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Wheeler-DeWitt equation and corrections to the inflationary spectrum

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The important thing is not to stop questioning. Curiosity has its own reason for existing. One cannot help but be in awe when one contemplates the mysteries of eternity, of life, of the marvellous structure of reality. It is enough if one tries to comprehend only a little of this mystery every day.

Albert Einstein

Abstract

In this thesis, within the context of the Wheeler-deWitt (WdW) equation, the quantisation of a minimally coupled inflaton field with constant potential is studied. This model captures significant features of the inflationary evolution. A Gaussian superposition of exact solutions to the homogeneous WdW equation is therefore taken into consideration, and the total wave function of the universe is formally obtained. Such a wave function naturally extends the semiclassical approach. We find interesting features of this state and, more importantly, we show that it may leave imprints in the inflationary power spectrum not present in the standard approach.

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Introduction

What happened at the beginning of the universe?

It is a very interesting question, because it deals with the initial physical state of the universe, and it opens a proving ground for high-energy physics. Most probably, until we have no observational evidence of it, a final answer cannot be given. Cosmic inflation, which consists in an accelerated expansion of space in the firsts instants of the universe, is widely accepted by the scientific community as an early phase of the universe, preceding the hot big bang [1, 2, 3]. Indeed, even though solid evidence of inflation is still missing, it naturally solves several fine-tuning problems that otherwise one must explain without postulating it. The mathematical framework of inflation was developed starting from a homogeneous scalar inflaton-gravity system. Subsequently, small perturbations around such a background and obeying the Mukhanov-Sasaki equation [4, 5] were taken into account. The standard approach to inflation is based on quantum field theory (QFT) in curved space-times [6, 7, 8], in particular, the homogeneous part of the system follows the classical evolution, while the perturbations are treated quantum mechanically. This semiclassical framework explains how the classical perturbations we observe today are generated at the end of inflation by quantum vacuum fluctuations. In fact, if one assumes an initial vacuum state in the quantum theory of the inflationary perturbations, due to the background dynamics, quantum excitations appear. These post-inflationary perturbations can then be connected with the anisotropies of the Cosmic-Microwave-Background (CMB), which is part of the radiation emitted when the universe had 300.000 years. In-

flation occurred very early and the energy involved is expected to be very large, up to the Planck energy or even higher. At such energies, classical general relativity and thus the description in terms of QFT on curved space-times is expected to break. A theory of quantum gravity should better describe what happened at the very beginning of the universe, however, it is still missing [9].

Canonical quantum gravity, which consists in expressing the matter-gravity system in the canonical formalism and then quantise it, is one of the earliest attempts to combine general relativity with quantum mechanics [10]. When applied to inflation, the canonical quantisation is applied to both homogeneous inflaton-gravity variables and the perturbations [11, 12, 13, 14, 15, 16]. A classical constraint equation then becomes the quantum equation that determines the wave function of the universe and it is called Wheeler-deWitt (WdW) equation. The WdW equation is generally not exactly solvable, apart from a few simplified cases, and a series of approximations are required to deal with it. One common approach consists in decomposing the wave function of the universe by the Born-Oppenheimer method, which separates the slow degrees of freedom (gravity) from the fast ones (matter) [17]. At this point, one obtains a system of two equations for the wave function describing the homogeneous variables and the infinite set of perturbations. The gravitational equation is still generally not solvable, and a WKB approximation of the gravitational wave function can be adopted. Such an approximation is justified by the expected semiclassical behaviour of the gravitational sector. Following this approximation, one can then introduce a time parametrisation for the evolution of the matter system, in particular, one obtains Schrödinger-like equations for the perturbations. If one then ignores the non-adiabatic terms suppressed as m_P^{-2} , the exact Schrödinger equations corresponding to the Mukhanov-Sasaki ones emerge. In this sense, canonical quantum cosmology can generalise the standard quantum perturbations theory, taking into account also the quantum evolution of the homogeneous background. Small corrections in the power spectra of inflationary perturbations are then obtained if one considers this

generalisation.

In this context, one expects that wave packets describing the homogeneous degrees of freedom should give corrections to the inflationary spectra. The original work of this thesis consists in the study of these corrections. The simplified model is that of an inflaton scalar field, minimally coupled to gravity, with a flat potential. This model predicts a non-realistic never ending inflationary evolution, but nevertheless, it captures several features of the inflationary dynamics. Moreover, a piecewise flat potential has been considered as a candidate for producing primordial black holes as dark matter. The homogeneous wave function is considered as a Gaussian packet, this choice reproduces a dynamics close to the classical one but with quantum variables. Finally, the calculation of how the quantum wave packet influences the observable power spectrum is presented.

The thesis is divided into three chapters:

Chapter 1: The standard model of cosmology is presented. In particular, the inflationary model is described within the framework of quantum perturbations on top of a classical background. The connection between this approach and some observable is also shown.

Chapter 2: Canonical quantisation of the inflaton-gravity system is described as the expected correct framework, in which some small deviations in the power spectra enter the scene.

Chapter 3: The specific model of canonical quantisation of the inflaton field with constant potential is presented as the original part of the thesis. This chapter shows how an exact quantum solution to the WdW equation gives corrections to the inflationary power spectrum.

Chapter 1

Standard cosmology

Since the seventeenth century, we have modeled the physical systems that we observe, such as the dynamics of an object, with mathematical frameworks. This procedure turns out to be extremely efficient; in fact, different observations of similar systems can be modeled by the same theory that predicts measurements with a sufficiently small error. A theoretical Physicist is mostly interested in understanding these theories, in particular how much the current theories agree with observations and if some better theories can be formulated.

The current mathematical framework that we use to describe the gravitational systems is differential geometry, and the corresponding physical theory is General Relativity. Space and time are modeled as a differentiable manifold $\mathcal{M}$ in which a metric tensor $g_{\mu\nu}$ is defined, it is a key ingredient in this theory; indeed, we can predict the dynamics of 'free falling' objects from it or describe physical systems on top of the background of gravity. The first goal of a specific gravitational model is then to derive the metric tensor, given a specific stress energy tensor $T_{\mu\nu}$, the object that, in principle, fully characterizes the gravitational content. The most successful general relativistic theory so far is Einstein's

theory of gravity, given in terms of the following Einstein's equations

$$R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = 8\pi GT_{\mu\nu} \quad (1.1)$$

with $R_{\mu\nu}$ the Ricci tensor, R the Ricci scalar, G is the Newton constant, $g_{\mu\nu}$ the metric tensor and $T_{\mu\nu}$ the stress energy tensor; in a generic coordinate system, and in four space-time dimensions, with $\mu, \nu = 0, 1, 2, 3$.

This thesis falls into the line of research whose ultimate goal is to accurately understand what happened at the very beginning of the universe.

In this first chapter, the standard picture of theoretical Cosmology is presented, the Manifold $\mathcal{M}$ is the entire universe, while the metric is obtained by solving the Einstein's equations (1.1), from the matter content $T_{\mu\nu}$ that we observe or more generally, take into consideration. Firstly, we will explain the Λ CDM model, and its shortcomings. Secondly, we shall explain how we can solve the Λ CDM puzzles by hypothesizing Cosmic Inflation. Finally we should see how inflation and the cosmological perturbation theory can help us in understanding structures formations and the inhomogeneities of the Cosmic Microwave Background and, we will explain how these perturbations can be generated as a quantum effect at the very beginning of the universe.

1.1 The standard model of the universe

1.1.1 Symmetries of the model

The first consideration we make is about the matter content of the universe. We model it with a simple shape; in this way it is manageable mathematically but at the same time sufficiently accurate with respect to the real world.

In practice, we follow the

COSMOLOGICAL PRINCIPLE

The universe is homogeneous and isotropic.

If there is a matter content with these symmetries, the metric tensor also enjoys them. Some motivations can be given that lead us to this choice: for example, the fact that at very large scales we see an isotropic universe, if we look very far away the amount of galaxies in a given solid angle is independent of the direction; the isotropy is much more precise (to about one part in 10^{-5}) in the cosmic-microwave background. Then, by following the

COPERNICAN PRINCIPLE

We are not a preferred observer in the universe

we can mathematically derive that the metric should also be homogeneous, hence follow the Cosmological principle. The most general homogeneous and isotropic metric is the **Friedmann–Lemaître–Robertson–Walker (FLRW) metric**,

$$ds^2 = dt^2 - a(t)^2 \left[\frac{dr^2}{1 - kr^2} + r^2(d\theta^2 + \sin^2 \theta d\phi^2) \right] \quad (1.2)$$

with $r \in [0, \infty]$, $t \in [-\infty, +\infty]$, $\theta \in [0, \pi]$, $\phi \in [0, 2\pi]$, $a(t)$ scale factor, a general function of time and $k = 0, \pm 1$. It is a specific choice of the chart adapted to observers comoving with the cosmic fluid, they are freely falling and described simply by fixed space coordinates r, θ, ϕ .

$k = 0, +1, -1$ correspond respectively to a spatially flat closed and open universe; the scale factor measures the distances at a given time.

The energy-momentum tensor of the (perfect) fluid takes the form

$$T^\mu{}_\nu = \text{diag}(\rho, -p, -p, -p) \quad (1.3)$$

where $p = p(t)$ is the pressure and $\rho = \rho(t)$ the energy density. For simplicity, we start by

considering a single type of cosmic fluid. The tensor $T^\mu{}_\nu$ satisfies the continuity equation

$$\nabla_\mu T^\mu{}_\nu = 0, \quad (1.4)$$

where ∇_μ is the covariant derivative. The equation $\nu = 0$ reads

$$\nabla_\mu T^\mu{}_0 = 0 \quad \Longrightarrow \quad \dot{\rho} + 3H(\rho + p) = 0. \quad (1.5)$$

Moreover, an equation of state for the fluid must be assumed

$$p = w \rho, \quad (1.6)$$

so that, with a specific and constant w , the following relation holds

$$\rho(a) \propto a^{-3(1+w)}. \quad (1.7)$$

This equation relates the energy density of a cosmic fluid with the scale factor, it will be useful in the realistic model that will be presented later on.

1.1.2 The dynamics of the metric

The 00 component of Einstein's equation is

$$G_{00} = 8\pi G_N T_{00} \quad \Longrightarrow \quad 3 \left(\frac{\dot{a}}{a} \right)^2 + \frac{3k}{a^2} = 8\pi G_N \rho \quad (1.8)$$

and is called **Friedmann equation**. The other equations: $G_{ii} = 8\pi G_N T_{ii}$ are satisfied by imposing the validity of the Friedmann equation at all times; thus the system is fully characterized by the two Eqs. (1.5,1.8).

The density parameter is defined as $\Omega \equiv \frac{8\pi G}{3H^2} \rho \equiv \frac{\rho}{\rho_{\text{crit}}}$, where $H = \frac{\dot{a}}{a}$ is the Hubble

parameter. The Eq. (1.8) can thus be written as

$$\Omega - 1 = \frac{k}{H^2 a^2} \quad (1.9)$$

and the following conclusions can be drawn

- $\rho < \rho_{\text{crit}} \iff \Omega < 1 \iff k = -1 \iff$ Open universe,
- $\rho = \rho_{\text{crit}} \iff \Omega = 1 \iff k = 0 \iff$ Flat universe,
- $\rho > \rho_{\text{crit}} \iff \Omega > 1 \iff k = +1 \iff$ Closed universe.

1.1.3 The Λ CDM model

In order to construct a realistic model for the universe evolution, we simultaneously consider the presence of different cosmic fluids, each one with its own equation of state. Then, the total energy-momentum tensor is given by the sum of the single tensors of the different cosmic fluids $T_{\nu}^{\mu}{}_{\text{tot}} = \sum_i T_{\nu}^{\mu}{}_{(i)} = \text{diag}\left(\sum_i \rho_i, \sum_i -p_i, \sum_i -p_i, \sum_i -p_i\right)$, where $\rho_i = \rho_i(t)$ and $p_i = p_i(t)$ is the density and pressure of the i -th fluid.

The Λ CDM model accounts for three different cosmic fluids:

- **Matter(dust)** with equation of state $w_m = 0$. It is considered as the ordinary Barionic matter that we observe in the universe, plus the so called **Cold Dark Matter(CDM)**, a fluid that gravitationally interacts as dust but whose origin is still not understood;
- **Radiation** with equation of state $w_r = \frac{1}{3}$;
- **Dark energy** with equation of state $w_{\Lambda} = -1$, which could explain the accelerated expansion that we observe today.

The total energy density is then

$$\rho_{\text{tot}} = \rho_m + \rho_r + \rho_\Lambda. \quad (1.10)$$

The observations seem to indicate a **flat universe**, and thus

$$\Omega_{\text{tot}}(t_0) \equiv \frac{\rho_{\text{tot}}(t_0)}{\rho_{\text{crit}}(t_0)} \simeq 1 \quad (1.11)$$

In particular we measure

$$\begin{aligned} \Omega_{r,0} &\simeq 9 \times 10^{-5}, \\ \Omega_{m,0} &\simeq 0.315, \\ \Omega_{\Lambda,0} &\simeq 0.685, \\ H_0 &\simeq 67.4 \text{ km s}^{-1} \text{ Mpc}^{-1}, \\ \Omega_{\text{tot},0} &= \Omega_{r,0} + \Omega_{m,0} + \Omega_{\Lambda,0} \simeq 1. \end{aligned}$$

The subscript 0, stands for the fact that these measurements refer to the values we observe today at t_0 . For the specific cosmic fluids in the Λ CDM model Eq. (1.7) becomes

$$\begin{aligned} \Omega_r &= \Omega_{r,0} \left(\frac{a}{a_0} \right)^{-4} \left(\frac{H_0}{H} \right)^2, \\ \Omega_m &= \Omega_{m,0} \left(\frac{a}{a_0} \right)^{-3} \left(\frac{H_0}{H} \right)^2, \\ \Omega_\Lambda &= \Omega_{\Lambda,0} \left(\frac{H_0}{H} \right)^2. \end{aligned}$$

The Friedmann Eq. (1.9), takes the form

$$H_0^2 \left[\Omega_{r,0} \left(\frac{a}{a_0} \right)^{-4} + \Omega_{m,0} \left(\frac{a}{a_0} \right)^{-3} + \Omega_{\Lambda,0} \right] = H^2, \quad (1.12)$$

with $k = 0$. This is a first order differential equation for the scale factor $a(t)$, it cannot be

solved exactly in closed form with simple elementary functions, but it can be integrated numerically. The intuition of this result is rather remarkable, by measuring some observable of our current universe (at a time t_0), we can obtain the evolution of the universe in the past.

