabla^2 E\right)=\frac{1}{3M_{PL}^2}\left(\dot{\bar{\phi}}\dot{\delta\phi}-\dot{\bar{\phi}}^2 A+V_{\bar{\phi}}\delta\phi\right). \tag{2.35}$$

- Momentum constraint

$$\partial_i\left(-\bar{H}A+\dot{D}+\frac{1}{3}\nabla^2\dot{E}+\frac{1}{2M_{PL}^2}\dot{\bar{\phi}}\delta\phi\right)=0\,. \tag{2.36}$$

- Equation of motion for the metric:
  - For the trace part:

$$\delta H=\dot{D}-\bar{H}A-\frac{1}{3}\frac{\nabla^2}{a}B\,, \tag{2.37}$$

    where we have used the identification $\bar{K}+\delta K\equiv -3(\bar{H}+\delta H)$. Note that the only function of (2.37) is to define the perturbation of the Hubble parameter.

  - For the traceless part:

$$\delta\tilde{A}^S_{ij}=\left(\partial_i\partial_j-\frac{1}{3}\delta_{ij}\nabla^2\right)\left(\frac{B}{a}+\dot{E}\right)\,. \tag{2.38}$$

    Similarly to (2.37), (2.38) only give us the definition of the perturbation of the scalar sector of $\tilde{A}_{ij}$ in terms of the quantities that appear in the metric (2.33). From now on, we will use (2.37) and (2.38) every time a δH or $\delta\tilde{A}^S_{ij}$ appears to avoid writing too many perturbation variables.

- Equation of motion for the extrinsic curvature
  - For the trace part:

$$\begin{aligned}&\ddot{D}-2\dot{\bar{H}}A-\bar{H}\dot{A}-\frac{1}{3}\frac{\nabla^2}{a}\dot{B}+2\bar{H}\dot{D}-2\bar{H}^2A-\frac{1}{3}\bar{H}\frac{\nabla^2}{a}B-\frac{1}{3}\frac{\nabla^2}{a^2}A\\&=-\frac{1}{3M_{PL}^2}\left(2\dot{\bar{\phi}}\dot{\delta\phi}-2\dot{\bar{\phi}}^2A-V_{\bar{\phi}}\delta\phi\right),\end{aligned} \tag{2.39}$$

  - For the traceless part:

$$\left(\partial_i\partial_j-\frac{1}{3}\delta_{ij}\nabla^2\right)\left(\frac{d}{dt}\left(\frac{B}{a}+\dot{E}\right)+3\bar{H}\left(\frac{B}{a}+\dot{E}\right)+\frac{1}{a^2}\left(A+D+\frac{1}{3}\nabla^2E\right)\right)=0\,. \tag{2.40}$$

Finally, and similarly to what we have done when studying the homogeneous equation of motion, we can perform the time derivative of the linearized Hamiltonian constraint (2.35) and insert the result in the equation of motion for the trace of the extrinsic curvature (2.39). The result is an equation of motion for the scalar field, as expected

$$\ddot{\delta\phi}+3\bar{H}\dot{\delta\phi}+V_{\bar{\phi}\bar{\phi}}\delta\phi+2V_{\bar{\phi}}A-\dot{\bar{\phi}}\left(\dot{A}-3\dot{D}+\frac{\nabla^2}{a^2}B\right)+\frac{2M_{PL}^2}{\dot{\bar{\phi}}}\frac{\nabla^2}{a^2}\left(-\bar{H}A+\dot{D}+\frac{1}{3}\nabla^2\dot{E}\right)=0\,. \tag{2.41}$$

Note that the last term of (2.41) can be further simplified by applying the operator $\delta^{ij}\partial_j$ to the linear momentum constraint (2.36). The final result for the linearized version of the KG equation is

$$\ddot{\delta\phi}+3\bar{H}\dot{\delta\phi}+V_{\bar{\phi}\bar{\phi}}\delta\phi-\frac{\nabla^2}{a^2}\delta\phi+2V_{\bar{\phi}}A-\dot{\bar{\phi}}\left(\dot{A}-3\dot{D}+\frac{\nabla^2}{a^2}B\right)=0\,. \tag{2.42}$$

In the vast majority of textbooks, the linearized KG equation (2.42) is obtained by perturbing the continuity equation $\nabla_\mu T^{\mu\nu}=0$. The reason we wanted to do it using solely the ADM equations is because we would like to remark that, in order to obtain the same form of the linearized KG equation as the one given by the continuity equation, we must use the momentum constraint to go from (2.41) to (2.42), which already give us a hint of its importance. Of course this does not happen when dealing with an exactly homogeneous and isotropic universe, where the momentum constraint does not play any role.

Once we have seen what are the linear equations describing small inhomogeneities in the scalar sector, it is important to have a physical intuition about what a scalar perturbation of the metric really means. By definition, a perturbation is the difference between the value of a quantity with respect to its value on the idealized FLRW background. This seems trivial, however, in order to make such a comparison, it is necessary to compute these two values at the same space-time point. Since the quantities to compare live in different space-times, we require a pointwise correspondence between them, which is given by a coordinate system x^μ such that the point P^b in the background space-time and the point P in the perturbed space-time, which have the same coordinate values, correspond to each other.

The freedom in the choice among these coordinate systems is called the gauge choice. Different gauges are related in linear perturbation theory (for gauge transformations beyond linear perturbation theory see for example [92]) via an infinitesimal gauge transformation of coordinates:

$$\tilde{x}^\mu=x^\mu+\delta x^\mu\,. \tag{2.43}$$

We can split the vector δx^μ into its time an space components $\delta x^\mu = (\lambda^0, \lambda^i)$, and, following the same idea as when we decomposed the perturbations in the metric, λ^i can be written as $\lambda^i = \lambda^i_\perp + \partial^i \eta$, where $\lambda^i_\perp$ is a 3-dimensional divergenless vector and η is a scalar function. In terms of these functions, the perturbed metric components of (2.33) transform as:

$$
\begin{aligned}
D \to \tilde{D} &= D + a\bar{H}\lambda^0 + \frac{1}{3}\nabla^2\eta \,, \\
A \to \tilde{A} &= A + a\bar{H}\lambda^0 + a\dot{\lambda}^0 \,, \\
E \to \tilde{E} &= E - \eta \,, \\
B \to \tilde{B} &= B + a\dot{\eta} - \lambda^0 \,.
\end{aligned} \tag{2.44}
$$

Finally, the scalar field perturbation transforms as:

$$
\delta\phi \to \tilde{\delta\phi} = \delta\phi + a\dot{\bar{\phi}}\lambda^0 \,. \tag{2.45}
$$

From (2.44) and (2.45) we can clearly see that the freedom on the choice of the gauge allows us to set two out of the five scalar perturbations to zero by choosing η and λ^0 accordingly. Some known choices of these parameters (gauge choices) are

- **Flat gauge:** In this gauge we are interested in choosing an exactly flat 3-dimensional hypersurface. In order to do so, it is clear from (2.33) that we must set $D_f = 0$ and $E_f = 0$, where the subscript f stands for flat gauge (we will follow the same notation for the rest of the gauges).

- **Newtonian gauge:** This gauge kills all the non-diagonal terms in the metric (2.33), reason why it is convenient to identify the D_N as the Newtonian gravitational potential of classical Newtonian gravity. This gauge is hence characterized by $B_N = 0$ and $E_N = 0$.

- **Synchronous gauge:** In this gauge the time lines are normal to the constant time hypersurfaces Σ_t, which means $A_s = 0$ and $B_s = 0$. Note that although the synchronous gauge completely fixes λ^0 when setting $A_s = 0$, it leaves some spatial freedom in η, the reason is that $B_s = 0$ only fixes $\dot{\eta}$ and not η itself. We can then say that the synchronous gauge as defined here does not completely fixes the gauge. This will not be a big issue for the rest of the thesis so we will not pay more attention to it.

- **Comoving gauge:** In this gauge the constant time hypersurfaces Σ_t are orthogonal to the fluid 4-velocity u_μ and hence $\delta\phi_c = 0$ and $B_c = 0$.

- **Uniform density gauge:** The definition of this gauge is simply to set the perturbation of the energy density to zero ($\delta\rho_{ud} = 0$). $\delta\rho$ in any gauge can be easily defined by means of the linearized Hamiltonian constraint of (2.35) as

$$\delta\rho \equiv \dot{\bar{\phi}}\dot{\delta\phi} - \dot{\bar{\phi}}^2 A + V_{\bar{\phi}}\delta\phi \tag{2.46}$$

Using the transformations rules of (2.44), one can also show that $\delta\rho$ trasforms as

$$\delta\rho \to \tilde{\delta\rho} = \delta\rho + a\dot{\bar{\rho}}\lambda^0 \,. \tag{2.47}$$

From (2.47) we see that setting $\delta\rho_{ud} = 0$ only fixes λ^0, in order to fix also η one usually sets $E_{ud} = 0$ to fully characterize the uniform density gauge.

- **Uniform Hubble gauge:** This gauge is defined by setting the perturbation in the Hubble rate to zero i.e. $\delta H_{uH} = 0$, where δH is defined in (2.37). It can be then shown then that δH transforms as

$$\delta H \to \tilde{\delta H} = \delta H + a\dot{\bar{H}}\lambda^0 + \frac{1}{3a}\nabla^2\lambda^0 \,. \tag{2.48}$$

The uniform Hubble gauge is usually supplemented by fixing (the time dependent part of) η by $B_{uH} = 0$ [93, 94].

- **Uniform N gauge:** In order to define this gauge we must first define the number of e-folds N, which quantifies the expansion of the universe in logarithmic scale such that $a \equiv e^N$, from where one can also show the following relation

$$dN = H\alpha dt \quad \to \quad N = \int H\alpha dt \,. \tag{2.49}$$

It is clear from (2.50) that the homogeneous and isotropic N is simply $\bar{N} = \int \bar{H}dt$ and that the perturbed δN is

$$\delta N = D - \frac{1}{3}\nabla^2 \int \frac{B}{a}dt \,, \tag{2.50}$$

which transforms as

$$\delta N \to \tilde{\delta N} = \delta N + a\bar{H}\lambda^0 + \frac{1}{3}\nabla^2 \int \frac{\lambda^0}{a}dt \,. \tag{2.51}$$

The uniform N gauge is usually supplemented by fixing (the time dependent part of) η by $B_{uN} = 0$ [95, 96].

Fixing λ^0 and η reduces the scalar degrees of freedom to three (which further reduces to two when using the ADM equations for a single scalar field), which can be written in terms of gauge invariant, and hence physical, variables: the two Bardeen potentials [86]

$$\Psi \equiv -D - \frac{1}{3}\nabla^2 E - aH^b\left(B + a\dot{E}\right)\,,$$
$$\Phi \equiv A + aH^b(B + a\dot{E}) + a\frac{d}{dt}(B + a\dot{E})\,, \tag{2.52}$$

and the Mukhanov-Sasaki (MS) variable [87, 88, 89]

$$Q \equiv \delta\phi - \frac{\dot{\bar{\phi}}}{\bar{H}}\left(D + \frac{1}{3}\nabla^2 E\right)\,. \tag{2.53}$$

Finally, a quantity of special interest which is proportional to the MS variable and hence it is also gauge invariant, is the comoving curvature perturbation, defined as

$$\mathcal{R} \equiv -\frac{\bar{H}}{\dot{\bar{\phi}}}Q = \left(D + \frac{1}{3}\nabla^2 E\right) - \frac{\bar{H}}{\dot{\bar{\phi}}}\delta\phi\,. \tag{2.54}$$

Let us also emphasise the name given to $\mathcal{R}$, i.e. "comoving curvature perturbation", the reason for this name is that in the comoving gauge, where $\delta\phi_c = 0$, $\mathcal{R} = \left(D + \frac{1}{3}\nabla^2 E\right)$ and hence it coincides with the curvature perturbation of the spatial metric. It is important then to remark that "comoving" appears in the name of $\mathcal{R}$ not because this quantity is defined only in one gauge, in fact it is a gauge invariant variable. Note that we could define any other gauge-invariant curvature perturbation in the same way, for example the "uniform density curvature perturbation" is

$$\mathfrak{z} \equiv \left(D + \frac{1}{3}\nabla^2 E\right) - \frac{\bar{H}}{\dot{\bar{\rho}}}\delta\rho\,. \tag{2.55}$$

and it coincides with the curvature perturbation of the spatial metric when we choose the uniform density gauge.

2.2.1.1 The Mukhanov-Sasaki equation

One could now write the linearized equations (2.35)-(2.40) in terms solely of the gauge invariant parameters (2.52)-(2.53). However, there exist even a more compact way of writing the relevant gauge invariant scalar degree of freedom: the MS equation. The idea is to combine the linearized hamiltonian constraint, the linearized KG for the scalar field and the integrated version of the linearized momentum constraint to obtain an equation of motion for the MS variable of (2.53), or equivalently for the comoving curvature perturbation of (2.54).

It is important to remark that we will use the integrated version of the momentum constraint when deriving the MS equation i.e. we will use

$$\int \partial_i \left(-\bar{H}A + \dot{D} + \frac{1}{3}\nabla^2 \dot{E} + \frac{1}{2M_{PL}^2}\dot{\bar{\phi}}\delta\phi \right) dx^i = 0\,, \tag{2.56}$$

which obviously leaves some freedom for a time dependent function that we will call $\dot{f}_1(t)$ for convenience:

$$-\bar{H}A + \dot{D} + \frac{1}{3}\nabla^2 \dot{E} + \frac{1}{2M_{PL}^2}\dot{\bar{\phi}}\delta\phi = \dot{f}_1(t)\,, \tag{2.57}$$

where $\dot{f}_1(t)$ is set by boundary conditions.

Combining now the the Hamiltonian constraint (2.35), the KG equation of the field (2.42) and the integrated momentum constraint (2.57) we get an equation of motion for the MS variable Q

$$\begin{aligned} \ddot{Q} + 3\bar{H}\dot{Q} + &\left[-\frac{\nabla^2}{a^2} + \bar{H}^2 \left(-\frac{3}{2}\epsilon_2 + \frac{1}{2}\epsilon_1\epsilon_2 - \frac{1}{4}\epsilon_2^2 - \frac{1}{2}\epsilon_2\epsilon_3 \right) \right] Q \\ &+ \frac{\dot{\bar{\phi}}}{\bar{H}} \left(\ddot{f}_1(t) + \bar{H}(3+\epsilon_2)\dot{f}_1(t) \right) = 0\,, \end{aligned} \tag{2.58}$$

or, written in terms of the comoving curvature perturbation $\mathcal{R}$

$$\frac{1}{a^3\epsilon_1}\frac{d}{dt}\left(a^3\epsilon_1 \left(\dot{\mathcal{R}} - \dot{f}_1(t) \right) \right) - \frac{\nabla^2}{a^2}\mathcal{R} = 0\,. \tag{2.59}$$

The expressions for the MS equation given in (2.58) and in (2.59) are not what one usually finds in the literature, the reason is that usually the boundary condition $\dot{f}_1(t) = 0$ is given for granted. It is important however to have in mind that this boundary condition is related with the assumption that the solution for the perturbations is well behaved in the long-wavelength limit. For the interested reader, Weinberg explains more in detail this "mild assumption" is his paper [97]. Setting $\dot{f}_1(t) = 0$ we finally obtain the most famous form for the MS equation, both for the variable Q

$$\ddot{Q} + 3\bar{H}\dot{Q} + \left[-\frac{\nabla^2}{a^2} + \bar{H}^2 \left(-\frac{3}{2}\epsilon_2 + \frac{1}{2}\epsilon_1\epsilon_2 - \frac{1}{4}\epsilon_2^2 - \frac{1}{2}\epsilon_2\epsilon_3 \right) \right] Q = 0\,, \tag{2.60}$$

and for $\mathcal{R}$

$$\frac{1}{a^3\epsilon_1}\frac{d}{dt}\left(a^3\epsilon_1\dot{\mathcal{R}} \right) - \frac{\nabla^2}{a^2}\mathcal{R} = 0\,. \tag{2.61}$$

Before proceeding with the solution of the MS equation it is worthy to mention that there is another gauge invariant equation that we have not used in the derivation of the

MS equation and that relates the two Bardeen potentials, this is the evolution equation for the traceless part of the extrinsic curvature (2.40) and it can be written as

$$\left(\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2\right)(\Phi - \Psi) = 0\,, \tag{2.62}$$

and hence, given the appropriate boundary conditions, $\Phi = \Psi$ if the matter content of the universe do not have anisotropic stress.

Once we know the equation of motion of the relevant scalar degrees of freedom ((2.60) or (2.61)), the next logical step is to try to solve it. In order to do so it is useful to define two new quantities

$$z \equiv a\frac{\dot{\phi}}{H}\,, \quad v \equiv aQ = -z\mathcal{R} \tag{2.63}$$

In terms of v and z, the MS equation can be written as

$$\ddot{v} + \bar{H}\dot{v} - \frac{\ddot{z} + \bar{H}\dot{z}}{z}v - \frac{\nabla^2}{a^2}v = 0\,, \tag{2.64}$$

which can be written in terms of the conformal time $d\tau = \frac{dt}{a}$ in a simpler way

$$v'' - \frac{z''}{z}v - \nabla^2 v = 0\,, \tag{2.65}$$

where a prime stands for the derivative with respect to conformal time and $\frac{z''}{z}$ can be written in terms of the SR parameters as follows

$$\frac{z''}{z} = \mathcal{H}^2\left(2 - \epsilon_1 + \frac{3}{2}\epsilon_2 - \frac{1}{2}\epsilon_1\epsilon_2 + \frac{1}{4}\epsilon_2^2 + \frac{1}{2}\epsilon_1\epsilon_2\right)\,, \tag{2.66}$$

where we have also introduced the conformal Hubble parameter $\mathcal{H} \equiv \frac{a'}{a} = a\bar{H}$.

In order to solve (2.65) we define the Fourier expansion of the field v:

$$v(t, \mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} v_{\mathbf{k}}(\tau)e^{i\mathbf{k}\cdot\mathbf{x}}\,, \tag{2.67}$$

where, according to the MS equation (2.65), the Fourier mode $v_{\mathbf{k}}$ must be a solution of the following equation

$$v_k'' + \left(k^2 - \frac{z''}{z}\right)v_k = 0\,, \tag{2.68}$$

where we have substituted the subscript **k** by its module $|\mathbf{k}| = k$, because (2.68) only depends on k.

By performing a simple change of variable $v_k \equiv (-\tau)^{1/2}s_k$, equation (2.68) can be written in a very convenient way as follows

$$\tau^2 s_k'' + \tau s_k' + \left(k^2\tau^2 - \nu^2\right) s_k = 0\,, \tag{2.69}$$

where $\nu^2 \equiv \frac{1}{4} + \frac{z''}{z}\tau^2$. Equation (2.69) has a analytical solution if and only if ν^2 is a constant, in this case (2.69) reduces to the well-known Bessel's differential equation and hence its solution can be written in terms of Bessel functions. It is then of crucial importance to know when ν^2 can be approximated as a constant, this will strongly depends on which of the inflationary regimes of section 2 we want to study. In the following we will show under which conditions ν is correctly assumed to be a constant:

First of all, it is very convenient to write τ in terms of $\mathcal{H} = a\bar{H}$ to see if the term $\frac{z''}{z}\tau^2$ is a constant. In the following we will do this for a general CR regime up to $\mathcal{O}(\epsilon_1)$. The first step is to use the definition of τ and integrate by parts

$$\tau = -\frac{1}{a\bar{H}} + \int \frac{da}{a^2\bar{H}}\epsilon_1\,. \tag{2.70}$$

Now we use the results of the end of section 2 to can write ϵ_1 as

$$\epsilon_1 = \epsilon_1^0 a^{-(6+2\kappa)} + \mathcal{O}\left(\epsilon_1^2\right)\,. \tag{2.71}$$

Using the solution of (2.71) we can integrate the second term in (2.70) again by parts such that

$$\int \frac{da}{a^2 H}\epsilon_1 = -\frac{\epsilon_1}{7\bar{H}a} - \frac{2\kappa}{7}\int \frac{da}{a^2 H}\epsilon_1 + \mathcal{O}\left(\epsilon_1^2\right)\,. \tag{2.72}$$

Combining (2.70) and (2.73) we get

$$\tau = -\frac{1}{\mathcal{H}}\left(1 + \frac{1}{2k+7}\epsilon_1\right) + \mathcal{O}\left(\epsilon_1^2\right)\,. \tag{2.73}$$

Finally, we can compute ν using the definition of $\frac{z''}{z}$ of (2.66)

$$\nu = \sqrt{\frac{1}{4} + \frac{z''}{z}\tau^2} = \frac{3}{2}\sqrt{1 - \frac{4}{9}\frac{V_{\bar{\phi}\bar{\phi}}}{\bar{H}^2}} - \frac{3(15+12\kappa+2\kappa^2)}{|3+2\kappa|\,(7+2\kappa)}\epsilon_1\,, \tag{2.74}$$

where we have used the following result

$$\frac{V_{\bar{\phi}\bar{\phi}}}{\bar{H}^2} = 6\epsilon_1 - \frac{3}{2}\epsilon_2 - 2\epsilon_1^2 - 2\epsilon_1^2 + \frac{5}{2}\epsilon_1\epsilon_2 - \frac{1}{4}\epsilon_1^2 - \frac{1}{2}\epsilon_2\epsilon_3\,. \tag{2.75}$$

Although we have just computed ν up to $\mathcal{O}(\epsilon_1)$, as we said before we are only interested in the cases in which ν is approximately constant, we can then distinguish two main cases

- SR: In this case we have that both κ and ϵ_i are constant if we ignore $\mathcal{O}\left(\epsilon_i^2\right)$ terms. We then have $\kappa \simeq -3$ and $\frac{V_{\bar{\phi}\bar{\phi}}}{\bar{H}^2} \simeq 6\epsilon_1 - \frac{3}{2}\epsilon_2$, which means that ν can be written as follows

$$\nu_{SR} = \frac{3}{2} + \epsilon_1 + \frac{1}{2}\epsilon_2 \,. \tag{2.76}$$

- Beyond SR: For any CR regime beyond SR (including USR), we have that κ is still constant but ϵ_1 strongly varies with time so we have to neglect all the terms proportional to ϵ_1, in this case we have $\frac{V_{\bar{\phi}\bar{\phi}}}{H^2} \simeq -3\kappa - \kappa^2$ and hence

$$\nu_{CR} = \frac{3}{2}\left|1 + \frac{2}{3}\kappa\right| \,. \tag{2.77}$$

Now that we know under which values of constant ν the MS equation has an analytical solution, we are finally in position to solve it in terms of Bessel functions. However, and following the usual approach of the literature, we will write the solution of (2.69) in terms of the Hankel functions, which are nothing but some functions constructed as the linear combination of the Bessel functions of first and second kind [98]. The solution for $v_k(\tau)$ is then

$$v_k(\tau) = C_1^k \sqrt{-\tau} H_\nu^{(1)}(-k\tau) + C_2^k \sqrt{-\tau} H_\nu^{(2)}(-k\tau) \,. \tag{2.78}$$

The next and final step is of course to specify C_1^k and C_2^k. In order to do so we must quantize the field v. As we will see, this quantization is performed in a completely analogy way with the quantization of the quantum harmonic oscillator. The first step is to promote the field v (or its Fourier transform v_k) to a quantum operator $\hat{v}$ ($v_{\mathbf{k}}$).

$$v \quad \rightarrow \quad \hat{v} \equiv \int \frac{d^3k}{(2\pi)^3} \left[v_k(\tau)\hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + v_k^\star(\tau)\hat{a}_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{x}} \right] \tag{2.79}$$

$$v_{\mathbf{k}} \quad \rightarrow \quad \hat{v}_{\mathbf{k}} \equiv v_k(\tau)\hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + v_k^\star(\tau)\hat{a}_{\mathbf{k}}^\dagger e^{-i\mathbf{k}\cdot\mathbf{x}} \,, \tag{2.80}$$

where the creation and annihilation operators $\hat{a}_{\mathbf{k}}^\dagger$ and $\hat{a}_{\mathbf{k}}$ must satisfy the canonical commutation relation:

$$\left[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}^\dagger\right] = (2\pi)^3 \, \delta\left(\mathbf{k} - \mathbf{k}'\right) \,. \tag{2.81}$$

The enforcement of condition (2.81) sets the correct normalization for the mode function, namely

$$i\left(v_k^\star v_k' - \left(v_k'\right)^\star v_k\right) = 1 \,, \tag{2.82}$$

which can be written in terms of the constants C_1^k and C_2^k as follows

$$|C_1^k|^2 - |C_2^k|^2 = \frac{\pi}{4} \,, \tag{2.83}$$

where we have used that $\left(H_\nu^{(1)}(x)\right)^\star = H_\nu^{(2)}(x)$ when ν is real, together with the useful simplification $H_{\nu-1}^{(1)}(x)H_\nu^2 - H_\nu^{(1)}(x)H_{\nu-1}^{(2)}(x) = \frac{4i}{\pi x}$.

The normalization condition (2.83) fixes one of the two constants in (2.78), in order to fix completely the mode function we must choose a vacuum state for the fluctuations. The standard choice is the so called Bunch-Davies vacuum [99]. It corresponds to the Minkowski vacuum of a comoving observer when all comoving scales are well inside the Hubble horizon, i.e when $k \gg a\bar{H}$, which accordingly with (2.73) also means $|k\tau| \gg 1$. In this limit the MS equation for the variable v_k (2.68) becomes simply

$$v_k'' + k^2 v_k = 0\,. \tag{2.84}$$

This is the equation of a simple harmonic oscillator with time-independent frequency for which the vacuum with the minimum energy state is defined by

$$\lim_{k\tau\to-\infty} v_k = \frac{e^{-ik\tau}}{\sqrt{2k}}\,. \tag{2.85}$$

We can now apply the limit $k\tau \to -\infty$ to the solution of the MS equation (2.78) and match it with (2.85). The result for the constants C_1^k and C_2^k is

$$C_1^k = \frac{\sqrt{\pi}}{2} i e^{\frac{i\pi}{4}(2\nu-1)}\,, \qquad C_2^k = 0\,, \tag{2.86}$$

which clearly satisfy the normalization condition (2.83). We are finally in a position to write down the full solution for the mode function v_k

$$v_k = \frac{\sqrt{\pi}}{2} i e^{\frac{i\pi}{4}(2\nu-1)} \sqrt{-\tau} H_\nu^{(1)}(-k\tau)\,. \tag{2.87}$$

Note that, although (2.83) must always be true if we want our solution to maintain its quantum nature, the constants in (2.86) can be different if we have some exotic feature in our inflationary model [100, 101, 102], for example, we show in appendix A that a transition between a SR and a USR inflationary regimes change the values of (2.86). This change in the value of C_1^k and C_2^k does not mean that we do not longer have an harmonic oscillator in the limit $k\tau \to -\infty$, it means that we have changed that state along the inflationary evolution.

2.2.1.2 Scalar power spectrum and spectral index

A very useful quantity to define at this point is the power spectrum. In order to define it we will compute the correlator $\langle 0|\hat{v}(\mathbf{x}_1, \tau_1)\hat{v}(\mathbf{x}_1, \tau_2)|0\rangle$. The result is

$$\langle 0|\hat{v}(\mathbf{x}_1,\tau_1)\hat{v}(\mathbf{x}_2,\tau_2)|0\rangle = \int \frac{d^3k_1 d^3k_2}{(2\pi)^6}\langle 0|\hat{v}_{\mathbf{k}_1}(\tau_1)\hat{v}_{\mathbf{k}_2}(\tau_2)|0\rangle$$
$$= \int \frac{d^3k_1 d^3k_2}{(2\pi)^3} v_{k_1}(\tau_1)v^\star_{k_2}(\tau_2)e^{i\mathbf{k}_1\cdot(\mathbf{x}_1-\mathbf{x}_2)}\delta\left(\mathbf{k}_1-\mathbf{k}_2\right) , \quad (2.88)$$

where in the second line we have used that (2.80), together with $a_{\mathbf{k}}|0\rangle = 0$ and $\langle 0|a^\dagger_{\mathbf{k}} = 0$. Now it is easier to proceed in polar coordinates, where $d^3k = k^2 dk \sin\theta d\theta d\varphi$, $\mathbf{k}_1 \cdot (\mathbf{x}_1 - \mathbf{x}_2) = kr\cos\theta$, and $r \equiv |\mathbf{x}_1 - \mathbf{x}_2|$. We can now integrate the delta function and the result is

$$\langle 0|\hat{v}(\mathbf{x}_1,\tau_1)\hat{v}(\mathbf{x}_2,\tau_2)|0\rangle = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \int_0^{\infty} \frac{dk}{(2\pi)^3} k^2 \sin\theta v_k(\tau_1)v^\star_k(\tau_2)e^{ikr\cos\theta} . \quad (2.89)$$

The integral of φ in (2.89) factorizes out and gives a factor of 2π, on the other hand, the integral of θ can be also computed as follows:

$$\int_0^{\pi} d\theta \sin\theta e^{ikr\cos\theta} = 2\frac{\sin kr}{kr} . \quad (2.90)$$

The final result of (2.89) is then

$$\langle 0|\hat{v}(\mathbf{x}_1,\tau_1)\hat{v}(\mathbf{x}_2,\tau_2)|0\rangle = \int_0^{\infty} \frac{dk}{2\pi^2} k^2 v_k(\tau_1)v^\star_k(\tau_2)\frac{\sin kr}{kr} . \quad (2.91)$$

In order to define the power spectrum we will set $\tau_1 = \tau_2 = \tau$ in (2.91), we then have

$$\langle 0|\hat{v}(\mathbf{x}_1,\tau)\hat{v}(\mathbf{x}_2,\tau)|0\rangle = \int_0^{\infty} \frac{dk}{2\pi^2} k^2 |v_k(\tau)|^2 \frac{\sin kr}{kr} \equiv \int_0^{\infty} \frac{dk}{2\pi^2} k^2 P_v(k,\tau)\frac{\sin kr}{kr}$$
$$\equiv \int_0^{\infty} \frac{dk}{k}\Delta_v(k,\tau)\frac{\sin kr}{kr} , \quad (2.92)$$

where we have defined both the power spectrum

$$P_v(k,\tau) \equiv |v_k(\tau)|^2 , \quad (2.93)$$

and the (sometimes more useful) dimensionless power spectrum

$$\Delta_v(k,\tau) \equiv \frac{k^3}{2\pi^2}|v_k(\tau)|^2 , \quad (2.94)$$

Note that the definition (2.93) coincides with the Fourier transform of the two point correlation function $\langle 0|\hat{v}(\mathbf{x}_1,\tau)\hat{v}(\mathbf{x}_2,\tau)|0\rangle$

$$
\begin{aligned}
P(k,\tau) &\equiv \int d^3r \langle 0|\hat{v}(\mathbf{x}+\mathbf{r},\tau)\hat{v}(\mathbf{x},\tau)|0\rangle e^{-i\mathbf{k}\cdot\mathbf{r}} \\
&= \int d^3r \left(\int \frac{d^3k'}{(2\pi)^3}|v_{k'}(\tau)|^2 e^{i\mathbf{k}'\cdot\mathbf{r}}\right) e^{-i\mathbf{k}\cdot\mathbf{r}} \\
&= \int d^3k' |v_{k'}(\tau)|^2 \left(\int \frac{d^3r}{(2\pi)^3} e^{i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')}\right) \\
&= \int d^3k' |v_{k'}(\tau)|^2 \delta(\mathbf{k}-\mathbf{k}') = |v_k(\tau)|^2 \,, \qquad (2.95)
\end{aligned}
$$

where in the second line we have used the result of (2.88) but making use of the delta function.