1.1.4 Behavior in Different Eras

From Eq.(1.12), one observes that the universe evolves through 3 different regimes:

- **Early universe (radiation-dominated):**

$$\Omega_r \gg \Omega_m, \Omega_\Lambda \quad \Rightarrow \quad a(t) \propto t^{1/2}.$$

The universe is governed by radiation, and **begins expanding** when $t \rightarrow 0$ and $a(t) \rightarrow 0$. If the Λ CDM model and GR are valid in such a limit, the evolution encounter a physical singularity. In that limit, however, one expects that the predictability of General relativity breaks down, we can still say that the model predicts a time in which the universe was extremely dense and hot, corresponding to the **Hot Big-bang**.

- **Intermediate era (matter-dominated):**

$$\Omega_m \gg \Omega_r, \Omega_\Lambda \quad \Rightarrow \quad a(t) \propto t^{2/3}.$$

The universe is governed by matter

- **Late universe (cosmological constant-dominated):**

$$\Omega_\Lambda \gg \Omega_r, \Omega_m \quad \Rightarrow \quad a(t) \propto e^{H_\Lambda t}$$

where $H_\Lambda = H_0\sqrt{\Omega_{\Lambda,0}}$. The universe is governed by dark energy and evolves with an accelerated expansion.

1.2 Problems in the Hot Big-Bang theory

Now that we have a specific model of the universe, we can compute, in principle, all the needed physical quantities. But, there are two big fine tuning problems in the Hot Big Bang/ Λ CDM theory; they are called flatness and horizon problem.

1.2.1 The flatness problem

We said that the current observations suggest that we live in a nearly flat universe, but, how can the universe evolve toward flatness in the Λ CDM model?

The Λ CDM model predicts a flat universe only if the density parameter is exactly 1 at all times, not only today

$$\Omega_{tot}(t) = 1. \quad (1.13)$$

An exact flat universe would be quite odd, it would mean that among all possible values of energy densities the universe has exactly chosen the critical value at all times.

Let us assume the possibility of having a generic density parameter today $\Omega_{tot}(t_0)$ and wonder its value in the past. The Friedmann Eq. (1.9) expressed in terms of the density parameter is

$$\frac{\Omega_{tot}(t) - 1}{\Omega_{tot}(t_0) - 1} = \frac{(a(t_0)H(t_0))^2}{(a(t)H(t))^2}. \quad (1.14)$$

The matter contents of the universe that dominated the past eras (matter and radiation) are responsible for an evolution with $\frac{1}{(a(t)H(t))}$, which is called **comoving Hubble radius**, that increases with time. This property can be shown by finding the comoving Hubble radius from the Friedmann equation, for simplicity during matter or radiation domination. For earlier and earlier times, the energy density gets closer to the critical value. If one

roughly estimates the Eq. (1.14) at the Planck scale

$$\begin{aligned}\frac{1}{T} &\propto a, \\ H(t_i) &\sim M_{\text{P}}, \\ T_i &\sim T_{\text{P}}, \\ T_0 &\simeq 2.7K, \\ H_0 &\simeq 10^{-60}M_P,\end{aligned}$$

the corresponding value of $\Omega_{\text{tot}}(t_i) - 1$ can be found to be

$$\Omega_{\text{tot}}(t_i) - 1 = (\Omega_{\text{tot}}(t_0) - 1) \frac{T_0}{H_0} \simeq (\Omega_{\text{tot}}(t_0) - 1) 10^{-58}. \quad (1.15)$$

This result clearly denotes a fine-tuning problem, since the initial density parameter must have a value extremely close to 1. It means that, if we stick to the Λ CDM model, either we accept this extreme fine tuning problem or try to solve it, for example, by assuming a new matter content that was present initially.

1.2.2 The horizon problem

At about 300.000 years after its beginning, the universe passed from a phase where it was optically "opaque" to a phase where it was optically "transparent", and this occurred when photons could start to propagate freely. This transition occurred when charged electrons and protons first became bound to form electrically neutral hydrogen atoms, this epoch is called recombination. Part of that radiation is still visible today, we call it **Cosmic Microwave Background (CMB)**. We see that radiation in every direction of the sky; it has a **Black-Body spectrum** which indicates that the universe was in thermal equilibrium. The temperature of the spectrum is almost exactly the same in

every direction

$$T_{CMB} = 2.72548 \pm 0.00057 K. \quad (1.16)$$

The relative differences are of order

$$\frac{\delta T}{T} \simeq 10^{-4}, 10^{-5}. \quad (1.17)$$

This is a great fact that confirms the Cosmological principle, assuming the Copernican principle, it means that originally the universe was extremely homogeneous and isotropic. However, within our current Λ CDM model, the space-time points that emitted the CMB with sufficiently different directions in the sky, were not in causal contact in their past.

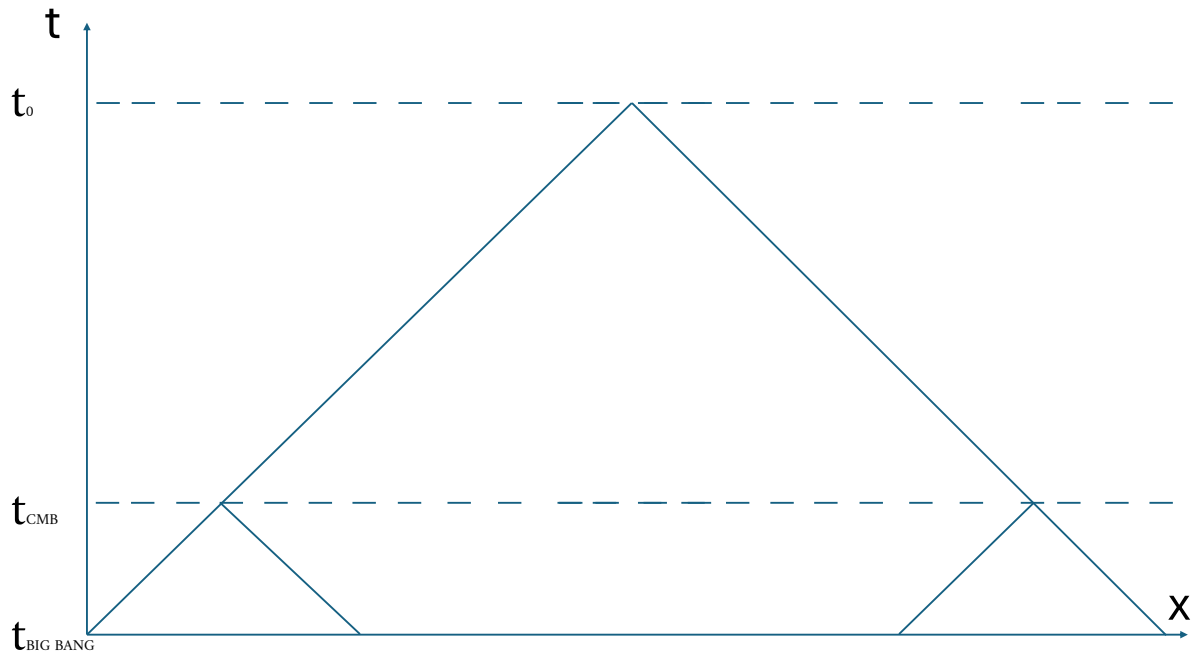


Figure 1.1: Pictorial representation of the horizon problem. The observer is located at the apex of the triangle. The two edges are the observed photons propagated along opposite directions; at the time of recombination, t_{CMB} , their past light cones did not intersect.

How is it possible that the CMB is extremely homogeneous, but it was originated in causally disconnected regions? This is called the horizon problem. The horizon problem

can be formally illustrated, by considering the radial light motion, in the flat case (one could derive an analog result also in the other cases). The following relation applies

$$dr = \frac{dt}{a(t)}. \quad (1.18)$$

From the Friedmann Eq. (1.12) follows

$$r(t_f; t_i) = \int_{a(t_i)}^{a(t_f)} \frac{da}{a^2 H_0 \sqrt{\Omega_{r,0} \left(\frac{a_0}{a}\right)^4 + \Omega_{m,0} \left(\frac{a_0}{a}\right)^3 + \Omega_{\Lambda,0}}}. \quad (1.19)$$

This function is the **comoving horizon**, it expresses the distance that light can travel from time t_i to time t_f . One can compute this integral numerically. In particular, if we calculate it between the initial time (Big-bang) and the time of recombination $r(t_{rec}; t_i)$, and between recombination and today $r(t_0; t_{rec})$, we have

$$\Delta\theta = \frac{r(t_{rec}; t_i)}{r(t_0; t_{rec})} \quad (1.20)$$

which is half the minimum angle between two directions pointing toward causally disconnected regions. The solid angle in the sky where the CMB could have been in causal contact in the past is then

$$\Delta\Omega = \pi(\Delta\theta)^2.$$

The correct numerical calculation leads to

$$\Delta\Omega \simeq 0.00127 sr, \quad (1.21)$$

it means that there are $\frac{4\pi}{0.00127} \simeq 10^4$ different causally disconnected patches in the CMB. Some intuition can be gained about this problem, looking at the single fluid generic case. We obtain the following:

$$a^{3/2(1+w)} \propto t, \quad (1.22)$$

then

$$dt/a = 3/2(1+w)a^{3/2(1+w)-2}da,$$

and finally

$$r(t_f; t_i) = \frac{3(1+w)}{1+3w} (a(t_f)^{1/2(1+3w)} - a(t_i)^{1/2(1+3w)}). \quad (1.23)$$

For the cases where $w > -1/3$, the comoving horizon is proportional to $a^k(t_f) - a^k(t_i)$ with $k > 0$, it grows with time for fixed t_i ; whereas for $w < -1/3$ the comoving horizon is proportional to $\frac{1}{a^k(t_i)} - \frac{1}{a^k(t_f)}$ with $k > 0$, it diverges in the limit $a(t_i) \rightarrow 0$ for any t_f . In the Λ CDM model the initial eras of the universe were dominated by matter and radiation, so they correspond to the $w > -1/3$ case and the model has slowly increasing comoving horizon, which leads to disconnected patches, as we have seen. On the other hand, if for some reason, initially the universe was dominated by a fluid with $w < -1/3$ we would have found a comoving horizon that increases and thus could possibly solve the horizon problem.

1.3 Cosmic Inflation

The previous problems can be formally solved by hypothesizing that at the very beginning of the universe cosmic inflation occurred. Cosmic inflation is the first stage of the universe; dominated by some form of matter that generates an accelerated expansion. After inflation one assumes that the Λ CDM model starts, beginning with the radiation era (Hot big-bang). This solution to the problems is currently largely accepted by the scientific community, although we still have no direct confirmation of inflation.

We will walk through this idea and see how this hypothesis solves the big-bang problems. Let us note that the flatness problem arises because of the increasing comoving Hubble radius $\frac{1}{(a(t)H(t))}$, while the horizon problem arises because the dynamics is initially governed by a fluid with $\omega > -1/3$. If we consider a general fluid w (for simplicity let $k = 0$),

combining the Friedmann Eq. (1.8) with the continuity Eq. (1.7) we get

$$H \propto a^{-\frac{3}{2}(1+w)}, \quad (1.24)$$

so that the comoving Hubble radius evolves according to

$$\frac{1}{aH} \propto a^{\frac{1}{2}(1+3w)}, \quad (1.25)$$

and it decreases in time if

$$\frac{d}{dt} \frac{1}{aH} < 0 \iff w < -1/3. \quad (1.26)$$

Moreover, it can be shown that the two conditions (1.26) are equivalent to

$$\ddot{a} > 0.$$

Therefore both problems can be solved by assuming the existence of an initial stage of the universe evolving in an accelerated way for a sufficiently long time, dominated by a cosmic fluid with $w < -1/3$. Clearly, a generic accelerated expansion is not a condition that completely fix the dynamics, we still have the freedom of choosing many different mechanisms giving rise to inflation.

1.3.1 Duration of inflation

The flatness problem is solved only for a sufficient duration of the inflationary expansion, that also addresses the horizon problem. As we already said, if we don't postulate a flat universe, we must consider an initial density curvature of order 1

$$\frac{(a(t_0)H(t_0))^2}{(a(t_i)H(t_i))^2} \simeq \frac{1}{\Omega_{\text{tot}}(t_0) - 1}. \quad (1.27)$$

In other terms

$$\left(\frac{a(t_0)}{a(t_{end})}\right)^2 \left(\frac{a(t_{end})}{a(t_i)}\right)^2 \left(\frac{H(t_0)}{H(t_{end})}\right)^2 \left(\frac{H(t_{end})}{H(t_i)}\right)^2 (\Omega_{\text{tot}}(t_0) - 1) \simeq 1, \quad (1.28)$$

where t_{end} stands for the time when inflation ends and t_i when it starts. If inflation is driven by a single fluid with equation of state w , from (1.24) we get the following relation

$$\frac{\dot{H}}{H^2} = -\frac{3}{2}(1 + \omega) \begin{matrix} \omega < -1/3 \\ > \end{matrix} -1. \quad (1.29)$$

Defining $\epsilon = -\frac{\dot{H}}{H^2}$ as the **first slow-roll parameter**, we then obtain

$$0 < \epsilon < 1 \iff \ddot{a} > 0.$$

Following (1.29), during inflation, we can assume that the rate of change of the Hubble parameter is not large

$$\left(\frac{H(t_{end})}{H(t_i)}\right)^2 \simeq 1.$$

We are then left only with the choice of the Hubble scale during inflation and its duration, with condition (1.28). For typical values of the Hubble parameter one has

$$\frac{H(t_0)}{H(t_{end})} \simeq 10^{-53}.$$

On the other hand, the final state of inflation, that corresponds to the initial state of the Λ CDM evolution, is given by

$$\frac{a(t_0)}{a(t_{end})} \simeq 10^{28}. \quad (1.30)$$

The duration of inflation is thus

$$\frac{a(t_{end})}{a(t_i)} \simeq 10^{26}. \quad (1.31)$$

The **e-folding number**, N , is defined by

$$a \equiv e^N, \quad (1.32)$$

and in terms of N , Eq. (1.31) becomes

$$N_{end} - N_i \simeq 60, \quad (1.33)$$

which is a quite known result. Moreover, since inflation must last long enough, the condition

$$|\eta_H| \equiv \left| \frac{\dot{\epsilon}}{H \epsilon} \right| < 1 \quad (1.34)$$

must be satisfied, where η_H is the **second slow-roll parameter**.