Finally, we can also consider the variance, or the 2-point correlator at the same spatial point $\mathbf{x}_1 = \mathbf{x}_2 = \mathbf{x}$ (or $\mathbf{r} = 0$). In this case we have from (2.88)

$$
\langle 0|\hat{v}(\mathbf{x},\tau)^2|0\rangle = \sigma_v^2(\mathbf{x},\tau) = \int \frac{d^3k}{(2\pi)^3} P_v(k,\tau)\,. \qquad (2.96)
$$

From (2.96) we can also see another useful interpretation of the power spectrum: If we consider the probability density function of all the quantum fluctuations with the same characteristic wavenumber k, then the power spectrum represents the variance of that probability density function.

In order to close this subsection we will also define here the spectral index, which is nothing more than the scale-dependence of the dimensionless power spectrum i.e.

$$
n_v - 1 \equiv \frac{d\log\Delta_v}{d\log k}\,. \qquad (2.97)
$$

Note that, although we have defined both the power spectrum (2.93) (or, equivalently the dimensionless power spectrum (2.94)) and the spectral index (2.97) for the variable v, we can generalize this definition for any other gauge invariant scalar variable such as the MS variable Q in (2.53), the comoving curvature perturbation $\mathcal{R}$ in (2.54) or the uniform density curvature perturbation ζ in (2.55).

2.2.1.3 The long-wavelength limit

Although in section 2.2.1.1 we paid more attention to the short-wavelength (or sub-Hubble) limit of quantum fluctuations in order to give reasonable initial conditions, we are usually more interested in the opposite regime, i.e. in the long-wavelength (or super-Hubble) limit. We will not describe in this thesis the precise relation between the long-wavelength limit of scalar power spectrum of (2.94) and the observed CMBR anisotropies, we will however explain qualitatively how the long-wavelength behaviour of the quantum fluctuations generated during inflation can actually affect the observable universe.

The idea is schematically shown in Fig. 2.1 and it is the following: the physical length of the quantum fluctuations generated during inflation get stretched according to $\lambda = a/k$ (where k is the comoving wavenumber) and always increase as the expansion of the universe proceeds. On the other hand we have that during inflation the Hubble radius is almost a constant (its rate of change is $\mathcal{O}(\epsilon_1)$). As a consequence, scales of interest today which start inflation in a sub-Hubble region, will eventually exit the Hubble horizon and start their super-Hubble evolution. Once inflation ends, the size of the Hubble radius starts increasing faster than the physical length of the quantum fluctuations, so there is a moment in which the fluctuations re-enter the Hubble radius and can affect the dynamics of our observable universe. As it can be seen in 2.1, the moment in which the a mode k (or λ) re-enters the Hubble radius, depends on when it exits it during inflation. The modes that exit the Hubble radius close to the end of inflation are the ones that will re-enter the horizon before, similarly, the further away from the end of inflation a mode is generated, the later will re-enter the Hubble radius.

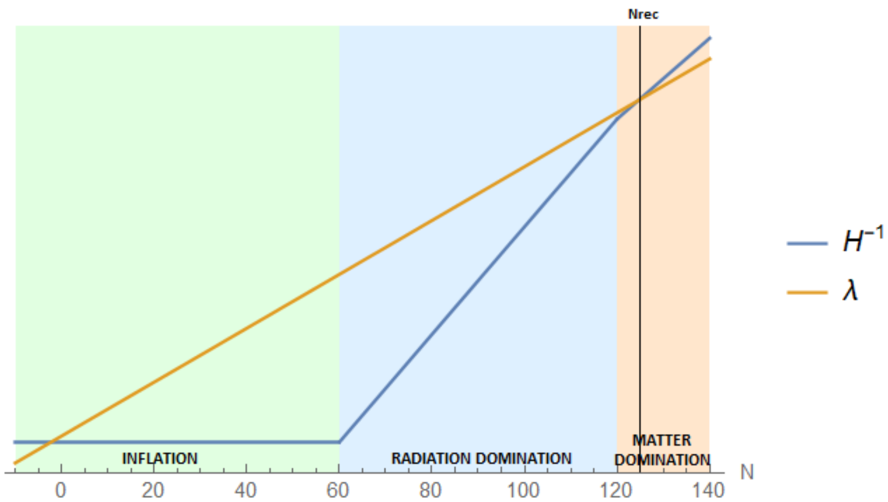

Fig. 2.1 Schematic representation of a mode (in orange) that exits horizon ~ 60 e-folds before the end of inflation and re-enter the horizon around the recombination epoch, when the CMBR is generated.

Once the importance of the long-wavelength limit of cosmological perturbation theory has been highlighted, we will compute the power spectrum of the comoving curvature perturbation $\mathcal{R}$ and we will see that, if some requirements are satisfied, it is fully consistent with the almost scale invariant power spectrum of the CMBR anisotropies.

Following (2.94), the dimensionless power spectrum for the comoving curvature perturbation is

$$\Delta_{\mathcal{R}} = \frac{k^3}{2\pi^2} |\mathcal{R}_k|^2 \,, \tag{2.98}$$

where $\mathcal{R}_k$ is given by (see (2.63) and (2.87))

$$\mathcal{R}_k = -\frac{v_k}{z} = -\frac{\bar{H}\sqrt{\pi}}{2a\dot{\bar{\phi}}} i e^{\frac{i\pi}{4}(2\nu-1)} \sqrt{-\tau} H_\nu^{(1)}(-k\tau) \,. \tag{2.99}$$

In order to know the long wavelength limit of (2.99) we will simply expand $H_\nu^{(1)}(-k\tau)$ around $k\tau \to 0$ and keep the leading order, the result is:

$$\mathcal{R}_k = -\frac{(1-i)2^{-\frac{3}{2}+\nu} e^{\frac{1}{2}i\pi\nu} \bar{H}\sqrt{-\tau}\Gamma[\nu]}{a\sqrt{\pi}\dot{\bar{\phi}}} (-k\tau)^{-\nu} \,. \tag{2.100}$$

Now let us remember that the solution of (2.99) is only valid when ν is a constant, which allow us to make some simplifications, these simplifications will again depend on the inflationary regime we want to study:

- Slow Roll:
  - Although $\nu^{SR} = \frac{3}{2} + \epsilon_1 + \frac{1}{2}\epsilon_2$ we will first explore the case in which we neglect all ϵ_i parameters for simplicity, in this case $\nu_0^{SR} = \frac{3}{2}$ and $\tau = -\frac{1}{aH}$. The dimensionless power spectrum in this case can be easily computed to be

    $$\Delta_{\mathcal{R}}^{SR} = \frac{\left(\bar{H}^0\right)^2}{8\pi^2 \epsilon_1^0 M_{PL}^2} \,. \tag{2.101}$$

    Note that in (2.101) we have written $\bar{H}^0$ and ϵ_1^0 instead of $\bar{H}$ and ϵ_1. The reason is that, in order to be consistent we need to compute all the quantities at zeroth order in ϵ_i and, since the rate of change of both $\bar{H}$ and ϵ_1 will include corrections of $\mathcal{O}(\epsilon_1)$, we must set these to quantities to a constant value, which we denote with a superscript "^{0}". It is also important to realize that, at this order, $\Delta_{\mathcal{R}}^{SR}$ does not depend on k and hence, from (2.97) we have that $n_{\mathcal{R}}^{SR} - 1 = \mathcal{O}(\epsilon_1)$, which means that the power spectrum is exactly scale invariant.
  - At leading order in SR parameters τ can be written as

    $$\tau \simeq -\frac{1}{a\bar{H}}(1+\epsilon_1^\star) = -\frac{1}{\mathcal{H}}(1+\epsilon_1^\star) = -\frac{a(\tau)}{a'(\tau)}(1+\epsilon_1^\star) \,, \tag{2.102}$$

    where we are using again that the rate of change of ϵ_1 is $\mathcal{O}(\epsilon_i^2)$ to evaluate ϵ_1 at some time $\tau^\star$. For observational reasons, the time $\tau^\star$ is usually chosen to be the value at which the pivot scale $k^\star$, which is the scale that re-enter the Hubble radius during recombination, crosses the Hubble radius during inflation. Similarly, we will denote by $\epsilon_1^\star$ and $H^\star$ the values of ϵ_1 and H at $\tau^\star$. Note that, although we are choosing the time $\tau^\star$ to be the time at which we evaluate the different quantities, this election is completely arbitrary.

Since $\epsilon_1^\star$ is a constant, we can now solve (2.102) to get

$$\log\left(\frac{a}{a^\star}\right) \simeq (1+\epsilon_1^\star)\log\left(\frac{\tau^\star}{\tau}\right) . \tag{2.103}$$

With the aid of (2.103), we can now write the approximate time dependence of ϵ_1 and $\bar{H}$ as follows

$$\begin{aligned}
\bar{H} &\simeq \bar{H}^\star + \left.\frac{d\bar{H}}{dN}\right|_{N=N^\star}(N-N^\star) \simeq \bar{H}^\star\left(1-\epsilon_1^\star\log\left(\frac{a}{a^\star}\right)\right) \simeq \bar{H}^\star\left(1-\epsilon_1^\star\log\left(\frac{\tau^\star}{\tau}\right)\right) , \\
\epsilon_1 &\simeq \epsilon_1^\star + \left.\frac{d\bar{H}}{dN}\right|_{N=N^\star}(N-N^\star) \simeq \epsilon_1^\star\left(1+\epsilon_2^\star\log\left(\frac{a}{a^\star}\right)\right) \simeq \epsilon_1^\star\left(1+\epsilon_2^\star\log\left(\frac{\tau^\star}{\tau}\right)\right)
\end{aligned} \tag{2.104}$$

Using these approximations in (2.99) we are left with

$$\Delta_{\mathcal{R}}^{SR} \simeq \frac{\left(\bar{H}^\star\right)^2}{2\epsilon_1^\star M_{PL}^2\pi^3}\Gamma\left[\nu\right](1-2\epsilon_1^\star)\left(1-(\epsilon_2^\star+2\epsilon_1^\star)\log\left(\frac{\tau^\star}{\tau}\right)\right)\left(-\frac{k\tau}{2}\right)^{3-2\nu} . \tag{2.105}$$

In order to obtain the dimensionless power spectrum of (2.105) we have only used the approximations of (2.102) and (2.104). The last thing we have to do is to use the value of ν^{SR} at leading order in SR parameters. From (2.76) we have

$$\nu^{SR} \simeq \frac{3}{2} + \epsilon_1^\star + \frac{\epsilon_2^\star}{2} , \tag{2.106}$$

where we have again evaluated the SR parameters at $\tau^\star$. Inserting this value for ν^{SR} in (2.105) and expanding at leading order in $\epsilon_1^\star$ and $\epsilon_2^\star$ we get the following dimensionless power spectrum

$$\begin{aligned}
\Delta_{\mathcal{R}}^{SR} \simeq \frac{\left(\bar{H}^\star\right)^2}{8\pi^2\epsilon_1^\star M_{PL}^2}\Big[1+ \\
2(1-\log 2-\gamma_E)\epsilon_1^\star + (2-\log 2-\gamma_E)\epsilon_2^\star - (2\epsilon_1^\star+\epsilon_2^\star)\log(-k\tau^\star))\Big] ,
\end{aligned} \tag{2.107}$$

where γ_E is the Euler-Mascheroni constant and it comes from the expansion of $\Gamma[\nu]$. In (2.107) the first line represents the leading order result and the second line the $\mathcal{O}(\epsilon_1)$ corrections. Surprisingly (or maybe not, as we will see later on), the $\mathcal{O}(\epsilon_1)$ corrections are completely time independent since all the variables that appear are evaluated at $\tau^\star$, which is a fixed value. We can then conclude that the power spectrum of the comoving curvature perturbation $\mathcal{R}$ during a SR phase of inflation is approximately a constant, being the only time dependence at $\mathcal{O}(\epsilon^2)$, where we cannot longer trust the analytical result of (2.99). Finally we can also compute the spectral index at leading order in SR parameters during SR:

$$n_{\mathcal{R}}^{SR} - 1 \equiv \frac{d\log\Delta_v}{d\log k} \simeq -2\epsilon_1^\star - \epsilon_2^\star\,. \tag{2.108}$$

The spectral index of (2.108) indicates that, during SR, the power spectrum is not exactly scale invariant but it is slightly red-tilted. The small red tilt comes from the fact that during SR both ϵ_1 and ϵ_2 are positive and much smaller than 1. This power spectrum is in perfect agreement with the latest observational data coming from Planck, where the power spectrum of the CMBR at large scales (the ones that can be explained by inflation as in Fig 2.1) is $n_s = 0.9649 \pm 0.0042$ [55].

This prediction of SR inflation about the spectral index is probably the biggest success of the inflationary theory since there are no that many mechanisms that can both solve the standards problem of Big-Bang cosmology and predict an slightly red tilted power spectrum for the anisotropies of the CMBR.

Finally, let us also compute the spectral index of (2.108) in an alternative and simpler way but that can lead to some confusions as we will see in other inflationary regimes. Let us consider the dimensionless power spectrum at zeroth order in SR parameters of (2.101) but without evaluating the quantities at $\tau^\star$ i.e.

$$\Delta_{\mathcal{R}}^{SR} = \frac{\bar{H}^2}{8\pi^2\epsilon_1 M_{PL}^2}\,. \tag{2.109}$$

Now, we will identify the characteristic scale of each mode with a crossing time, like this we have that $k = aH$ and hence we can write the following

$$\frac{d\log k}{dN} = 1 - \epsilon_1 \quad \rightarrow \quad d\log k = (1-\epsilon_1)dN\,, \tag{2.110}$$

and hence the spectral index would be

$$n_{\mathcal{R}}^{SR} - 1 = \frac{1}{\Delta_{\mathcal{R}}(1-\epsilon_1)}\frac{d\Delta_{\mathcal{R}}}{dN} \simeq -2\epsilon_1^\star - \epsilon_2^\star\,, \tag{2.111}$$

which coincides with the true spectral index of (2.108). The reason why the two methods coincide is because the true power spectrum of (2.107) is exactly a constant at superhorizon scales and hence the rate at which the modes exit the horizon coincides with the k-dependence of the power spectrum. As we will show in the following, this is however only true in this case, reason why we will not use this method anymore.

- Beyond SR:

In this case ϵ_1 has a strong dependence with time so we cannot consider $\mathcal{O}(\epsilon_1)$ corrections in an analytical way. Neglecting $\mathcal{O}(\epsilon_1)$ terms simplifies considerably the computations since in this case $\tau = -\frac{1}{aH}$. The dimensionless scalar power spectrum for a generic CR inflationary regime can then be written as

$$\Delta_{\mathcal{R}}^{CR} = \frac{\bar{H}^2}{8\pi^2\epsilon_1 M_{PL}^2}\left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2\left(\frac{k}{2aH}\right)^{3-2\nu_{CR}}\,, \tag{2.112}$$

where ν^{CR} is a constant given by (2.77). We can now distinguish different behaviours of the power spectrum depending on the value of ν^{CR}.

  – Ultra-Slow-Roll (USR): As explained in section 2, in this case we have $\kappa = 0$ and hence $\nu^{USR} = \frac{3}{2}$. The power spectrum then takes exactly the same form as the one for SR at zeroth order in SR parameters i.e.

$$\Delta_{\mathcal{R}}^{USR} = \frac{\bar{H}^2}{8\pi^2\epsilon_1 M_{PL}^2}\,. \tag{2.113}$$

There is however a crucial difference between (2.101) and (2.113). In order to see this difference it is better to compute the time derivative of (2.113)

$$\frac{d\Delta_{\mathcal{R}}^{USR}}{dN} = -\Delta_{\mathcal{R}}^{USR}(2\epsilon_1 + \epsilon_2)\,. \tag{2.114}$$

While in the case of SR at zeroth order both ϵ_1 (that comes from the time derivative of $\bar{H}$) and ϵ_2 (that comes from the time derivative of ϵ_1) are neglected, in the case of USR we can only neglect ϵ_1 but not ϵ_2 because in this case it is $\epsilon_2^{CR} \sim \mathcal{O}(1)$, more concretely $\epsilon_2^{USR} \simeq -6$. Now, since the ϵ_2 term comes from the time derivative of ϵ_1, it means that, in order to be fully consistent we must take $\bar{H}$ in (2.113) to be exactly a constant (that we will call $\bar{H}_0$) but ϵ_1 to be a time dependent function. The final power spectrum in USR is then

$$\Delta_{\mathcal{R}}^{USR} = \frac{\bar{H}_0^2}{8\pi^2 \epsilon_1 M_{PL}^2} \,. \tag{2.115}$$

We can finally compute the spectral index of (2.115), which is trivially

$$n_{\mathcal{R}}^{USR} - 1 = 0 \,, \tag{2.116}$$

because $\Delta_{\mathcal{R}}^{USR}$ does not have any k-dependence. Note that if we were using the simplification of (2.111) we would get $n_{\mathcal{R}}^{USR} - 1 \simeq -\epsilon_2^{USR} \simeq 6$, which is completely wrong as it can be seen above. As anticipated before, this faliure is a consequence of the time evolution of the power spectrum at superhorizon scales, but more importantly, it tell us that the k-dependence and time dependence are not always interchangeable.

– Other cases of CR: As already mentioned many times, both SR and USR are special cases of a more general regime of CR in which $\kappa = \frac{V_{\bar{\phi}}}{\bar{H}\dot{\bar{\phi}}}$ is a constant. The value of ν in this case is given by (2.77) $\left(\nu_{CR} = \frac{3}{2}\left|1 + \frac{2}{3}\kappa\right|\right)$. Using also the time dependence of ϵ_1 when κ is a constant given by (2.71) we can write the power spectrum of (2.112) in a very convenient way as

$$\Delta_{\mathcal{R}}^{CR} = C a^{3\left(1+\frac{2}{3}\kappa+\left|1+\frac{2}{3}\kappa\right|\right)} k^{3\left(1-\left|1+\frac{2}{3}\kappa\right|\right)} \,, \tag{2.117}$$

where

$$C = \frac{\bar{H}_0^{3\left|1+\frac{2}{3}\kappa\right|-1}}{8\pi^2 \epsilon_1^0 M_{PL}^2} 2^{3\left(\left|1+\frac{2}{3}\kappa\right|-1\right)} \left(\frac{\Gamma\left[\frac{3}{2}\left|1+\frac{2}{3}\kappa\right|\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2 \,, \tag{2.118}$$

is a constant. From (2.117) we can see the general behaviour, both in time and in k, of the power spectrum depending on the value of κ.

 * Time dependence:
   · $\Delta_{\mathcal{R}}^{CR}$ is a constant if $\kappa \leq -\frac{3}{2}$.
   · $\Delta_{\mathcal{R}}^{CR}$ grows with time as $a^{6+4\kappa}$ if $\kappa > -\frac{3}{2}$.
 * k-dependence: The spectral index is

$$n_{\mathcal{R}}^{CR} - 1 = 3\left(1 - \left|1 + \frac{2}{3}\kappa\right|\right) \,, \tag{2.119}$$

from there we can deduce the following:

   · $n_{\mathcal{R}}^{CR} - 1 > 0$ and hence the power spectrum is blue-tilted for $-3 < \kappa < 0$.
   · $n_{\mathcal{R}}^{CR} - 1 < 0$ and hence the power spectrum is red-tilted for $\kappa < -3$ or $\kappa > 0$.

· $n_{\mathcal{R}}^{CR} - 1 = 0$ and hence the power spectrum is scale invariant for $\kappa = -3$ (SR) and $\kappa = 0$ (USR), as we already knew.

· In the same way that SR and USR have the same k-dependence, the power spectrum of any two inflationary regimes characterized by κ_1 and κ_2 will have the same k-dependence if the following relation is satisfied:

$$3 + \kappa_1 = -\kappa_2 \,, \tag{2.120}$$

which represent a nice duality that has been explored recently [103].

Both the time and k-dependence of the general power spectrum $\Delta_{\mathcal{R}}^{CR}$ of (2.117) are represented schematically in Fig. 2.2, where one can clearly see the duality of (2.120).

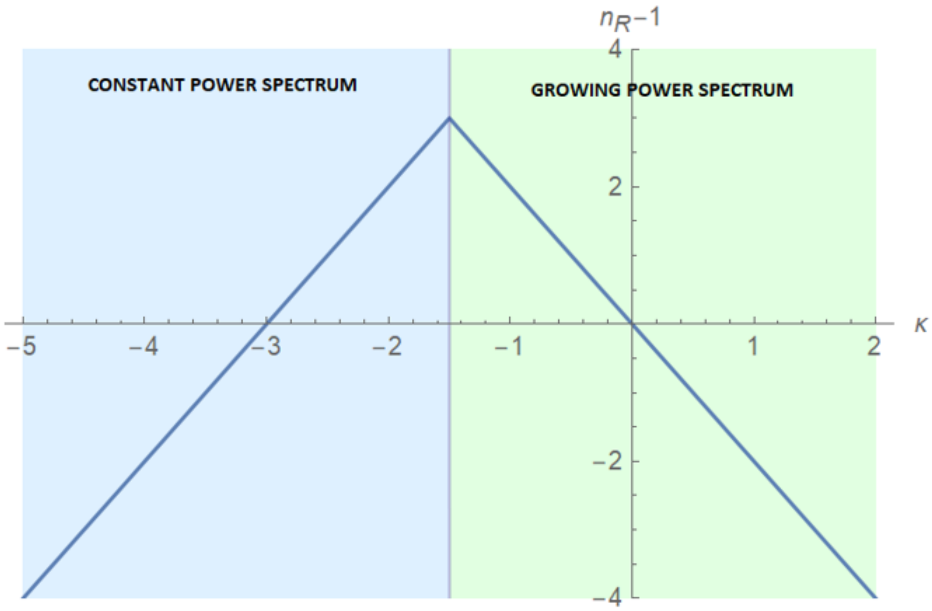

Fig. 2.2 Dependence of $n_{\mathcal{R}} - 1$ with the parameter κ and dependence of the power spectrum with time.

We will conclude this section by computing the behaviour of the curvature perturbation in the long-wavelength limit in an alternative way. Although this could seem a bit repetitive, we will see along the thesis that it is actually worthy. If we go back to the MS equation for $\mathcal{R}$ (2.61) in Fourier space and we take the long-wavelength limit ($k \to 0$) we have:

$$\frac{d}{dt}\left(a^3 \epsilon_1 \dot{\mathcal{R}}_k\right) = 0 \,, \tag{2.121}$$

whose solution is obviously

$$\mathcal{R}_k(k \to 0) = C_1(k) + C_2'(k) \int \frac{dt}{a^3 \epsilon_1}\,, \tag{2.122}$$

where $C_1(k)$ and $C_2'(k)$ are k-dependent constants specified by initial conditions that we will not set at the moment.

If we consider $\bar{H} = \bar{H}_0$ to be a constant (so we are neglecting $\mathcal{O}(\epsilon_1)$ corrections) and we assume that we are in a CR regime (so ϵ_1 behaves as (2.71)), we can easily integrate the second term of (2.122) and get

$$\mathcal{R}_k(k \to 0) \simeq C_1(k) + C_2(k) a^{3+2\kappa}\,. \tag{2.123}$$

Solution (2.123) is composed of two modes, a constant one ($C_1(k)$) and a time-dependent one (proportional to $C_2(k)$), which decays when $\kappa < -\frac{3}{2}$ and grows when $\kappa > -\frac{3}{2}$. We can then say the following

- The constant mode dominates after a while for $\kappa \leq -\frac{3}{2}$.
- The growing mode dominates after a while for $\kappa > -\frac{3}{2}$.

In order to fully specify the solution (2.123), we must specify the constants $C_1(k)$ and $C_2(k)$, in the following we will see how

- In the limit in which ν is constant and hence the full MS equation has an analytical solution, we can set the constants $C_1(k)$ and $C_2(k)$ accordingly with the $k \to 0$ limit of the analytical solution i.e. with (2.100). From (2.117) we can write $\mathcal{R}_k$ as

  $$\mathcal{R}_k(k \to 0) = c(k) a^{\frac{3}{2}\left(1+\frac{2}{3}\kappa+\left|1+\frac{2}{3}\kappa\right|\right)}\,, \tag{2.124}$$

  where

  $$c(k) \equiv \sqrt{C} k^{\frac{3}{2}\left(1-\left|1+\frac{2}{3}\kappa\right|\right)}\,, \tag{2.125}$$

  and C is defined in (2.118).

  Comparing (2.123) and (2.124) we can set $C_1(k)$ and $C_2(k)$ depending on the value of κ:

  - If $\kappa \leq -\frac{3}{2}$ we have $C_1(k) = c(k)$ and $C_2(k)$ must be k-suppressed with respect to $C_1(k)$.
  - If $\kappa > -\frac{3}{2}$ we have $C_2(k) = c(k)$ and $C_1(k)$ must be k-suppressed with respect to $C_2(k)$.

    These results support the idea that, in single-regime inflationary scenarios, the mode that do not dominate the long-wavelength evolution of $\mathcal{R}_k$ must also be k-suppressed.

- Since (2.122) is an exact solution, we would expect that both modes are present in the $k \to 0$ limit, the reason why we are killing one of them when comparing with the analytical solution is not because the other one is k-suppressed, but because it cannot be compared with the analytical solution (2.122). Because the analytical solution of the MS equation is generically only valid up to $\mathcal{O}(\epsilon_1)$ we can say the following:
  - If $\kappa \leq -\frac{3}{2}$ we have $C_1(k) = \mathcal{O}(1)$ and $C_2'(k) = \mathcal{O}(\epsilon_1)$, but of the same order in k as $C_1(k)$.
  - If $\kappa > -\frac{3}{2}$ we have $C_2'(k) = \mathcal{O}(1)$ and $C_1(k) = \mathcal{O}(\epsilon_1)$, but of the same order in k as $C_1(k)$.

  This means that there is no reason to think that the non-dominating mode is also $k-$suppressed in the long wavelength limit.

Although the scalar sector of fluctuations during inflation is the most relevant one, it is important to explore also the vectorial and tensorial sectors, at least to justify why we will not pay much attention to them in this thesis.

2.2.2 Vectorial sector

Using the decomposition of (2.29) and (2.32) the vectorial sector of the linearized metric of (2.27) is

$$ds_V^2 = -dt^2 + 2a(t)B_i^V dx^i + a^2(t)\left[\delta_{ij} - (\partial_j E_i + \partial_i E_j)\right] dx^i dx^j \,, \tag{2.126}$$

where (as a reminder) $\partial^i B_i^V = 0$ and $\partial^i E_i = 0$. The gauge transformation of these variables with the notation below (2.43) in which $\tilde{x}^i = x^i + \lambda_\perp^i + \partial^i \eta$ and $\tilde{t} = t + \lambda^0$ is

$$\begin{aligned} B_i^V \to& \tilde{B}_i^V = B_i^V - a\left(\lambda_\perp\right)_i \,, \\ E_i \to& \tilde{E}_i = E_i - \left(\lambda_\perp\right)_i \,. \end{aligned} \tag{2.127}$$

The combination $\dot{E}_i - \frac{B_i^V}{a}$ is called the gauge invariant vector perturbation. Now we can study the evolution of this gauge invariant quantity with the ADM equations of section (1.3). More concretely, combining equations (2.22) and (2.24) when the matter content is given by a single scalar field we get the following equation of motion at linear order

$$\frac{d}{dt}\left(\dot{E}_i - \frac{B_i^V}{a}\right) + 3\bar{H}\left(\dot{E}_i - \frac{B_i^V}{a}\right) = 0 \,. \tag{2.128}$$

From (2.128) we can clearly see that the gauge invariant vector perturbation always decay in during inflation, reason why we will forget about it for the rest of the thesis.

2.2.3 Tensorial sector

Finally, we will explore the tensorial sector. By using the decomposition of (2.32) again, we can write the tensorial part of the linearized metric of (2.27) as

$$ds_T^2 = -dt^2 + a^2(t)\left[\delta_{ij} - h_{ij}\right] , \tag{2.129}$$

where (accordingly with (2.32)) $\partial^i E_{ij}^T = 0$ and $\delta^{ij} E_{ij}^T = 0$. Tensor perturbations at linear order are automatically gauge invariant so we do not have to worry about the gauge issue in this case. The next step is to use again the relevant ADM equations of section 1.3 and linearize its tensorial part. In this case the relevant equations are again (2.22) and (2.24), combining the two in a universe filled with a scalar fluid with the stress-energy tensor of (2.2) we get

$$\ddot{h}_{ij} + 3\bar{H}\dot{h}_{ij} - \frac{\nabla^2}{a^2} h_{ij} = 0\,, \tag{2.130}$$

where the term $\frac{\nabla^2}{a^2} h_{ij}$ comes from $R_{ij}^{(3)}$ in (2.24). Equation (2.130) is a wave equation and hence it describes the evolution of gravitational waves in an expanding universe. We will see in the following that these gravitational waves are produced by quantum fluctuations during inflation, however they decay at superhorizon scales with the expansion of the universe. The reason that we will pay more attention to them than to the vector modes is that, as we will see, the amplitude of these gravitational waves at recombination may still be large enough to leave distinctive signatures in B-modes of CMB polarization.

The way of solving (2.130) closely follows what we did with the MS equation of (2.60), in fact, the only difference between the equation for h_{ij} and the one for Q are the ϵ-dependent terms in (2.60). First we will define the Fourier transform of h_{ij} as

$$h_{ij} = \int \frac{d^3k}{(2\pi)^3} \sum_{s=+,\times} e_{ij}^s(k) h_{\mathbf{k}}^s e^{i\mathbf{k}\cdot\mathbf{x}} \tag{2.131}$$

where $+$ and $\times$ represent the two polarizations and $e_{ij}^+(k)$ and $e_{ij}^\times(k)$ are the two polarization tensors. Each one of the modes will then follow the following equation

$$\ddot{h}_k^s + 3H\dot{h}_k^s + \frac{k^2}{a^2} h_k^s = 0\,. \tag{2.132}$$

Now, we will do a convenient change of variable $v_k^s = \frac{a}{2} M_{PL} h_k^s$ such that we can write (2.132) in a much more familiar way using conformal time τ i.e.

$$(v_k^s)'' + \left(k^2 - \frac{2}{\tau^2}\right) v_k^s = 0\,, \tag{2.133}$$

which is the same equation as for the scalar modes (2.68) but with $\frac{z''}{z} = \frac{2}{\tau^2}$ or, in other words, with $\nu = \frac{3}{2}$.