1.3.2 Inflaton field

We should ask ourselves what kind of matter generates inflation. The inflaton matter is the dominant type of matter present during inflation and its energy density is the leading one with respect to the other cosmic fluids (from Eq. 1.7). Moreover, there should exist a mechanism that explains how the ordinary matter is generated after inflation. The chosen matter content which drives inflation is often considered as the inflaton scalar field, which can describe how particles are generated afterwards. Let us consider a single scalar field $\phi = \phi(t)$ spatially homogeneous and isotropic, minimally coupled to gravity

$$S = \int d^4x \sqrt{-g} \left[-\frac{1}{16\pi G} R + \frac{1}{2} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - V(\phi) \right]. \quad (1.35)$$

where the dynamics is essentially determined by the shape of the potential and the initial conditions of the inflaton field. The explicit equations of motion of the inflaton-gravity system can be calculated by varying the action. The metric is flat (for simplicity) and of

FRWL type:

$$ds^2 = dt^2 - a^2(t)(dx^2 + dy^2 + dz^2). \quad (1.36)$$

Then the action then takes the following form

$$S = \frac{1}{2}L^3 \int dt \left[-\frac{6a\dot{a}^2}{8\pi G_N} + a^3\dot{\phi}^2 - 2a^3V(\phi) \right] \quad (1.37)$$

with $L^3 = \int d^3x$. The continuity equation $\nabla_\mu T^\mu_0 = 0$ gives

$$\ddot{\phi} + 3H\dot{\phi} + V'(\phi) = 0, \quad (1.38)$$

with $V'(\phi) = \frac{dV(\phi)}{d\phi}$. The Friedmann equation is

$$H^2 = \frac{8\pi G_N}{3} \left(\frac{1}{2}\dot{\phi}^2 + V(\phi) \right). \quad (1.39)$$

The condition for inflation to occur is $\epsilon \leq 1$

$$\epsilon \equiv -\frac{\dot{H}}{H^2} = \frac{4\pi G \dot{\phi}^2}{H^2}, \quad (1.40)$$

$$\epsilon \ll 1 \iff \dot{\phi}^2 \ll V(\phi). \quad (1.41)$$

Conditions (1.41) and $\eta_H \ll 1$ are called **slow roll conditions**, since the velocity of the field is small (compared to the potential) and must remain small for ~ 60 e-folds. In the slow roll approximation, the dynamical equations take the form

$$3H\dot{\phi} \simeq -V'(\phi), \quad (1.42)$$

$$H^2 \simeq \frac{8\pi G_N}{3} V(\phi). \quad (1.43)$$

One can often solve these equations analytically and obtain the inflationary evolution as solution. We next consider the two main categories of inflation: large and small field inflation.

1.3.3 Different types of inflation

During inflation the field velocity satisfies

$$\dot{\phi}^2 \ll V(\phi),$$

and inflation ends when

$$\dot{\phi}^2 \simeq V(\phi).$$

If the number of e-foldings is close to 60, we can say that the model under consideration is compatible with inflation.

Large Field

A model of inflation is called "large field" when $\Delta\phi$, the difference between the value of the field at the beginning and at the end of inflation, is larger than the Planck mass. A typical example of large field inflation is given by monomial potentials

$$V(\phi) = \lambda\phi^n. \tag{1.44}$$

From Eq. (1.40), using the approximations (1.42-1.43) we get

$$\epsilon \ll 1 \iff \phi \gg \sqrt{\frac{n^2}{4} \frac{1}{8\pi G}} \equiv \frac{n}{\sqrt{2}} M_P. \tag{1.45}$$

Inflation starts at $\phi_{in} \gg \frac{n}{\sqrt{2}}M_P$, one sets ϕ_{in} such that when it reaches ϕ_{end} , $N \simeq 60$ occurred, after some calculation one could find the following

$$\Delta\phi > M_P. \quad (1.46)$$

Small Field

In contrast, an inflaton model is "small field" when

$$\Delta\phi < M_P. \quad (1.47)$$

Some typical potentials, leading to "small field" inflation are

$$V(\phi) = V_0(1 - \alpha e^{-k\phi})^2. \quad (1.48)$$

Let us recap the overall picture; we said that inflation occurred at the beginning of the universe, nevertheless we are not completely satisfied, because there is no direct observational evidence for it, and even if it happened, we do not have a specific inflation's dynamic. The Cosmological principle well describes the early universe because the CMB is extremely homogeneous. However, the CMB is not exactly isotropic, and the temperature slightly differs, with relative differences of order $\frac{\delta T}{T} \simeq 10^{-4}, 10^{-5}$. Moreover the homogeneous FLRW solution cannot account for the structures observed in the universe. We can thus improve our knowledge of the early universe by considering also inhomogeneities in the model. A viable inflationary model must predict the observed features (anisotropies) of the CMB, and inhomogeneities in the large scale structures. We shall then begin also considering the evolution of the perturbations in the metric tensor and energy momentum tensor.

1.4 Cosmological perturbations

Fortunately, primordial inhomogeneities are expected to be tiny, meaning that we can consider small perturbations and expand to the first order on the homogeneous and isotropic model. When the standard cosmological perturbation theory is presented, one usually splits the problem into a homogeneous part, governed by a homogeneous and isotropic matter content and metric tensor, and the perturbation part, in which there are small perturbations in the matter and background.

1.4.1 Cosmological perturbations of the metric

As a first thing we introduce the description of perturbation in the metric tensor. We henceforth work with the conformal time

$$d\eta = \frac{dt}{a(t)}. \quad (1.49)$$

The perturbed metric is

$$ds^2 = (g_{\alpha\beta}^{(0)} + \delta g_{\alpha\beta}(x^\gamma)) dx^\alpha dx^\beta, \quad |\delta g_{\alpha\beta}| \ll |g_{\alpha\beta}^{(0)}|, \quad (1.50)$$

where the background metric tensor is the flat FRWL metric

$$g_{\alpha\beta}^{(0)} dx^\alpha dx^\beta = a^2(\eta) (d\eta^2 - \delta_{ij} dx^i dx^j). \quad (1.51)$$

The perturbations are assumed to be small, we thus neglect quadratic order in δg . The background enjoys rotational and translational symmetry in the space coordinates. In this way we can decompose the metric perturbations into scalar, vector and tensor per-

turbations under these symmetries.

$$\delta g_{00} = 2a^2 \phi \quad (1.52)$$

$$\delta g_{0i} = a^2 (B_{,i} + S_i), \quad S^i_{,i} = 0 \quad (1.53)$$

$$\delta g_{ij} = a^2 (2\psi \delta_{ij} + 2E_{,ij} + 2F_{(i,j)} + h_{ij}) \quad (1.54)$$

$$\text{with: } F^i_{,i} = 0, \quad h^i_i = 0, \quad h^i_{j,i} = 0, \quad (1.55)$$

where the latin indices take the values 1,2,3.

Scalar perturbations are described by four scalar functions, ϕ , ψ , B , and E . One can verify that they are generated by inhomogeneities in the energy density. They play a central role in cosmology because they can lead to gravitational instabilities, potentially giving rise to the formation of cosmic structures.

Vector perturbations are represented by the two vector fields S_i and F_i . They are associated with the rotational motions of the fluid, they decay rapidly, and are typically negligible from a cosmological perspective.

Tensor perturbations h_{ij} have no Newtonian counterpart. They correspond to gravitational waves, which are intrinsic degrees of freedom of the gravitational field.

To the first order scalar, vector and tensor perturbations are decoupled and thus can be studied separately.

The total degrees of freedom are: four coming from the scalar perturbations, four from the vectorial and two from the tensorial ones; leading to a total of ten. These are not all physical degrees of freedom, since part of them can be removed by a suitable choice of coordinates.

1.4.2 Coordinate transformation

Giving a metric, a new metric that is physically equivalent to the starting one can be obtained by doing a coordinate transformation. All the relevant physical quantities will be the same. Since we are simultaneously dealing with an infinite set of different metrics (1.50), we want to have a systematic way of separating them into different physically inequivalent sets. For each one of such sets we want to choose a unique representative, by ‘fixing the gauge’, i.e. by selecting a particular set of coordinates. We restrict ourselves

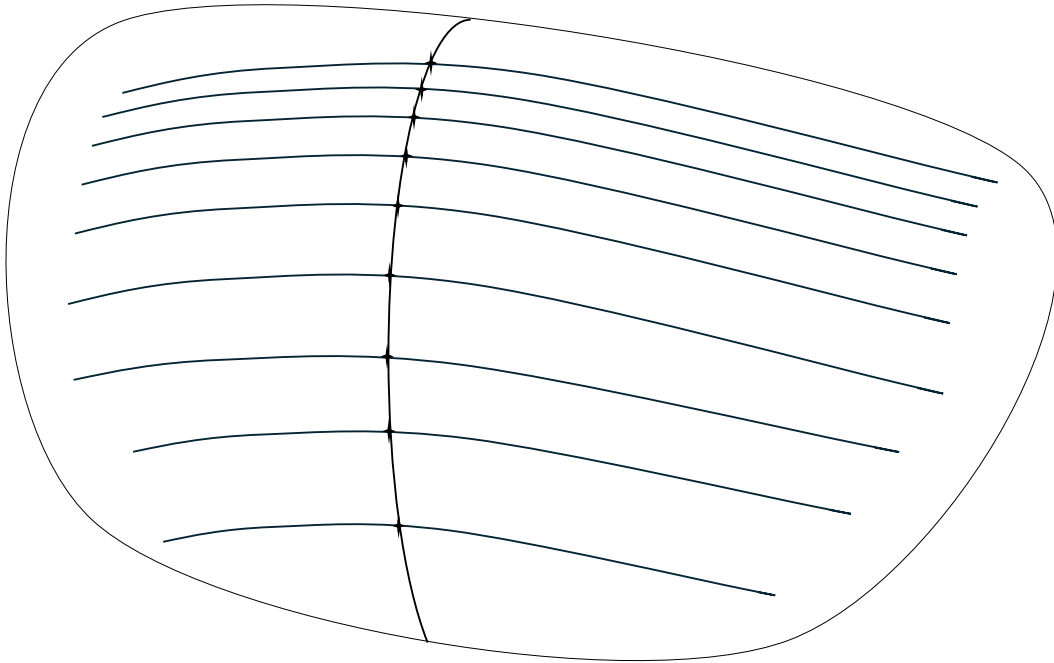


Figure 1.2: *Pictorial representation of the gauge-fixing procedure. The points represent the set of all perturbed metrics described by Eq. (1.50). Each horizontal line corresponds to a class of metrics related by coordinate transformations and therefore physically equivalent. The vertical line represents the gauge-fixing condition, which selects a unique representative from each equivalence class, given by the intersection of the lines.*

to infinitesimally small changes of coordinates, the **diffeomorphisms**

$$x^\alpha \rightarrow \tilde{x}^\alpha = x^\alpha + \xi^\alpha. \quad (1.56)$$

Giving the metrics (1.50), the change coordinates (1.56) leads to the following

$$\tilde{g}_{\alpha\beta}(\tilde{x}^\rho) = \frac{\partial x^\gamma}{\partial \tilde{x}^\alpha} \frac{\partial x^\delta}{\partial \tilde{x}^\beta} g_{\gamma\delta}(x^\rho) \approx g_{\alpha\beta}^{(0)}(x^\rho) + \delta g_{\alpha\beta} - g_{\alpha\delta}^{(0)} \xi^\delta{}_{,\beta} - g_{\gamma\beta}^{(0)} \xi^\gamma{}_{,\alpha}, \quad (1.57)$$

where only the terms linear in δg and ξ are kept. The metric is split into background and perturbation parts

$$\tilde{g}_{\alpha\beta}(\tilde{x}^\rho) = g_{\alpha\beta}^{(0)}(\tilde{x}^\rho) + \delta \tilde{g}_{\alpha\beta}(\tilde{x}^\rho), \quad (1.58)$$

since

$$g_{\alpha\beta}^{(0)}(x^\rho) \approx g_{\alpha\beta}^{(0)}(\tilde{x}^\rho) - g_{\alpha\beta,\gamma}^{(0)} \xi^\gamma, \quad (1.59)$$

the following relation is obtained

$$\delta \tilde{g}_{\alpha\beta} = \delta g_{\alpha\beta} - g_{\alpha\beta,\gamma}^{(0)} \xi^\gamma - g_{\gamma\beta}^{(0)} \xi^\gamma{}_{,\alpha} - g_{\alpha\delta}^{(0)} \xi^\delta{}_{,\beta}. \quad (1.60)$$

The spatial components of the infinitesimal vector ξ^α are written as

$$\xi^i = \xi_\perp^i + \zeta^i, \quad (1.61)$$

with $\xi_\perp^i$ is a 3-vector with 0 divergence, and ζ a scalar function. This implies the following gauge transformation of the metric perturbations

$$\delta \tilde{g}_{00} = \delta g_{00} - 2a(a \xi^0)', \quad (1.62)$$

$$\delta \tilde{g}_{0i} = \delta g_{0i} + a^2 (\xi_i'^\perp + \zeta'_{,i} - \xi_{,i}^0), \quad (1.63)$$

$$\delta \tilde{g}_{ij} = \delta g_{ij} + a^2 \left(2 \frac{a'}{a} \delta_{ij} \xi^0 + 2 \zeta_{,ij} + \xi_{i,j}^\perp + \xi_{j,i}^\perp \right) \quad (1.64)$$

From this result, we can discuss how different types of perturbations behave under a small change of coordinates and then how to fix the gauge.