The way of quantizing and solving (2.133) is identical to the way we did for (2.68) in section 2.2.1.1. Thus, we will not repeat the procedure here. If we chose again the Bunch-Davies vacuum as initial condition we will get the same solution as in (2.87) but with $\nu = \frac{3}{2}$ i.e.

$$v_k^s = \frac{e^{-ik\tau}}{\sqrt{2}k^{3/2}} \left(-\frac{1}{\tau}\right)(i - k\tau) \ . \tag{2.134}$$

Similarly to what we did in section 2.2.1.3 we are interested in the long-wavelength limit ($k\tau \to 0$) of the solution so, the second term in the last parenthesis of (2.134) can be safely neglected. The dimensionless power spectrum of v_k^s in the long-wavelenght limit is then

$$\Delta_{v^s} = \frac{\left(\bar{H}^\star\right)^2 a^2}{4\pi^2} \,, \tag{2.135}$$

where we have used the following approximations (valid at zeroth order in ϵ_1): $\tau \simeq -\frac{1}{a\bar{H}}$ and $\bar{H} \simeq \bar{H}^\star$. Undoing the change of variable that we did before $\left(v_k^s = \frac{a}{2} M_{PL} h_k^s\right)$ we can easily compute the power spectrum for a single polarization mode during inflation in the long wavelength to obtain

$$\Delta_{h^s} = \frac{\left(\bar{H}^\star\right)^2}{\pi^2 M_{PL}^2} \,, \tag{2.136}$$

which means that the total dimensionless power spectrum of the gravitational waves (or tensor fluctuations) is

$$\Delta_h = 2\Delta_{h^s} = \frac{2\left(\bar{H}^\star\right)^2}{\pi^2 M_{PL}^2} \,. \tag{2.137}$$

Tensor fluctuations are often normalized relative to the amplitude of the scalar fluctuations $\Delta_{\mathcal{R}}$ by means of the so-called tensor-to-scalar ratio, which is defined as:

$$r \equiv= \frac{\Delta_t}{\Delta_{\mathcal{R}}} = 16\epsilon_1^\star \,. \tag{2.138}$$

Since $\epsilon_1^\star \ll 1$ (see (2.108) and discussion below) we have that the tensor modes are highly suppressed with respect to the scalar modes. This is also in agreement with observations in the CMB, in fact, the latest constraint in r is $r < 0.056$ [55].

2.2.4 Beyond linear cosmological perturbation theory.

Although we will not explore higher orders in cosmological perturbation theory in this thesis it is important at least to comment qualitatively some interesting differences between linear and second (or higher) orders in cosmological perturbation theory:

- As we have shown in the previous sections, at linear order in cosmological perturbation theory, the scalar, vectorial and tensorial sectors evolve independently, which make them relatively easy to handle. This is no longer true already at second order, where the second order perturbations start mixing with the first order perturbations squared, probably the most known example of this effect are the scalar induced gravitational waves (GW). The possibility of the existence of these GW was first noticed in 1967 [104] and it was later rediscovered in the 90's [105, 106]. The idea goes as follows:

  Let us choose the Newtonian gauge[3] for simplicity and expand the metric up to first order in the scalar part and up to second order in the tensorial part (we will ignore the vectorial part), the result is:

$$ds^2 = -(1+2\Phi)dt^2 + a^2(t)\left[(1-2\Phi)\delta_{ij} + h_{ij} + \frac{1}{2}h_{ij}^{(2)}\right]dx^i dx^j \,, \quad (2.139)$$

  where Φ is one of the Bardeen potentials without anisotropic stress. Apart form the first order scalar fluctuations in (2.139) we have the fluctuation of the scalar field i.e. $\phi = \bar{\phi} + \delta\phi$. It can be shown that the scalar fluctuations of the metric in Newtonian gauge are suppressed with respect to the scalar field fluctuations [107]. Thus, from now on we will only consider fluctuations of the field.

  In (2.139) we have defined $h_{ij}^{(2)}$ as the second order tensor perturbation, we will not derive the equation of motion for $h_{ij}^{(2)}$ here because it can be found in the literature (see for example [108] for a review) so, we will rather give some intuitive idea: while h_{ij} follow the equation given by (2.130), $h_{ij}^{(2)}$ follow a similar equation but with a source term proportional to the Bardeen's potential squared i.e something like:

$$\ddot{h}_{ij}^{(2)} + 3\bar{H}\dot{h}_{ij}^{(2)} - \frac{\nabla^2}{a^2}h_{ij}^{(2)} \propto \partial_i\delta\phi\partial_j\delta\phi \,. \quad (2.140)$$

  Without caring too much about the evolution of these fluctuations, we can already see that the dimensionless scalar power spectrum induces gravitational waves with a power spectrum

$$\Delta_{h^{(2)}} \propto \Delta_{\delta\phi}^2 \sim \epsilon_1^2 \Delta_{\mathcal{R}}^2 \quad (2.141)$$

  For the CMBR modes, $\Delta_{\mathcal{R}}^2$, and so $\Delta_{h^{(2)}}$, is small . It is nevertheless true that,

[3]We remind the reader that the Bardeen potentials of (2.52) in this gauge take the following form: $\Phi = A$, $\Psi = -D$

as we will justify later on, there is no reason a priori to expect the amplitude of the power spectrum at CMB scales to be the same at all scales. Can in this case $\Delta_{\mathcal{R}}$ grow enough such that $\Delta_{h^{(2)}}$ can be observable? The answer is yes, this can happen both during [102] and after [108] inflation, and it represents a very active research topic that we will not further explore here.

In the same way that first order scalar fluctuations squared can act as a source term in the equation of motion for second order tensor fluctuations, we also have that first order tensor fluctuations squared affect the equation of motion of second order scalar fluctuations. Similarly, the second order vector fluctuations, would also acquire some source terms coming from first order tensor and scalars fluctuations and so on.

- Another important effect that appears at higher order in the scalar sector of cosmological perturbation theory is the the existence of non-gaussianities. In order to better understand this point let us take a slightly different approach to cosmological perturbation theory. In the approach taken in this thesis (see section (2.2.1)), we have extracted the ADM equations form the action (1.7) and we have perturbed them over a FLRW background, another option is to perturb the ADM action up to second order directly and then extract the first order equations of motion. This is the approach taken for example in [91]. In this case the perturbed action for the scalar sector is

$$S^{(2)} = \frac{1}{2}\int d^x \left[(v')^2 - \partial^i v \partial_i v + \frac{z''}{z} v^2 \right] , \tag{2.142}$$

from where the variational principle give us the MS equation for v that we already know (2.65).

A free theory like this one is fully characterized by the power spectrum of (2.93), and hence the PDF for the perturbations is Gaussian.

If we want to study the non-Gaussian features of our probability distribution we must include interaction terms in our Hamiltonian, which only appear a next-to-leading order in cosmological perturbation theory. Apart from the non-Gaussianities, which are studied via the bispectrum, trispectrum etc [109, 110, 111, 112], the interaction Hamiltonian also include one-loop corrections to the scalar power spectrum, whose effects in the case in which the tree level power spectrum grows have been a hot topic lately [113, 114, 115, 116, 117, 118, 119, 120, 121, 122].

- Finally, we will end this section by mentioning that the gauge issue of linear cosmological perturbation theory, gets increasingly more complicated at higher orders, loosing a bit the difference between what is an observable and what is not.

For example, while tensor fluctuations at first order are gauge invariant and hence we can identify then unequivocally with GW, this is not longer true with tensor fluctuations at second order **Acquaviva:2002ud, Chang:2020tji**, a natural question then arises: In the case of scalar induced gravitational waves, what is exactly what we expect to detect? this has also been a very active topic for discussion lately [123, 124, 125, 126, 127] that we will not further discuss here.

2.2.4.1 Why should we go beyond linear cosmological perturbation theory?

In sections 2.2.1.3 and 2.2.3 we have already seen that, if we accept inflation as the mechanism responsible for the inhomogeneities of the CMBR, a period of SR at the beginning of inflation is needed in order to have an almost scale invariant power spectrum. In order to obtain all the inflationary predictions for the CMBR we have used linear cosmological perturbation theory combined with quantum field theory. The reason is that both the amplitude of the power spectrum and the non-gaussianities measured at the CMBR are too small to generate a relevant amount of large fluctuations.

The interest of large fluctuations resides on the fact that, once they re-enter the horizon after inflation, they can gravitationally collapse and lead to the formation of black holes. Those are the so-called Primordial Black Holes (PBHs). PBHs play a crucial role in the understanding of our universe, for example, they represent natural candidates not only for dark matter [128], but also as the seed of supermassive BHs at the center of massive galaxies [129]. Apart from that, we will see in the following that they can even probe the missing scales of inflation. For the interested reader, we recommend [130] for a nice review on PBHs.

In order to form enough PBH that could represent for example a significant fraction of the dark matter we need to exponentially enhance the amplitude of the power spectrum on scales which are not probed by the CMBR, for which a violation of SR is needed. We have already seen that USR predicts such a growth in the power spectrum, which make the generation of large inhomogeneities more and more probable. As it can be schematically seen in Fig. 2.3, where we assume for simplicity Gaussian statistics, a growth of the power spectrum means a growth in the value of the variance of the PDF for the curvature perturbation, which means that, non-perturbative values for example of order $\mathcal{R} \sim 1$, which are unreachable for the CMBR scales (they are $\sim 3 \times 10^4\sigma$ away), become "only" $\sim 30\sigma$ away if the power spectrum is $\Delta_{\mathcal{R}} \sim \mathcal{O}\left(10^{-3}\right)$. Note also that, as we justified before, the growth of the power spectrum necessary for the formation of PBH might also have the effect of the formation of scalar induced gravitational waves, reason why it is sometimes claimed that the formation of PBH always have a (possibly detectable) GW counterpart [131, 132].

It is then clear that, if we want to generate a non-negigible amount of PBH and at

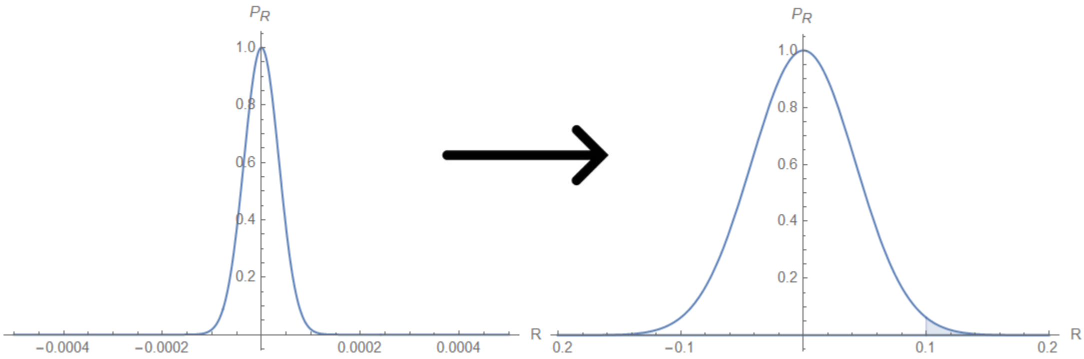

Fig. 2.3 Evolution of the PDF of the curvature perturbation $P(\mathcal{R})$ if the power spectrum grows by a factor $\sim 10^6$, the values of $\mathcal{R}$ coloured in blue could eventually collapse forming a PBH.

the same time satisfy the constraints given by the CMBR, we must abandon the SR regime after generating the inhomogeneities responsible for the CMBR . In Fig. 2.4 we show a very similar figure as Fig. 2.1 where we include a mode (in green) which is generated after the generation of the CMB anisotropies (in orange) and that, as a consequence, re-enters the horizon before recombination, where there are no known observational constraints on the power spectrum. The power spectrum of the green modes is precisely the one that can grow if we violate the SR regime and can lead to the non-negligible generation of large inhomogeneities which can form PBH when it re-enter the horizon (at N_{PBH}).

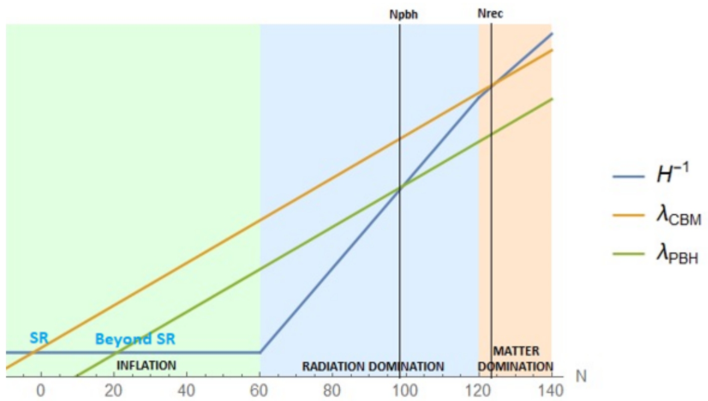

Fig. 2.4 Schematic representation of the mode (in orange) that could explain the CMB data and for which a SR period of inflation is required and of the mode (in green) that could be responsible for the formation of PBH and for which SR must be violated.

Although a growth of the power spectrum beyond SR can be predicted in the context of linear perturbation theory, as we have done in section 2.2.1, the precise study of the inhomogeneities located in the tail of the PDF, which are the ones of interest for PBH, must be done in a fully non-perturbative way. In fact, the Gaussian assumption for the PDF of scalar fluctuations is only justified in the case of linear perturbation theory. One expects higher order in perturbation theory (and even non-perturbative) terms to lead to a non-Gaussian PDF for $\mathcal{R}$. Any non-Gaussianity affect the tail of the PDF of $\mathcal{R}$ can exponentially affect the production of PBH. This is the reason why a very precise description of higher orders in cosmological perturbation theory and/or non-perturbative effects, is of crucial importance for the computation of masses and abundances of PBH.

Having presented the well-known linear cosmological perturbation theory and having motivated why it is important to go beyond it, we are finally in position to start studying some very useful non-perturbative methods that we can use in inflation.

2.3 Gradient expansion.

We have already talked about how the characteristic scale of inhomogeneities λ becomes larger than the Hubble radius as inflation proceeds. We show in Fig. 2.5 an intuitive representation of how this process happen: during inflation the Hubble radius $(H)^{-1}$ stays approximately constant and the exponential expansion of the universe stretches more and more the characteristic wavelength of the fluctuations until it becomes much larger than the Hubble radius. i.e. $\lambda \gg (H)^{-1}$. In this limit, as it can be seen in Fig. 2.5, the effect of the fluctuation can be seen as a constant shift of the background dynamics of $(H)^{-1}$ (from the dotted line to the solid line in the right-hand side of Fig. 2.5). This suggests that, in the long-wavelenght limit , one can consider small patches to be approximately homogeneous and isotropic, this is the main assumption of gradient expansion.

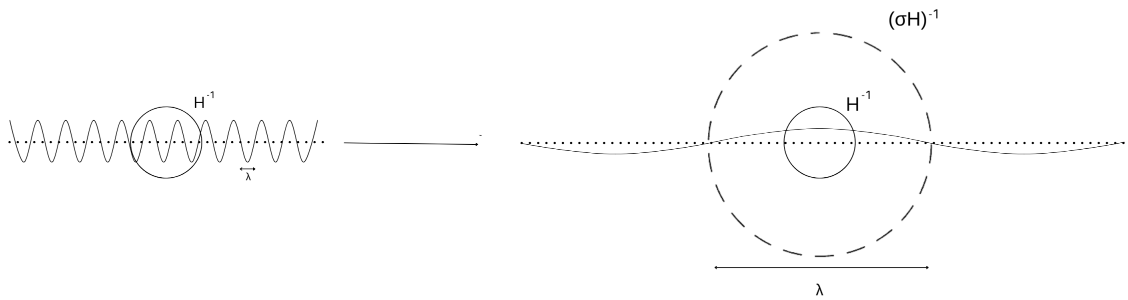

Fig. 2.5 Evolution of the wavelength λ of the different modes during inflation.

The gradient expansion approximation [133, 134, 135, 136, 137, 138, 139, 140, 141, 93] then consists in considering small patches of the universe which can be approximately described by a local FLRW geometry. By choosing some local coordinates $(t_l, \mathbf{x})$, this geometry may be described by the following metric

$$ds_l^2 = -dt_l^2 + a_l^2(t_l)\,\delta_{ij} dx_l^i dx_l^i\,, \tag{2.143}$$

where the subscript l denotes a local patch (the solid circle in Fig. 2.5). We can also define the local Hubble parameter as $H_l \equiv \frac{\partial_{t_l} a_l}{a_l}$.

As already anticipated, the patch is chosen in a way that the characteristic scale of inhomogeneities, which we call it λ, is much larger than $(H_l)^{-1}$. One can then define an expansion parameter $\sigma \equiv (H_l \lambda)^{-1} \ll 1$.

Reversing the argument, at leading order in σ, each patch of the universe of size $(\sigma H_l)^{-1}$ (the coarse grained scale) is approximately described by an homogeneous FLRW universe. Higher order terms in σ expansion will instead capture local inhomogeneities.

Contrary to the linear cosmological perturbation theory approach, the gradient expansion is valid for any amplitude of local over-densities, as wavelength of the fluctuation is large enough for the gradients to be negligible, in this sense we can say that linear cosmological perturbation theory is valid at leading order in the amplitude of the inhomogeneities but at all orders in k and that leading order in gradient expansion is valid at leading order in k but at all orders in the amplitude of the inhomogeneities.

Note that the assumption on which the gradient expansion is based on implies that a patch can be found such that any spatial gradient would introduce an order σ. In other words, for a generic function X, $\partial_i X \sim X \times \mathcal{O}(\sigma)$. This is because a function which is approximately homogeneous in local coordinates can be written as $X(t, \sigma x^i)$ with $\sigma \ll 1$. Thus, we have

$$\partial_i X(t, \sigma x^i) = \sigma \frac{\partial}{\partial\left(\partial x^i\right)} X\left(t, \sigma x^i\right) = \sigma \left.\frac{\partial}{\partial\left(\partial x^i\right)} X\left(t, \sigma x^i\right)\right|_{\sigma=0} + \mathcal{O}\left(\sigma^2\right) , \quad (2.144)$$

and, since $\left.\frac{\partial}{\partial(\partial x^i)} X\left(t, \sigma x^i\right)\right|_{\sigma=0}$ can be of the same order as $X\left(t, \sigma x^i\right)$, we can generically write

$$\partial_i X \sim X \times \mathcal{O}\left(\sigma\right) . \quad (2.145)$$

2.3.1 Naive leading order in gradient expansion.

Usually, when performing gradient expansion we will be comparing different patches, each one with local coordinates as in (2.143). For better comparison between patches it is necessary to define a set of coordinates which is valid for all the different patches at the same time, the most logical set of coordinates which allow us to compare different patches in a non-perturbative way is given by the ADM line element presented in section (1.2):

$$ds^2 = -\alpha^2(t,\mathbf{x})dt^2 + a^2(t)e^{2\zeta(t,\mathbf{x})}\tilde{\gamma}_{ij}(t,\mathbf{x})\left[dx^i + \beta^i(t,\mathbf{x})dt\right]\left[dx^j + \beta^j(t,\mathbf{x})\right] . \tag{2.146}$$

The coordinates $(t, \mathbf{x})$ in (2.146) are common for all the different patches such that the differences between patches are now given by differences into the lapse function α, the shift vector β^i and the rest of the functions. The most important point is then to give the correct order in gradient expansion to each one of these functions. Naively we could demand that all physical quantities do not vanish at leading order in gradient expansion i.e.

$$\begin{aligned} {}_{(0)}\alpha(t) - 1 \sim \mathcal{O}(\sigma^0)\,, \qquad {}_{(0)}\zeta(t) \sim \mathcal{O}(\sigma^0)\,, \qquad {}_{(0)}\beta^i(t) \sim \mathcal{O}(\sigma^0) \\ {}_{(0)}\phi(t) \sim \mathcal{O}(\sigma^0) \qquad \tilde{\gamma}_{ij} - \delta_{ij} \sim \mathcal{O}(\sigma)\,, \end{aligned} \tag{2.147}$$

where the subscript (0) reminds the reader that we are at leading order in gradient expansion and the time-only dependence is because any spatial dependence would introduce higher order in gradient expansion effects. Note that in the order estimation of (2.147) we have included also the field. The reason why $\tilde{\gamma}_{ij} - \delta_{ij} \sim \mathcal{O}(\sigma)$ is because we will only focus on scalar modes and the traceless part of the scalar part of the spatial metric will always contain some spatial derivatives, we will further explore this point later on.

We can now derive the equations of motion at leading order in gradient expansion by inserting the order estimation of (2.147) into the ADM equations (2.19)-(2.24) of section 1.2. The only two relevant equations that do not vanish at leading order in gradient expansion are

$$\left(\frac{\bar{H} + {}_{(0)}\dot{\zeta}}{{}_{(0)}\alpha}\right)^2 = \frac{1}{3M_{PL}^2}\left(\frac{{}_{(0)}\dot{\phi}^2}{2\,{}_{(0)}\alpha^2} + V\left({}_{(0)}\phi\right)\right)\,, \tag{2.148}$$

$$\frac{1}{{}_{(0)}\alpha}\frac{d}{dt}\left(\frac{\bar{H} + {}_{(0)}\dot{\zeta}}{{}_{(0)}\alpha}\right) + \left(\frac{\bar{H} + {}_{(0)}\dot{\zeta}}{{}_{(0)}\alpha}\right)^2 = -\frac{1}{3M_{PL}^2}\left(\frac{{}_{(0)}\dot{\phi}^2}{{}_{(0)}\alpha^2} - V\left({}_{(0)}\phi\right)\right)\,. \tag{2.149}$$

Note that under the redefinition $dt_l = {}_{(0)}\alpha dt$ and $H_l = \frac{\bar{H} + {}_{(0)}\dot{\zeta}}{{}_{(0)}\alpha}$, equations (2.148) and (2.149) coincide with the equations of motion of an exactly homogeneous and isotropic FLRW universe (see (2.4) and (2.5)) but in local coordinates. This is not surprising because our assumption is precisely that at leading order in gradient expansion the metric in local coordinates is precisely (2.143), i.e. a FLRW metric.

Since the justification of the order in gradient expansion of each variable given in

(2.147) is a bit hand-waving (and we will see later on it is not completely true), it is worthy to perform a consistency check. It consist in linearizing the equations of motion of the local patch (2.148) and (2.149) and check if the solution obtained in this way coincides with the solution obtained in the long-wavelength limit of linear cosmological perturbation theory, i.e. (2.122). In order to do so we will perturb ${}_{(0)}\alpha$, ${}_{(0)}\zeta$ and ${}_{(0)}\phi$ at linear order:

$$\begin{aligned}
{}_{(0)}\alpha &\simeq 1 + A^{gr} \,, \\
{}_{(0)}\zeta &\simeq D^{gr} \,, \\
{}_{(0)}\phi &\simeq \bar{\phi} + \delta\phi^{gr} \,,
\end{aligned} \tag{2.150}$$

where the subscript gr indicates that we are linearizing only the equations at leading order in gradient expansion and not whole set of ADM equations, note also that we are only focused in the scalar part. Inserting (2.150) into (2.148) and (2.149) we get

$$2\bar{H}\left(\dot{D}^{gr} - \bar{H}A^{gr}\right) = \frac{1}{3M_{PL}^2}\left(\dot{\bar{\phi}}\dot{\delta\phi}^{gr} - \dot{\bar{\phi}}^2 A^{gr} + V_{\bar{\phi}}\delta\phi^{gr}\right) \,, \tag{2.151}$$

$$\ddot{D}^{gr} - 2\dot{\bar{H}}A^{gr} - \bar{H}\dot{A}^{gr} + 2\bar{H}\dot{D}^{gr} - 2\bar{H}^2 A^{gr} = -\frac{1}{3M_{PL}^2}\left(2\dot{\bar{\phi}}\dot{\delta\phi}^{gr} - 2\dot{\bar{\phi}}^2 A^{gr} - V_{\bar{\phi}}\delta\phi^{gr}\right) \,, \tag{2.152}$$

For convenience, let us write (2.151) in a more suggestive way

$$HA^{gr} - \dot{D}^{gr} - \frac{\dot{\phi}^{gr}}{2M_{PL}^2}\delta\phi = \frac{\epsilon_1}{3-\epsilon_1}\dot{\mathcal{R}}^{gr} \,, \tag{2.153}$$

where we have defined the "gradientless" version of the comoving curvature perturbation as $\mathcal{R}^{gr} \equiv D^{gr} - \frac{H}{\dot{\bar{\phi}}}\delta\phi^{gr}$.

Now we can combine (2.151),(2.152) and (2.153) as we did in section 2.2.1.1 when obtaining equation (2.59). Following the same notation as in (2.59), we have $\dot{f}_1(t) = \frac{\epsilon_1}{3-\epsilon_1}\dot{\mathcal{R}}$ and therefore the equation of motion for $\mathcal{R}^{gr}$ is [4]

$$\frac{d}{dt}\left(\frac{3a^3\epsilon_1}{3-\epsilon_1}\dot{\mathcal{R}}_k^{gr}\right) = 0 \,, \tag{2.154}$$

whose solution is obviously

$$\mathcal{R}_k^{gr} = c_1(k) + c_2(k)\int \frac{3-\epsilon_1}{3a^3\epsilon_1}dt \,. \tag{2.155}$$

[4] Equation (2.154) take the same form in Fourier space and in real space because of the absence of spatial gradients, we will use the Fourier space version for better comparision with the results in section 2.2.1.3.

If we compare the solution for $\mathcal{R}$ in the long-wavelength limit (2.122) with (2.155) we can see that they are not exactly the same. This was already noted almost 25 years ago [142, 143] but it is worthy to explore this difference in detail and see how it affects our leading order in gradient expansion.

The first thing one could think is that the difference between (2.122) and (2.155) is $\mathcal{O}(\epsilon_1)$ so it is not very important. However, this is not completely true, the reason is that we have not said anything about the constants $c_1(k)$ and $c_2(k)$, these constants must be set in such a way that the solution (2.155) represents the $k \to 0$ limit of a solution with $k \neq 0$ as we did in section 2.2.1.3. One way of imposing this condition is by using the boundary condition given by the momentum constraint, i.e. using (2.57), which is equivalent to impose the right-hand side of (2.153) to be identically zero, or, in other words $\dot{\mathcal{R}}_k = 0$.

The constant $c_2(k)$ must then vanish in order to satisfy the boundary condition imposed by the momentum constraint meaning that, the term proportional to $c_2(k)$ in (2.155) is not the $k \to 0$ limit of a solution with $k \neq 0$ and hence it is not a physical solution. We can then conclude that the solution for the comoving curvature perturbation $\mathcal{R}$ that comes from the linearization of the naive leading order in gradient expansion is:

$$R^{gr} = c_1(k)\,, \tag{2.156}$$

i.e. always a constant. We have then lost the time dependent mode. As we saw in section (2.2.1.3), this mode is negligible if $\kappa \leq -\frac{3}{2}$. However, for $\kappa > -\frac{3}{2}$ the constant mode is actually the negligible one so in this case we have lost the relevant mode.

The reason why this naive leading order in gradient expansion fails to reproduce the time dependent mode can clearly be guessed if we write the linear Hamiltonian constraint of (2.35) in the following suggestive way

$$\bar{H}A - \dot{D} - \frac{1}{2}\nabla^2\dot{E} - \frac{\dot{\bar{\phi}}}{2M_{PL}^2} = \frac{\epsilon_1}{3-\epsilon_1}\dot{\mathcal{R}} + \frac{1}{\bar{H}(3-\epsilon_1)}\frac{\nabla^2}{a^2}\Psi\,. \tag{2.157}$$

Again, the only way that the Hamiltonian constraint (2.157) and the linear momentum constraint (2.57) are compatibles is if the right-hand side of (2.157) identically vanish, which implies

$$\dot{\mathcal{R}} = -\frac{1}{\bar{H}\epsilon_1}\frac{\nabla^2}{a^2}\Psi\,. \tag{2.158}$$

From (2.158) we can clearly see what went wrong with the naive leading order gradient expansion: a spatial gradient does not necessarily means a k-suppresion, in fact, if we compare (2.158) with the solution of the MS equation in the long wavelength limit (2.122) we have

$$\nabla^2\Psi = C_2'(k)\frac{\bar{H}}{a}\,, \tag{2.159}$$

where $C_2'(k)$ is not generically k-suppressed, as we saw in section 2.2.1.3.

The reason why the naive leading order in gradient expansion does not give us the time-dependent mode is that, when giving the order estimation of (2.147), we have automatically set any quantity with a spatial gradient equal to zero. On the other hand, from (2.159) we can see that, although it decays with time, $\nabla^2\Psi$ does not vanish in the $k \to 0$ limit. Something that decays with time could seem harmless, however these decaying (but not k-suppressed) functions can become dangerous when multiplied by function that grows in time, as it is the case in (2.158), where $\frac{1}{\epsilon_1}$ can be a growing function. In fact, neglecting $\nabla^2\Psi$ in (2.158) means killing the growing mode of $\mathcal{R}$ when $\kappa = \frac{V_{\bar{\phi}}}{\bar{H}\dot{\bar{\phi}}} > -\frac{3}{2}$.

As far as we know, all the previous work on gradient expansion during inflation use the naive approximation presented in this section, this is why in section 2.3 we will formulate for the first time a consistent leading order in gradient expansion that takes care of the terms that, although contain a spatial derivative, do not vanish in the $k \to 0$ limit. However, before that, we will present in the next section an alternative way of interpreting these decaying (but not $k-$suppressed terms) based on symmetries of the Einstein equations [78].

2.3.2 Symmetries in the long-wavelength limit

In the previous section we have shown that the time dependent mode of $\mathcal{R}$ is related with terms with spatial derivatives that do not vanish in the $k \to 0$ limit. In this section we will give an alternative proof of this phenomena showing that both modes of $\mathcal{R}$ are related to a symmetry of the perturbative equations in the Newtonian gauge, generalizing Weinberg's procedure to determine the constant mode of $\mathcal{R}$ [97].