Scalar perturbations

The scalar perturbations are

$$ds^2 = a^2 \left[(1 + 2\phi) d\eta^2 + 2B_{,i} dx^i d\eta - ((1 - 2\psi)\delta_{ij} - 2E_{,ij}) dx^i dx^j \right], \quad (1.65)$$

these scalar quantities transform as in Eqs. (1.62, 1.63, 1.64) and more explicitly as

$$\tilde{\phi} = \phi - \frac{1}{a}(a\xi^0)', \quad (1.66)$$

$$\tilde{B} = B + \zeta' - \xi^0, \quad (1.67)$$

$$\tilde{\psi} = \psi + \frac{a'}{a}\xi^0, \quad (1.68)$$

$$\tilde{E} = E + \zeta. \quad (1.69)$$

Thus, only ξ^0 and ζ enter the transformations. Different metrics, specified by the four scalar potentials (ϕ, B, ψ, E) , are not all physically inequivalent; indeed, we can perform coordinate transformation, with different ξ^0 and ζ , and end up with different but equivalent metrics. A systematic way to fix the gauge is to choose specific ξ^0 and ζ and for example, eliminate two of the four potentials. If we choose $E = B = 0$ we are dealing with the so called **Conformal Newtonian Gauge**

$$ds^2 = a^2 \left[(1 + 2\phi) d\eta^2 - ((1 - 2\psi)\delta_{ij}) dx^i dx^j \right]. \quad (1.70)$$

Otherwise, we can work with two gauge invariant quantities

$$\Phi \equiv \phi - \frac{1}{a} [a(B - E)']', \quad (1.71)$$

$$\Psi \equiv \psi + \frac{a'}{a}(B - E'), \quad (1.72)$$

which are called Bardeen potentials. This shows that there are only two physical scalar degrees of freedom.

Vector Perturbations

The metric with the vector perturbations takes the form

$$ds^2 = a^2[d\eta^2 + 2S_i dx^i d\eta - (\delta_{ij} - F_{i,j} - F_{j,i})dx^i dx^j] \quad (1.73)$$

and the vectors transform as

$$\tilde{S}_i = S_i + \xi'_{\perp i}, \quad (1.74)$$

$$\tilde{F}_i = F_i + \xi_{\perp i}. \quad (1.75)$$

The gauge invariant quantity is thus

$$\bar{V}_i = S_i - F'_i. \quad (1.76)$$

This shows that only two of the four independent functions of S_i and F_i characterize physical perturbations.

Tensor Perturbations

$$ds^2 = a^2 [d\eta^2 - (\delta_{ij} + h_{ij})dx^i dx^j] \quad (1.77)$$

One could check that the tensor perturbation h_{ij} is already gauge invariant and represents gravitational waves.

We are now able to count the total number of physical degrees of freedom, there are two d.o.f. for each type of perturbation, leading to a total of six.

1.4.3 Linearized Einstein's equations

The evolutions of the perturbations are governed by the linearized Einstein's equations.

The full equations are

$$G_{\beta}^{\alpha} \equiv R_{\beta}^{\alpha} - \frac{1}{2}g_{\beta}^{\alpha}R = 8\pi G T_{\beta}^{\alpha}, \quad (1.78)$$

the Einstein tensor can be expanded as

$$G_{\beta}^{\alpha} = G_{\beta}^{(0)\alpha} + \delta G_{\beta}^{\alpha} + \dots, \quad (1.79)$$

for a metric with small perturbations, with $\delta G_{\beta}^{\alpha}$ denoting the terms linear in the metric perturbations. The energy-momentum tensor can be split in a similar way, and the linearized equations for perturbations are

$$\boxed{\delta G_{\beta}^{\alpha} = 8\pi G \delta T_{\beta}^{\alpha}} \quad (1.80)$$

which are the governing equations for the perturbations. The calculation of the background quantities leads to

$$G_0^{(0)0} = \frac{3\mathcal{H}^2}{a^2}, \quad (1.81)$$

$$G_i^{(0)0} = 0, \quad (1.82)$$

$$G_j^{(0)i} = \frac{1}{a^2}(2\mathcal{H}' + \mathcal{H}^2)\delta_j^i, \quad (1.83)$$

with $\mathcal{H} \equiv \frac{a'}{a}$. One could derive the transformation laws for the perturbations of the energy momentum tensor and verify that the following objects are gauge invariant

$$\delta \bar{T}_0^0 = \delta T_0^0 - \left(T_0^{(0)0} \right)' (B - E') \quad (1.84)$$

$$\delta \bar{T}_i^0 = \delta T_i^0 - \left(T_0^{(0)0} - \frac{T_k^{(0)k}}{3} \right) (B - E')_{,i} \quad (1.85)$$

$$\delta \bar{T}_j^i = \delta T_j^i - \left(T_j^{(0)i} \right)' (B - E'). \quad (1.86)$$

Similarly

$$\delta \bar{G}_0^0 = \delta G_0^0 - \left(G_0^{(0)0} \right)' (B - E') \quad (1.87)$$

$$\delta \bar{G}_i^0 = \delta G_i^0 - \left(G_0^{(0)0} - \frac{G_k^{(0)k}}{3} \right) (B - E')_{,i} \quad (1.88)$$

$$\delta \bar{G}_j^i = \delta G_j^i - \left(G_j^{(0)i} \right)' (B - E'). \quad (1.89)$$

The tensor $\delta \bar{T}_\beta^\alpha$ can be decomposed into scalar, vector and tensor perturbations. Each type of perturbation of the energy-momentum tensor contributes only to the evolution of the corresponding type of metric perturbations. For scalar perturbations, the dynamical Eqs. (1.80) can be expressed in terms of $\delta \bar{G}_\alpha^\beta$ and of the Bardeen potentials (1.71-1.72); the advantage of this formulation is that the evolution equations can be written entirely in terms of gauge invariant variables. After some algebra, one obtains

$$\nabla^2 \Psi - 3\mathcal{H}(\Psi' + \mathcal{H}\Phi) = 4\pi G a^2 \delta \bar{T}_0^0, \quad (1.90)$$

$$(\Psi' + \mathcal{H}\Phi)_{,i} = 4\pi G a^2 \delta \bar{T}_i^0, \quad (1.91)$$

$$\begin{aligned} \delta_j^i \left[\Psi'' + \mathcal{H}(2\Psi + \Phi)' + (2\mathcal{H}' + \mathcal{H}^2)\Phi + \frac{1}{2}\nabla^2(\Phi - \Psi) \right] \\ - \frac{1}{2}(\Phi - \Psi)^{,i}_{,j} = -4\pi G a^2 \delta \bar{T}_j^i. \end{aligned} \quad (1.92)$$

These equations are given in a general coordinate system. From the last equation, we see that

$$\Phi = \Psi \quad (1.93)$$

if there is no anisotropic stress in the matter perturbation, namely if $\delta\bar{T}_j^i = 0$ for $i \neq j$. For vector perturbations, after following an analogous procedure, the equations that govern the dynamics are

$$\nabla^2 \bar{V}_i = 16\pi G a^2 \delta\bar{T}_i^0{}_{(V)}, \quad (1.94)$$

$$(\bar{V}_{i,j} + \bar{V}_{j,i})' + 2\mathcal{H}(\bar{V}_{i,j} + \bar{V}_{j,i}) = -16\pi G a^2 \delta\bar{T}_j^i{}_{(V)}, \quad (1.95)$$

with $\bar{V}_i$ given by (1.76) and where $\delta\bar{T}_\alpha^\beta{}_{(V)}$ is the vector part of the energy momentum tensor. Equivalently, the equation for the tensor perturbations is

$$h_{ij}'' + 2\mathcal{H}h_{ij}' - \nabla^2 h_{ij} = 16\pi G a^2 \delta\bar{T}_j^i{}^{(T)}, \quad (1.96)$$

$\delta\bar{T}_j^i{}^{(T)}$ is the part of the energy-momentum tensor that has the same structural form as h_{ij} , i.e. the tensor perturbation of it.

The dynamical equations that we have obtained are used to calculate the evolution of the perturbations, from a post-inflationary phase to the time in which the CMB was emitted; during all this period perturbations are linear. Let us now specialize the study of the cosmological perturbation in the presence of the inflaton field.

1.4.4 Inflaton field perturbations

In inflationary cosmology driven by a single scalar field, we can decompose

$$\phi(\eta, x) = \phi_0(\eta) + \delta\phi(\eta, x). \quad (1.97)$$

The gauge-invariant perturbation associated to the scalar field is

$$\bar{\delta}\phi \equiv \delta\phi - \phi'_0(B - E'). \quad (1.98)$$

From the action (1.35) we can derive the energy-momentum tensor of the inflaton

$$T_{\mu\nu} = \partial_\mu\phi\partial_\nu\phi - g_{\mu\nu}\left(\frac{1}{2}\partial_\sigma\phi\partial^\sigma\phi - V(\phi)\right). \quad (1.99)$$

The gauge-invariant perturbations for the energy-momentum tensor of a scalar field are derived through (1.84,1.85,1.86)(condition (1.93) is satisfied). The equations of motion for the scalar perturbations reduce to

$$\nabla^2\Phi - 3\mathcal{H}\Phi' - (\mathcal{H}' + 2\mathcal{H}^2)\Phi = 4\pi G\left(\phi'_0\bar{\delta}\phi' + V'a^2\bar{\delta}\phi\right), \quad (1.100)$$

$$\Phi' + \mathcal{H}\Phi = 4\pi G\phi'_0\bar{\delta}\phi, \quad (1.101)$$

$$\Phi'' + 3\mathcal{H}\Phi' + (\mathcal{H}' + 2\mathcal{H}^2)\Phi = 4\pi G\left(\phi'_0\bar{\delta}\phi' - V'a^2\bar{\delta}\phi\right), \quad (1.102)$$

where primes denote differentiation with respect to the conformal time η , except on the potential, where $V' = dV/d\phi$. On subtracting the first equation (1.100) from the third (1.102) and using the second (1.101) to eliminate $\bar{\delta}\phi$, we obtain the following second-order partial differential equation governing the classical evolution of the potential Φ :

$$\Phi'' + 2\left(\mathcal{H} - \frac{\phi''_0}{\phi'_0}\right)\Phi' - \nabla^2\Phi + 2\left(\mathcal{H}' - \mathcal{H}\frac{\phi''_0}{\phi'_0}\right)\Phi = 0. \quad (1.103)$$

Once this equation is solved, the expression for $\bar{\delta}\phi$ follows from the previous relations.

1.4.5 Connection between perturbations and observables

We will give a rough explanation to the connection between the scalar and tensor perturbations, at the end of inflation, and the observables.

Scalar perturbations

Using the inflaton energy-momentum tensor, one can obtain the equations governing the evolution of the scalar perturbations (1.90,1.91,1.92). These calculations are the crucial ones to connect the post-inflationary perturbations spectrum to that at decoupling. Indeed the primordial perturbations evolve and leave an imprint on the CMB anisotropies. The perturbation field $\Phi(\mathbf{k}, \eta)$, such that

$$\Phi(\mathbf{x}, \eta) = \int \frac{d^3k}{(2\pi)^{3/2}} \Phi(\mathbf{k}, \eta) e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (1.104)$$

is mainly responsible for the inhomogeneities of the CMB that we see today. A perturbation mode $\Phi(\mathbf{k}, \eta)$ with momentum $\mathbf{k}$ is called **super-horizon** if

$$k < aH, \quad (1.105)$$

while it is **sub-horizon** if

$$k > aH. \quad (1.106)$$

One typically finds that when a mode is super-horizon $\Phi(\mathbf{k}, \eta)$ does not evolve significantly. Since the comoving Hubble radius always increases after inflation, all the modes that are super-horizon at the time that the CMB was emitted

$$k < (aH)|_{\eta_{CMB}} \quad (1.107)$$

were super-horizon from the time in which they crossed it, during inflation. This implies that these modes remain basically constant from inflation to η_{CMB} . In this way, we can connect straightforwardly some anisotropies in the CMB with the primordial perturbations. The evolution of the other modes can be calculated numerically. Treating $\Phi(\mathbf{k}, \eta)$ as a random field, one finds that the expectation value of the product of two Fourier

modes is

$$\langle \Phi(\mathbf{k}, \eta_{CMB}) \Phi^*(\mathbf{k}', \eta_{CMB}) \rangle = |\Phi(\mathbf{k}, \eta_{CMB})|^2 \delta^{(3)}(\mathbf{k} - \mathbf{k}') \quad (1.108)$$

for small and Gaussian inhomogeneities, as one usually considers. The dimensionless power spectrum is defined as

$$\Delta_{\Phi}^2(k) \equiv \frac{k^3}{2\pi^2} |\Phi_k|^2. \quad (1.109)$$

After some calculations, for the modes satisfying (1.107), a rough estimate of the deviation of the Planckian temperature from a given direction n with respect to the mean temperature, observed today η_0 , can be obtained

$$\frac{\Delta T}{T_0}(n, \eta_0) \simeq \frac{3}{10} \int \frac{d^3 k}{(2\pi)^{3/2}} \Phi(k, \eta_i) e^{-iknr}. \quad (1.110)$$

Conversely, by measuring the temperature, one can infer the scalar perturbation at η_{CMB} , and relate it with the perturbations at the end of inflation.

There is another observable connected with the CMB: its polarization. Before recombination begins, the radiation field has only dipole anisotropy, and therefore polarization cannot be generated. Since recombination is not instantaneous, the photons start to propagate with some other scattering; thus, polarization is generated. The polarization induced at the last scattering surface is characterized by the symmetric traceless tensor field $P_{ab}(\mathbf{n})$ on the celestial sphere; with $a, b=1, 2$. The two free components can be characterized by

$$E(\mathbf{n}) \equiv P^{;ab}_{ab}, \quad B(\mathbf{n}) \equiv P_{b;ac}{}^a \epsilon^{cb}, \quad (1.111)$$

with ; covariant derivative with respect to the Euclidean metric on the 2 sphere and ϵ is the two-dimensional skew-symmetric Levi-Civita “tensor”. The result is that the scalar perturbations cause the generation of E-modes, while the tensor perturbations generate both E-modes and B-modes.

Tensor Perturbations

Primordial tensor perturbations give an extremely small contribution to the inhomogeneities of the temperature in the CMB and they have not been detected yet. The polarization of light might be the best observable to measure primordial tensor modes, in particular the B-mode polarization. In future we hope to measure the B-mode polarization, and from them, infer the amplitude of gravitational waves at that time, and using equation (1.96) obtain the post-inflationary tensor perturbations.

1.5 Quantum origin of the primordial perturbations

We have illustrated how the post-inflationary perturbations evolve and how they connect with observations. But what is the origin of these perturbations? A striking result of the inflation model is that these perturbations can be explained by a quantum effect occurring during inflation. In particular, if we quantize the perturbations during inflation, and assume an initial vacuum state; the perturbations will inevitably carry some excitations at the end of inflation. This type of phenomenon, which naturally explains the primordial post-inflationary classical perturbations, leads to a nearly scale invariant spectrum, and is possible in the background of cosmic inflation. Thus, the inhomogeneities of the CMB we are observing can be an indirect evidence of inflation.

In what follows we first consider a toy model, and a small quantum field fluctuation $\delta\varphi$, in a fixed de Sitter background, which is an eternal exponentially growing universe. The realistic procedure will be presented in the following subsection 1.5.2

1.5.1 Quantization of perturbations in a de Sitter background

The following model is made of a de Sitter background with a test massless scalar field $\delta\varphi$

$$S = \int d^4x \sqrt{-g} \frac{1}{2} g^{\mu\nu} \partial_\mu \delta\varphi \partial_\nu \delta\varphi, \quad (1.112)$$

with the flat FLRW metric (1.36) and the scale factor behaves as

$$a(\eta) = -\frac{1}{H\eta}. \quad (1.113)$$

The action (1.112) becomes

$$S = \frac{1}{2} \int d\eta d^3x a^2 [(\delta\varphi')^2 - (\nabla\delta\varphi)^2]. \quad (1.114)$$

If we define

$$u = a\delta\varphi, \quad (1.115)$$

and add a total time derivative $\frac{d}{d\eta} \frac{a'u^2}{a}$ to the action. After some calculations, the action becomes

$$S = \frac{1}{2} \int d\eta d^3x \left[(u')^2 - (\nabla u)^2 + \frac{a''}{a} u^2 \right]. \quad (1.116)$$

This action, equivalently describes a field u with a time-dependent mass in Minkowski space-time

$$m^2 = -\frac{a''}{a} = -\frac{2}{\eta^2}. \quad (1.117)$$

The equation of motion in momentum space is

$$u_k'' + \left(k^2 - \frac{a''}{a} \right) u_k = 0, \quad (1.118)$$

and can be solved exactly, in the de Sitter case, by

$$u_k(\eta) = A(k) e^{-ik\eta} \left(1 - \frac{i}{k\eta}\right) + B(k) e^{ik\eta} \left(1 + \frac{i}{k\eta}\right). \quad (1.119)$$

We see that in the sub-horizon limit ($k \gg aH \iff -k\eta \gg 1$), the solution behaves like a plane wave and the fluctuation oscillates as in flat spacetime. In the super-horizon limit ($k \ll aH \iff -k\eta \ll 1$), the mode $\delta\varphi_k$ remains approximately constant.

Canonical quantisation of the field

The canonical momentum π conjugate to u is $\pi = u'$. Canonical quantisation consists in promoting the field u and the momentum π to operators $\hat{u}$ and $\hat{\pi}$ in the Hilbert space of the theory. Following canonical quantisation rules, we impose the canonical commutation relations at equal times

$$[\hat{u}(\eta, \vec{x}), \hat{u}(\eta, \vec{x}')] = 0, \quad (1.120)$$

$$[\hat{\pi}(\eta, \vec{x}), \hat{\pi}(\eta, \vec{x}')] = 0, \quad (1.121)$$

$$[\hat{u}(\eta, \vec{x}), \hat{\pi}(\eta, \vec{x}')] = i \delta^{(3)}(\vec{x} - \vec{x}'). \quad (1.122)$$

The Fourier transform of the $\hat{u}$ operator is

$$\hat{u}(\eta, \vec{x}) = \int \frac{d^3k}{(2\pi)^{3/2}} \left[\hat{a}_{\vec{k}} u_k(\eta) e^{i\vec{k}\cdot\vec{x}} + \hat{a}_{\vec{k}}^\dagger u_k^*(\eta) e^{-i\vec{k}\cdot\vec{x}} \right] = \int \frac{d^3k}{(2\pi)^{3/2}} \hat{u}_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}, \quad (1.123)$$

where $k = |\vec{k}|$. The creation-annihilation operators $\hat{a}_{\vec{k}}, \hat{a}_{\vec{k}}^\dagger$ satisfy

$$[\hat{a}_{\vec{k}}, \hat{a}_{\vec{k}'}^\dagger] = \delta^{(3)}(\vec{k} - \vec{k}'), \quad (1.124)$$

$$[\hat{a}_{\vec{k}}, \hat{a}_{\vec{k}'}] = [\hat{a}_{\vec{k}}^\dagger, \hat{a}_{\vec{k}'}^\dagger] = 0, \quad (1.125)$$

and $u_k(\eta)$ satisfies the equation (1.118). Using the relation (1.122) where we insert the operator (1.123) and the momentum operator, and using (1.124), the Wroskian condition follows

$$u_k u_k^{*'} - u_k^* u_k' = i. \quad (1.126)$$

A preferred state $|0\rangle$, called the vacuum state, is defined; it is the state that satisfies the condition

$$\hat{a}_{\vec{k}}|0\rangle = 0. \quad (1.127)$$

The choice of vacuum is not unique in curved spacetime, since the notion of particles depends on the choice of mode functions. The operators $\hat{a}_{\vec{k}}, \hat{a}_{\vec{k}}^\dagger$ depend on the specific evolution of the fields $u_k(\eta)$, in particular, it can be shown that choosing a different basis for the solutions leads to a different vacuum state. In other words, different choices of constants of integration in the solutions of (1.118) yield different annihilation and creation operators and different vacuum states. A preferred choice for the mode functions is the Bunch-Davies prescription, the respective vacuum is the **Bunch-Davies (BD) vacuum**. The BD modes reflect the choice of having a Minkoskian vacuum when the effect of the curvature is negligible. In our case, these modes are plane waves when they are far sub horizon

$$k^2 \gg \frac{a''}{a} \iff k \gg aH \iff k \gg -\frac{1}{\eta} \implies u_{k,BD}(\eta) \rightarrow \frac{1}{\sqrt{2k}} e^{-ik\eta}. \quad (1.128)$$

To this end we select

$$B(k) = 0 \quad (1.129)$$

with the correspondent

$$A(k) = \frac{1}{\sqrt{2k}}, \quad (1.130)$$

coming from the Wroskian condition (1.126). The mode functions is therefore

$$u_k = \frac{e^{-ik\eta}}{\sqrt{2k}} \left(1 - \frac{i}{k\eta} \right). \quad (1.131)$$

Now, we can compute the two point function

$$\langle \hat{u}_{\vec{k}} \hat{u}_{\vec{k}'} \rangle \equiv \langle 0 | \hat{u}_{\vec{k}} \hat{u}_{\vec{k}'} | 0 \rangle = |u_{\vec{k}}|^2 \delta^{(3)}(\vec{k} + \vec{k}'). \quad (1.132)$$

As we have seen, the fundamental observable of the physical predictions is the dimensionless power spectrum. For the modes u , it has the following form

$$\Delta_u(\vec{k}, \eta) \equiv \frac{k^3}{2\pi^2} |u_{\vec{k}}|^2, \quad (1.133)$$

in an equivalent way with definition (1.109). This means that the modulus square of the classical solution determines the variance of quantum fluctuations. If we look at the field two point function, we should consider the calculation

$$\langle 0 | \hat{\delta}\varphi(\vec{x}) \hat{\delta}\varphi(\vec{y}) | 0 \rangle = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{x}-\vec{y})} \frac{2\pi^2}{k^3} P_{\delta\varphi}(k), \quad (1.134)$$

with

$$P_{\delta\varphi}(k) = \frac{k^3}{2\pi^2} \frac{|u_k|^2}{a^2}. \quad (1.135)$$

For $-k\eta \ll 1$ (super-horizon modes)

$$P_{\delta\varphi}(k) \simeq \left(\frac{H}{2\pi} \right)^2. \quad (1.136)$$

This is a scale invariant power spectrum: for a de Sitter universe, the amplitude of the fluctuation on scales larger than Hubble length does not depend on the time at which the fluctuations crosses the horizon.

However, this result is not realistic since we are not considering the metric perturbations, i.e. the backreaction on the metric, that will be included in the following section.

1.5.2 Quantizing the perturbation in the realistic model

We split the full action (1.35)

$$S = S^{(0)}[g_{\mu\nu}^{(0)}, \phi_0] + S^{(2)}[g_{\mu\nu}^{(0)}, \delta g_{\mu\nu}, \phi_0, \delta\phi], \quad (1.137)$$

where $\phi = \phi_0 + \delta\phi$ and $g_{\mu\nu} = g_{\mu\nu}^{(0)} + \delta g_{\mu\nu}$. The term $S^{(1)}$ is linear in perturbations and vanishes by imposing the homogeneous equations of motion.

Scalar perturbations

The second order action can be written as that of a scalar field with a time-dependent mass in Minkowski spacetime and has the form

$$S^{(2)} = \frac{1}{2} \int d\eta d^3x \left[(v')^2 - (\vec{\nabla}v)^2 + \frac{z''}{z} v^2 \right] \quad (1.138)$$

with

$$v = a \left(\delta\bar{\phi} + \frac{\phi'_0}{\mathcal{H}} \Phi \right), \quad z = \frac{a \phi'_0}{\mathcal{H}} = \frac{a \dot{\phi}_0}{H} = a \sqrt{\frac{\epsilon}{4\pi G}}. \quad (1.139)$$

The gauge invariant variable v is called Mukhanov-Sasaki variable. It represents the single gauge invariant scalar degree of freedom describing primordial scalar fluctuations. The momentum space equation of motion is

$$v_k'' + \left(k^2 - \frac{z''}{z} \right) v_k = 0, \quad (1.140)$$

and is called **Mukhanov-Sasaki equation**. When $k^2 \gg \frac{z''}{z}$, which in slow roll inflation corresponds to sub-horizon modes $k^2 \gg (aH)^2$, the solution is

$$v_k(\eta) = A(k) e^{-ik\eta} + B(k) e^{ik\eta}, \quad (1.141)$$

and the BD prescription fixes the integration constants to be $A(k) = \frac{1}{\sqrt{2k}}$ and $B(k) = 0$. While, in the super-horizon limit $k^2 \ll (aH)^2$ one has

$$v_k(\eta) = C(k) z(\eta) + D(k) z(\eta) \int^\eta \frac{d\eta'}{z^2(\eta')}. \quad (1.142)$$

In the long wavelength limit, and when slow roll conditions are satisfied, the second contribution is negligible and the above solution reduces to

$$v_k(\eta) = C(k) z(\eta). \quad (1.143)$$

The integration constant $C(k)$ can be estimated by matching the absolute value of the solutions at the horizon crossing $k = aH$, in particular

$$|C(k) z|_{k=aH} = \frac{1}{\sqrt{2k}} \quad \Rightarrow \quad v_k(\eta) = \frac{z(\eta)}{(z\sqrt{2k})|_{k=aH}}. \quad (1.144)$$

The preferred gauge invariant quantity is the comoving curvature perturbation

$$\mathcal{R} = \frac{v}{z} = \frac{\mathcal{H}}{\phi'_0} \bar{\delta}\phi + \Phi. \quad (1.145)$$

Computing the power spectrum of $\mathcal{R}$ is important because this quantity, in the super-horizon limit, from the Hubble radius crossing during inflation, until it re-enters the horizon after the end of inflation, is conserved. In this way, one computes first the power spectrum of $\mathcal{R}$ and then the power spectrum of the scalar perturbations, if needed (Eq. 1.109). Upon quantising the theory, as we have seen in the subsection 1.5.1, we find that

its power spectrum is

$$P_{\mathcal{R}}(k) = \frac{k^3}{2\pi^2} \frac{|v_k|^2}{z^2}. \quad (1.146)$$

If we now insert (1.144) in (1.146) we obtain

$$P_{\mathcal{R}}(k) \simeq \frac{1}{4\pi^2} \frac{H^4}{\dot{\phi}_0^2} \Big|_{k=aH} = \frac{1}{8\pi^2 M_{\text{P}}^2} \frac{H^2}{\epsilon} \Big|_{k=aH}. \quad (1.147)$$