In Newtonian gauge, the metric can be written as:

$$ds^2 = -(1+2A_N)dt^2 + a^2(1+2D_N)\delta_{ij}dx^i dx^j\,. \tag{2.160}$$

The scalar set of perturbed Einstein's equations in this gauge is

- Hamiltonian constraint

$$-3\bar{H}^2 A_N + 3\bar{H}\dot{D}_N - \frac{\nabla^2}{a^2}D_N = \frac{1}{2M_{pl}^2}\left(\dot{\bar{\phi}}\delta\dot{\phi}_N - \dot{\bar{\phi}}^2 A_N + V'(\bar{\phi})\delta\phi_N\right)\,. \tag{2.161}$$

- Momentum constraint

$$\partial_i \left(-\bar{H} A_N + \dot{D}_N + \frac{\dot{\bar{\phi}}}{2M_{pl}^2} \delta\phi_N \right) = 0 \,. \tag{2.162}$$

- Trace of the spacial Einstein equations

$$6\dot{\bar{H}} A_N + 3\bar{H}\dot{A}_N - 3\ddot{D}_N + \frac{\nabla^2}{a^2} A_N + 6\bar{H}^2 A_N - 6\bar{H}\dot{D}_N = \frac{1}{M_{pl}^2}\left(2\dot{\bar{\phi}}\delta\dot{\phi}_N - 2\dot{\bar{\phi}}^2 A_N - V'(\bar{\phi})\delta\phi_N\right) \,. \tag{2.163}$$

- Traceless part of the spacial Eisntein equations

$$\left(\partial_i \partial_j - \frac{1}{3}\delta_{ij}\nabla^2\right)(A_N + D_N) = 0 \tag{2.164}$$

One can show that the above equations are invariant under the following fields re-definitions

$$\begin{aligned} \tilde{A}_N &= A_N - \dot{\lambda}^0 \,, \\ \tilde{D}_N &= D_N - H\lambda^0 - \frac{1}{3}\nabla^2\lambda \,, \\ \delta\tilde{\phi} &= \delta\phi - \dot{\bar{\phi}}\lambda^0 \,, \end{aligned} \tag{2.165}$$

where

$$\lambda = -x^2 \frac{f_1(t)}{2} + f_2(t) \,, \tag{2.166}$$

and

$$\lambda^0(t, \vec{x}) = -a^2(t) x^2 \frac{\dot{f}_1(t)}{2} + f_3(t) \,. \tag{2.167}$$

As we shall see, the function $f_1(t)$ is going to be of perturbative order. Note that, although the field redefinition contain potentially non-perturbative terms (those proportional to $x^2 \equiv \delta_{ij} x^i x^j$) the Einstein's equations do not contain any x^2. This term either cancels out or is removed by a Laplacian. Thus, in this sense, the proposed field re-definition keeps the equations at linear order.

It is interesting to note that, in the UV, those fields redefinition are related to the change of coordinates

$$t \to t + \lambda^0(t, \vec{x}), \qquad x^i \to x^i + \partial_i \lambda(t, \vec{x}) \,, \tag{2.168}$$

which takes a Friedmann geometry in Newtonian form [**?**]. Those coordinate transformation may only be extended to the IR if and only if $\dot{f}_1 = 0$. The relation between the coordinate transformation and the symmetry of the Einstein's equations in Newtonian gauge was the starting point of the Weinberg procedure in [97].

Both tilded and un-tilded functions solve the *same* equations and so are, possibly different, solutions of the *same* system. Then, because we are only considering linear differential equations, the difference between the tilded and un-tilded solutions would still represent a solution. Moreover, because this solution is homogeneous, it will be related to perturbations in the long-wavelength limit.

Different solutions are selected by considering specific boundary and/or initial conditions. The boundary conditions, as we are going to see, are related to the momentum constraint, while the initial conditions to the Bunch-Davies vacuum. The latter will ultimately fix the evolution equation of the variable we would like to consider.

The comoving curvature perturbation $\mathcal{R}$ in Newtonian gauge is

$$\mathcal{R} = \hat{D}_N - \frac{\bar{H}}{\dot{\bar{\phi}}}\delta\hat{\phi}_N \,, \tag{2.169}$$

where hatted functions are a solution of the linear Einstein equations before imposing any boundary or initial conditions.

We can then consider

$$\mathcal{R} = (\tilde{D}_N - D_N) - \frac{\bar{H}}{\dot{\bar{\phi}}}(\delta\bar{\phi}_N - \delta\phi_N) = f_1(t) \,. \tag{2.170}$$

This is simply telling us that, until boundary conditions are imposed, the most generic solution of $\mathcal{R}$ is a generic function of time.

The boundary conditions of our set of differential equations are the integrated version of the momentum constraint. As before, we fix the integrated momentum to zero for the untilded variables

$$-\bar{H}A_N + \dot{D}_N + \frac{\dot{\bar{\phi}}}{2M_{pl}^2}\delta\phi_N = 0 \,. \tag{2.171}$$

While the transformation from un-tilded to tilded variables leave invariant the equations of motion, they change the boundary conditions (the integrated momentum) into

$$-\bar{H}\tilde{A}_N + \dot{\tilde{D}}_N + \frac{\dot{\bar{\phi}}}{2M_{pl}^2}\delta\tilde{\phi}_N - \dot{f}_1(t) = 0 \,.$$

This does not represent a problem as the integration of the momentum constraint precisely leaves the freedom of adding a time-dependent function.

Combining (2.161), (2.163) and the second line of (2.172) we get the following equation:

$$\ddot{\tilde{Q}} + 3\bar{H}\dot{\tilde{Q}} + \left[-\frac{\nabla^2}{a^2} + \bar{H}^2\left(-\frac{3}{2}\epsilon_2 + \frac{1}{2}\epsilon_1\epsilon_2 - \frac{1}{4}\epsilon_2^2 - \frac{1}{2}\epsilon_2\epsilon_3\right)\right]\tilde{Q} + \\ + \frac{\dot{\bar{\phi}}}{\bar{H}}\left(\ddot{f}_1(t) + \bar{H}(3+\epsilon_2)\dot{f}_1(t)\right) = 0\,. \quad (2.172)$$

A solution is such that the tilde MS equation is satisfied, i.e.

$$\ddot{\tilde{Q}} + 3\bar{H}\dot{\tilde{Q}} + \left[-\frac{\nabla^2}{a^2} + \bar{H}^2\left(-\frac{3}{2}\epsilon_2 + \frac{1}{2}\epsilon_1\epsilon_2 - \frac{1}{4}\epsilon_2^2 - \frac{1}{2}\epsilon_2\epsilon_3\right)\right]\tilde{Q} = 0\,, \quad (2.173)$$

leaving

$$\ddot{f}_1(t) + \bar{H}(3+\epsilon_2)\dot{f}_1(t) = 0\,. \quad (2.174)$$

The solution of this equation is

$$f_1(t) = C_1 + C_2\int e^{-\int \bar{H}(3+\epsilon_2)dt}dt\,, \quad (2.175)$$

implying, in Fourier space and in the $k \to 0$ limit

$$\mathcal{R}_k = C_1^k + C_2^k\int e^{-\int \bar{H}(3+\epsilon_2)dt}dt\,. \quad (2.176)$$

Because $\mathcal{R}_k$ follows a second order differential equation, the solutions (2.176) represent the whole set of solutions and the constant C_i^k can now be fixed by initial conditions.

Thus, we have proven that both decaying(growing) and constant modes, are related to a hidden symmetry of the perturbed Einstein equations in Newtonian gauge, extending the analysis of Weinberg.

2.3.3 Leading order in gradient expansion

The first thing to emphasise is that, in the same way as we can set a quantity to zero in linear perturbation theory by specifying a gauge, the leading order in gradient expansion of each one of the functions in (2.146) will also depend on the choice for the 3+1 decomposition of the metric. In our case we will only explore choice of hypersurfaces which are well behaved in the $k \to 0$ limit. In order to define this well-behaved hypersurfaces we will again make use of linear perturbation theory. As we have seen in (2.159), the term which contains a gradient but does not vanish in the $k \to 0$ limit is $\nabla^2\Psi$. This term can be written in terms of the gauge invariant variables as (see (2.52))

$$\nabla^2\Psi = -\nabla^2 D - \frac{1}{3}\nabla^2\nabla^2 E - a\bar{H}\nabla^2 B - a^2\bar{H}\nabla^2\dot{E}\,. \quad (2.177)$$

The way we will define a "well-behaved" gauge will be clear with an example.

Imagine that we choose the Newtonian gauge in which $B_N = E_N = 0$, in this case the important term in the $k \to 0$ limit would be $\nabla^2 D_N$. Now, if we go to the linear equations of motion of (2.35)-(2.40), we see that we have terms like $\dot{D}_N$ in the equations of motion. Thus, if we have that $\nabla^2 D_N \sim \mathcal{O}(\sigma^0)$, then $D_N \sim \mathcal{O}(\sigma^{-2})$ and hence we have divergent terms when $\sigma \to 0$. This is what we will define as a ill-behaved gauge in the limit $k \to 0$. On the other hand, let us study for example the flat gauge where $\nabla^2 \Psi = -a\bar{H}\nabla^2 B_f$. The main difference in this case is that every time that B_f appear in the linear equations of motion of (2.35)-(2.40), it does as $\nabla^2 B_f$ and never as B_f alone so we do not have any divergent term. The flat gauge would then be an example of a well-behaved gauge in the $k \to 0$ limit.

With this in mind we can finally formulate the leading order in gradient expansion: the key point is that, as it can be straightforwardly shown, the local metric (2.146) can be written with a coordinate redefinition as follows[5]

$$ds_l^2 = -\,{}_{(0)}\alpha^2 dt^2 + a^2(t) e^{2\,{}_{(0)}\zeta} \delta_{ij} \left(dx^i + {}_{(0)}\beta^i dt\right)\left(dx^j + {}_{(0)}\beta^j dt\right) \,, \qquad (2.178)$$

with the conditions

1. ${}_{(0)}\alpha = {}_{(0)}\alpha(t)\,,$
2. ${}_{(0)}\beta^i = b(t) x^i\,,$
3. ${}_{(0)}\zeta = {}_{(0)}\zeta(t)\,.$

It is important to remark that, although it is written in different coordinates, the metric (2.265) is still a FLRW metric. One could be worried about the fact that a homogeneous and isotropic metric contains terms outside the diagonal, however, following [144] we know that a space-time is homogeneous and isotropic if:

1. All constant time hypersurfaces Σ_t are constant curvature spaces. In our case the hypersurfaces Σ_t are simply Euclidean and this condition is trivially satisfied.
2. The extrinsic curvature of the hypersurfaces is homogeneous and isotropic. Using the definition of extrinsic curvature of (1.6) together with the conditions for ${}_{(0)}\alpha$, ${}_{(0)}\beta^i$ and ${}_{(0)}\gamma_{ij}$ specified below (2.265), we can see that the extrinsic curvature only depends on time and hence this condition is also satisfied.

[5] Note that we are only considering scalar fluctuations when performing this redefinition. If we want to study inflation in a fully non-perturbative way, we should also take into account vector and tensor perturbations. This is because, although they are independent at linear order in perturbation theory, this is no longer true at higher orders as justified in section 2.2.4. The reason why we do not include vector and tensor perturbations here is because, although at this level it would be straightforward, it is not possible when applying gradient expansion to stochastic inflation as we will see later on. In this sense we are formulating a gradient expansion which is non-perturbative only for the scalar sector in the case in which tensor and vector fluctuations are negligible.

Note that the x-dependence in ${}_{(0)}\beta^i$ is already showing that the order estimation that we did in (2.147) is not correct. The new (and correct) order estimation is now the following:

$$
\begin{aligned}
{}_{(0)}\alpha(t) - 1 \sim \mathcal{O}(\sigma^0)\,, \qquad {}_{(0)}\zeta(t) \sim \mathcal{O}(\sigma^0)\,, \qquad {}_{(0)}\beta^i(t) \sim \mathcal{O}(\sigma^{-1}) \\
{}_{(0)}\phi(t) \sim \mathcal{O}(\sigma^0) \qquad \tilde{\gamma}_{ij} - \delta_{ij} \sim \mathcal{O}(\sigma)\,, \qquad (2.179)
\end{aligned}
$$

It is now important to make some comments about the last line, as before ${}_{(0)}\phi(t)$ has been added to take into account the expansion of the scalar field, which is generically non-zero at the background level. Furthermore, note that here the condition $\tilde{\gamma}_{ij} - \delta_{ij} \sim \mathcal{O}(\sigma)$ implies a further condition on the scalar part of $\tilde{\gamma}_{ij}$, in fact, using the expansion of the exponential of a matrix we can write

$$
\tilde{\gamma}_{ij} = e^{-2M_{ij}} \simeq \delta_{ij} - 2M_{ij} + \mathcal{O}(\sigma^2)\,. \qquad (2.180)
$$

Now, M_{ij} must be traceless by definition (see footnote 2). Focusing only in the scalar part of M_{ij} we can then write

$$
\tilde{\gamma}_{ij} - \delta_{ij} \simeq -2\left(\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2\right) C + \mathcal{O}(\sigma^2)\,, \qquad (2.181)
$$

where C is a scalar function. This immediataly implies that $\left(\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2\right) C \sim \mathcal{O}(\sigma)$. It is very important to remark that this condition is not in contradiction with $\nabla^2 C \sim \mathcal{O}(\sigma^0)$ [6].

As before, different functions for ${}_{(0)}\alpha$, ${}_{(0)}\beta^i$ and ${}_{(0)}\zeta$ will give different FLRW patches as long as they satisfy the conditions given below (2.265). We can then relate the different locally homogeneous and isotropic patches by knowing the different non-perturbative functions for ${}_{(0)}\alpha$, ${}_{(0)}\beta^i$ and ${}_{(0)}\zeta$ that lead to each one of them. Of course, in the same way as in perturbation theory, the value of ${}_{(0)}\alpha$, ${}_{(0)}\beta^i$ and ${}_{(0)}\zeta$ will depend on the gauge choice and on the solution for the ADM equations.

We will now explicitly compare the naive leading order in gradient expansion of section 2.3.1 with the correct leading order in gradient expansion presented above. In order to do so let us choose the spatially flat gauge, i.e. ${}_{(0)}\zeta_f = 0$ and expand the ADM

[6] Take for example $C = \mathbf{x}\cdot\mathbf{x}g(t,\sigma\mathbf{x})$, where g is an arbitrary function. In this case we have:

$$
\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2 C = \mathcal{O}(\sigma)\,,
$$

$$
\frac{1}{3}\nabla^2 C = 2\, g(t,\sigma\mathbf{x})|_{\sigma=0} + \mathcal{O}(\sigma)\,,
$$

and hence both $\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2 C$ and $\partial^j\left(\partial_i\partial_j - \frac{1}{3}\delta_{ij}\nabla^2 C\right) = \partial^j\left(\frac{2}{3}\nabla^2 C\right)$ are of order σ.

Hamiltonian constraint (2.19) with both the naive order estimation of (2.147) and with the correct order estimation of (2.179). In the naive case we just have to take (2.148) and set ${}_{(0)}\zeta_f = 0$ i.e.

$$\left(\frac{\bar{H}}{{}_{(0)}\alpha_f}\right)^2 = \frac{1}{3M_{PL}^2}\left(\frac{{}_{(0)}\dot{\phi}_f^2}{2\,{}_{(0)}\alpha_f^2} + V\left({}_{(0)}\phi_f\right)\right). \tag{2.182}$$

On the other hand, for the order estimation of (2.179) we must take also into account some spatial derivatives, leading to the following result

$$\left(\frac{\bar{H}}{{}_{(0)}\alpha_f} - \frac{1}{3\,{}_{(0)}\alpha_f}\partial_i\,{}_{(0)}\beta^i_f\right)^2 = \frac{1}{3M_{PL}^2}\left(\frac{1}{2}\left(\frac{1}{{}_{(0)}\alpha_f}\,{}_{(0)}\left(\left(\partial_t - \beta^i_f\partial_i\right)\phi_f\right)\right)^2 + V\left({}_{(0)}\phi_f\right)\right), \tag{2.183}$$

where we can clearly see the presence of the new terms proportional to β^i_f. Equation (2.183) can also be reduced to the Hamiltonian constraint of a homogeneous and isotropic universe in local coordinates with the following redefinitions

$$H_l \equiv \frac{\bar{H}}{{}_{(0)}\alpha_f} - \frac{1}{3\,{}_{(0)}\alpha_f}\partial_i\,{}_{(0)}\beta^i_f\,, \tag{2.184}$$

$$\frac{d\phi_l}{dt_l} \equiv \frac{1}{{}_{(0)}\alpha_f}\,{}_{(0)}\left(\left(\partial_t - \beta^i_f\partial_i\right)\phi_f\right). \tag{2.185}$$

Note that, although the redefinition (2.185) could seem a bit weird since it contains a spatial derivative of the field, it is actually what one would expect. In fact, the operator $\frac{d}{dt_l} \equiv \frac{1}{{}_{(0)}\alpha_f}\,{}_{(0)}\left(\partial_t - \beta^i_f\partial_i\right)$ is precisely the Lie derivative of the orthogonal vector n^μ to the spatial hypersurface Σ_t (see Fig. 1.1), which is what a local observer would interpret as the time, this Lie derivative then plays the role of a time derivative in local coordinates.

2.3.3.1 Role of the momentum constraint in gradient expansion.

Another very important aspect that we observe when including terms proportional to $\partial_i\,{}_{(0)}\beta^i_f$ in gradient expansion is that the momentum constraint acquire a very important role. In order to see why let us again make use of linear perturbation theory. The first thing to realize is that, although the momentum constraint itself contains spatial derivatives and hence it should not appear at leading order in gradient expansion, the integrated version, which in flat gauge is

$$\bar{H}A_f - \frac{\dot{\bar{\phi}}}{2M_{PL}^2}\delta\phi_f = 0\,, \tag{2.186}$$

is actually important at leading order in gradient expansion so in principle it should always be taken into account at this order.

However, in the naive version of the leading order in gradient expansion, the momentum constraint does not play any important role for the dynamics of the system, the reason is that we can obtain a equation of motion for the gauge invariant variable $\mathcal{R}^{gr}$ (see (2.154)) without need of this constraint. The only role of the momentum constraint in this case is to set the initial conditions (more concretely, to set $c_2(k) = 0$, as we saw in section 2.3.1). In other words, in the naive leading order in gradient expansion we can set the initial conditions such that they satisfy the momentum constraint and evolve the system without worrying anymore about it [145].

This is no longer true if we include terms proportional to $\partial_{i\,(0)}\beta^i_f$, in this case we cannot write a single equation for $\mathcal{R}$ using only the Hamiltonian constraint (2.35) and the evolution equation of the extrinsic curvature (2.39). In fact, if we try to do that we can use (2.157) together with (2.57) and (2.59) to find the following equation

$$\frac{d}{dt}\left[\frac{3a^3\epsilon_1}{3-\epsilon_1}\left(\dot{\mathcal{R}} + \frac{1}{3\bar{H}}\frac{\nabla^2}{a^2}\Psi\right)\right] = 0\,. \tag{2.187}$$

The fact that (2.187) does not only depends on $\mathcal{R}$ but also on $\nabla^2\Psi$ tell us that we need another equation to describe the correct dynamics of $\mathcal{R}$: the momentum constraint. It is then clear that if we include terms with spatial derivatives but that do not vanish in the $k \to 0$ limit in gradient expansion, we must also take into account the momentum constraint when describing the evolution of the gauge invariant variables, playing a more important role than giving only some initial conditions, as in the naive case.

The two main differences between the naive leading order in gradient expansion and the correct leading order in gradient expansion are the following:

1. The inclusion of terms with spatial derivatives that do not vanish in the limit $k \to 0$.
2. The role of the momentum constraint, which becomes important to describe the dynamics of the long-wavelength.

Although gradient expansion is a powerful tool to study large inhomogeneities during inflation it still needs a mechanism to give the initial conditions. As shown in section 2.2.1.1, initial conditions are given in the short-wavelength limit, were we impose the Bunch-Davies vacuum, however gradient expansion is not valid in the short-wavelength limit. This is the reason why gradient expansion is usually combined with some other formalism able to provide initial conditions. The rest of the thesis is devoted to two different ways of combining gradient expansion with linear perturbation theory to obtain a consistent way to describe inflationary inhomogeneities in a non-perturbative way: the δN formalism and the stochastic approach to inflation.

2.4 δN formalism.

The δN formalism is a tool that uses the definition of the number of e-folds $N = \int H dt$ for computing the evolution of cosmological perturbations at super-horizon scales [146, 147, 148, 140, 149, 150, 151].

The local number of e-folds in a given super-horizon patch is

$$N_l = \int_{t_l(t^0,\mathbf{x})}^{t_l(t^e,\mathbf{x})} H_l(t_l) dt_l \simeq \int_{t^0}^{t^e} H_l(t)\alpha(t) dt\,, \tag{2.188}$$

where α is the lapse function of each super-horizon patch defined as $dt_l = \alpha_l dt$ and we have expanded everything at leading order in gradient expansion. Note that this definition of N is not gauge invariant as it depends on the specific gauge relating the local to the background coordinates.

We will start by enunciating the δN formalism in its linear version such that afterwards it will be straightforward to formulate the non-perturbative version. If we now perturb (2.188) with respect to a FLRW background we get the expression for the number of e-folds in a perturbed universe

$$N_l \simeq \int_{t^0}^{t^e} \left(\bar{H} + \dot{D} - \frac{\nabla^2}{3} \left(\frac{B}{a} \right) \right) dt\,, \tag{2.189}$$

where we have no fixed yet any gauge and we are keeping the term $\frac{\nabla^2}{3}\left(\frac{B}{a}\right)$ because, as we saw in the previous subsection, it might play an important role in the $k \to 0$ limit. A gauge transformation (2.43) would lead to

$$\int_{\bar{t}^0}^{t^e} \left(\bar{H} + \dot{D} - \frac{\nabla^2}{3} \left(\frac{B}{a} \right) \right) dt \longrightarrow \int_{t^0}^{t^e} \left(\bar{H} + \frac{d}{dt}\left(D - \bar{H}\lambda^0\right) - \frac{\nabla^2}{3} \left(\frac{B}{a} \right) - \frac{\nabla^2}{3} \left(\frac{\lambda^0}{a^2} \right) \right) dt\,. \tag{2.190}$$

We will choose ξ^0 to be next to leading order in gradient expansion[7]. With this in mind, the number of e-folds transform as:

$$N_p \to N_p - \bar{H}\xi^0\Big|_{t^e} + \bar{H}\xi^0\Big|_{t^0} \tag{2.191}$$

If $\bar{H}\xi^0\Big|_{t^e}$ and $\bar{H}\xi^0\Big|_{t^e}$ represent different gauges, let us say gauge $\mathcal{A}$ and $\mathcal{B}$, we will say that we have chosen an interpolating gauge between $\mathcal{A}$ and $\mathcal{B}$ and we will write $N_{\mathcal{A}}^{\mathcal{B}}$.

We then finally define δN as follows

$$\delta N \equiv N_{\mathcal{A}}^{\mathcal{B}} - N_{\mathcal{A}'}^{\mathcal{B}'}\,. \tag{2.192}$$

In the following we are going to see that, depending on the gauges chosen for $\mathcal{A}$ and

[7]This is only possible in the well behaved gauges defined in section (2.3.3)

$\mathcal{B}$ we can recover both the uniform density curvature perturbation $\mathfrak{z}$ defined in (2.55) or the comoving curvature perturbation $\mathcal{R}$ defined in (2.54).

- The curvature perturbation at uniform density ζ is obtained by choosing $\mathcal{A}$ and $\mathcal{B}$ respectively in flat and uniform density gauges while $\mathcal{A}'$ and $\mathcal{B}'$ in flat gauge.

  Indeed, with this choice

$$\delta N_\zeta = N_f^{ud} - N_f^f = \left(D - \bar{H}\xi_{ud}^0\right)\Big|_{t^e} . \tag{2.193}$$

  Now because in the uniform density we have $(\delta\rho - \dot{\bar{\rho}}\lambda_{ud}^0)\Big|_{t^e} = 0$, we get

$$\delta N_{\mathfrak{z}} = N_f^{ud} - N_f^f = \left(D - \frac{\bar{H}}{\dot{\bar{\rho}}}\delta\rho\right)\Bigg|_{t^e} = \mathfrak{z}(t^e)\,, \tag{2.194}$$

  where the last equality comes by fixing η such that $E = 0$.

- The comoving curvature perturbation $\mathcal{R}$ is instead obtained by taking $\mathcal{A}$ and $\mathcal{B}$ to be flat and comoving gauges, while $\mathcal{A}'$ and $\mathcal{B}'$ are flat gauges.

  Then we get, similarly as before,

$$\delta N_{\mathcal{R}} = N_f^c - N_f^f = \left(D - \frac{\bar{H}}{\dot{\bar{\phi}}}\delta\phi\right)\Bigg|_{t^e} = \mathcal{R}(t^e)\,, \tag{2.195}$$

Having clarified that the choice of gauges actually determines the curvature perturbation that we reproduce with the δN formalism. In most lecture notes and textbooks about inflation one can find that the uniform density curvature perturbation $\mathfrak{z}$ and the comoving curvature perturbation $\mathcal{R}$ are actually equivalent in the limit $k \to 0$ [152, 153, 154]. However, let us take a closer look to it. Combining the linear Hamiltonian and momentum constraints (see (2.35) and (2.57)) it is straightforward to get the following relation

$$\mathfrak{z} = \mathcal{R} + \frac{1}{3\bar{H}^2\epsilon_1}\frac{\nabla^2}{a^2}\Psi \tag{2.196}$$

From (2.196) one can clearly that the reason $\mathfrak{z}$ is usually assumed to be equal to $\mathcal{R}$ in the limit $k \to 0$ is actually the same reason why the naive gradient expansion of section (2.3.1) fails to reproduce the correct $k \to 0$ evolution of $\mathcal{R}$: the assumption that in the limit $k \to 0$, every quantity that contains a spatial derivative must vanish. In fact, if we introduce the relation (2.158) into (2.196) we get

$$\mathfrak{z} = \mathcal{R} - \frac{\dot{\mathcal{R}}}{3\bar{H}}\,, \tag{2.197}$$

from where it is clear that $\mathfrak{Z}$ and $\mathcal{R}$ exponentially differ if $\mathcal{R}$ grows with time i.e. when $\kappa = \frac{V_{\bar{\phi}}}{\bar{H}\dot{\bar{\phi}}} > -\frac{3}{2}$.

The conclusion is that, although during SR (and regimes where $\kappa = \leq -\frac{3}{2}$) the difference between $\mathfrak{Z}$ and $\mathcal{R}$ decays with time and hence it can be neglected, in other cases as USR this is no longer true so one must be very careful with the gauge choice when defining the δN formalism.

The formulation of the δN formalism presented in this section can be generalized to include non-linear effects using gradient expansion at leading order, where the metric is given by (2.265). In this case, the number of e-folds in a local patch specified by **x** is

$$N_l = \int_{t^0}^{t^e} {}_{(0)}H_l(t, \mathbf{x})\, {}_{(0)}\alpha(t, \mathbf{x})\big|_{\mathbf{x}=\text{constant}}\, dt\,. \tag{2.198}$$

In (2.201), H_l is identified with the trace of extrinsic curvature as

$$K \equiv -3H_l\,. \tag{2.199}$$

We can then compute ${}_{(0)}K$ (and hence ${}_{(0)}H_l$) by expanding at leading order in gradient expansion its definition of (1.6), the result is

$${}_{(0)}H_l = \frac{1}{{}_{(0)}\alpha}\left(\bar{H} + {}_{(0)}\zeta - \frac{1}{3}\partial_i\, {}_0\beta^i\right) \tag{2.200}$$

The number of e-folds in (2.201) can be then written as follows:

$$N_l = \int_{t^0}^{t^e}\left(\bar{H} + {}_{(0)}\zeta - \frac{1}{3}\partial_i\, {}_0\beta^i\right) dt\,, \tag{2.201}$$

which is the non-perturbative version of expression (2.189). We note that, even if it is of leading order in gradient expansion [94], $\partial_i\, {}_0\beta^i$ always decays at the inverse volume with time as we have shown in (2.159). Because in this case we do not have any growing function multiplying $\partial_i\, {}_0\beta^i$ we will simply neglect it. The number of e-folds takes a very simple form

$$N_l(t^0, t^e, \mathbf{x}) = \bar{N}(t^0, t^e) + {}_{(0)}\zeta(t^e, \mathbf{x}) - {}_{(0)}\zeta(t^e, \mathbf{x})\,, \tag{2.202}$$

where we are explicitly keeping the **x**-dependence to specify that the N_l computed in different patches, contrary to $\bar{N} \equiv \int_{t^0}^{t^e} \bar{H}$, which is the same for all the patches. Note that this means that once we specify a patch by choosing **x**, N_l does not depend on **x** anymore, which is in concordance with the leading order in gradient expansion assumption, in which each patch behaves as a $FLRW$ universe and hence it only depends on t_l.

As in linear case, we can choose a gauge transformation that interpolates different hypersurfaces for the initial and final times. If we now define a non-linear version of the δN formalism (let us call it ΔN) in the same way as we did in (2.194) and (2.195) we get

$$\Delta N_{\mathfrak{Z}} = {}_{(0)}\zeta_{ud}(t^e, \mathbf{x}) \,, \tag{2.203}$$

$$\Delta N_{\mathcal{R}} = {}_{(0)}\zeta_{c}(t^e, \mathbf{x}) \,, \tag{2.204}$$

Whether ${}_{(0)}\zeta_{ud}$ and ${}_{(0)}\zeta_c$ are respectively the non-linear generalization of the uniform density curvature perturbation $\mathfrak{Z}$ and of the comoving curvature perturbation $\mathcal{R}$ is however still an open problem.

2.4.1 δN formalism in terms of inflation initial conditions

The δN described in the previous section is really of little practical use. The reason is that in order to get the ΔN, one would need to know already the solution of the locally perturbed metric in terms of background coordinates.