This function can be rewritten via the e.o.m. in terms of different quantities, for example, during slow-roll inflation (1.42,1.43) it is a function of the potential at the crossing time

$$P_{\mathcal{R}}(k) \simeq \frac{1}{12\pi^2 M_{\text{P}}^6} \left(\frac{V^3}{V'^2} \right) \Big|_{k=aH}. \quad (1.148)$$

Tensor Perturbations

The starting point is the action (1.35) with the perturbed metric

$$ds^2 = a^2(\eta) \left[d\eta^2 - (\delta_{ij} + h_{ij}) dx^i dx^j \right], \quad (1.149)$$

where the tensor $h_{ij}(\eta, \mathbf{x})$ represents gravitational waves. To quadratic order in tensor fluctuations, the action takes the form

$$S^{(2)} = \frac{M_{\text{Pl}}^2}{8} \int d\eta d^3x a^2 \left[(h'_{ij})^2 - (\nabla h_{ij})^2 \right]. \quad (1.150)$$

The tensor h_{ij} can be decomposed as

$$h_{ij}(\eta, \mathbf{x}) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \left[h_k^+(\eta) \epsilon_{ij}^+(\mathbf{k}) + h_k^\times(\eta) \epsilon_{ij}^\times(\mathbf{k}) \right], \quad (1.151)$$

where the polarization tensors satisfy

$$\epsilon_{ij}^\lambda = \epsilon_{ji}^\lambda, \quad k_i \epsilon_{ij}^\lambda = 0, \quad \epsilon_{ii}^\lambda = 0, \quad \lambda = +, \times. \quad (1.152)$$

If we define

$$v_k^\lambda = \frac{aM_{\text{P}}}{2} h_k^\lambda, \quad (1.153)$$

the equation of motion in momentum space is

$$v_k^{\lambda''} + \left(k^2 - \frac{a''}{a} \right) v_k^\lambda = 0, \quad (1.154)$$

and we can use the results previously illustrated to conclude that the power spectrum on super-Hubble scales is

$$\mathcal{P}_T = 2 \times \frac{4}{M_{\text{P}}^2} \times \left(\frac{H}{2\pi} \right)^2 \bigg|_{k=aH}, \quad (1.155)$$

where the factor 2 accounts for the two polarizations and the second factor comes from the normalization as a canonical scalar field. We obtain that the tensorial power spectrum is

$$\mathcal{P}_T = \frac{2}{3\pi^2} \left(\frac{V}{M_{\text{P}}^4} \right) \bigg|_{k=aH}. \quad (1.156)$$

1.5.3 Connection between primordial quantum fluctuations and the CMB spectrum

The important physical quantities, which must be calculated when studying a specific inflationary model, are the two power spectrum (1.147) and (1.155). They can be related to anisotropies of the Planckian spectrum of the CMB. Their spectral indices quantify the deviation from scale invariance, and for scalar perturbations we have

$$n_s - 1 = \frac{d \ln \mathcal{P}_{\mathcal{R}}(k)}{d \ln k} \bigg|_{k=k_*}, \quad (1.157)$$

where k_* is the pivot scale, which is a typical reference scale. In the slow-roll approximation, and at horizon crossing ($k = aH$), the following relation holds

$$d \ln k = d \ln(aH) \simeq d \ln a. \quad (1.158)$$

Using the dynamical equations in the slow-roll approximation, we get

$$\frac{d\phi}{d \ln a} = \frac{\dot{\phi}}{H} \simeq -\frac{V'}{3H^2} \simeq -M_{\text{P}}^2 \frac{V'}{V}. \quad (1.159)$$

The slow-roll parameters can also be defined in terms of the scalar field potential $V(\phi)$:

$$\epsilon_V = \frac{M_{\text{P}}^2}{2} \left(\frac{V'}{V} \right)^2, \quad (1.160)$$

$$\eta_V = M_{\text{P}}^2 \frac{V''}{V}. \quad (1.161)$$

For the slow-roll models, the two definitions are linked as follow

$$\epsilon \simeq \epsilon_V, \quad \eta_H \simeq \eta_V - \epsilon_V, \quad (1.162)$$

and from (1.148) we obtain

$$n_s - 1 = (-6\epsilon_V + 2\eta_V)|_{aH=k_*}. \quad (1.163)$$

For tensor perturbations, the spectral index is defined as

$$n_T = \frac{d \ln \mathcal{P}_T(k)}{d \ln k} \Big|_{k=k_*}. \quad (1.164)$$

and from (1.156) we have

$$n_T = -2\epsilon|_{aH=k_*}. \quad (1.165)$$

Another useful quantity, which is often compared to observation, is the tensor-to-scalar ratio, given by

$$r = \frac{\mathcal{P}_T}{\mathcal{P}_\mathcal{R}} = 16 \epsilon|_{aH=k_*}, \quad (1.166)$$

which is proportional to the slow-roll parameter. If we combine the above result with (1.165), we find the consistency relation

$$r = -8 n_T, \quad (1.167)$$

which relates two observable quantities. The tensorial spectrum has never been observed, we have, however, derived some observational upper bound for the tensor-to-scalar ratio.

This bound, with the observed scalar spectrum, constraints the possible dynamics of inflation. In this sense not every inflation model can generate what we observe in the CMB. The standard calculations therefore treat the homogeneous variables in a classical way. This framework is generalized in the following chapter, where both homogeneous and inhomogeneous variables are quantised and the inflaton-gravity system is fully quantised.

Chapter 2

Canonical quantisation of the inflaton-gravity system

In chapter 1, we have studied the standard picture of inflation, modeled within the framework of Quantum field theory in a curved space-time. Inflation is a physical phenomenon that occurred in the very early stages of the universe, where the scale factor was much smaller than today and the energy densities extremely higher. In principle, the energy involved at the very beginning of inflation could be very large, up to the Planck energy or even higher, where the framework of QFT in curved space-times is expected to break-down. For this reason, the beginning of the universe should be better described by a theory of quantum gravity. Finding a theory of quantum gravity is one of the biggest challenges of modern theoretical physics; a consolidated, fundamental description of gravity at Planckian energies is certainly missing. However, canonical quantum gravity is one of the earliest theoretical attempts to combine GR with quantum mechanics. It consists of expressing the classical dynamics of the matter-gravity system in the canonical formalism and quantising it. While it is commonly believed that well above Planckian energy, canonical quantum gravity should break down and must be replaced by some new theory, one still expects that the well established formalism of quantum field theory applied to

GR leads to a consistent theoretical description of the gravitational interactions almost up to Planck scales. It is then suitable for describing an early universe phenomenon such as inflation. In this second chapter, we will present the standard procedure to canonically quantise the inflaton model. Firstly, we will write down the action of the classical system; secondly, the Hamiltonian formalism is presented followed by the full quantisation of the system, the semi-classical limit is then studied; finally, the connection between this limit and the paradigm of QFT in curved space-times is presented.

2.1 Classical system

Let us consider a minimally coupled scalar field (inflaton matter) on a curved, spatially flat, space-time described by the usual action (1.35). It can be decomposed into a homogeneous part plus fluctuations around it. The fluctuations of the metric $\delta g_{\mu\nu}$ are defined by

$$g_{\mu\nu} = g_{\mu\nu}^{(0)} + \delta g_{\mu\nu}, \quad (2.1)$$

where $g_{\mu\nu}^{(0)} = \text{diag}[a^2(\eta)(1, -1, -1, -1)]$ is the flat FRWL metric. The perturbations can be described by the Eqs. (1.52, 1.53, 1.54). As we have already discussed, only the scalar and tensor fluctuations “survive” the inflationary expansion. The four degrees of freedom (d.o.f.) of the scalar sector mix with the inflation fluctuation $\delta\phi(x, \eta)$, defined by $\phi(x, \eta) \equiv \phi_0(\eta) + \delta\phi(x, \eta)$. One can either rewrite these four scalar perturbations in terms of just two Bardeen’s potentials (1.71, 1.72) or fix the gauge and set two of them at zero. Finally, using the equations of motion, the scalar sector can be collectively described by a single field $v(x, \eta)$. In particular, we use the uniform curvature gauge, then the gauge invariant Mukhanov field (1.139), becomes $v(\mathbf{x}, \eta) = a(\eta) \delta\phi(\mathbf{x}, \eta)$, where we used the e.o.m. (1.103). Its Fourier transform, $v_{\mathbf{k}}$, can be decomposed into two parts $v_{1,\mathbf{k}} \equiv \text{Re}(v_{\mathbf{k}})$, $v_{2,\mathbf{k}} \equiv \text{Im}(v_{\mathbf{k}})$.

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The tensor fluctuations are already gauge invariant and given by

$$ds^2 = a^2(\eta) \left[d\eta^2 - (\delta_{ij} + h_{ij}) dx^i dx^j \right], \quad (2.2)$$

with $\partial^i h_{ij} = 0, \delta^{ij} h_{ij} = 0$. Only two physical degrees of freedom remain $h_{(+)}$ and $h_{(\times)}$. Then, on defining $v_{1,\mathbf{k}}^{(\lambda)} \equiv \frac{a\sqrt{M_P}}{\sqrt{2}} \text{Re}(h_{\mathbf{k}}), v_{2,\mathbf{k}}^{(\lambda)} \equiv \frac{a\sqrt{M_P}}{\sqrt{2}} \text{Im}(h_{\mathbf{k}})$, one can describe the tensor perturbations in a manner similar to that of the scalar perturbations. The effective action of the homogeneous inflaton-gravity system plus the inhomogeneous perturbations finally is

$$\begin{aligned} S = \int d\eta \Big\{ & L^3 \left[-\frac{m_P^2}{2} a'^2 + \frac{a^2}{2} (\phi_0'^2 - 2V(\phi_0)a^2) \right] \\ & + \frac{1}{2} \sum_{i=1}^2 \sum_{\mathbf{k} \neq 0} \left[v_{i,\mathbf{k}}'(\eta)^2 + \left(-k^2 + \frac{z''}{z} \right) v_{i,\mathbf{k}}(\eta)^2 \right] \\ & + \frac{1}{2} \sum_{i=1}^2 \sum_{\lambda=+,\times} \sum_{\mathbf{k} \neq 0} \left[\left(v_{i,\mathbf{k}}^{(\lambda)'}(\eta) \right)^2 + \left(-k^2 + \frac{a''}{a} \right) \left(v_{i,\mathbf{k}}^{(\lambda)}(\eta) \right)^2 \right] \Big\} \end{aligned} \quad (2.3)$$

with $m_p = \sqrt{6}M_P$, $z \equiv a\sqrt{\epsilon_1}$, $\epsilon_1 \equiv -\frac{H'}{aH^2}$, $H = \frac{a'}{a^2}$, $L^3 \equiv \int d^3x$ and the prime denotes differentiation with respect to conformal time. Notice that we have introduced an unspecified length L arising from the integration of homogeneous variables over a flat 3-space, $L^3 = \int d^3x$. In the following, we shall set $L = 1$, which is equivalent to replacing $a \rightarrow a/L, \eta \rightarrow \eta L, v \rightarrow \sqrt{Lv}, k \rightarrow k/L$.

2.2 The Wheeler-deWitt equation: Canonical quantisation

In order to illustrate the quantisation procedure in detail, without losing generality, we single out the homogeneous part and one real scalar field for the perturbations in (2.3)

$$S = \int d\eta \left[-\frac{m_P^2}{2} a'^2 + \frac{a^2}{2} (\phi_0'^2 - 2V(\phi_0)a^2) + \frac{1}{2} \sum_{k \neq 0} (v_k'(\eta)^2 - \omega_k^2 v_k(\eta)^2) \right] \equiv \int d\eta \mathcal{L}_{\text{tot}}. \quad (2.4)$$

where $\omega_k^2(\eta) = k^2 + m^2(\eta)$ is time dependent and it is such that $m^2(\eta) = -\frac{z''}{z}$ for scalar perturbations and $m^2(\eta) = -\frac{a''}{a}$ for tensor perturbations.

The necessary choice of a time direction along which evolution can be described is at the foundation of the canonical formalism. However, the choice of such a foliation remains largely arbitrary and, furthermore, the same foliation can still be parameterised by different times and spatial coordinates. The diffeomorphism invariance of classical GR leads to a series of constraints at the quantum level for the universe wave function: **the Wheeler-DeWitt (WdW) equation**, associated with time re-parametrization invariance, and three momentum constraints related to the invariance with respect to spatial coordinates parametrization. When the formalism is applied to homogenous matter-gravity systems, such as those relevant for cosmology, the momentum constraints are trivially satisfied and one is simply left with the WdW equation.

The latter logic can be implemented by rewriting the above action in terms of an arbitrary time parameter τ with $N(\tau)d\tau = a(\eta)d\eta$, with $N(\tau)$ the lapse function.

$$\begin{aligned}
S &= \int d\tau \frac{N}{a} \left[-\frac{m_{\text{P}}^2}{2} \frac{a^2 \dot{a}^2}{N^2} + \frac{a^4}{2} \left(\frac{\dot{\phi}_0^2}{N^2} - 2V(\phi_0) \right) \right. \\
&\quad \left. + \frac{1}{2} \sum_{k \neq 0}^{\infty} \left(\frac{a^2 \dot{v}_k^2}{N^2} - \omega_k^2 v_k^2 \right) \right] \\
&\equiv \int d\tau \tilde{\mathcal{L}}_{\text{tot}}.
\end{aligned} \tag{2.5}$$

the dot here indicates the derivative with respect to τ . The lapse function N plays the role of a Lagrange multiplier in the action, and the variation of the action with respect to N leads to the following equation of motion

$$0 = \frac{\delta \tilde{\mathcal{L}}_{\text{tot}}}{\delta N} = \frac{m_{\text{P}}^2 a \dot{a}^2}{N^2} - \frac{a^3 \dot{\phi}_0^2}{2N^2} - a^3 V - \sum_{k \neq 0}^{\infty} \left[\frac{a \dot{v}_k^2}{2N^2} + \frac{\omega_k^2 v_k^2}{2a} \right], \tag{2.6}$$

having the form of a constraint equation.