By using the separate universe approach more seriously, however, one might hope to obtain the curvature perturbations just by solving the evolution equations in a local FRW universe and subtract the number of e-folds of the background [155, 156, 157, 158, 159, 160, 161]. The difference between the evolution of one patch to another would then be related to different initial conditions. The idea goes as follows: let us write the equations for the evolution of each patch in its local coordinates of (2.143) i.e.

$$H_l^2 = \frac{1}{3M_{PL}^2}\left(\frac{\left(\frac{d\phi_l}{dt_l}\right)^2}{2} + V\left(\phi_l\right)\right) \,, \tag{2.205}$$

$$\frac{d^2\phi_l}{dt_l^2} + 3H_l\frac{d\phi_l}{dt_l} + V_{\phi_l}\left(\phi_l\right) = 0 \,, \tag{2.206}$$

Now let us write these equations in terms of the local number of e-folds $dN_l \equiv H_l dt_l$ and combine them to get a simple equation for ϕ_l

$$\frac{d^2\phi_l}{dN_l^2} + \left(3 - \left(\epsilon_1\right)_l\right)\frac{d\phi_l}{dN_l} + M_{PL}^2\left(3 - \left(\epsilon_1\right)_l\right)\frac{V_{\phi_l}\left(\phi_l\right)}{V\left(\phi_l\right)} = 0 \tag{2.207}$$

where we have defined which the local ϵ_1 parameter as

$$\left(\epsilon_1\right)_l \equiv \frac{1}{2M_{PL}^2}\left(\frac{d\phi_l}{dN_l}\right)^2 \tag{2.208}$$

The equation of motion (2.207) is a closed equation for ϕ_l and hence it can be solved in terms of two initial conditions, one for the value of the field ϕ_l^0 and another one for the value of the velocity $\pi_l^0 \equiv \left.\frac{d\phi_l}{dN_l}\right|_{N_l=N_l^0}$, both at initial local time $N_l = N_l^0$. The solution at some final time $N_l = N_l^e$ can be written as

$$\phi_l^e = \phi_l^e \left(N_l^e, \phi_l^0(\mathbf{x}), \pi_l^0(\mathbf{x}) \right) \,, \tag{2.209}$$

where we have explicitly written the **x**-dependence of the initial conditions to indicate, although the evolution of each patch once the initial conditions are defines is completely deterministic, the initial conditions themselves are different for each patch.

Now, let us set the initial hypersurface to be flat and the final one to be comoving, as we do when computing $\delta N_{\mathcal{R}}$ in (2.195). In this case we have the following identifications

- $N_l^e = N_f^c$ because by our gauge choice, the number of e-fold of the local patch corresponds to the number of e-folds from a flat to a comoving hypersurface.
- $\phi_l^0(\mathbf{x})$ and $\pi_l^0(\mathbf{x})$ correspond to initial values given in a flat hypersurface, so we will label them by ϕ_f^0 and π_f^0, having always in mind that they are different for each patch.
- Finally, $\phi_l^e = \bar{\phi}^e$ because the final hypersurface is comoving and hence the field in this hypersurface is the same as the value of the field in a fictitious unperturbed background[8].

With this in mind, and although it is not always doable in an analytic way, we can in principle invert (2.209) and write it as follows

$$N_f^c = N_f^c \left(\bar{\phi}^e, \phi_f^0, \pi_f^0 \right) \,. \tag{2.210}$$

Now we can follow the same procedure for the fictitious global background and write the following

$$\bar{N} = \bar{N} \left(\bar{\phi}^e, \bar{\phi}^0, \bar{\pi}^0 \right) \,, \tag{2.211}$$

with the main difference that in this case, $\bar{\phi}^0$ and $\bar{\pi}^0$ are global initial conditions that do not depend on the specific patch and hence they are **x** independent. Inserting (2.210) and (2.211) into (2.202) we can finally compute the curvature perturbation, in this case ${}_{(0)}\zeta_c$.

In order to make this point even clearer we will solve ${}_{(0)}\zeta_c$ for USR, where an

[8]The reason why we say there that the unperturbed background is fictitious is because, contrary to what happens in cosmological perturbation theory, where we perturb over a physical background, if we want to study inhomogeneities in a non-perturbative way it does not exists the concept of background. We can however still define a fictitious background that would correspond to a fictitious universe with no inhomogeneities.

analytical solution at leading order in SR parameters is possible to obtain[9]. The local equation for the field (2.207) in this case is

$$\frac{d^2\phi_l}{dN_l^2} + 3\frac{d\phi_l}{dN_l} = 0\,, \tag{2.212}$$

whose solution is

$$\phi_l^e = \frac{1}{3}\left(1 - e^{-3N_l^e}\right)\pi^0(\mathbf{x}) + \phi^0(\mathbf{x})\,. \tag{2.213}$$

We can now solve (2.213) and use the identifications below (2.209), the result is

$$N_f^c = \frac{1}{3}\log\left[\frac{\pi_f^0}{\pi_f^0 + 3\phi_f^0 - 3\bar{\phi}^e}\right]\,. \tag{2.214}$$

In the same way, the solution for the fictitious background is

$$\bar{\phi}^e = \frac{1}{3}\left(1 - e^{-3\bar{N}}\right)\pi^0 + \phi^0\,, \tag{2.215}$$

and hence $\bar{N}$ would be

$$\bar{N} = \frac{1}{3}\log\left[\frac{\pi^0}{\pi^0 + 3\phi^0 - 3\bar{\phi}^e}\right]\,. \tag{2.216}$$

We can then compute the non-linear comoving curvature perturbation as:

$${}_{(0)}\zeta_c = \Delta N_{\mathcal{R}} = N_f^c - \bar{N} = \frac{1}{3}\left(\log\left[\frac{\pi_f^0}{\pi_f^0 + 3\phi_f^0 - 3\bar{\phi}^e}\right] - \log\left[\frac{\bar{\pi}^0}{\bar{\pi}^0 + 3\bar{\phi}^0 - 3\bar{\phi}^e}\right]\right)\,. \tag{2.217}$$

As a consistency check, we can expand $\pi_f^0 = \pi^0 + \delta\pi_f$ and $\phi_f^0 = \phi^0 + \delta\phi_f$ and show that we can recover the linear result. In order to do so we need the solution of $\delta\phi_f$ in the long wavelength limit. By definition of flat gauge we know that $\delta\phi_f = Q$, where Q is the solution of the MS equation defined in (2.53). Its solution at superhorizon scales is

$$Q_k = i\frac{\bar{H}_0}{\sqrt{2}k^{3/2}}\,, \tag{2.218}$$

where $\bar{H}_0$ is a constant, which implies that $\delta\pi_f^0 = \frac{dQ}{dN} = 0$ so we can neglect it. If we now expand (2.217) up to linear order in $\delta\phi_f = Q$ we get

[9] In fact, the formulation itself of the δN formalism forbid us to include $\mathcal{O}(\epsilon_1)$ terms in USR. The reason is that, when formulating the δN formalism we have neglected decaying terms as $\partial_i\,{}_{(0)}\beta^i$, for example in (2.201). Now, since ϵ_1^{USR} also decays with time, it would be inconsistent to include $\mathcal{O}(\epsilon_1)$ terms and at the same time neglect $\partial_i\,{}_{(0)}\beta^i$.

$$
\begin{aligned}
{}_{(0)}\zeta_c =& \Delta N_{\mathcal{R}} = N_f^c - \bar{N} = \frac{1}{3}\left(\log\left[\frac{\bar{\pi}^0}{\bar{\pi}^0 + 3(\bar{\phi}^0 + Q) - 3\bar{\phi}^e}\right] - \log\left[\frac{\bar{\pi}^0}{\bar{\pi}^0 + 3\bar{\phi}^0 - 3\bar{\phi}^e}\right]\right) \\
&\simeq -\frac{Q}{\bar{\pi}^0 + 3\bar{\phi}^0 - 3\bar{\phi}^e} = -\frac{Q}{\bar{\pi}^e} = -\frac{\bar{H}_0}{\dot{\bar{\phi}}^e} Q = \mathcal{R}(t^e)\,,
\end{aligned}
\tag{2.219}
$$

where in the last line we have used the equation of motion (2.213) to set $3\left(\bar{\phi}^0 - \bar{\phi}^e\right) = \bar{\pi}^0 - \bar{\pi}^e$. From (2.219) we get that, at linear level, ${}_{(0)}\zeta_c(t^e) \simeq \mathcal{R}(t^e)$, as expected.

Note that it we would like to recover ${}_{(0)}\zeta_{ud}$ instead of ${}_{(0)}\zeta_c$, we should solve the continuity equation of the local patch i.e.

$$
\frac{d\rho_l}{dt_l} = -3H_l\left(\rho_l + p_l\right) \tag{2.220}
$$

This continuity equation (2.220) can be easily obtained from (2.205) and (2.206) taking into account that the pressure p and the energy density ρ of the local field take the same form as its unperturbed values i.e. the same form as in (2.3). The solution of (2.220) can in principle be written as

$$
\rho_l = \rho_l(N_l, \rho^0(\mathbf{x}))\,, \tag{2.221}
$$

where there is only one initial value because (2.220) is a first order differential equation. We can now follow the same procedure and get the uniform density curvature perturbation using the δN formalism but this time giving perturbed initial values to the energy density rather than to the field.

Based on the results above, it seems that the δN formalism is a very powerful tool to compute the curvature perturbation in a non-perturbative way using only the local equations of motion, however there are some aspects that must be taken into account when claiming that the δN formalism is a non-perturbative method:

- We have indicated above that, by consistency, if we ignore decaying terms like $\partial_{-}, (0)\beta^i$ when constructing the δN formalism in section 2.4, we must also ignore any other function that decays, such as $\left(\epsilon_1\right)_l$ during USR. However and although the time evolution of $\left(\epsilon_1\right)_l$ will always decay, its initial value will strongly depend on the initial conditions, which are different for each patch. Could we find a patch in which the perturbation of the velocity is so large such that $\left(\epsilon_1\right)_l$ plays an important role in the first stages of the evolution of the patch? The answer is that this is perfectly possible in a fully non-perturbative way where the initial conditions can reach arbitrarily high values, those are of course rare events that happen in the tail of the PDF for initial conditions, however, those are precisely the events of interest for PBH formation as explained in Section (2.2.4).

- Although in the example of this section we have computed the value of the ${}_{(0)}\zeta_c$, this is rather meaningless, being the relevant quantity the PDF of ${}_{(0)}\zeta_c$. Assuming that we know the PDF of the initial conditions, the PDF of ${}_{(0)}\zeta_c$ is trivial to compute:

$$P\left({}_{(0)}\zeta_c\right) = P(\phi_0^f)\frac{d\phi_0^f}{d\,{}_{(0)}\zeta_c} \tag{2.222}$$

  where we have assumed that the only important perturbed initial value is the field (and not the velocity) and where the last derivative is performed by knowing the non-perturbative relation between ϕ_0^f and ${}_{(0)}\zeta_c$ that the δN formalism provides, for example (2.217) in the case of USR.

  From (2.222) it is clear that, in order to know $P\left({}_{(0)}\zeta_c\right)$ it is not enough with knowing the relation between ϕ_0^f and ${}_{(0)}\zeta_c$ given by the δN formalism, we also need some knowledge about the $P(\phi_0^f)$. The approach usually taken in the literature is to assume $P(\phi_0^f)$ to be gaussian [162, 103, 163], however, we have already seen in section 2.2.4 that any higher order in cosmological perturbation theory effect introduces non-Gaussianities. The assumption of Gaussianity for $P(\phi_0^f)$ automatically implies that the initial values are given in the context of linear perturbation theory.

From the two points aroused above we can extract a very important conclusion: the δN formalism (at least the one that we presented here) is not able to describe the curvature perturbation generated by non-perturbative initial conditons, failing then to describe large enough values for ${}_{(0)}\zeta_c$ which are very deep in the tail of the PDF(let us say ${}_{(0)}\zeta_c \sim 1$). In this sense we will say that, although the δN formalism is non-linear, in the sense that it can include efects of order $\delta\phi, \delta\phi^2, \delta\phi^3, ...$ (where $\delta\phi$ is small enough) in the expression for ${}_{(0)}\zeta_c$, it fails to describe fully non-perturbative effects.

In the next section we will present an attempt to include non-perturbative effects in the PDF of $\delta\phi$, the stochastic approach to inflation.

2.5 Stochastic approach to inflation.

Firstly introduced by Starobinsky [164] , the hope of the stochastic approach to inflation is that it incorporates quantum corrections to the inflationary dynamics in a non-perturbative way. This approach combines the two approximations schemes presented until now to study the evolution of inhomogeneities in a non-perturbative way. The idea is to split the variables of interest (let us say X) into two parts: an infrared (IR) part that contains all the inhomogeneities with characteristic wavelength larger that some coarse-grained scale $(\sigma H)^{-1}$ (σ is the same parameter as the one used in gradient expansion) and a ultraviolet (UV) part, which encompasses inhomogeneities with characteristic scale smaller than $(\sigma H)^{-1}$ (or characteristic wavenumber k bigger than $\sigma a H$). The success of the stochastic formalism resides on the fact that, as we will see later on, it allows to reduce a quantum problem into a statistical one.

Since the UV part starts evolving well inside the coarse grained scale defined by $(\sigma H)^{-1}$, we will assume that the perturbations did not have enough time to grow enough such that they are still perturbatively small. Thus, one can use linear perturbation theory to describe it, where initial conditions are well defined. The IR part instead can be large, however, since the IR part only contains long wavelengths, the leading order in gradient expansion can be used there. As we will see, whenever an UV mode exits the coarse-grained scale, it will act as a kick for the IR part, solving the initial condition problem of gradient expansion and constantly modifying the background evolution of the local patch.

The stochastic formalism is then a mathematical framework that, in principle, allow us to study the inhomogeneities generated during inflation in a non-perturbative way, reason why it is widely used when studying PBHs formation (see for example [165, 166] among others). To see how stochastic inflation works and why it is called "stochastic" we will derive the formalism step by step.

Since the stochastic formalism uses gradient expansion for the IR part, it should be already clear now that we will have different stochastic equations depending on if we are using the naive leading order in gradient expansion of section 2.3.1 or the more precise gradient expansion or 2.3.3. The stochastic formalism that uses the naive leading order in gradient expansion is the most widely used in the literature [164, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 166, 185, 186, 187] so we will start with its derivation. After that, we will take advantage of the stochastic equations just derived to present a stochastic formalism based on the gradient expansion of section (2.3.3) [94].

Before starting with the derivation let us empathize the gauge that we will use: the uniform-N gauge. The perturbative definition of this gauge has been already presented in section (2.2.1) and it correspond to the following choice for the perturbative parameters

$$D_{uN} = 0\,, \qquad B_{uN} = 0\,. \tag{2.223}$$

The choice (2.223) can be promoted to a choice of non-perturbative quantities at leading order in gradient expansion. Focusing only on the scalar part we would have

$${}_{(0)}\zeta_{uN} = 0\,, \qquad \beta^i_{uN} = 0\,. \tag{2.224}$$

2.5.1 Stochastic approach based on the naive leading order in gradient expansion.

As we have already indicated, this is the stochastic formalism most widely used in the literature due to its simplicity. However, as one can guess, the stochastic formalism presented in this section will have a limited range of validity [188], the reason is that it is based on the naive leading order in gradient expansion, which, as seen in section 2.3.1, fails to exactly reproduce the long-wavelength limit of perturbation theory. At the end of this section we will talk more about the range of validity of this naive stochastic formalism.

First of all, it is very important to realize that in the naive leading order in gradient expansion, both the uniform-N gauge and the spatially flat gauge are equivalent, which leads to many authors to use the uniform-N gauge for the IR part and the spatially flat gauge for the UV part [95]. Let us see why: from the definition of the MS variable (2.53) we have

$$Q = \delta\phi_f = \delta\phi_{ud} - \frac{1}{3}\nabla^2 E_{ud}\,. \tag{2.225}$$

As shown in section 2.3.1, in the naive separate universe approach we always neglect any term that comes with a spatial derivative so in this case we have

$$Q^{gr} = \delta\phi_f^{gr} = \delta\phi_{ud}^{gr} \tag{2.226}$$

The main consequence of (2.226) is that, under the naive leading order in gradient expansion, we can express all the scalar fluctuations only in terms of the field inhomogeneities not only in the spatially flat gauge, but also in the uniform-N gauge. For non-linear generalizations of this variables see [189, 190].

In the same way we can easily check that if we apply the order estimation of (2.147), together with the condition ${}_{(0)}\zeta_{uN} = {}_{(0)}\zeta_f = 0$, to the all the ADM equations, the only two relevant equations are:

$$\left(\frac{\bar{H}}{{}_{(0)}\alpha_{uN}}\right)^2 = \frac{1}{3M_{PL}^2}\left(\frac{{}_{(0)}\dot{\phi}_{uN}^2}{2\,{}_{(0)}\alpha_{uN}^2} + V\left({}_{(0)}\phi_{uN}\right)\right)\,, \tag{2.227}$$

$$\frac{1}{{}_{(0)}\alpha_{uN}}\frac{d}{dt}\left(\frac{\bar{H}}{{}_{(0)}\alpha_{uN}}\right) + \left(\frac{\bar{H}}{{}_{(0)}\alpha_{uN}}\right)^2 = -\frac{1}{3M_{PL}^2}\left(\frac{{}_{(0)}\dot{\phi}_{uN}^2}{{}_{(0)}\alpha_{uN}^2} - V\left({}_{(0)}\phi_{uN}\right)\right)\,, \tag{2.228}$$

which are the same for the flat and the uniform-N gauge.

Before continuing, let us remind the reader that the equivalence between these two gauges in only valid if we neglect all the spatial gradient, which, as seen in section

2.4.1, it generically fails at $\mathcal{O}(\epsilon_1)$.

We will now properly start with the derivation of the stochastic formalism, during this section, and although it is not compulsory, we will work using the number of e-folds $N \equiv \int \bar{H} dt$ as time variable[10]. Another important aspect is that, in order not to overload notation, we will suppress the subscript uN indicating the gauge we are using, such that in the following, unless otherwise stated, a variable without a subscript that indicates the gauge is a variable in the uniform-N gauge.

The stochastic formalism presented in this subsection is based on the naive leading order in gradient expansion for the IR part and on linear perturbation theory for the UV part. To illustrate this we will consider in detail the equation of motion for the trace the extrinsic curvature (2.23) in uniform-N gauge, which can be written using the variables of the ADM metric (1.23) as:

$$-3\frac{\bar{H}}{\alpha}\frac{\partial}{\partial N}\left(\frac{\bar{H}}{\alpha}\right)-\left(\frac{\bar{H}}{2\alpha}\right)^2\frac{\partial\tilde{\gamma}_{ij}}{\partial N}\frac{\partial\tilde{\gamma}^{ij}}{\partial N}-3\left(\frac{\bar{H}}{\alpha}\right)^2+D_kD^k\alpha-\frac{1}{M_{PL}^2}\left(\left(\frac{\bar{H}}{\alpha}\right)^2\left(\frac{\partial\phi}{\partial N}\right)^2-V(\phi)\right)=0\,. \tag{2.229}$$

Note that (2.229) is an exact equation in the uniform-N gauge. We will now apply the approximations mentioned above.

The first thing to do is to split the variables of interest into their IR and UV part. In this case we only have two variables to split:

$$\begin{aligned}\alpha &= \alpha^{IR} + \alpha^{UV}\,,\\ \phi &= \phi^{IR} + \phi^{UV}\,.\end{aligned} \tag{2.230}$$

Note that in (2.230) we are not considering $\frac{\partial\tilde{\gamma}_{ij}}{\partial N}$ as a variable of interest not only because $\tilde{\gamma}_{ij} = \delta_{ij}$ in at leading order in naive gradient expansion, but also because $\frac{\partial\tilde{\gamma}_{ij}}{\partial N}\frac{\partial\tilde{\gamma}^{ij}}{\partial N} \sim \mathcal{O}(\sigma^2)$ in gradient expansion and quadratic in perturbation theory so it does not play any role even if we were using the more precise formulation of gradient expansion.

Due to the perturbative nature of the UV variables, we will expand (2.229) keeping

[10]Note that we can use any time variable we want because we will use the coordinates of a fictitious global background, i.e. the coordinates of (2.265). If we would instead use local coordinates (as in (2.143)), we would be interested in using an unperturbed time variable, being N the natural choice in the uniform-N gauge.

only linear terms in UV and isolate them in the right hand side of the equation getting[11]

$$
\begin{aligned}
&-3\frac{\bar{H}}{\alpha^{IR}}\frac{\partial}{\partial N}\left(\frac{\bar{H}}{\alpha^{IR}}\right)-3\left(\frac{\bar{H}}{\alpha^{IR}}\right)^{2}+D^{k}D_{k}\alpha^{IR}-\frac{1}{M_{PL}^{2}}\left(\left(\frac{\bar{H}}{\alpha^{IR}}\right)^{2}\left(\frac{\partial\phi^{IR}}{\partial N}\right)^{2}-V\left(\phi^{IR}\right)\right)\\
&=-3\frac{\bar{H}^{2}}{\left(\alpha^{IR}\right)^{3}}\frac{\partial\alpha^{UV}}{\partial N}+\left(\frac{9\bar{H}^{2}}{\left(\alpha^{IR}\right)^{4}}\frac{\partial\alpha^{IR}}{\partial N}-\frac{6\bar{H}}{\left(\alpha^{IR}\right)^{3}}\left(\frac{\partial\bar{H}}{\partial N}\right)\right)\alpha^{UV}-\frac{6\bar{H}^{2}}{\left(\alpha^{IR}\right)^{3}}\alpha^{UV}-\frac{\nabla^{2}}{a^{2}}\alpha^{UV}\\
&+\frac{1}{M_{PL}^{2}}\left[2\left(\frac{\bar{H}}{\alpha^{IR}}\right)^{2}\frac{\partial\phi^{IR}}{\partial N}\frac{\partial\phi^{UV}}{\partial N}-2\frac{\bar{H}^{2}}{\left(\alpha^{IR}\right)^{3}}\left(\frac{\partial\phi^{IR}}{\partial N}\right)^{2}\alpha^{UV}-V_{\phi}\left(\phi^{IR}\right)\phi^{UV}\right].
\end{aligned}
\tag{2.231}
$$

Now, since the IR variables are well outside the Hubble horizon, we will use the naive leading order in gradient expansion for them for them so $\alpha^{IR} = {}_{(0)}\alpha^{IR}$ and $\phi^{IR} = {}_{(0)}\phi^{IR}$. Since $\alpha^{IR} \sim \mathcal{O}(\sigma^0)$ and hence $D_k D^k \alpha^{IR} \sim \mathcal{O}(\sigma^2)$ we have:

$$
\begin{aligned}
&-3\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\frac{\partial}{\partial N}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)-3\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^{2}-\frac{1}{M_{PL}^{2}}\left(\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^{2}\left(\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\right)^{2}-V\left({}_{(0)}\phi^{IR}\right)\right)\\
&=-3\frac{\left(\bar{H}\right)^{2}}{\left({}_{(0)}\alpha^{IR}\right)^{3}}\frac{\partial\alpha^{UV}}{\partial N}+\left(\frac{9\left(\bar{H}\right)^{2}}{\left({}_{(0)}\alpha^{IR}\right)^{4}}\frac{\partial\,{}_{(0)}\alpha^{IR}}{\partial N}-\frac{6\bar{H}}{\left({}_{(0)}\alpha^{IR}\right)^{3}}\left(\frac{\partial\bar{H}}{\partial N}\right)\right)\alpha^{UV}-\frac{6\bar{H}^{2}}{\left({}_{(0)}\alpha^{IR}\right)^{3}}\alpha^{UV}\\
&-\frac{\nabla^{2}}{a^{2}}\alpha^{UV}+\frac{1}{M_{PL}^{2}}\left[2\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^{2}\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\frac{\partial\phi^{UV}}{\partial N}-2\frac{\bar{H}^{2}}{\left({}_{(0)}\alpha^{IR}\right)^{3}}\left(\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\right)^{2}\alpha^{UV}-V_{\phi}\left({}_{(0)}\phi^{IR}\right)\phi^{UV}\right].
\end{aligned}
\tag{2.232}
$$

where the left-hand side coincides with the naive leading order in gradient expansion expression of (2.228), as expected.

The schematic decomposition of (2.230) is effectively done in Fourier space, where the splitting into IR ($k > \sigma a_l H_l$) and UV ($k < \sigma a_l H_l$) is more explicit. We will then introduce a window function in Fourier space, the most common choice for the window function is simply the Heaviside theta which, as we will see later on, lead to white noises in the final stochastic system.

It is also fair to mention that the choice of the Heaviside theta as the window function present an important problem: the real-space smoothing window function associated with the sharp Heaviside theta cutoff in Fourier space decays too slow at large distances, which translates into the fact that the noises correlators at large spatial separations are not independent on the choice of the window function [191]. In this thesis we will avoid this problem by computing correlators always at the same space point. Furthermore, the choice of a more realistic window function would lead to coloured noises, for which the stochastic system is very difficult to solve, both numerically and analytically.

[11]Note that this is the same as we did in linear perturbation theory of section 2.2 but using the ADM metric of (1.23) as a background metric.

We have the following decomposition for a generic function X.

$$X^{IR}(N,\mathbf{x}) \equiv \int \frac{d\mathbf{k}}{(2\pi)^3}\Theta\left(\sigma a_l(N)H_l(N)-k\right)\hat{\mathcal{X}}^{IR}_{\mathbf{k}}(N,\mathbf{x}),$$
$$X^{UV}(N,\mathbf{x}) \equiv \int \frac{d\mathbf{k}}{(2\pi)^3}\Theta\left(k-\sigma a_l(N)H_l(N)\right)\hat{\mathcal{X}}^{UV}_{\mathbf{k}}(N,\mathbf{x}), \tag{2.233}$$

where, similarly as in linear perturbation theory (see (2.80)),$\mathcal{X}^{UV}_{\mathbf{k}}(t,\mathbf{x})$ is define as the following hermitian operator:

$$\hat{\mathcal{X}}^{UV}_{\mathbf{k}}(N,\mathbf{x}) = X_{\mathbf{k}}(N)\hat{a}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}} + X^{\star}_{\mathbf{k}}(N)\hat{a}^{\dagger}_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{2.234}$$

where $X_{\mathbf{k}}(N)$ is the solution of the evolution equation for the perturbation X over the local background defined by (2.265) and $a_{\mathbf{k}}$ and $a^{\dagger}_{\mathbf{k}}$ are the usual creation and annihilation operators which follow the commutation relation given in (2.81).

Note that, in the spirit of gradient expansion, the splitting is done in the local cosmological coarse-grained scale $(\sigma H_l)^{-1}$, which generically differs form the one of the background, for example in uniform-N gauge we have $H_l = \frac{H^b}{{}_{(0)}\alpha^{IR}}$.

Inserting the definition of X^{UV} of (2.233) into (2.232) we get:

$$\begin{aligned}
&-3\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\frac{\partial}{\partial N}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)-3\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2-\frac{1}{M^2_{PL}}\left(\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2\left(\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\right)^2-V\left({}_{(0)}\phi^{IR}\right)\right)\\
&=3\frac{\bar{H}^2}{\left({}_{(0)}\alpha^{IR}\right)^3}\frac{\partial}{\partial N}\left(\sigma a\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)\int\frac{d\mathbf{k}}{(2\pi)^{3/2}}\delta\left(k-\sigma a\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)\boldsymbol{\alpha}^{UV}_{\mathbf{k}}\\
&-\frac{2}{M^2_{PL}}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\frac{\partial}{\partial N}\left(\sigma a\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)\int\frac{d\mathbf{k}}{(2\pi)^{3/2}}\delta\left(k-\sigma a\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)\varphi^{UV}_{\mathbf{k}}\\
&+\int\frac{d\mathbf{k}}{(2\pi)^{3/2}}\Theta\left(k-\sigma a\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)\Bigg\{-3\frac{\bar{H}^2}{\left({}_{(0)}\alpha^{IR}\right)^3}\frac{\partial\boldsymbol{\alpha}^{UV}_{\mathbf{k}}}{\partial N}\\
&+\left(\frac{9\bar{H}^2}{\left({}_{(0)}\alpha^{IR}\right)^4}\frac{\partial\,{}_{(0)}\alpha^{IR}}{\partial N}-\frac{6\bar{H}}{\left({}_{(0)}\alpha^{IR}\right)^3}\left(\frac{\partial\bar{H}}{\partial N}\right)\right)\boldsymbol{\alpha}^{UV}_{\mathbf{k}}-\frac{6\bar{H}^2}{\left({}_{(0)}\alpha^{IR}\right)^3}\boldsymbol{\alpha}^{UV}_{\mathbf{k}}+\frac{k^2}{a^2}\boldsymbol{\alpha}^{UV}_{\mathbf{k}}\\
&\frac{1}{M^2_{PL}}\left[2\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\frac{\partial\varphi^{UV}_{\mathbf{k}}}{\partial N}-\frac{2\bar{H}^2}{\left({}_{(0)}\alpha^{IR}\right)^3}\left(\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\right)^2\boldsymbol{\alpha}^{UV}_{\mathbf{k}}-V_{\phi}\left({}_{(0)}\phi^{IR}\right)\varphi^{UV}_{\mathbf{k}}\right]\Bigg\},
\end{aligned} \tag{2.235}$$

where $\boldsymbol{\alpha}^{UV}_{\mathbf{k}}$ and $\varphi^{UV}_{\mathbf{k}}$ are operators defined as in (2.234).

The right-hand side of (2.235) has two different terms:

1. The second integral (terms multiplying the Heaviside theta) is the evolution equation for the extrinsic curvature linearized over a local FLRW patch defined by ${}_{(0)}\alpha^{IR}$ and ${}_{(0)}\phi^{IR}$. Once the Bunch-Davies vacuum is chosen for that patch, this term can be consistently set to zero. Note that the solution of this term, when

combined with all the terms proportional to the Heaviside theta in the rest of the ADM equations, is precisely what give us the functions $X_{\mathbf{k}}$ in (2.234).

2. The first two integrals, proportional to a Dirac delta, can be seen as boundary conditions and hence they will act as the initial conditions missing when using only gradient expansion.

We then get:

$$
\begin{aligned}
&-3\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\frac{\partial}{\partial N}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)-3\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2-\frac{1}{M_{PL}^2}\left(\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2\left(\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\right)^2-V\left({}_{(0)}\phi^{IR}\right)\right)\\
&=-3\frac{\bar{H}^2}{\left({}_{(0)}\alpha^{IR}\right)^3}\xi_3+\frac{2}{M_{PL}^2}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\xi_1\,, \qquad (2.236)
\end{aligned}
$$

where we have defined ξ_1 and ξ_3 as:

$$
\begin{aligned}
\xi_1 &\equiv -\frac{\partial}{\partial N}\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)\int\frac{d\mathbf{k}}{(2\pi)^{3/2}}\delta\left(k-\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)\varphi_{\mathbf{k}}^{UV}\,,\\
\xi_3 &\equiv -\frac{\partial}{\partial N}\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)\int\frac{d\mathbf{k}}{(2\pi)^{3/2}}\delta\left(k-\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)\boldsymbol{\alpha}_{\mathbf{k}}^{UV}\,. \qquad (2.237)
\end{aligned}
$$

Note that $\varphi_{\mathbf{k}}^{UV}$ and $\boldsymbol{\alpha}_{\mathbf{k}}^{UV}$ are computed in the flat or uniform-N gauge, which in this approximation are interchangeable.

We will characterize and give a the physical interpretation to the quantities ξ_1 and ξ_3 but for the moment let us focus on the construction of the stochastic system.

If we now follow the same procedure explained above with the Hamiltonian constraint we get:

$$
6\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2-\frac{2}{M_{PL}^2}\left[\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2\left(\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\right)^2+V\left({}_{(0)}\phi^{IR}\right)\right]=\frac{2}{M_{PL}^2}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\xi_1\,, \qquad (2.238)
$$

which can be solved for $\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2$ i.e.

$$
\left(\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)^2=\frac{V\left({}_{(0)}\phi^{IR}\right)}{3M_{PL}^2-\frac{1}{2}\left(\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\right)^2-\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\xi_1}\,. \qquad (2.239)
$$

Finally, and although it is redundant, it is worthy to write also the stochastic equation of motion for the field, which is obtained in the same way:

$$\frac{\partial^2 {}_{(0)}\phi^{IR}}{\partial N^2} + \left(3 + \frac{\frac{\partial}{\partial N}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)}{\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}}\right)\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N} + \frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)^2}$$

$$= -\frac{\partial \xi_1}{\partial N} - \xi_2 - \left(3 + \frac{\frac{\partial}{\partial N}\left(\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)}{\frac{\bar{H}}{{}_{(0)}\alpha^{IR}}}\right)\xi_1 + \frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N}\frac{\xi_3}{{}_{(0)}\alpha^{IR}}\,, \tag{2.240}$$

where ξ_2 is defined similarly to ξ_1 and ξ_3:

$$\xi_2 \equiv -\frac{\partial}{\partial N}\left(\sigma a \frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)\int \frac{d\mathbf{k}}{(2\pi)^{3/2}}\delta\left(k - \sigma a \frac{\bar{H}}{{}_{(0)}\alpha^{IR}}\right)\frac{\partial \varphi^{UV}_{\mathbf{k}}}{\partial N}\,. \tag{2.241}$$

As anticipated before, the usage of the uniform-N gauge and the naive leading order in gradient expansion ensures that all the scalar inhomogeneities are encoded in the scalar field. This becomes clearer once we realize that we can write the system (2.236)-(2.240) in terms only of the scalar field. Inserting (2.236) and (2.239) into (2.240) and neglecting ξ_i^2 terms because they are quadratic in perturbation theory we get:

$$\frac{\partial^2 {}_{(0)}\phi^{IR}}{\partial N^2} + \left(3 - \frac{1}{2M_{PL}^2}\left(\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N}\right)^2\right)\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N} + \left(3M_{PL}^2 - \frac{1}{2}\left(\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N}\right)^2\right)\frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)}$$
$$-\frac{\partial \xi_1}{\partial N} - \xi_2 - \left[3 - \frac{1}{2M_{PL}^2}\left(\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N}\right)^2 - \frac{1}{M_{PL}^2}\left(\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N}\right)^2 - \frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)}\left(\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N}\right)\right]\xi_1\,, \tag{2.242}$$

which can be conveniently written if we use an auxiliary variable ${}_{(0)}\pi^{IR}$:

$${}_{(0)}\pi^{IR} = \frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N} + \xi_1\,,$$
$$\frac{\partial\, {}_{(0)}\pi^{IR}}{\partial N} + \left(3 - \frac{\left({}_{(0)}\pi^{IR}\right)^2}{2M_{PL}^2}\right){}_{(0)}\pi^{IR} + M_{PL}^2\left(3 - \frac{\left({}_{(0)}\pi^{IR}\right)^2}{2M_{PL}^2}\right)\frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)} = -\xi_2\,. \tag{2.243}$$

The system of (2.243) is the stochastic system most widely used in the literature. However, and in the same way as the naive leading order gradient expansion in which (2.243) is based on, it contains an important limitation: it neglects terms with spatial derivatives that do not vanish in the $k \to 0$ limit. The consequences of neglecting these terms are not as dramatic as what we showed in section (2.2.1.3) because in this case these terms are never multiplied by a growing function so they always decay, however, it is important to keep the stochastic formalism consistent with this fact, which is not always easy, specially when dealing with numerical solutions, where the decaying terms are usually hidden in the solution.

A conservative guess to keep the formalism within its regime of validity would be to neglect all the terms proportional to ${}_{(0)}\epsilon_1^{IR} \equiv \frac{\left({}_{(0)}\pi^{IR}\right)^2}{2M_{PL}^2}$, because in regimes beyond SR, these terms are time dependent and can actually be of the same order of the neglected terms. In this case the stochastic system would be:

$$\begin{aligned} {}_{(0)}\pi^{IR} &= \frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N} + \xi_1\,, \\ \frac{\partial\, {}_{(0)}\pi^{IR}}{\partial N} + 3\, {}_{(0)}\pi^{IR} + 3M_{PL}^2 \frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)} &= -\xi_2\,. \end{aligned} \tag{2.244}$$

Neglecting terms proportional to ${}_{(0)}\epsilon_1^{IR}$ could seem like a good approximation. However, as already justified at the end of section 2.4.1, this approximation actually neglects possible important non-perturbative effects. Furthermore, even in the case in which we restrict ourselves to the perturbative regime, we can have non-negligible ϵ_1 effects, for example during a transition between SR and USR (further studied in appendix A), where ϵ_1 has to grow enough such that the field can overcome the flat part of the potential. For those reasons, if we want to formulate a stochastic formalism able to consistently take care of non-perturbative effects, we must formulate a stochastic formalism based on the correct leading order in gradient expansion of section (2.3.3).

2.5.2 Stochastic formalism valid at all orders in SR parameters.

As claimed above, the naive leading order in gradient expansion of section 2.3.1 generically fails to give the correct long-wavelength evolution of the inhomogeneities at $\mathcal{O}(\epsilon_1)$. On the other hand, the correct gradient expansion of section 2.3.3 solves this problem by including both terms with spatial derivatives and the momentum constraint, this is why in this section we will construct a stochastic formalism based on the correct gradient expansion.

First of all, it is important to remark that some of the affirmations we did about the uniform-N gauge at the beginning of section (2.5.1) are no longer correct, more concretely, we cannot longer study the scalar inhomogeneities in terms solely of the inflaton field. This is clear form linear perturbation theory where the MS variable can be written as in (2.225). If we insist on using the uniform-N gauge we must also take into account the contribution from E when studying scalar perturbations.

We could also use spatially flat gauge in this case and forget about E, however, in this case we should take into account all the terms proportional to $\left({}_{(0)}\beta_f\right)^i$ that appear for example in (2.183), this is why we will keep using the uniform-N gauge, where

$\beta^i_{uN} = 0$.

One can easily check that the stochastic equations for the evolution of the extrinsic curvature (2.236), for the Hamiltonian constraint (2.239) and for the evolution of the field (2.240) do not change when including E and hence the stochastic system is still the one given by (2.243). The only difference is given by the inclusion of the momentum constraint (1.22), which, in uniform-N gauge can be written as:

$$D^j \left(-\frac{H^b}{2\alpha} \frac{\partial \tilde{\gamma}_{ij}}{\partial N} \right) - \frac{2}{3} D_i K = -\frac{1}{M_{PL}^2 \alpha} \frac{\partial \phi}{\partial N} \partial_i \phi \,, \tag{2.245}$$

where we have used the evolution equation for $\tilde{\gamma}_{ij}$ (2.22) to eliminate $\tilde{A}_{ij}$. Splitting (2.245) into IR and UV and using the decomposition of $\tilde{\gamma}_{ij}$ explained around (2.181) to keep only $\mathcal{O}(\sigma)$ terms in the IR part (remember that the $\mathcal{O}(\sigma^0)$ information from the momentum constraint can only be extracted if we write the momentum constraint up to $\mathcal{O}(\sigma)$), we can write the stochastic equation for the momentum constraint:

$$_{(0)}\partial_i \left(\frac{\partial}{\partial N} \left(\frac{1}{3} \nabla^2 C^{IR} \right) \right) - \frac{_{(0)}\partial_i \alpha^{IR}}{_{(0)}\alpha^{IR}} + \frac{\partial \, _{(0)}\phi^{IR}}{\partial N} \frac{_{(0)}\partial_i \phi}{2M_{PL}^2} = -\partial_i \xi_4 \,, \tag{2.246}$$

where ξ_4 is defined similarly to ξ_1, ξ_2 and ξ_3 i.e.

$$\xi_2 \equiv -\frac{\partial}{\partial N} \left(\sigma a \frac{H^b}{_{(0)}\alpha^{IR}} \right) \int \frac{d\mathbf{k}}{(2\pi)^{3/2}} \delta \left(k - \sigma a \frac{H^b}{_{(0)}\alpha^{IR}} \right) \left(-\frac{k^2}{3} \mathcal{C}^{UV}_{\mathbf{k}} \right) \,. \tag{2.247}$$

With the addition of the stochastic equation (2.246) to the system of (2.243) obtained before, we have a stochastic formalism able to describe the non-linear evolution of scalar inhomogeneities at all orders in SR parameters and, in principle, in a non-perturbative way.

However, it is not all good news: firstly, since the construction of the gradient expansion in section 2.3, we have been neglecting possible interactions scalar-tensor or scalar-vector, reason why the stochastic formalism constructed here will not take these interactions into account either. Secondly, we do not exactly know how to extract the $\mathcal{O}(\sigma^0)$ information form (2.246) in a fully non linear way. Finally, we do not know which is the combination of $_{(0)}\phi^{IR}$ and $\nabla^2 C^{IR}$ that give us the correct and non-perturbative and gauge invariant quantity that describe scalar inhomogeneities i.e. we do not have a non-linear generalization of the MS variable[12]. The first issue is beyond the scope

[12] A non-linear gauge invariant variable at leading order in terms of the quantities of metric (2.146) in gradient expansion has been defined in [189, 190] as:

$$\partial_i Q^{NL} \equiv \partial_i \phi + \frac{1}{\alpha} \frac{\partial \phi}{\partial N} \partial_i \zeta$$

However, the variable above does not include the term proportional to $\nabla^2 E$ in its linearization. Reason of this thesis, but the second and third ones can be solved, at least approximately, by imposing that both the momentum constraint and the non-linear generalization of the MS variable match their linear counterpart when the global background is subtracted. In this way, the $\mathcal{O}(\sigma^0)$ information of (2.246) can be straightforwardly extracted and the whole system of stochastic equations based on the correct gradient expansion of section 2.3.3 and hence valid at all orders in SR parameters is:

$$\begin{aligned}
&{}_{(0)}\pi^{IR} = \frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N} + \xi_1\,,\\
&\frac{\partial\,{}_{(0)}\pi^{IR}}{\partial N} + \left(3 - \frac{\left({}_{(0)}\pi^{IR}\right)^2}{2M_{PL}^2}\right){}_{(0)}\pi^{IR} + \left(3M_{PL}^2 - \frac{\left({}_{(0)}\pi^{IR}\right)^2}{2}\right)\frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)} = -\xi_2\,,\\
&\frac{\partial}{\partial N}\left(\frac{1}{3}\,{}_{(0)}\nabla^2 C^{IR}\right) - \left(H^b\sqrt{\frac{3M_{PL}^2 - \frac{\left({}_{(0)}\pi^{IR}\right)^2}{2}}{V\left({}_{(0)}\phi^{IR}\right)}} - 1\right) + \frac{1}{2_{PL}^2}\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\left({}_{(0)}\phi^{IR} - \phi^b\right) = -\xi_4\,,
\end{aligned} \tag{2.248}$$

where we have used the Hamiltonian constraint to eliminate ${}_{(0)}\alpha^{IR}$ in the last equation. Note that ξ_1,ξ_2 and ξ_4 are constructed in the uniform-N gauge, which is no longer equivalent to the spatially flat gauge[13].

Finally, as suggested in [193, 194, 195], we can define the non-linear counterpart of the MS variable of (2.53) at leading order in gradient expansion as:

$$Q^{IR} = {}_{(0)}\phi^{IR} - \phi^b - \frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N}\frac{1}{3}\,{}_{(0)}\nabla^2 C^{IR}\,, \tag{2.249}$$

where we remind the reader that ${}_{(0)}\phi^{IR}$ and ${}_{(0)}\nabla^2 C^{IR}$ are both in the uniform N gauge.

2.5.3 Characterization of the noises

The interpretation of ξ_1, ξ_2 and ξ_4 in (2.248) as classical noises is not trivial because they are, strictly speaking, quantum operators. In order to see how they are effectively classical, we can compute the two-point correlation function of ξ_1 for example at equal space point, the result is:

---

why this variable can be only interpreted as a non-linear generalization of Q^{gr} in (2.226).

[13]To see the gauge transformation between spatially flat and uniform-N gauges in linear theory one can see [95] , where it is claimed that the differences between those two gauges is always of higher order in gradient expansion, however, this conclusion is reached by considering the value of ϵ_1 at horizon crossing (ϵ_1^* there) to be constant with k, which is generically not a good approximation beyond SR. In fact in [192] it is shown numerically that the difference between $\delta\phi_f$ and $\delta\phi_{\delta N}$ can be $\mathcal{O}(\epsilon_1)$ in regimes of interest for PBH formation, in agreement with the differences between the naive and the correct gradient expansion remarked in this thesis.

$$\langle 0 \left| \xi_1(N_1)\xi_1(N_2) \right| 0 \rangle = \frac{1}{2\pi^2}\frac{\partial}{\partial N}\left(\sigma a \frac{H^b}{{}_{(0)}\alpha^{IR}}\right)\left(\sigma a \frac{H^b}{{}_{(0)}\alpha^{IR}}\right)^2 \left| \delta\phi(N_1)_{k=\left(\sigma a \frac{H^b}{{}_{(0)}\alpha^{IR}}\right)} \right|^2 \delta\left(N_1 - N_2\right) , \tag{2.250}$$

where we have used a similar procedure as when defining the scalar power spectrum in (2.92), with the only difference that the existence of a Dirac delta function in ξ_1 allow us to perform the integral in k.

From (2.250) we see that $\delta\phi_{\mathbf{k}}$, which is the solution for the field perturbation over the local patch of size $\left(\sigma a \frac{H^b}{{}_{(0)}\alpha^{IR}}\right)^{-1}$, is evaluated at the coarse-grained scale , i.e. well outside the Hubble horizon. It can then be shown that at those scales, any perturbation that started from a coherent vacuum state has evolved into a highly squeezed state [196, 197] , which means that we can consider $\left| \delta\phi(N)_{k=\left(\sigma a \frac{H^b}{{}_{(0)}\alpha^{IR}}\right)} \right|^2$ as the power spectrum of a classical random variable, whose time evolution is consistent with probabilities conserved along classical trajectories. One way to check that this statement is true is simply to compute the following quantity:

$$r_k \equiv \left(\delta\phi_k \left(\frac{\partial \delta\phi_k}{\partial N}\right)^\star - \delta\phi_k^\star \frac{\partial \delta\phi_k}{\partial N}\right)_{k=\left(\sigma a \frac{H^b}{{}_{(0)}\alpha^{IR}}\right)} \tag{2.251}$$

At sub-Hubble scales, where the quantum nature of the field is important, r_k is given by (2.82). On the other hand, it can be shown that at super-Hubble scales $r_k \to 0$, meaning that the field can now be described as a classical (but probabilistic) variable.

Once this is clarified, we are now in position to describe ξ_1 as a classical white noise[14] with variance given in (2.250). Furthermore, since the field fluctuations are Gaussian to a good level of approximation, the variance computed in (2.250) is enough to fully characterize ξ_1.

Finally, in order to characterize the system (2.243) we also need:

[14]Its "white" nature is due to the presence of $\delta\left(N_1 - N_2\right)$ in the two-point correlator. Note that this is a consequence of the the choice of the Heaviside theta function as Window function, any other choice would lead to coloured noises, which are much more difficult to deal with, both analytically and numerically

$$
\begin{aligned}
&\langle 0\left|\xi_1(N_1)\xi_2(N_2)\right|0\rangle = \langle 0\left|\xi_2(N_1)\xi_1(N_2)\right|0\rangle^* = \\
&\frac{1}{2\pi^2}\frac{\partial}{\partial N}\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)^2\left(\delta\phi(N_1)_{k=\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)}\frac{\partial\delta\phi^*(N_1)_{k=\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)}}{\partial N}\right)\delta\left(N_1-N_2\right)\,, \\
&\langle 0\left|\xi_2(N_1)\xi_2(N_2)\right|0\rangle = \frac{1}{2\pi^2}\frac{\partial}{\partial N}\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)^2\left|\frac{\partial\delta\phi(N_1)_{k=\left(\sigma a\frac{H^b}{{}_{(0)}\alpha^{IR}}\right)}}{\partial N}\right|^2\delta\left(N_1-N_2\right)\,,
\end{aligned}
\tag{2.252}
$$

and similarly with the noise ξ_4

The characterization of ξ_1, ξ_2 and ξ_4 as white noises give us now a intuitive picture of the physics behind the stochastic formalism. As explained before, different functions for ${}_{(0)}C^{IR}$ and ${}_{(0)}\phi^{IR}$ (in uniform-N gauge) describe the evolution of different FLRW patches, the way of getting these different functions is now clear if we see ξ_1, ξ_2 and ξ_4 as random variables. For example, the evolution of a specific patch, let us call it ${}^1FLRW$, will be given by ${}^{1}_{(0)}C^{IR}$ and ${}^{1}_{(0)}\phi^{IR}$, whose specific form will be determined by the random values that the noises ${}^1\xi_1$, ${}^1\xi_2$ and ${}^1\xi_4$ will pick at each time step. Now, if we want to describe a second patch ${}^2FLRW$, we just have to solve again the stochastic equation with different random values for the noises ${}^2\xi_1$, ${}^2\xi_2$ and ${}^2\xi_4$, always satisfying the statistics described by (2.250) and (2.252). Like this, we can describe the evolution of an ensemble of FLRW patches by solving many times the same stochastic equation with different random values for the noises. The correlators between these patches are described by statistical moments of the IR variables.

Once we know how the noise behave (its white nature) and what are the equations of motion for the system ((2.244) or (2.248), depending on the precision we are looking for), the only thing left to fully characterize the system is the computation of the modes function that enter into the noises such as $\delta\phi_k^{UV}$. In order to know these functions, the system we have to solve is given by all the terms proportional to the Heaviside theta that we sent to zero when constructing the stochastic system (see (2.235) and the discussion below), those terms represent the equation of motion of the scalar perturbations over the local background so they take exactly the same form as (2.35)-(2.40) but in local coordinates. These terms can be combined in the same way as in standard linear perturbation theory and obtain a MS equation for Q_k^{UV}:

$$
\frac{\partial^2 Q_k^{UV}}{\partial N_l^2}+\left(3-(\epsilon_1)_l\right)\frac{\partial Q_k^{UV}}{\partial N_l}+\left[\frac{k^2}{H_l^2a_l^2}+\left(-\frac{3}{2}(\epsilon_2)_l+\frac{1}{2}(\epsilon_1)_l(\epsilon_2)_l-\frac{1}{4}(\epsilon_2)_l^2-\frac{1}{2}(\epsilon_2)_l(\epsilon_3)_l\right)\right]Q_k^{UV}=0\,.
\tag{2.253}
$$

Before proceeding, let us remark here that (2.253) is precisely the reason why the stochastic formalism is able, in principle, to include non-perturbative effects. The point is that, although the form of (2.253) is the same as in linear perturbation theory, all the local terms that appear in that equation can be non-perturbatively different from its background value. In this sense, the noises, although they are constructed using linear perturbation theory, can give a cumulative effect to the variables of the local patch that can reach non-perturbative values.

One could think that, because (2.253) is the usual MS equation, we can solve it in the same way as we did in section 2.2.1.1. Unfortunately this is not true, the reason is that all the local quantities that appear in (2.253) are actually stochastic quantities. For example, in uniform-N gauge we have

$$N_l = N\,, \qquad a_l = a\,, \qquad H_l = \frac{\bar{H}}{{}_{(0)}\alpha^{IR}}$$
$$\left(\epsilon_1\right)_l = \frac{\left({}_{(0)}\pi^{IR}\right)^2}{2M_{PL}^2}\,, \quad \left(\epsilon_i\right)_l = \frac{\partial\left(\epsilon_{i-1}\right)_l}{\partial N}\,, \tag{2.254}$$

which means that the functional form of the solution of (2.253) is not the same as the functional form of the usual MS equation (2.266), where all the quantities are deterministic.

2.5.3.1 Approximation for the noises and consequences.

We can clearly see that the local quantities that appear in (2.253) depend on the stochastic IR quantities that of (2.244) or (2.248). We then face a huge problem: In order to characterize the noises we must solve the stochastic system and in order to solve the stochastic system we must characterize the noises. This makes the stochastic system very difficult to handle, both analitically and numerically. Although there are numerical algorithms capable of solving the system exactly[15] [192] , they are generically very computationally expensive so the most reasonable way of facing the problem is via some approximations:

- The first approximation would consist on neglecting all $\mathcal{O}\left(\left(\epsilon_i\right)_l\right)$ terms. This would be equivalent to solve the mode function Q_k^{UV} over an exactly de-Sitter background i.e.
$$\frac{\partial^2 Q_k^{UV}}{\partial N^2} + 3\frac{\partial Q_k^{UV}}{\partial N} + \frac{k^2}{a^2 H_l^2}Q_k^{UV} = 0\,, \tag{2.255}$$

[15] It is true, however, that in [192] , the authors solve numerically the stochastic formalism based on the naive leading order in gradient expansion, so even if the numerical algorithm presented in [192] represents the most accurate solution for stochastic inflation, it can still be improved by its promotion to the system (2.248).

which in terms of the global coordinates would be

$$\frac{\partial^2 Q_k^{UV}}{\partial N^2} + 3\frac{\partial Q_k^{UV}}{\partial N} + \left({}_{(0)}\alpha^{IR}\right)^2 \frac{k^2}{a^2 \bar{H}_0^2} Q_k^{UV} = 0\,, \tag{2.256}$$

where we are setting $\bar{H} = \bar{H}_0$ because we are neglecting ϵ_1 corrections.

The MS equation of (2.256) still depends on the stochastic quantity ${}_{(0)}\alpha^{IR}$, however, its only dependence is in the k-dependent part of the equation, which will be suppressed when we evaluate the solution at $k = \sigma a \frac{\bar{H}}{{}_{(0)}\alpha^{IR}}$, where $\sigma \ll 1$. We can then say that, at least approximately, the long wavelength solution of (2.256) has the same functional form as in the deterministic case (when $\nu = \frac{3}{2}$) (2.218) i.e.

$$Q_k^{UV} \simeq i \frac{\bar{H}_0}{{}_{(0)}\alpha^{IR}\sqrt{2}k^{3/2}}\,. \tag{2.257}$$

Note that equation (2.256) is implicitly assuming that $\nu = \frac{3}{2}$, so this approximation would in principle only be valid for SR and USR, both at leading order in ϵ_1, for which the stochastic formalism of section 2.5.1 is enough. At this level of approximation we also have that the mode function that appear in (2.250) and (2.252) is $(\delta\phi_k)_{uN} = (\delta\phi_k)_f = Q_k^{UV}$, so the variances of the noises can be straightforwardly computed:

$$\langle \xi_1(N_1)\xi_1(N_2)\rangle = \left(\frac{\bar{H}_0}{2\pi}\right)^2 \delta(N_1 - N_2)\,, \tag{2.258}$$

$$\langle \xi_1(N_1)\xi_2^\star(N_2)\rangle = \langle \xi_1^\star(N_1)\xi_2(N_2)\rangle = 0\,, \tag{2.259}$$

$$\langle \xi_2(N_1)\xi_2(N_2)\rangle = 0\,. \tag{2.260}$$

With the variances of (2.260) we can write the system of (2.244) in the regimes in which the equation (2.256) can be approximately valid i.e. in SR and in USR

- SR: In this case we must neglect the term proportional to the acceleration because it would be of higher order in ϵ_i:

$$\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N} + M_{PL}^2 \frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)} = \frac{\bar{H}_0}{2\pi}\xi(N)\,, \tag{2.261}$$

  where we define $\xi(N)$ as a white noise with unit variance i.e. $\langle \xi(N_1)\xi(N_2)\rangle = \delta\left(N_1 - N_2\right)$.

- USR:

$$
\begin{aligned}
{}_{(0)}\pi^{IR} &= \frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N} + \xi_1 \,, \\
\frac{\partial\, {}_{(0)}\pi^{IR}}{\partial N} &+ 3\, {}_{(0)}\pi^{IR} = 0 \,,
\end{aligned}
\tag{2.262}
$$

which can be further simplified if we solve the deterministic second equation of (2.262)

$$
\frac{\partial\, {}_{(0)}\phi^{IR}}{\partial N} = \pi_0 e^{-3N} + \frac{\bar{H}_0}{2\pi}\xi(N) \,. \tag{2.263}
$$

This approximation is widely used in the literature [198, 199, 184, 178], in fact, equation (2.261) is the one that Starobinsky used in his first paper about stochastic inflation [164]. However, it is really important to have in mind the consequences of this approximation:

- First, it is only valid for exact SR and USR for which it is not very useful when studying realistic single field inflationary scenarios that aim to reproduce the CMB observations (so they need a phase of SR) and to create a non-negligible PBH abundance (so they need, for example, a phase of USR). The reason is that in these scenarios there would be a SR-USR transition that cannot be explained with this approximation (see appendix A for a detailed study of the SR-USR transiton in linear perturbation theory).
- The second and most important consequence is that, as we have already claimed before, there is no reason a priori to think that the smallness of the $(\epsilon_1)_l$ is still true beyond perturbation theory, which means that the MS equation (2.256) can only represent an accurate description of the evolution of inhomogeneities in a local patch during SR (or USR) and in the perturbative regime.

• Another reasonable approximation that one could think of is to characterize the noises by the value of the mode functions that they would take in a fictitious deterministic background, which is the same for all the different local patches. This deterministic background would be given by a line element of the form

$$
ds^2 = -dt^2 + a^2(t)\delta_{ij}dx^i dx^j \,. \tag{2.264}
$$

The line element (2.264) is different from the line element for the real stochastic background of a local path given by (2.265), which in uniform-N gauge is given by

$$ds_l^2 = -\left({}_{(0)}\alpha^{IR} \right)^2 dt^2 + a^2(t)\delta_{ij}dx^i dx^j \,, \tag{2.265}$$

where ${}_{(0)}\alpha^{IR}$ is a stochastic variable that differ from one patch to another.

Using the line element of (2.264), the equation of motion for the mode functions is obviously the well-known MS equation

$$\frac{\partial^2 Q_k^{UV}}{\partial N^2} + (3-\epsilon_1)\frac{\partial Q_k^{UV}}{\partial N} + \left[\frac{k^2}{\bar{H}^2 a^2} + \left(-\frac{3}{2}\epsilon_2 + \frac{1}{2}\epsilon_1\epsilon_2 - \frac{1}{4}\epsilon_2^2 - \frac{1}{2}\epsilon_2\epsilon_3\right)\right] Q_k^{UV} = 0\,, \tag{2.266}$$

where $\bar{H}$ and ϵ_i are deterministic variables, contrary to what happens in the realistic case of (2.253). This approximation at least it is not restricted to SR or USR and it is valid for any inflationary regime. However, by computing the noises over a fictitious deterministic background rather than over the real stochastic one, we are actually loosing all the power of stochastic inflation to describe inhomogeneities beyond linear perturbation theory. In fact, the approximation of solving (2.266) instead of (2.253) is equivalent to say that

$$X^{IR} - \bar{X} \sim \mathcal{O}\left(X^{UV}\right)\,, \tag{2.267}$$

where X^{IR} is any stochastic IR variable and $\bar{X}$ is its counterpart computed in a deterministic background. In this way, the approximation (2.267) is telling us that this version of the stochastic formalism can only reproduce the already well-known results of linear perturbation theory in the long-wavelength limit. In the following we will show, for the sceptical reader, that this is indeed the case.

The following demonstration will be done at leading order in ϵ_1 for any CR regime without transitions, we will then use the system of (2.244), the reason is that in this case we can perform the analysis analytically, which makes the demonstration more understandable. In the next chapter we will present numerical results that also support this claim using the improved stochastic system of (2.248) during a non-analytical SR-USR transition.

If we call $\Delta_Q^{CR}(k,N)\big|_{k=\sigma a\bar{H}}$ to the power spectrum of the variable Q^{UV} computed with equation (2.266) and evaluated at $k=\sigma a\bar{H}$ we can easily write the variances (2.250) and (2.252) as follows

$$\begin{aligned}
\langle \xi_1(N_1)\xi_1(N_2)\rangle &= \Delta_Q^{CR}(k,N_1)\big|_{k=\sigma a\bar{H}}\,\delta(N_1-N_2)\,,\\
\langle \xi_1(N_1)\xi_2^\star(N_2)\rangle = \langle \xi_1^\star(N_1)\xi_2(N_2)\rangle &= \frac{1}{2}\,\frac{d\Delta_Q^{CR}(k,N_1)}{dN}\bigg|_{k=\sigma a\bar{H}}\delta(N_1-N_2)\,,\\
\langle \xi_2(N_1)\xi_2(N_2)\rangle &= \Delta_{\pi_Q}^{CR}(k,N_1)\Big|_{k=\sigma a\bar{H}}\,\delta(N_1-N_2)\,.
\end{aligned} \tag{2.268}$$

The power spectrum $\Delta_Q^{CR}(k,N_1)\big|_{k=\sigma a\bar{H}}$ and $\Delta_{\pi_Q}^{CR}(k,N_1)\Big|_{k=\sigma a\bar{H}}$ can be computed using the result for the power spectrum of $\mathcal{R}$ in section (2.2.1) (see (2.112)), the result is

$$\begin{aligned}
\Delta_Q^{CR}(k,N_1)\big|_{k=\sigma a\bar{H}} &= \left(\frac{\bar{H}_0}{2\pi}\right)^2\left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2\left(\frac{\sigma}{2}\right)^{3-2\nu_{CR}}\,,\\
\Delta_{\pi_Q}^{CR}(k,N_1)\Big|_{k=\sigma a\bar{H}} &= \left(\frac{3}{2}-\nu_{CR}\right)^2\left(\frac{\bar{H}_0}{2\pi}\right)^2\left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2\left(\frac{\sigma}{2}\right)^{3-2\nu_{CR}}\,,
\end{aligned} \tag{2.269}$$

so the stochastic system to solve can be written as:

$$\begin{aligned}
\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N} &= {}_{(0)}\pi^{IR} + \frac{\bar{H}}{2\pi}\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}}\xi(N)\,,\\
\frac{\partial\,{}_{(0)}\pi^{IR}}{\partial N} + 3\,{}_{(0)}\pi^{IR} + 3M_{PL}^2\frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)} &= -\left(\frac{3}{2}-\nu_{CR}\right)\frac{\bar{H}}{2\pi}\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}}\xi(N)\,,
\end{aligned} \tag{2.270}$$

where $\langle\xi(N_1)\xi(N_2)\rangle = \delta(N_1-N_2)$.