The system Hamiltonian is

$$\mathcal{H} = -\frac{N \pi_a^2}{2am_{\text{P}}^2} + \frac{N \pi_{\phi}^2}{2a^3} + a^3 NV + \sum_{k \neq 0}^{\infty} \left[\frac{N \pi_k^2}{2a} + \frac{N \omega_k^2}{2a} v_k^2 \right], \tag{2.7}$$

where we have introduced the canonical momenta associated to the variables

$$\pi_N = 0, \quad \pi_a = -\frac{m_{\text{P}}^2 a \dot{a}}{N}, \quad \pi_{\phi} = \frac{a^3 \dot{\phi}_0}{N}, \quad \pi_k = \frac{a \dot{v}_k}{N}. \tag{2.8}$$

We now observe that the Hamiltonian is proportional to the constraint (2.6)

$$0 = \frac{\delta \tilde{\mathcal{L}}_{\text{tot}}}{\delta N} = \frac{\mathcal{H}}{N}. \tag{2.9}$$

which is then called the Hamiltonian constraint.

Having described the system in the Hamiltonian formalism, we are ready to canonically quantise it. The Hamiltonian constraint becomes the WdW equation by substituting canonical quantities with operators.

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Once the system is quantised a natural ingredient emerges, the wave function of the universe Ψ . The Copenhagen interpretation of quantum mechanics assumes that the operation of measurement of some property of a system makes the wave function collapse in a non-deterministic way. This interpretation does not necessarily hold for the wave function of the universe, since it is not a microscopic quantum mechanical system, with no measurement apparatus external to it, and it present only one realization of the universe. It is often claimed that the WdW equation is an elegant quantum equation for the universe wave function, which leads to no really quantitative predictions. Nevertheless, the universe wave function contains information on how the universe began and how it expands evolving from a state with quantum properties to a state which has an increasingly classical behaviour.

Until this chapter the background geometry has been treated classically, now we are quantising the background itself. In compact form, the WdW equation reads

$$\hat{\mathcal{H}}|\Psi\rangle = 0. \quad (2.10)$$

In the coordinate representation, the operators act as (setting $\hbar = 1$)

$$\langle a, \phi_0, \{v_k\} | \hat{a} \Psi \rangle = a \Psi(a, \phi_0, \{v_k\}), \quad (2.11)$$

$$\langle a, \phi_0, \{v_k\} | \hat{\pi}_a \Psi \rangle = -i \frac{\partial}{\partial a} \Psi(a, \phi_0, \{v_k\}), \quad (2.12)$$

$$\langle a, \phi_0, \{v_k\} | \hat{\phi}_0 \Psi \rangle = \phi_0 \Psi(a, \phi_0, \{v_k\}), \quad (2.13)$$

$$\langle a, \phi_0, \{v_k\} | \hat{\pi}_{\phi_0} \Psi \rangle = -i \frac{\partial}{\partial \phi_0} \Psi(a, \phi_0, \{v_k\}), \quad (2.14)$$

$$\langle a, \phi_0, \{v_k\} | \hat{v}_k \Psi \rangle = v_k \Psi(a, \phi_0, \{v_k\}), \quad (2.15)$$

$$\langle a, \phi_0, \{v_k\} | \hat{\pi}_k \Psi \rangle = -i \frac{\partial}{\partial v_k} \Psi(a, \phi_0, \{v_k\}). \quad (2.16)$$

The Wheeler-deWitt equation becomes

$$\left[\frac{1}{2m_{\text{P}}^2} a^{-l} \partial_a a^{-j} \partial_a a^{-i} - \frac{1}{2a^2} \frac{\partial^2}{\partial \phi_0^2} + a^4 V + \sum_k \hat{H}_k \right] \Psi(a, \phi_0, \{v_k\}) = 0. \quad (2.17)$$

with $i = -l - j$ and

$$\hat{H}_k = -\frac{1}{2} \frac{\partial^2}{\partial v_k^2} + \frac{\omega_k^2}{2} v_k^2. \quad (2.18)$$

The first term of the equation arises because of ordering ambiguities, for example, at the classical level $\pi_a = \frac{1}{a} \pi_a a$, but when quantised $\hat{\pi}_a \Psi = -i \frac{\partial}{\partial a} \Psi \neq -i \frac{1}{a} \frac{\partial}{\partial a} a \Psi$ (in coordinate representation). We will focus on the standard choice: $i = j = l = 0$.

2.2.1 Born-Oppenheimer decomposition

Despite its simple form, solving the Wheeler–DeWitt equation is an extremely difficult task, except in very special cases, and therefore suitable approximations are required. Even in the absence of perturbations, the strong coupling between matter and gravitational degrees of freedom makes the problem highly non-trivial. A useful approximation scheme is provided by the Born–Oppenheimer (BO) method, originally introduced in molecular physics to separate slow (heavy) and fast (light) degrees of freedom. In quantum cosmology, this separation is naturally suggested by the hierarchy between the Planck mass and matter energy scales, allowing gravity to play the role of the slow subsystem and matter the fast one.

It consists in factorising the wave function of the universe into a product

$$\Psi(a, \phi_0, \{v_k\}) = \psi(a) \chi(a, \phi_0, \{v_k\}). \quad (2.19)$$

with $\psi(a)$ is the wave function for the homogeneous gravitational sector and $\chi(a, \phi_0, \{v_k\})$ is that for matter (homogeneous plus perturbations). The matter wave function can be further factorized into an homogeneous inflaton $\chi_0(a, \phi_0)$ factor and a part for each mode

k of the perturbation $\chi_k(a, v_k)$

$$\chi(a, \phi_0, \{v_k\}) = \chi_0(a, \phi_0) \prod_{k \neq 0}^{\infty} \chi_k(a, v_k) = \prod_{k=0}^{\infty} \chi_k. \quad (2.20)$$

The above factorization leads to the following set of partial differential equations, which are equivalent to the Wheeler-deWitt equation:

Gravity equation

$$\left[\frac{1}{2m_{\text{P}}^2} \frac{\partial^2}{\partial a^2} + \langle \hat{H}^{(M)} \rangle \right] \tilde{\psi} = -\frac{1}{2m_{\text{P}}^2} \langle \frac{\partial^2}{\partial a^2} \rangle \tilde{\psi}, \quad (2.21)$$

and matter Equation

$$\tilde{\psi}^* \tilde{\psi} \left(\hat{H}^{(M)} - \langle \hat{H}^{(M)} \rangle \right) \tilde{\chi} + \frac{1}{m_{\text{P}}^2} \left(\tilde{\psi}^* \frac{\partial \tilde{\psi}}{\partial a} \right) \frac{\partial \tilde{\chi}}{\partial a} = \frac{1}{2m_{\text{P}}^2} \tilde{\psi}^* \tilde{\psi} \left(\left\langle \frac{\partial^2}{\partial a^2} \right\rangle - \frac{\partial^2}{\partial a^2} \right) \tilde{\chi}, \quad (2.22)$$

with

$$\hat{H}^{(M)} \equiv -\frac{1}{2a^2} \frac{\partial^2}{\partial \phi_0^2} + a^4 V + \sum_k \hat{H}_k \quad (2.23)$$

and

$$\psi = \exp\left(-i \int^a A(a') da'\right) \tilde{\psi}, \chi = \exp\left(i \int^a A(a') da'\right) \tilde{\chi}, A = -i \langle \chi | \frac{\partial}{\partial a} | \chi \rangle. \quad (2.24)$$

The sign $\langle \hat{O} \rangle$ stands for $\langle \hat{O} \rangle = \langle \tilde{\chi} | \hat{O} | \tilde{\chi} \rangle$ and each mode is individually normalized by $\langle \chi_k | \chi_k \rangle = \int dv_k \chi_k^* \chi_k = 1$. We can now multiply the matter equation by $\prod_{j \neq k} \langle \tilde{\chi}_j |$, and split it into a set of equations, each governing the dynamics of a single mode k of the matter field:

$$\begin{aligned} \tilde{\psi}^* \tilde{\psi} \left[\hat{H}_k - \langle \tilde{\chi}_k | \hat{H}_k | \tilde{\chi}_k \rangle \right] \tilde{\chi}_k + \frac{1}{m_{\text{P}}^2} \left(\tilde{\psi}^* \frac{\partial \tilde{\psi}}{\partial a} \right) \frac{\partial \tilde{\chi}_k}{\partial a} \\ = \frac{1}{2m_{\text{P}}^2} \tilde{\psi}^* \tilde{\psi} \left[\left\langle \tilde{\chi}_k \left| \frac{\partial^2}{\partial a^2} \right| \tilde{\chi}_k \right\rangle - \frac{\partial^2}{\partial a^2} \right] \tilde{\chi}_k. \end{aligned} \quad (2.25)$$

If we divide the latter equation by $|\tilde{\psi}|^2$, we obtain

$$\left[\hat{H}_k - \langle \tilde{\chi}_k | \hat{H}_k | \tilde{\chi}_k \rangle \right] \tilde{\chi}_k + \frac{1}{m_{\text{P}}^2 \tilde{\psi}} \left(\frac{\partial \tilde{\psi}}{\partial a} \right) \frac{\partial \tilde{\chi}_k}{\partial a} = \frac{1}{2m_{\text{P}}^2} \left[\left\langle \tilde{\chi}_k \left| \frac{\partial^2}{\partial a^2} \right| \tilde{\chi}_k \right\rangle - \frac{\partial^2}{\partial a^2} \right] \tilde{\chi}_k. \quad (2.26)$$

2.2.2 WKB Approximation

The WKB approximation is justified by the (heavy) quasi-classical behaviour of the gravitational d.o.f. This approximation gives a systematic way to solve the gravitational wave equation, order by order in m_P^{-1} .

One starts from the following ansatz for the gravitational wave function

$$\tilde{\psi} = \exp \left(i m_{\text{P}} \{ S_0 + \frac{S_1}{m_P} + O(m_{\text{P}}^{-2}) \} \right). \quad (2.27)$$

If we plug this function in (2.21), neglecting the right hand side of it, which is proportional to $\frac{1}{m_P^2}$ and thus negligible to the first order equations, we obtain

$$\left[\frac{1}{2m_{\text{P}}^2} \left(i \frac{d^2 S}{da^2} - \left(\frac{dS}{da} \right)^2 \right) + \langle \hat{H}^{(M)} \rangle \right] \tilde{\psi}(a) = 0. \quad (2.28)$$

with $S = m_{\text{P}} \{ S_0 + \frac{S_1}{m_P} + o(m_{\text{P}}^{-2}) \}$.

At the zero-th order (m_P^0), the equation reads

$$\left(\frac{dS_0}{da} \right)^2 = 2 \langle \hat{H}^{(M)} \rangle, \quad (2.29)$$

and has the form of the Hamilton-Jacobi equation. The classical Friedmann equation

$$-\frac{m_{\text{P}}^2}{2} a'^2 + \langle \hat{H}^{(M)} \rangle = 0, \quad (2.30)$$

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can then be recovered. To this end, we identify $m_P \frac{dS_0}{da}$ with the classical momentum conjugate to the scale factor, given by $p_a = -m_P^2 a'$. The solution of Eq. (2.29) is

$$S_0 = \pm \int da \sqrt{2\langle \hat{H}^{(M)} \rangle} = \pm \int da m_P a'. \quad (2.31)$$

To first order (m_P^{-1}), Eq. (2.28) is

$$i \frac{d^2 S_0}{da^2} = 2 \frac{dS_1}{da} \frac{dS_0}{da}, \quad (2.32)$$

with solution

$$S_1 = -i \ln |p_a|^{-1/2} + \text{const.} \quad (2.33)$$

The first order approximate solution is therefore the following

$$\begin{aligned} \tilde{\psi}(a) &= \exp(im_P S_0 + iS_1) \\ &= \frac{1}{\sqrt{m_P^2 a'}} \left[c_1 \exp\left(i \int^a m_P^2 a' da\right) + c_2 \exp\left(-i \int^a m_P^2 a' da\right) \right]. \end{aligned} \quad (2.34)$$

2.2.3 Introduction of time

The WdW equation has no time dependence, since it is derived from time parametrization invariance. However, in the semi-classical limit, we can introduce time in a natural way, by considering the scale factor evaluated on the classical trajectory $a = a_{\text{cl}}(\eta)$, $\tilde{\chi}_k(\eta, v_k) \equiv \tilde{\chi}_k(a_{\text{cl}}(\eta), v_k)$.

In the equations for the matter (inflaton) wave function, time emerges through the gravitational wave function as follow

$$\frac{1}{m_P^2 \tilde{\psi}} \frac{\partial \tilde{\psi}}{\partial a} \partial_a = -i a'_{\text{cl}} \frac{\partial}{\partial a} - \frac{1}{2m_P^2} \frac{a''_{\text{cl}}}{a_{\text{cl}}'^2} \partial_a = -i \frac{\partial}{\partial \eta} - \frac{1}{2m_P^2} \frac{a''_{\text{cl}}}{a_{\text{cl}}'^2} \partial_a. \quad (2.35)$$

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Thus the BO decomposition leads to the emergence of time in the semiclassical limit of the gravitational sector. The second term (which is proportional to $\frac{1}{m_P^2}$) can be thought as a quantum correction to the emergence of time.