On the other hand, and for better comparison, we can schematically write the leading order in ϵ_1 stochastic equations where the noises are correctly computed over the local stochastic background with (2.253) as

$$\begin{aligned}
\frac{\partial\,{}_{(0)}\phi^{IR}}{\partial N} &= {}_{(0)}\pi^{IR} + \sqrt{\left(\Delta_Q^{CR}\big|_{k=\sigma a H_l}\right)_l}\,\xi(N)\,,\\
\frac{\partial\,{}_{(0)}\pi^{IR}}{\partial N} + 3\,{}_{(0)}\pi^{IR} + 3M_{PL}^2\frac{V_\phi\left({}_{(0)}\phi^{IR}\right)}{V\left({}_{(0)}\phi^{IR}\right)} &= \sqrt{\left(\Delta_{\pi_Q}^{CR}\Big|_{k=\sigma a H_l}\right)_l}\,\xi(N)\,,
\end{aligned} \tag{2.271}$$

where we are denoting by $\left(\Delta_Q^{CR}\big|_{k=\sigma a H_l}\right)_l$ to the local power spectrum that appear in the right hand side of (2.250) (and similarly with $\left(\left.\Delta^{CR}_{\pi_Q}\right|_{k=\sigma a H_l}\right)_l$) when the local MS equation (2.253). Since we are only able to compute this local power spectrum numerically [192], we cannot say much about its functional form, what we know for sure is that this quantity will depend on the stochastic IR variables. Schematically we can write the following

$$\left(\left.\Delta^{CR}_{Q}\right|_{k=\sigma a H_l}\right)_l = f_1\left({}_{(0)}\phi^{IR},\ {}_{(0)}\pi^{IR}\right) \tag{2.272}$$

meaning that the noises will generically depend on the dynamics of the local background. On the other hand, the power spectrum computed over the deterministic background only depend on the background time N[16] i.e.

$$\left.\Delta^{CR}_{Q}\right|_{k=\sigma a \bar{H}} = f_2\left(\bar{\phi}, \bar{\pi}\right) \tag{2.273}$$

As an illustrative example, let us imagine a one dimensional standard stochastic equation such as

$$dx = a(x)dt + b(x)dW(t)\,, \tag{2.274}$$

where $W(t)$ is the standard Brownian motion and hence $\frac{dW(t)}{dt} \equiv \xi(t)$. Based on what we have said above, we would say that the approximation (2.267) would modify the stochastic equation (2.273) as

$$\begin{aligned} dx &= a(x)dt + b(x)dW(t)\,, \\ &\downarrow \\ dx &\simeq a(x)dt + b(\bar{x})dW(t) \end{aligned} \tag{2.275}$$

where $\bar{x}$ is the solution of $d\bar{x} = a(\bar{x})dt$. Unfortunately, as we will see in the following, the approximation (2.280) is actually inconsistent, the reason is that, in order to approximate $b(x) \simeq b(\bar{x})$ in a stochastic equation, we need the noise to be small i.e. $b(x) = \epsilon B(x)$, where $\epsilon \ll 1$ so we can treat ϵ as an expansion parameter, if we do that we will see that the approximation (2.280) is actually inconsistent with the order expansion in ϵ.

The equation to solve is

[16] In our case of CR, the power spectrum evaluated at $k = \sigma a \bar{H}$ is constant with time but it could generically depend on N (or $N(\bar{\phi}, \bar{\pi})$).

$$dx = a(x)dt + \epsilon B(x)dW(t)\,, \tag{2.276}$$

where ϵ is a small parameter. We now assume that the solution $x(t)$ of (2.276) can be written as follows

$$x(t) = x_0(t) + \epsilon x_1(t) + \epsilon^2 x_2(t) + \dots \tag{2.277}$$

and hence

$$\begin{aligned} a(x) =& a\left(\bar{x}(t) + \sum_{m=1}^{\infty} \epsilon^m x_m\right) = \sum_{p=0}^{\infty} \frac{d^p a(\bar{x})}{d\bar{x}^p} \left(\sum_{m=1}^{\infty} \epsilon^m x_m\right) \\ & a(\bar{x}) + \epsilon \left(x_1 \frac{da(\bar{x})}{d\bar{x}}\right) + \epsilon^2 \left(x_2 \frac{da(\bar{x})}{d\bar{x}} + \frac{1}{2} x_1^2 \frac{d^2 a(\bar{x})}{d\bar{x}^2}\right) + \dots . \end{aligned} \tag{2.278}$$

Although it is not easy to write explicitly the full set of terms in general, it is easy to see that, for $n \geq 1$, the term proportional to ϵ^n will only depend linearly on x_n. We can now insert the expansion (2.278) for $a(x)$ and a equivalent expansion for $B(x)$ into (2.276) and equate coefficients of like powers of ϵ. We then obtain an infinite set of Stochastic differential equations:

$$\begin{aligned} d\bar{x} &= a(\bar{x})dt \\ dx_1 &= \frac{da(\bar{x})}{d\bar{x}} x_1 dt + B(\bar{x})dW(t) \\ dx_2 &= \left(\frac{da(\bar{x})}{d\bar{x}} x_2 + \frac{1}{2}\frac{d^2 a(\bar{x})}{d\bar{x}^2} x_1^2\right) dt + \frac{dB(\bar{x})}{d\bar{x}} x_1 dW(t) \\ &\vdots \end{aligned} \tag{2.279}$$

From (2.279) we can clearly see that if $B(x)$ depends generically on x, the approximation $B(x) \simeq B(\bar{x})$, where $\bar{x}$ is the deterministic value of x (or leading order in small noise approximation), is actually equivalent to the perform a small noise approximation up to next to leading order. This means that the correct way of writting the approximation of (2.280) is

$$
\begin{aligned}
dx =& a(x)dt + b(x)dW(t)\,, \\
&\downarrow \\
d(\bar{x} + \epsilon x_1) =& \left(a(\bar{x}) + \frac{da(\bar{x})}{d\bar{x}} x_1 \right) dt + \epsilon B(\bar{x}) dW(t)\,,
\end{aligned}
\tag{2.280}
$$

which can be solved order by order.

If we go back to our system of equations, it is now clear that the system (2.270) is actually inconsistent and that the only way of solving (2.271) consistently is doing it order by order in the small noise approximation, being the system for the leading order

$$
\begin{aligned}
\frac{\partial \bar{\phi}}{\partial N} =& \bar{\pi}\,, \\
\frac{\partial \bar{\pi}}{\partial N} =& -3\bar{\pi} - 3M_{PL}^2 \frac{V_{\bar{\phi}}}{V}\,,
\end{aligned}
\tag{2.281}
$$

and the system for the first order

$$
\begin{aligned}
\frac{\partial\, {}_{(0)}\phi_1^{IR}}{\partial N} =&\ {}_{(0)}\pi_1^{IR} + \frac{\bar{H}_0}{2\pi} \frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]} \left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}} \xi(N)\,, \\
\frac{\partial\, {}_{(0)}\pi_1^{IR}}{\partial N} + 3\, {}_{(0)}\pi_1^{IR} + 3M_{PL}^2 \frac{V_{\bar{\phi}\bar{\phi}}\left(\bar{\phi}\right)}{V\left(\bar{\phi}\right)}\, {}_{(0)}\phi_1^{IR} =& -\left(\frac{3}{2} - \nu_{CR}\right) \frac{\bar{H}_0}{2\pi} \frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]} \left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}} \xi(N)\,,
\end{aligned}
\tag{2.282}
$$

such that the final solution is ${}_{(0)}\phi^{IR} = \bar{\phi} + \epsilon\, {}_{(0)}\phi_1^{IR}$. The only thing left to do is to check that the statistics properties of ${}_{(0)}\phi_1^{IR}$ are actually the same as the ones predicted by linear perturbation theory.

Note that, in order to be consistent with the CR regime in which $\nu_{CR} = \frac{3}{2}\sqrt{1 - M_{PL}^2 \frac{4}{3} \frac{V_{\bar{\phi}\phi}}{V}}$ is a constant, we must also set $M_{PL}^2 \frac{V_{\bar{\phi}\phi}}{V} = \frac{1}{12}\left(9 - 4\nu_{CR}^2\right)$ to be a constant. The system of (2.282) can then be rewritten as

$$
\begin{aligned}
\frac{\partial\, {}_{(0)}\phi_1^{IR}}{\partial N} =&\ {}_{(0)}\pi_1^{IR} + \frac{\bar{H}_0}{2\pi} \frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]} \left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}} \xi(N)\,, \\
\frac{\partial\, {}_{(0)}\pi_1^{IR}}{\partial N} + 3\, {}_{(0)}\pi_1^{IR} + \frac{1}{12}\left(9 - 4\nu_{CR}^2\right) {}_{(0)}\phi_1^{IR} =& -\left(\frac{3}{2} - \nu_{CR}\right) \frac{\bar{H}_0}{2\pi} \frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]} \left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}} \xi(N)\,,
\end{aligned}
\tag{2.283}
$$

The system of (2.283) is actually a 2-dimensional Ornstein–Uhlenbeck process with constant coefficients, which is a very well known system and for which an exact analytical solution solution exists [200]. The solution of (2.283) is

$$\begin{pmatrix} {}_{(0)}\phi_1^{IR}(N) \\ {}_{(0)}\pi_1^{IR}(N) \end{pmatrix} = \chi(N) \begin{pmatrix} \phi_0 \\ \pi_0 \end{pmatrix} + \int_0^N \chi(N')\mu(N')dW(N') \tag{2.284}$$

where

$$\chi(N) = \begin{pmatrix} e^{-\frac{3}{2}N}\left(\cosh\left[\nu_{CR}N\right] + \frac{3\sinh[\nu_{CR}N]}{2\nu_{CR}}\right) & e^{-\frac{3}{2}N}\frac{3\sinh[\nu_{CR}N]}{\nu_{CR}} \\ -e^{-\frac{3}{2}N}\frac{\left(9-\nu_{CR}^2\right)\sinh[\nu_{CR}N]}{4\nu_{CR}} & e^{-\frac{3}{2}N}\left(\cosh\left[\nu_{CR}N\right] - \frac{3\sinh[\nu_{CR}N]}{2\nu_{CR}}\right) \end{pmatrix} \tag{2.285}$$

is the solution of the homogeneous equation without noises and $\mu(N)$ is

$$\beta(N) = \begin{pmatrix} \frac{\bar{H}_0}{2\pi}\frac{\Gamma[\nu_{CR}]}{\Gamma\left[\frac{3}{2}\right]}\left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}} \\ -\left(\frac{3}{2}-\nu_{CR}\right)\frac{\bar{H}_0}{2\pi}\frac{\Gamma[\nu_{CR}]}{\Gamma\left[\frac{3}{2}\right]}\left(\frac{\sigma}{2}\right)^{\frac{3}{2}-\nu_{CR}} \end{pmatrix} \tag{2.286}$$

We can also compute the full probability distribution at leading order in small noise expansion, in fact, from the solution (2.284) we clearly see that the variable ϕ_1 (or π_1) and the noise ξ are in linear correspondence, which means that, since ξ is Gaussian, ϕ_1 (or π_1) must also be Gaussian. The covariance matrix for this Gaussian PDF can be obtained by computing the 2-point correlator of (2.284), the different components of the covariance matrix are:

$$\begin{aligned}
\sigma_{\phi_1}^2(N) &= \langle {}_{(0)}\phi_1^{IR}(N)^2\rangle - \langle {}_{(0)}\phi_1^{IR}(N)\rangle^2 = \left(\frac{\bar{H}_0}{2\pi}\right)^2\left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2\left(\frac{\sigma}{2}\right)^{3-2\nu_{CR}}\frac{1-e^{-N(3-2\nu_{CR})}}{3-2\nu_{CR}} \\
\sigma_{\pi_1}^2(N) &= \langle {}_{(0)}\pi_1^{IR}(N)^2\rangle - \langle {}_{(0)}\pi_1^{IR}(N)\rangle^2 = \left(\frac{\bar{H}_0}{2\pi}\right)^2\left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2\left(\frac{\sigma}{2}\right)^{3-2\nu_{CR}}\frac{1-e^{-N(3-2\nu_{CR})}}{4}(3-2\nu_{CR}) \\
\sigma_{\phi_1\pi_1}(N) &= \sigma_{\pi_1\phi_1}(N) = \langle {}_{(0)}\phi_1^{IR}(N)\,{}_{(0)}\pi_1^{IR}(N)\rangle - \langle {}_{(0)}\phi_1^{IR}(N)\rangle\langle {}_{(0)}\pi_1^{IR}(N)\rangle \\
&= -\left(\frac{\bar{H}_0}{2\pi}\right)^2\left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2\left(\frac{\sigma}{2}\right)^{3-2\nu_{CR}}\frac{1-e^{-N(3-2\nu_{CR})}}{2}
\end{aligned} \tag{2.287}$$

Using the results of (2.269), one can easily check that the variances computed in (2.287) are actually the same variances one would expect from linear perturbation theory i.e.

$$
\begin{aligned}
\sigma^2_{\phi_1}(N) &= \int_{k=\sigma a(0)H}^{\sigma a(N)H} \Delta_Q^{CR}(k,N)\frac{dk}{k} \\
&= \left(\frac{\bar{H}_0}{2\pi}\right)^2 \left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2 \left(\frac{1}{a\bar{H}_0}\right)^{3-2\nu_{CR}} \int_{k=\sigma a(0)H}^{\sigma a(N)H} k^{3-2\nu_{CR}}\frac{dk}{k}\,, \\
\sigma^2_{\pi_1}(N) &= \int_{k=\sigma a(0)H}^{\sigma a(N)H} \Delta_{\pi_Q}^{CR}(k,N)\frac{dk}{k} \\
&= \frac{1}{4}(3-2\nu_{CR})^2 \left(\frac{\bar{H}_0}{2\pi}\right)^2 \left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2 \left(\frac{1}{a\bar{H}_0}\right)^{3-2\nu_{CR}} \int_{k=\sigma a(0)H}^{\sigma a(N)H} k^{3-2\nu_{CR}}\frac{dk}{k}\,, \\
\sigma_{\phi_1\pi_1}(N) &= \frac{1}{2}\int_{k=\sigma a(0)H}^{\sigma a(N)H} \frac{d\Delta_{\pi_Q}^{CR}(k,N)}{dN}\frac{dk}{k} \\
&= -\frac{1}{2}(3-2\nu_{CR}) \left(\frac{\bar{H}_0}{2\pi}\right)^2 \left(\frac{\Gamma\left[\nu_{CR}\right]}{\Gamma\left[\frac{3}{2}\right]}\right)^2 \left(\frac{1}{a\bar{H}_0}\right)^{3-2\nu_{CR}} \int_{k=\sigma a(0)H}^{\sigma a(N)H} k^{3-2\nu_{CR}}\frac{dk}{k}\,,
\end{aligned}
\tag{2.288}
$$

where the integration limits are set according to what we compute in the stochastic formalism, i.e. the variance of the IR modes when they start receiving kicks at $k = \sigma a(0)\bar{H}_0$ and where $a(0) = 1$ according to our convention $N_0 = 0$.

Once the variances for each variable have been computed, and knowing that our PDF is Gaussian, we can finally write down the probability distribution for $P(\phi, \pi; N)$ at leading order in the small noise approximation [200]:

$$
P(\phi,\pi;N) = \frac{1}{2\pi\sigma_\phi\sigma_\pi\sqrt{1-\rho^2}}\exp\left\{-\frac{1}{2(1-\rho^2)}\left[\left(\frac{\phi-\bar{\phi}}{\sigma_\phi}\right)^2 + \left(\frac{\pi-\bar{\pi}}{\sigma_\pi}\right)^2 - 2\rho\frac{\left(\phi-\bar{\phi}\right)\left(\pi-\bar{\pi}\right)}{\sigma_\phi\sigma_\pi}\right]\right\}, \tag{2.289}
$$

where $\rho = \frac{\sigma_{\phi\pi}}{\sigma_\phi\sigma_\pi}$ here represents the correlation coefficient. In this case it is easy to check that the correlation coefficient is $\rho \pm 1$, depending on the sign of $\left(\frac{3}{2} - \nu_{CR}\right)$, namely $\rho = 1$ if $\nu_{CR} > \frac{3}{2}$ and $\rho = -1$ if $\nu_{CR} > \frac{3}{2}$. In this case the PDF of (2.289) is degenerate and can be written as:

$$
P(\phi,\pi;N) = \delta\left(\frac{\pi-\bar{\pi}}{\sigma_\pi} \mp \frac{\phi-\bar{\phi}}{\sigma_\phi}\right)\frac{1}{\sqrt{2\pi}\sigma_\phi\sigma_\pi}e^{-\frac{1}{8}\left(\frac{\pi-\bar{\pi}}{\sigma_\pi}\pm\frac{\phi-\bar{\phi}}{\sigma_\phi}\right)^2}\,, \tag{2.290}
$$

where the upper case corresponds to $\rho = 1$ and the lower one to $\rho = -1$. As already justified in section (2.2.4), the PDF of (2.290) is precisely what we obtain in linear perturbation theory. With this we have demonstrated that if we use a stochastic formalism in which the noises are computed in a deterministic background, we are actually doing linear perturbation theory and hence loosing all the power of this (hopefully) non-perturbative description of inflation. Higher orders in this small noise expansion in the context of stochastic inflation have been explored in the literature [201, 202, 203], however, as shown here, this is nothing more than computing higher orders in perturbation theory.

Finally, we will end this section by noticing that, although the stochastic system of (2.270) is actually inconsistent, this inconsistency can however give some information when comparing the results from the stochastic formalism with the ones of linear perturbation theory, in fact, since we know that the correlations functions calculated with the stochastic system of (2.270) will coincide, up to second order in perturbation theory, to the ones calculated in linear perturbation theory, any inconsistency between the two approaches will signal the break-down of perturbation theory.

2.6 Stochastic approach vs δN formalism.

In this section we will emphasize the similarities and differences between the two non-linear mathematical frameworks presented in sections 2.4 (δN) and 2.5 (stochastic formalism). For better comparison we will use the naive stochastic formalism presented in section 2.5.1, the reason is that the δN formalism requires terms with spatial derivatives but that do not vanish in the $k \to 0$ such as $\partial_i\, {}_{(0)}\beta^i$ to be neglected so it can only be consistently compared with a stochastic formalism in which we also neglect these kind of terms.

Both the stochastic approach and the δN formalism complete gradient expansion by giving some natural initial conditions that come from linear perturbation theory. One of the main differences of these approaches are actually the quantity they are computing: while the aim of the stochastic formalism presented in section 2.5.1 is the computation of the PDF for the inhomogeneities of the long-wavelength field ${}_{(0)}\phi^{IR}$, the δN formalism of section 2.4.1 assumes a known initial distribution of ${}_{(0)}\phi^{IR}$ and computes the PDF of ${}_{(0)}\zeta$ from there. It is then reasonable to try to formulate some kind of δN formalism that uses as initial condition the PDF for ${}_{(0)}\phi^{IR}$ provided by the stochastic formalism instead of the one provided by linear perturbation theory. This is the so-called stochastic δN formalism [204].

We will not explain into detail the stochastic δN here because we are only introducing it for better comparison between the classical δN formalism of section 2.4.1 and the stochastic formalism. The schematic idea can however be seen in Fig. 2.6:

- The classical δN (left panel) starts from the linear PDF for ${}_{(0)}\phi^{IR}$[17] (dashed lines) and evolve in a deterministic from there until reaching a fixed value $\bar{\phi}^e$ (orange solid line). The PDF of ${}_{(0)}\zeta_c$ is then related with the PDF of N at ${}_{(0)}\phi^{IR} = \bar{\phi}^e$ as shown in (2.4.1)

- On the other hand, the trajectories for ${}_{(0)}\phi^{IR}$ in the stochastic δN formalism (dashed lines of the right panel), which also start from the linear PDF for ${}_{(0)}\phi^{IR}$, receive stochastic kicks at every time step such the PDF of ${}_{(0)}\phi^{IR}$ changes with time. In this case the PDF of ${}_{(0)}\zeta_c$ will be related with the first passage time of each stochastic trajectory through $\bar{\phi}^e$ (orange solid line).

Note also that, for better visualization, we have also plotted in Fig. 2.6 with a blue solid line what the trajectory of the field of the fictitious background without perturbations.

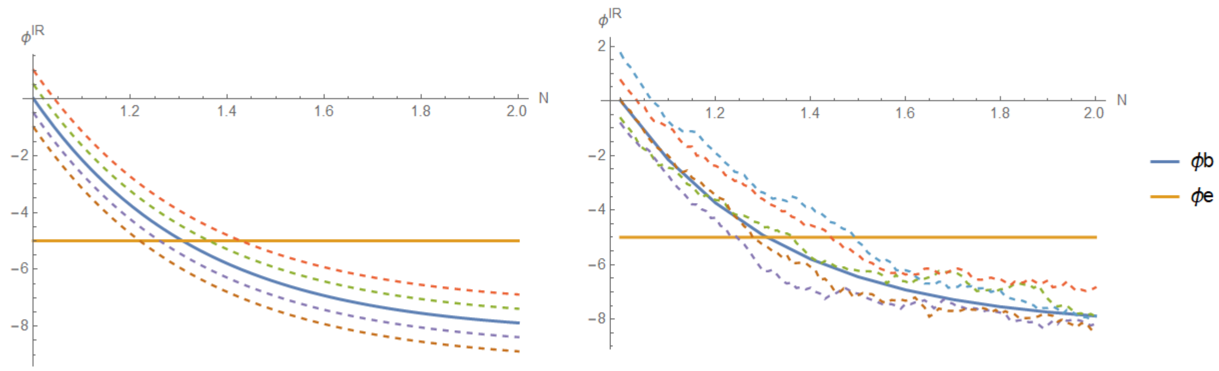

Fig. 2.6 Classical δN formalism vs stochastic δN formalism.

From the comparison between the classical δN formalism and the stochastic δN formalism we can clearly see the improvement of the latter over the former, the stochastic δN formalism could, in principle, start from a fully non-linear PDF for the field ${}_{(0)}\phi^{IR}$ which is described by the stochastic equations of (2.244), on the other hand, the classical δN formalism usually starts from the linear Gaussian PDF for ${}_{(0)}\phi^{IR}$[18].

2.7 Numerical results.

In section 2.5.3.1 we have shown that the PDF for the ${}_{(0)}\phi^{IR}$ obtained with a stochastic system in which the noises are computed in a fictitious deterministic background

[17] Note that, in this schematic example we are fully characterizing the trayectores with different initial conditions in ${}_{(0)}\phi^{IR}$, however, as justified in section 2.4.1, the classical trajectory could also depend on ${}_{(0)}\pi^{IR}$. In this case we should also give some intitial conditions to ${}_{(0)}\pi^{IR}$ that follow the PDF of linear perturbation theory.

[18] Note that the classical δN formalism could be improved if the initial conditions for ${}_{(0)}\phi^{IR}$ (and ${}_{(0)}\pi^{IR}$) were given at higher order in perturbation theory, including for example non-Gaussianities. This is automatically done in the stochastic δN formalism

exactly corresponds with the PDF computed in linear perturbation theory. This demonstration has been done analytically by the usage of the small noise approximation at leading order in $\mathcal{O}(\epsilon_1)$ during a CR regime. By construction, we of course expect this correspondence between the stochastic approach with deterministic noises and linear perturbation theory to hold at all orders in SR parameters and for any inflationary regime, however it is important to check it numerically. Also, as already mentioned at the end of section 2.5.3.1, we can also (inconsistently) use the full non-linear equation of motion for ${}_{(0)}\phi^{IR}$ while computing the noises in a deterministic background and compare the result with the one of linear perturbation theory, if we detect some important differences between the two methods it would mean a break-down of perturbation theory itself. Finally, it is also important to check the improvement that the new stochastic formalism of section 2.5.2 represents with respect to the naive one of section 2.5.1.

In order to check all the aspects mentioned above during this thesis we have developed a very accurate numerical code able to compute some statistical properties of the inhomogeneities using both the "new" stochastic formalism of 2.5.2 and the naive one of section 2.5.1 and compare them with the numerical results from linear perturbation theory. Although with this code we can compute any correlator of the long-wavelength scalar variable Q^{IR} of (2.249) as a function of the number of e-folds N, we will focus with the two-point correlation function, which is basically the variance of the PDF for Q^{IR} and hence it is related with the power spectrum.

2.7.1 Numerical computation in linear perturbation theory

In linear perturbation theory we must compute:

$$\langle Q(N)Q(N)\rangle = \int_{\sigma a(N=0)H(N=0)}^{\sigma a(N)H(N)} \frac{dk}{k}\Delta_Q(k,N)\,, \tag{2.291}$$

where Q_k is given by the solution of (2.266) in a deterministic background. The limits in (2.291) correspond to the selection of modes inside the coarse grained scale (defined by $k = \sigma a(N)H(N)$) from the beginning of inflation ($N = 0$). This anti-Fourier transformation from the power spectrum is needed in order to compare (2.291) with the real space correlator coming from the stochastic formalism.

In order to find (2.291) we numerically solve the MS equation for many values of k between the two integration limits in (2.291). After that, we perform a numerical integration in the k direction. In Fig. 2.7 this procedure is schematically explained. Each blue line in Fig. 2.7 corresponds to the solution of the MS equation $Q_{\mathbf{k}}(N)$ with fixed wave number k in a generic Slow-Rolling background. The grey plane represents the plane in which each k-mode exits the coarse-grained scale. The idea is to integrate from $k = \sigma H(N = 0)$ to $k = \sigma a(N)H(N) = \sigma e^N H(N)$ i.e. in the direction followed by the grey arrow. This means that the value of $\langle Q^{lin}(N_\star)Q^{lin}(N_\star)\rangle$ at time $N_\star$ will be the integral of the exponential of the blue surface (it is the exponential because we have plotted the log of the power spectrum for better visualization) from the $\log(\sigma H(0))$ plane up to the grey plane along the line where $N = N_\star$. For example, for $N_\star = 10$ we will be integrating the red line.

In the stochastic formalism, the IR part of the field receives stochastic kicks from $N = 0$ onward. Thus the first k-mode from which the IR field receives a kick is the one with $k = \sigma a(N = 0)H(N = 0)$.

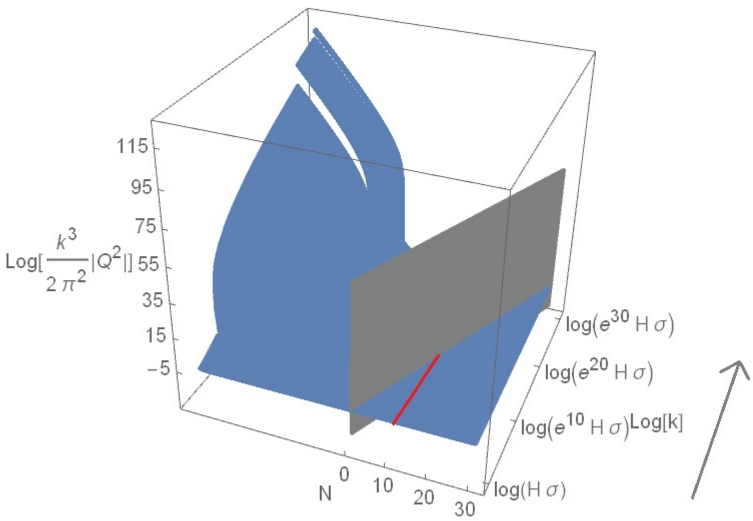

Fig. 2.7 Numerical procedure followed in order to compute (2.291)

As we did around (2.109), whenever $\Delta_Q(k, N)$ does not depend on N, one can do a very useful approximation, which consists in evaluating the power spectrum at coarse-grained scale crossing, i.e. at $k = \sigma aH$, and assume that this value does not change with time. This would allow us to write (2.291) as

$$\langle Q(N)Q(N)\rangle = \int_0^N \Delta(k = \sigma a(N')H(N'))dN'. \tag{2.292}$$

In this case one could write the power spectrum as the derivative with respect of the number of e-folds N of the correlator in real space.

$$\mathcal{P}(k) = \frac{d}{dN}\langle Q^{lin}(N)Q^{lin}(N)\rangle, \tag{2.293}$$

Graphically, this would correspond to perform the integral (2.292) in the direction N (x axis in Fig 2.7) by calculating the value of power spectrum only in the point in which blue and grey surfaces of Fig. 2.7 cross. However, this technique cannot be used if the power spectrum evolves with time [205]. Thus, unfortunately, the approximation (2.293) cannot be used with the full numerical result, in fact it can be used at zeroth order in ϵ_1 in SR and USR but not in any transition between them nor in CR.

2.7.2 Stochastic evolutions

In the stochastic approach, where the variables are statistical and non-linear, we can define a "non-linear" perturbation as $\Delta Q^{IR} = Q^{IR} - \overline{Q^{IR}}$, where $\overline{Q^{IR}}$ is the mean value of the variable Q^{IR}. With this definition it is clear that the correlator $\langle Q^{IR}(N)Q^{IR}(N)\rangle$ in real space at the same time N is the statistical variance of the stochastic variable Q^{IR}.

We will compute Var$(Q^{IR}(N))$ by simulating the system of stochastic equations many times where the noises will take values distributed Gaussianly with variances computed in different ways depending on which stochastic formalism we are using

- If we use the naive or "old" stochastic formalism of section 2.5.1 i.e. the system of (2.244), we will compute the noises as done in section 2.5.3.1 i.e. using (2.268) and (2.269).

- If we use our "new" stochastic formalism based on the correct leading order in gradient expansion of section 2.5.2 i.e. the system of (2.248), we will compute the noises by solving numerically the linear equations presented in section 2.2.1 in uniform-N gauge, which at all orders in $\mathcal{O}(\epsilon_1)$ is not equivalent to the flat gauge anymore. The noises ξ_1, ξ_2 and ξ_4 will then be proportional to the power spectrum of $\delta\phi_{uN}$, $\frac{\partial\delta\phi_{uN}}{\partial N}$ and $\nabla^2 E_{uN}$, respectively, of course these power spectrum must be evaluated at wavenumber $k = \sigma a(N)\bar{H}(N)$ and at coarse-grained crossing time, i.e. when blue and grey surfaces of Fig. 2.7 cross each other. Another option is to solve numerically the MS equation (2.266) and perform a gauge transformation from flat to uniform-N gauge as in [192].

We will then run the system of stochastic equations many times until we have enough statistics to give a trustworthy value for Var$(Q^{IR}(N))$. Since with the "new" stochastic formalism we are able to compute variables with precision $\epsilon_1 \ll 1$, we are interested in a very precise numerical method for the resolution of stochastic differential equations.

In the context of ordinary differential equations, we could think on using a Runge-Kutta 4 method, where the total accumulated error is $\mathcal{O}(h_n^4)$, where h_n is the time step of our simulation, and hence it is quite accurate. However, when trying to extrapolate the ordinary Runge-Kutta method to stochastic differential equations everything becomes more complicated.

As we know, any ordinary Runge-Kutta method is based on Taylor expansion of the true solution of the ordinary differential equation around different points. If we try to do the same with the solution of a stochastic differential equation, we will find that the Taylor expansion in this case is not as trivial as in the deterministic case [206] , which makes the construction of any numerical method for the solution of stochastic differential equations more and more complicated. There has been however some recent development in the construction of such methods, for our simulation we will use a Runge-Kutta method adapted for stochastic equations which was first developed in [207] . This algorithm is presented in 2.7.2.1 and it is of order 1.5 in strong convergence and of order 3 in weak convergence, where

- Strong convergence for a stochastic numerical method means that the total accumulated error between the different true trajectories and the simulated trajectories is $\mathcal{O}(h_n^s)$, where s is the order of strong convergence.
- Weak convergence for a stochastic numerical method means that the total accumulated error between the true statistical properties of the stochastic system and simulated statistical properties is $\mathcal{O}(h_n^w)$, where w is the order of weak convergence.

The reason why there are two order of convergence in the stochastic numerical methods is basically because we have a deterministic part of the equation and a stochastic part. While the specific trajectories of the system will be different depending on the specific random values that the stochastic part takes, the statistical properties of the system will only depend on the statistical properties of the noise and not on the specific values that it takes.

2.7.2.1 Numerical algorithm for the stochastic simulation

For the stochastic equations that we want to simulate, i.e. the ones of (2.248), the noises are:

- Additive, meaning that their variance only depend on the time variable and not on the stochastic variables themselves. This is a consequence of solving the linear equations over a deterministic background.
- Completely correlated, which means that there is effectively only one noise, the reason is that $\delta\phi_{uN}$, $\frac{\partial\delta\phi_{uN}}{\partial N}$ and $\nabla^2 E_{UN}$ are not independent functions, they are related by the linear equations of section 2.2.1. In the same way, the noises ξ_1, ξ_2 and ξ_4 are not independent either.

We will then present in this section the stochastic algorithm of [207] adapted to additive and correlated noises. We denote by $X = (X_t)_{t\in\mathcal{I}}$ (where $\mathcal{I} = [t_0, T]$ for some $0 \le t_0 < T < \infty$) the solution of the d-dimensional system of stochastic differential equations (SDE) (2.294).

$$X_t = X_{t_0} + \int_{t_0}^{t} a(s, X_s)ds + \sum_{j=1}^{m} \int_{t_0}^{t} b^j(s, X_s)dW_s^j, \tag{2.294}$$

with an m-dimensional driving Weiner process $(W_t)_{t\ge 0} = \left((W_t^1, ..., W_t^m)^T\right)_{t\ge 0}$.

In our case we have completely correlated noises and hence $m = 1$. A further simplification can be done to (2.294) by imposing the additivity of the noises, which translates into $b(s, X_s) = b(s)$. Under these simplifications, the algorithm used in order to numerically solve (2.294) is an order 1.5 strong Stochastic Runge- Kutta (SRK) method defined by the initial condition $Y_0 = X_{t_0}$ and:

$$Y_{n+1} = Y_n + \sum_{i=1}^{s} \alpha_i a\left(t_n + c_i^{(0)}h_n, H_i^{(0)}\right)h_n + \sum_{i=1}^{s}\left(\beta_i^{(1)} I_{(1)} + \beta_i^{(2)}\frac{I_{(1,0)}}{h_n}\right) b\left(t_n + c_i^{(1)}h_n\right), \tag{2.295}$$

for $n = 0, 1, ..., N-1$ with stages

$$H_i^{(0)} = Y_n + \sum_{j=1}^{s} A_{ij}^{(0)} a\left(t_n + c_j^{(0)}h_n, H_j^{(0)}\right)h_n + \sum_{j=1}^{s} B_{ij}^{(0)} b\left(t_n + c_j^{(1)}h_n\right)\frac{I_{(1,0)}}{h_n}, \tag{2.296}$$

for $i = 1, ..., s$. In the algorithm described above h_n is the time step, $I_{(1)}$ and $I_{(1,0)}$ are some Îto stochastic integrals that will be specified in (2.297), and α_i, $c_i^{(0)}$, $c_i^{(1)}$, $\beta_i^{(1)}$, $\beta_i^{(2)}$, $A_{ij}^{(0)}$ and $B_{ij}^{(0)}$ are some constants that characterize the method, they are usually written in a compact way using the so-called Butcher tableau:

$c^{(0)}$	$A^{(0)}$	$B^{(0)}$	$c^{(1)}$
	α^T	${\beta^{(1)}}^T$	${\beta^{(2)}}^T$

Table 2.1 Butcher tableau of a generic stochastic Runge-Kutta method

The specific entries of the Butcher tableau 2.1 used in the SRK method of strong order 1.5 and weak order 3 are written down in Table 2.2:

Once the Butcher tableau is specified, the only thing left is to define the stochastic Îto integrals $I_{(1)}$ and $I_{(1,0)}$

$$I_{(1)} = \int_{t_n}^{t_{n+1}} dW_s; \qquad I_{(1,0)} = \int_{t_n}^{t_{n+1}}\int_{t_n}^{s} dW_u ds. \tag{2.297}$$

One can easily compute the expected value, the variance and the correlation of the

$$
\begin{array}{c|ccc|ccc|ccc}
0 & & & & & & & 1 & & \\
1 & 1 & & & 0 & & & 0 & & \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & & 1 & \frac{1}{2} & & 0 & & \\
\hline
 & \frac{1}{6} & \frac{1}{6} & \frac{2}{3} & 1 & 0 & 0 & 1 & -1 & 0
\end{array}
$$

Table 2.2 Butcher tableau of the stochastic Runge-Kutta method that we use in our simulation.

integrals defined in (2.297) getting:

$$
\begin{gathered}
E\left(I_{(1)}\right) = 0 \qquad E\left(I^2_{(1)}\right) = h_n^2 \\
E\left(I_{(1,0)}\right) = 0 \qquad E\left(I^2_{(1,0)}\right) = \frac{1}{3}h_n^3 \qquad E\left(I_{(1,0)}I_{(1)}\right) = \frac{1}{2}h_n^2.
\end{gathered} \tag{2.298}
$$

The statistical behavior of (2.298) can be implemented numerically by defining two independent $N(0;1)$[19] random variables U_1 and U_2. In this case we have:

$$
I_{(1)} = U_1\sqrt{h_n} \qquad I_{(1,0)} = \frac{1}{2}h_n^{3/2}\left(U_1 + \frac{1}{\sqrt{3}}U_2\right) \tag{2.299}
$$

It is important to remark that if one do a naive extension of the Runge-Kutta method from deterministic equations to stochastic equations one would get a precision similar to the Euler-Maruyama method, which is of strong order 0.5 and weak order 1 and that basically consist on adding a random part to the deterministic Euler method. This was firstly noticed in [208] and it can be numerically seen in Fig. 2.8, where we show in magenta the analytical solution of the tochastic equation $dX(t) = \lambda X(t)dt + \nu X(t)dW_t$ where $\lambda = 2$, $\nu = 1$ and $X(0) = 1$, the dashed lines of Fig. 2.8 represent numerical simulations of the same equation: In red we see the numerical solution obtained with the Euler-Maruyama method, in blue we see the numerical solution obtained with a naive stochastic extension of the third order Runge-Kutta for deterministic equations in which a random part is simply added to the deterministic solution solution, finally, in green we see the numerical solution obtained with the stochastic Runge-Kutta method proposed in [207] and explained above. One can clearly see that the precision is highly improved by the usage of the stochastic Runge-Kutta method explained here.

2.7.3 Numerical results for a non-analytic potential.

Once we have explained the numerical procedure that we will follow to compare the correlator $\langle Q^2 \rangle$ computed in linear perturbation theory with the variance Var(Q^{IR})

[19] $N(0;1)$ refers to a random variable that follows a normal distribution with mean 0 and variance 1

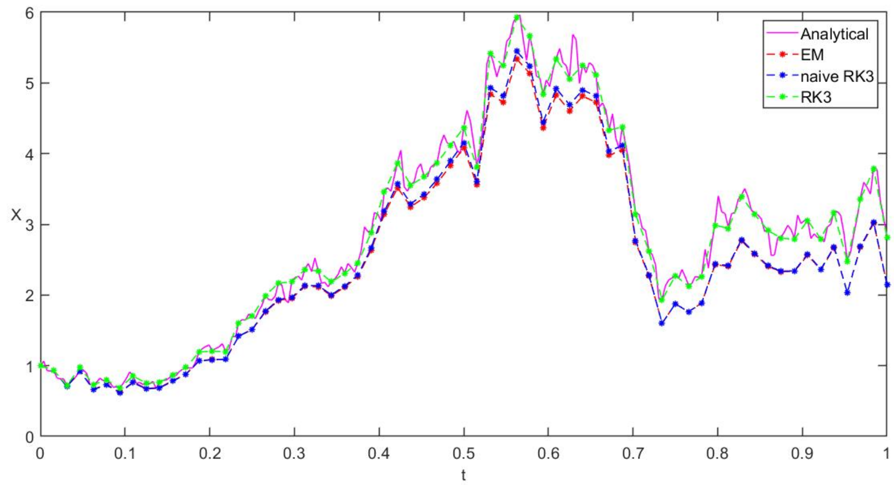

Fig. 2.8 Comparison of different numerical methods for the solution of stochastic differential equations

obtained with the stochastic approach we will apply this procedure to an inflationary model in which the potential contains an inflection point, which means that it will go from a SR to a USR regime and back to a secondary SR regime and hence the power spectrum will experience a growth that can help in the context of PBH formation of generation of scalar induced gravitational waves, as justified in section 2.2.4.

The potential used to simulate the SR-USR-SR transition is a cubic potential containing an inflection point at $\phi = \phi_0 = 1$, i.e.

$$V(\phi) = V_0 \left(1 + \beta \left(\phi - \phi_0\right)^3\right) , \tag{2.300}$$

where the parameters chosen are $V_0 = 1 \times 10^{-8}$ and $\beta = 0.8$.

The transition between these two regimes is quite interesting as it is the regime in which we could expect some difference between the IR part of "old" and "new" stochastic equations. As justified before, the difference between the two stochastic approaches is $\mathcal{O}(\epsilon_1)$, however, in order for the the inflaton field to overshoot the inflection point of the potential (2.300), ϵ_1 grows until reaching values only slightly smaller than one. In Fig. 2.9 we show the results that we expected, namely that the fully numerical linear perturbation theory correlator of (2.291) (yellow dashed line) exactly coincides with the correlator from the "new" stochastic formalism of (2.248) (blue solid line) while disagreeing with the correlator computed with the naive stochastic formalism of (2.244) (purple solid line), which is only valid at leading order in ϵ_1. Note that Fig. 2.9 is also telling us that perturbation theory in this model is under control.

We have then numerically demonstrated two very important facts

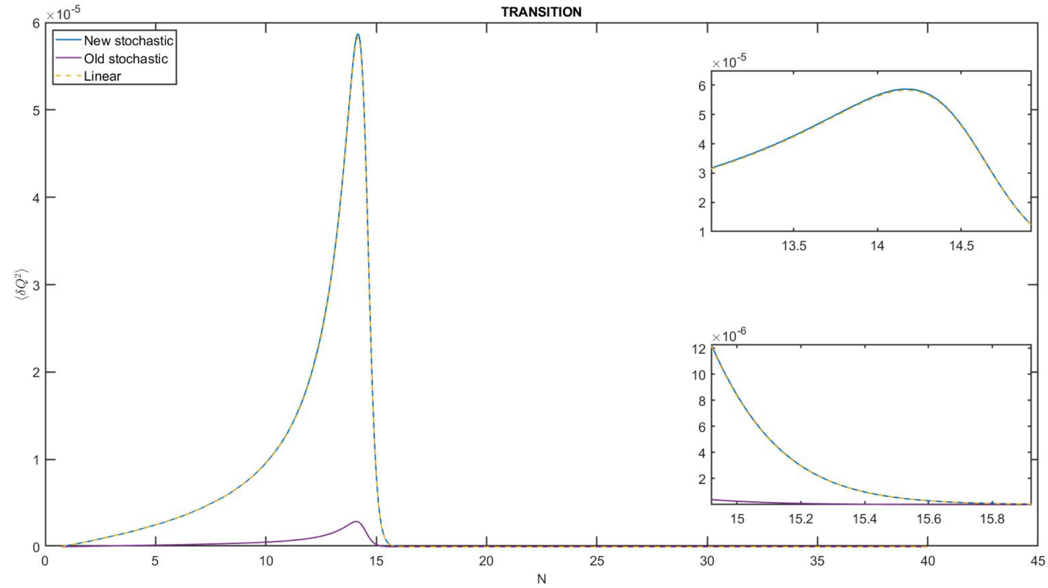

Fig. 2.9 Comparison between two point correlator $\langle Q^2 \rangle$ computed with the different stochastic formalism of sections 2.5.1 and 2.5.2 and computed in linear perturbation theory.

- A stochastic formalism in which the noises are computed in a deterministic background must reproduce the same results that we know from linear perturbation theory. This was already checked in section 2.5.3.1 but only for CR inflationary regimes and at leading order in ϵ_1, here we have do it at all orders in ϵ_1 and for a non-analytical SR-USR-SR transition.

- A stochastic formalism as the one presented in section 2.5.2, i.e. based on a gradient expansion that do not neglect terms with spatial derivatives that do not vanish in the $k \to 0$ limit nor the momentum constraint, which has been first developed for the first time during this thesis is needed in order to study most of the realistic inflationary scenarios of interest for PBH formation of generation of scalar induced gravitational waves.

CHAPTER 3

Conclusions

This thesis has been devoted to the study of different mathematical framework that aim to describe the inhomogeneities generated during cosmological inflation in a non-perturbative way. In this section we will recapitulate the most important findings and results of the thesis:

- In sections 2 and 2.2, we compute, using linear perturbation theory, the power spectrum of the comoving curvature perturbation $\Delta_{\mathcal{R}}$ in the long-wavelength limit, which is constant in time and scale-invariant in the SR regime, as expected. Beyond SR, there is a much richer landscape of possibilities. If we define $\kappa = \frac{V_{\bar{\phi}}}{\bar{H}\dot{\bar{\phi}}}$, we have:
  - Time dependence:
    - $\Delta_{\mathcal{R}}$ is constant if $\kappa \leq -\frac{3}{2}$.
    - $\Delta_{\mathcal{R}}$ grows with time as $a^{6+4\kappa}$ if $\kappa > -\frac{3}{2}$.
  - k-dependence:
    - $\Delta_{\mathcal{R}}$ is blue-tilted for $-3 < \kappa < 0$.
    - $\Delta_{\mathcal{R}}$ is red-tilted for $\kappa < -3$ or $\kappa > 0$.
    - $\Delta_{\mathcal{R}}$ is scale invariant for $\kappa = -3$ (SR) and $\kappa = 0$ (USR).

  The approach of considering SR as a specific case of the more general CR where κ is a constant also helps to identify when some approaches valid for SR, fail when studying inflationary regimes beyond it. For example, the identification $k = a\bar{H}$ when computing the spectral index is a specific feature of SR and it does not hold beyond it.

- With the motivation that the power spectrum can grow both in time and in k beyond SR, the second part of this chapter, composed of sections 2.3, 2.4, 2.5, 2.6 and 2.7, studies different attempts to describe inflationary inhomogeneities in a non-perturbative way.

First we show that if we want to correctly describe with global coordinates the evolution of different homogeneous and isotropic patches in the context of leading order in gradient expansion, we must take care of both terms with spatial derivatives that do not vanish in the $k \to 0$ limit (sometimes called non-local terms) and of the momentum constraint of general relativity: we showed in section 2.3.1 that, if those terms are not taken into account, only the linear constant mode of the comoving curvature perturbation is reproduced. For $\kappa > -\frac{3}{2}$ however, the non-constant mode dominates. In section 2.3.3 we consistently formulate the leading order in gradient expansion such that also the decaying (or growing) mode is reproduced. In section 2.3.2, we find those modes to be related to a new symmetry of the perturbative Einstein equations in the long-wavelength limit that arises when taking into account terms with spatial derivatives in the long-wavelength limit and in Newtonian gauge.

We then turn our attention to the δN formalism, which in principle can deliver the PDF of the comoving (uniform density) curvature perturbation given some initial conditions for the field (energy density). In section (2.4.1), we clarify that whenever the initial conditions are provided in the context of linear perturbation theory, as it is usually the case, the final result for the curvature perturbation can only describe perturbative physics.

The main result of this thesis is the development of the stochastic approach to inflation at all orders in ϵ_i (the SR parameters): firstly we re-derive the stochastic formalism typically used in the literature from first principles in section 2.5.1, realizing two important aspects:

- It is not able to reproduce the two modes that appear in linear perturbation theory in the limit $k \to 0$. Because the stochastic formalism is constructed such that the dynamical variable is the field, the mode that we lose by using the naive leading order in gradient expansion is never the growing one, however we still lose terms proportional to $\mathcal{O}(\epsilon_1)$, which can become important at linear order in some inflationary models, as we show numerically in section 2.7, and in the non-perturbative part of the PDF of the inhomogeneities.
- It is formulated using the uniform-N gauge, which is equivalent to the flat gauge at leading order in ϵ_1 and hence in this case both gauges are interchangeable.

Using the correct leading order in gradient expansion which takes into account non-local terms and the momentum constraint of general relativity, we derive for the first time in section 2.5.2 a stochastic formalism which is able to describe the correct long-wavelength behaviour of inflationary inhomogeneities at all orders in SR parameters. We do this using again the uniform-N gauge but taking into account that at this level of precision, this gauge is not longer equivalent to the flat gauge.

Although the formulation of the improved stochastic formalism of section 2.5.2 is very promising, the practical computation of any statistical quantity by solving this stochastic system is very difficult, the reason is that, generically, in order to solve the stochastic system we must characterize the noises. Since the noises are computed with linear perturbation theory techniques over a stochastically corrected background, rather than over a deterministic background, it is clear that in order to characterize the noises we must know the solution of the stochastic system. This difficulty is usually overcome via some approximations, the principal one is to compute the noises over a deterministic global background rather than over the true stochastic local background. We show analytically for pure CR inflationary models in section 2.5.3.1 and numerically for a transient SR-USR-SR inflationary model in section 2.7 that this approximation is actually equivalent to linear perturbation theory or, in other words, if we approximate the true local stochastic background by a global deterministic one, we are loosing all the power of the stochastic approach to inflation to explore the non-perturbative region of the PDF.

Based on the results of this thesis, it is then clear that there is still a long way to go in order to correctly describe inflationary inhomogeneities in a non-perturbative way, whose statistical properties are crucial for the description of different observables such as PBH or scalar induced GW. However, this thesis represents the first step to achieve this objective: the comprehension of the different mathematical frameworks which aim to describe inflation in a non-perturbative way and their limitations.

Appendices

Appendix A

Transition between Slow-Roll and Constant-Roll regimes

In this appendix we will study the behaviour of the MS variable Q in the transition between a SR regime, necessary in order to explain the inhomogeneities of the CMBR, and a constant-ν regime in which the power spectrum $\Delta_{\mathcal{R}}$ grows with time in the long wavelength limit and hence it can be of interest for PBH formation or the generation of scalar induced GW. As justified in section 2.2.1.3, this growth of the power spectrum of $\mathcal{R}$ will take place if $\kappa = \frac{V_{\bar{\phi}}}{H\dot{\bar{\phi}}} > -\frac{3}{2}$. We will make this study at neglecting all ϵ_1 terms[1], which means that the transition can be written in terms of ϵ_2 as

$$\epsilon_2^{SR} \simeq 0 \quad \Longrightarrow \quad \epsilon_2^{CR} = -6 + 2\kappa < -3\,. \tag{A.1}$$

Usually the way these transitions are studied [100] is by modeling the behavior of ϵ_2 as a sharp transition from ϵ_2^{SR} to ϵ_2^{CR} at conformal time τ_1 i.e. as[2]

$$\epsilon_2(\tau) = \epsilon_2^{SR}\Theta(\tau_1 - \tau) + \epsilon_2^{CR}\Theta(\tau - \tau_1)\,. \tag{A.2}$$

In this case we will take a slightly different approach motivated by [101], instead of imposing the sharp transition in ϵ_2 as in (A.2), we will to it in ν itself i.e.

$$\nu(\tau) = \nu^{SR}\Theta(\tau_1 - \tau) + \nu^{CR}\Theta(\tau - \tau_1)\,, \tag{A.3}$$

where $\nu^{SR} = \frac{3}{2}$. One could think that (A.2) and (A.3) are equivalent, however, from (2.66) and (2.74) and neglecting ϵ_1 terms we have

$$\nu^{CR} \simeq \sqrt{\frac{9}{4} + \frac{3}{2}\epsilon_2^{CR} + \frac{1}{4}\left(\epsilon_2^{CR}\right)^2 - \tau\frac{1}{2}\frac{d\epsilon_2^{CR}}{d\tau}}\,, \tag{A.4}$$

where we have used the definition of ϵ_3 i.e. $\frac{d\epsilon_2}{dN} = \epsilon_2\epsilon_3$. From (A.4) it is clear that (A.2) and (A.3) are not exactly equivalent, indeed if the time evolution of ϵ_2^{CR} is described by

[1] This is a slightly inconsistent approach as we will see later on, however it will already give us some relevant information.

[2] During inflation $\tau \in (-\infty, 0)$ so the smaller value for τ the sooner stages of inflation. Since the Heaviside theta function $\Theta(\tau_1 - \tau)$ in (A.2) is 1 for $\tau < \tau_1$, it is clear that (A.2) describes a starting SR regime followed by a CR regime.

$$\frac{3}{2}\epsilon_2^{CR} + \frac{1}{4}\left(\epsilon_2^{CR}\right)^2 - \tau\frac{1}{2}\frac{d\epsilon_2^{CR}}{d\tau} = \nu^2 - \frac{9}{4}\,, \tag{A.5}$$

we can have a analytical solution for the MS equation (which requires ν to be a constant) even for time dependent ϵ_2. We will then study regimes in which (A.3) is satisfied but in which

$$\epsilon_2(\tau) = \epsilon_2^{SR}\Theta(\tau_1 - \tau) + \epsilon_2^{CR}(\tau)\Theta(\tau - \tau_1)\,, \tag{A.6}$$

where $\epsilon_2^{CR}(\tau)$ is the solution of (A.5), which can be written as:

$$\epsilon_2^{CR}(\tau) = \frac{\left(3 - 2\nu^{CR}\right)\left(3 + \epsilon_2^{CR}\big|_{\tau_1} + 2\nu^{CR}\right) - \left(3 + 2\nu^{CR}\right)\left(3 + \epsilon_2^{CR}\big|_{\tau_1} - 2\nu^{CR}\right)\left(\frac{\tau}{\tau_1}\right)^{2\nu}}{-\left(3 + \epsilon_2^{CR}\big|_{\tau_1} + 2\nu^{CR}\right) + \left(3 + \epsilon_2^{CR}\big|_{\tau_1} - 2\nu^{CR}\right)\left(\frac{\tau}{\tau_1}\right)^{2\nu}}\,, \tag{A.7}$$

where

$$\epsilon_2^{CR}\big|_{\tau_1} \equiv \lim_{\tau\to\tau_1^+}\epsilon_2(\tau)\,. \tag{A.8}$$

Note that, by definition we also have

$$\lim_{\tau\to\tau_1^-}\epsilon_2(\tau) = \epsilon_2^{SR} = 0\,, \tag{A.9}$$

which makes $\epsilon_2(\tau)$ generically discontinuous. The time dependence of $\epsilon_2(\tau)$ is such that it goes from $\epsilon_2 = -3+2\nu^{CR}$ to $\epsilon_2 = -3-2\nu^{CR}$, which are the two constant values of ϵ_2 that satisfy (A.5), in a smooth way (as an hyperbolic tangent).

Now that we know what is the time dependence of ϵ_2, it is also interesting to derive the time dependence of ϵ_1, which can be shown to be:

$$\epsilon_1(\tau) = \epsilon_1^{SR}\Theta(\tau_1 - \tau) + \epsilon_2^{CR}(\tau)\Theta(\tau - \tau_1)\,, \tag{A.10}$$

where we will set $\epsilon_1^{SR} = \epsilon_1^0$ to be a small constant and

$$\epsilon_1^{CR}(\tau) = \frac{\epsilon_1^0}{16\left(\nu^{CR}\right)^2}\left(\left(3 + \epsilon_2^{CR}\big|_{\tau_1} + 2\nu^{CR}\right)\left(\frac{\tau}{\tau_1}\right)^{\frac{1}{2}\left(3-2\nu^{CR}\right)} - \left(3 + \epsilon_2^{CR}\big|_{\tau_1} - 2\nu^{CR}\right)\left(\frac{\tau}{\tau_1}\right)^{\frac{1}{2}\left(3+2\nu^{CR}\right)}\right)^2\,. \tag{A.11}$$

It is important to remark that, contrary to what happens with $\epsilon_2(\tau)$, $\epsilon_1(\tau)$ is always a continous funciton at $\tau = \tau_1$.

With the ingredients above we are finally in position to compute the MS variable Q after the transition. The procedure to follow is quite simple and straightforward but tedious, this is the reason why we will only explain the procedure here and write down the results of interest.

Basically, what we have to do is simply to write down the solutions in both regimes and apply some matching conditions at $\tau = \tau_1$.

Although we will compute Q_k in this appendix, the matching conditions are better understood if we use the comoving curvature perturbation $\mathcal{R}_k$, for which the MS equation takes a very simple form (see (2.61)), in conformal time τ we can write :

$$\frac{1}{a^2\epsilon_1}\frac{d}{d\tau}\left(a^2\epsilon_1\frac{d\mathcal{R}}{d\tau}\right) + k^2\mathcal{R} = 0\,. \tag{A.12}$$

For the first matching condition we will obviously impose the continuity of the $\mathcal{R}_k$ i.e.

$$\lim_{\tau\to\tau_1^-}\mathcal{R}_k = \lim_{\tau\to\tau_1^+}\mathcal{R}_k\,. \tag{A.13}$$

Now, the second matching condition straightforwardly follows form inserting (A.13) into (A.12). Taking into account that both a and ϵ_1 are continuous at $\tau = \tau_1$ we have

$$\lim_{\tau\to\tau_1^-}\frac{d\mathcal{R}_k}{d\tau} = \lim_{\tau\to\tau_1^+}\frac{d\mathcal{R}_k}{d\tau}\,. \tag{A.14}$$

The solution for the SR region will be the one that we got in section 2.2.1.1 using the Bunch-Davies vacuum as initial condition, i.e. (2.87) with $\nu = \frac{3}{2}$:

$$\mathcal{R}_k^{SR} = \frac{e^{-ik\tau}\bar{H}_0}{2\sqrt{\epsilon_1^0}M_{PL}k^{3/2}}\left(i - k\tau\right)\,. \tag{A.15}$$

On the other hand, the solution in the CR region is a more general solution where no vacuum is imposed i.e.

$$\mathcal{R}_k^{CR} = \frac{H\tau\sqrt{-\tau}}{M_{PL}\sqrt{2\epsilon_1^{CR}(\tau)}}\left(C_1(k)H_\nu^{(1)}(-k\tau) + C_2(k)H_\nu^{(2)}(-k\tau)\right)\,, \tag{A.16}$$

where $\epsilon_1^{CR}(\tau)$ is given by (A.11).

We can now apply the matching conditions (A.13) and (A.14) and obtain the constants $C_1(k)$ and $C_2(k)$, the solution for Q_k^{CR} will then be

$$Q_k^{CR} = -H\tau\sqrt{-\tau}\left(C_1(k)H_\nu^{(1)}(-k\tau) + C_2(k)H_\nu^{(2)}(-k\tau)\right)\,. \tag{A.17}$$

The expressions for $C_1(k)$ and $C_2(k)$ are very cumbersome so we will not write them here. We will only study some of its most interesting limits:

- It is important to remark that the approximation taken in this appendix, in which ϵ_2^{CR} might have some time dependence, allow us to study smoother transitions than the ones usually studied in the literature. We can then distinguish two limiting cases for completely sharp or very smooth transitions
  - If $\epsilon_2^{CR}\big|_{\tau_1}$ is set to be the final value in which we want ϵ_2 to saturate, i.e. $\epsilon_2^{CR}\big|_{\tau_1} = -3 - 2\nu^{CR}$, then we are in the limit of sharp transition in which ϵ_2 is of the form of

(A.2). This case is widely studied in the literature and our results for Q_k^{CR} perfectly match the well known results [100].

- If, on the other hand, we set $\epsilon_2^{CR}\big|_{\tau_1} \simeq 0$ (not exactly zero because in some case we would not have a transition), then we are making ϵ_2 in (A.6) an almost continuous function, which is the case studied in [101].

- Apart from the limits regarding the value of $\epsilon_2^{CR}\big|_{\tau_1}$, we also have different limiting cases in the evolution of Q_k^{CR} according to where are the modes with respect to the Hubble radius when the transition occurs at τ_1:

  - For the modes which are deep in the horizon when the transition occurs i.e. $-k\tau_1 \to \infty$ we recover the same result as if we were using the Bunch-Davies vacuum in the CR phase i.e. the result from (2.86).
  - For the modes which are already well outside the horizon when the transition occurs i.e. $-k\tau \lesssim -k\tau_1 << 1$ (remember that we need $\tau > \tau_1$ to use the CR solution of (A.17)) we have the following behaviour.

$$Q_k^{CR} \simeq i\frac{\bar{H}_0}{4\nu\sqrt{2}k^{3/2}} \left(\left(3+\epsilon_2^{CR}\big|_{\tau_1}+2\nu^{CR}\right)\left(\frac{\tau}{\tau_1}\right)^{\frac{1}{2}\left(3-2\nu^{CR}\right)} - \left(3+\epsilon_2^{CR}\big|_{\tau_1}-2\nu^{CR}\right)\left(\frac{\tau}{\tau_1}\right)^{\frac{1}{2}\left(3+2\nu^{CR}\right)}\right). \tag{A.18}$$

This is the regime that we wanted to remark in this appendix because it makes very clear the point that something that is decaying is not always $k-$suppressed. For example, in the sharp SR-USR transition in which $\nu^{CR} = \frac{3}{2}$ and $\epsilon_2^{CR}\big|_{\tau_1} = -6$ we have

$$Q_k^{USR} \simeq i\frac{\bar{H}_0}{\sqrt{2}k^{3/2}}\left(\frac{\tau}{\tau_1}\right)^3 = \frac{\bar{H}_0}{\sqrt{2}k^{3/2}}e^{-3(N-N_1)}\,. \tag{A.19}$$

  - There are many others intermediate regimes that depend on the specific form of $C_1(k)$ and $C_2(k)$ and that generate some very important features in the power spectrum, such as the famous k^4-growth [100]. We will not enter into these regimes because they have been widely studied and the main point of this appendix was the behaviour of (A.18)

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