In the equation for the perturbations (2.26), we can eliminate the term $\langle \tilde{\chi}_k | \hat{H}_k | \tilde{\chi}_k \rangle$ by defining a re-phase wave function:

$$|\chi_k\rangle_s \equiv \exp\left(-i \int^\eta \langle \tilde{\chi}_k | \hat{H}_k | \tilde{\chi}_k \rangle d\eta'\right) |\tilde{\chi}_k\rangle. \quad (2.36)$$

This, immediately implies

$$\begin{aligned} i\partial_\eta |\chi_k\rangle_s - \hat{H}_k |\chi_k\rangle_s &= \exp\left[i \int^\eta \langle \tilde{\chi}_k | \hat{H}_k | \tilde{\chi}_k \rangle d\eta'\right] \frac{1}{2m_P^2} \left[\partial_a^2 - \frac{a''}{(a')^2} \partial_a \right. \\ &\quad \left. - \left\langle \tilde{\chi}_k \left| \partial_a^2 - \frac{a''}{(a')^2} \partial_a \right| \tilde{\chi}_k \right\rangle \right] |\tilde{\chi}_k\rangle \\ &\equiv \frac{1}{2m_P^2} \left[\hat{\Omega}_k - \langle \hat{\Omega}_k \rangle_s \right] |\chi_k\rangle_s, \end{aligned} \quad (2.37)$$

with $\langle \hat{O} \rangle_s \equiv {}_s\langle \chi_k | \hat{O} | \chi_k \rangle_s$. The operator $\hat{\Omega}_k$ has the following form

$$\hat{\Omega}_k = \frac{1}{(a')^2} \frac{d^2}{d\eta^2} + \left[\frac{2i \langle \hat{H}_k \rangle_s}{(a')^2} - \frac{2a''}{(a')^3} \right] \frac{d}{d\eta}, \quad (2.38)$$

it has a nonlinear structure, since it depends on χ_k and χ_k^* through multiplicative factors of the form $\langle \hat{O} \rangle_s$. To first order, neglecting the terms proportional to $\frac{1}{m_P^2}$, a Schrödinger-like equation emerges

$$i\partial_\eta |\chi_k\rangle_s = \hat{H}_k |\chi_k\rangle_s. \quad (2.39)$$

The following section illustrates that the latter equation is the analog of the Mukhanov-Sasaki Eq. (1.140)

2.3 Recovery of the standard picture

The Eq. (2.39) reads

$$i\partial_\eta \chi_{k,s}(\eta, v_k) = \left[-\frac{1}{2} \frac{\partial^2}{\partial v_k^2} + \frac{\omega_k^2}{2} v_k^2 \right] \chi_{k,s}(\eta, v_k). \quad (2.40)$$

in the coordinate representation. We search for an invariant operator $\hat{I}(\eta)$ that satisfies the equation

$$\frac{d\hat{I}}{d\eta} = \frac{\partial \hat{I}}{\partial \eta} + \frac{1}{i} [\hat{I}, \hat{H}_k] = 0. \quad (2.41)$$

The eigenstates of the invariant operator $\hat{I}$, multiplied by a proper phase factor, are a complete set of solutions to the Schrödinger equation. A possible candidate for this invariant is the quadratic invariant

$$\hat{I}(\eta) = \frac{1}{2} \left[\frac{1}{\rho(\eta)^2} \hat{v}_k^2 + (\rho(\eta) \hat{\pi}_k - \rho(\eta)' \hat{v}_k)^2 \right], \quad (2.42)$$

where $\rho(\eta)$ is a real time-dependent function. By substituting this ansatz into the invariance condition (2.41), one can verify that $\rho(\eta)$ must satisfy the Ermakov-Pinney equation

$$\rho(\eta)'' + \omega^2(\eta) \rho(\eta) = \frac{1}{\rho^3(\eta)}. \quad (2.43)$$

The linear part of Eq. (2.43) is exactly the Mukhanov-Sasaki equation that we previously obtained (1.140), with the substitution of $\rho(\eta)$ with v_k . We can search for the eigenfunctions of the invariant operator $\hat{I}(\eta)$ defined in Eq. (2.42). These eigenfunctions can be obtained by noting that the invariant operator can be expressed in terms of time-dependent creation and annihilation operators:

$$\hat{I}(\eta) = \left(\hat{a}^\dagger(\eta) \hat{a}(\eta) + \frac{1}{2} \right) \quad (2.44)$$

where the operators $\hat{a}(\eta)$ and $\hat{a}^\dagger(\eta)$ are given by:

$$\hat{a}(\eta) = \frac{1}{\sqrt{2}} \left[\frac{\hat{v}_k}{\rho(\eta)} + i(\rho(\eta)\hat{\pi}_k - \rho'(\eta)\hat{v}_k) \right] \quad (2.45)$$

$$\hat{a}^\dagger(\eta) = \frac{1}{\sqrt{2}} \left[\frac{\hat{v}_k}{\rho(\eta)} - i(\rho(\eta)\hat{\pi}_k - \rho'(\eta)\hat{v}_k) \right] \quad (2.46)$$

and satisfy the commutation relation $[\hat{a}(\eta), \hat{a}^\dagger(\eta)] = 1$. The ground state of the invariant, $|0, \eta\rangle$, is then defined by the action of the annihilation operator

$$\hat{a}(\eta)|0, \eta\rangle = 0. \quad (2.47)$$

Through the creation operator, we can then obtain the entire spectrum of the number operator $\hat{N}(\eta) = \hat{a}(\eta)^\dagger \hat{a}(\eta)$

$$\hat{N}(\eta)|n; \eta\rangle = n|n; \eta\rangle. \quad (2.48)$$

The eigenstates of the invariant operator in the position space are $\chi_n(v_k, \eta) = \langle v_k | n; \eta \rangle$, and after some calculations

$$\chi_n(v_k, \eta) = \frac{1}{\sqrt{2^n n!}} \chi_0(v_k, \eta) \mathcal{H}_n \left[\frac{v_k}{\rho(\eta)} \right], \quad (2.49)$$

with $\mathcal{H}_n$ Hermite polynomials of order n and

$$\chi_0(v_k, \eta) = \left[\frac{1}{\pi \rho(\eta)^2} \right]^{\frac{1}{4}} \exp \left\{ \frac{i}{2} \left[\frac{\rho'(\eta)}{\rho(\eta)} + \frac{i}{\rho(\eta)^2} \right] v_k^2 \right\}. \quad (2.50)$$

We then require that these functions multiplied by a phase factor $\alpha_n(\eta)$ are a solution of the Schrödinger Eq. (2.40), we obtain the equation

$$\frac{d\alpha_n(\eta)}{d\eta} = \langle n; \eta | \left[i \frac{\partial}{\partial \eta} - \hat{H}_k(\eta) \right] | n; \eta \rangle \quad (2.51)$$

and its solution is

$$\alpha_n(\eta) = -(n + \frac{1}{2}) \int_0^\eta \frac{d\eta'}{\rho(\eta')^2}. \quad (2.52)$$

The general solution of (2.40) is therefore

$$|\chi(\eta)_k\rangle_s = \sum_{n=0}^{\infty} C_n e^{i\alpha_n(\eta)} |n; \eta\rangle \quad (2.53)$$

or equivalently

$$\chi_{k,s}(v_k, \eta) = \sum_{n=0}^{\infty} C_n e^{i\alpha_n(\eta)} \chi_n(v_k, \eta). \quad (2.54)$$

We have found the solution of the Schrödinger equation and shown that it is a function of the solution of the Ermakov-Pinney Eq. (2.43), which, in turn, depends on the background dynamics.

2.3.1 Equivalence between the two expectation values of interest

Let us calculate the following expectation value

$$\langle 0, \eta | \hat{v}_k^2 | 0, \eta \rangle = \int_{-\infty}^{+\infty} v_k^2 |\chi_0(v_k, \eta)|^2 dv_k. \quad (2.55)$$

By inserting the function (2.50) in the last expression we find

$$\langle 0, \eta | \hat{v}_k^2 | 0, \eta \rangle = \frac{1}{\sqrt{\pi}\rho} \int_{-\infty}^{+\infty} dv_k v_k^2 e^{-\frac{v_k^2}{\rho^2}} = \frac{\rho^2}{2}. \quad (2.56)$$

The variable $\rho = \rho(\eta)$ satisfies the Ermakov-Pinney (EP) Eq. (2.43). Let us imagine that we know the solution of the Mukhanov-Sasaki equation

$$v_k(\eta)'' + \omega^2(\eta)v_k(\eta) = 0, \quad (2.57)$$

which in general takes complex values and can thus be written as

$$v_k(\eta) = \frac{\rho(\eta)}{\sqrt{2}} e^{-i\theta(\eta)}. \quad (2.58)$$

If we assume that the solution $v_k(\eta)$ satisfies the Wronskian condition (1.126), the following holds

$$\theta' = \frac{1}{2|v_k|^2}. \quad (2.59)$$

The function $\rho(\eta)$ with condition (2.59) automatically solves the EP equation

$$\rho(\eta)'' + \omega^2(\eta)\rho(\eta) = \frac{1}{\rho^3(\eta)}. \quad (2.60)$$

We can now write

$$\rho(\eta) \longleftrightarrow \sqrt{2}|v_k|, \quad (2.61)$$

and substituting this result in (2.56) we find

$$\langle \hat{v}_k^2 \rangle \longleftrightarrow |v_k|^2 \quad (2.62)$$

which is the usual expectation value we had in the previous chapter, the one obtained when the perturbations are quantised on top of a classical background, for example as in (1.132). All the formalism developed in this chapter leads to a generalization of the semiclassical one, hence we can include some or all the terms that we have neglected previously and find suitable corrections to the standard procedure. However, in general, there are some deviations already coming at this level if one knows exactly the wave function of the universe. As a toy model, we will consider a scenario in which we know the analytical solutions to the WdW equation and see how these quantum corrections emerge.

Chapter 3

Flat potential inflation

The whole machinery we have constructed in the previous chapter can be implemented in a specific inflaton model. Realistic inflationary models generally admit neither an exact classical solution nor a fully quantum solution, but nevertheless one can study their evolution through some reasonable approximation, as we have already discussed in the previous chapters. Here, we want to consider a model having exact solutions and where the quantum dynamics is close to the classical one. The aim of this work is the theoretical understanding of how an exact quantum solution to the Wheeler-DeWitt equation can influence the classical power spectrum giving some deviations with respect to the standard approach. In particular, we stick to the model of a minimally coupled inflaton field with a constant potential. It is a toy model that captures several features of the inflationary spectra and, moreover, it is one of the potentials that have been studied as possible mechanisms for the production of primordial black holes as dark matter. We then see how a Gaussian superposition of solutions to the WdW equation leave an imprint on the observable power spectrum.

In this chapter, we start by considering the homogeneous part of the system, since its classical and quantum dynamics are not affected by the perturbations at leading order; we then obtain the equations governing the perturbations and understand how the quan-

tum wave packet influences the observable power spectrum. We finally calculate how a generic superposition of expanding solutions gives the same result to the leading order.

3.1 Classical homogeneous dynamics

The specific model we shall consider is that of a homogeneous inflaton field $\phi = \phi(\eta)$ minimally coupled to gravity and with a flat potential. Following the action (1.35) with $V = V_0$ and the flat FRLW metric (1.36), the momenta are

$$\pi_a = -6M_P^2 a', \quad \pi_\phi = a^2 \phi', \quad (3.1)$$

where π_ϕ is a constant of motion, it is one parameter that labels a specific classical trajectory. The Friedmann equation, for the expanding universe is then

$$H = \frac{1}{\sqrt{3}M_P} \sqrt{\frac{\pi_\phi^2}{2a^6} + V_0}, \quad (3.2)$$

with H the Hubble parameter. It can be solved in cosmic time

$$a(t) = \left[a_0^3 \cosh \left(\frac{\sqrt{3V_0}}{M_P} (t - t_0) \right) + \sqrt{a_0^6 + \frac{\pi_\phi^2}{2V_0}} \sinh \left(\frac{\sqrt{3V_0}}{M_P} (t - t_0) \right) \right]^{\frac{1}{3}}, \quad (3.3)$$

with $a_0 = a(t_0)$. We observe that it cannot be solved analytically in conformal time η .

We immediately note that for $\pi_\phi = 0$ the solution describes a deSitter space-time

$$a(t) = a_0 e^{\sqrt{\frac{V_0}{3}} \frac{t-t_0}{M_P}}, \quad (3.4)$$

and for a general $\pi_\phi \neq 0$, in the large t limit the background quickly approaches a deSitter space-time

$$a(t) \simeq \left(\frac{a_0^3 + \sqrt{a_0^6 + \frac{\pi_\phi^2}{2V_0}}}{2} \right)^{1/3} e^{\sqrt{\frac{V_0}{3}} \frac{t-t_0}{M_P}}, \quad (3.5)$$

with

$$H^2 - H_{dS}^2 \propto \frac{\pi_\phi^2}{a^6}. \quad (3.6)$$

The first slow roll parameter is

$$\epsilon_1 = -\frac{H'}{aH^2} = \frac{3\pi_\phi^2}{\pi_\phi^2 + 2a^6V_0}, \quad (3.7)$$

while the second slow roll parameter is

$$\eta_H = \frac{\epsilon_1'}{aH\epsilon_1} = -12 \frac{a^6V_0}{\pi_\phi^2 + 2a^6V_0}. \quad (3.8)$$

This model exhibits inflation if $\epsilon_1 < 1$ when $a^3 > \frac{|\pi_\phi|}{\sqrt{V_0}}$, but the second slow roll parameter, in that regime of the scale factor, takes the values inside the interval $(-6, -4)$, and for this reason it is not standard slow-roll inflation. Intuitively, we can think about this model as a never ending inflation that approaches the deSitter limit.

3.2 Quantum homogeneous dynamics

The Hamiltonian constraint is the following

$$\mathcal{H} = \frac{\pi_\phi^2}{2a^2} - \frac{\pi_a^2}{2m_P^2} + a^4V_0 = 0, \quad (3.9)$$

with $m_P^2 = 6M_P^2$. New variables are defined as

$$A \equiv \ln(m_P a), \quad F \equiv \phi/m_P, \quad (3.10)$$

and $V_0 = \lambda m_P^4$. The theory is canonically quantised and the Wheeler-DeWitt(WdW) equation emerges, after choosing a convenient ordering of the kinetic term, the WdW equation takes the form

$$\{\partial_A^2 - \partial_F^2 + 2\lambda e^{6A}\}\Psi(A, F) = 0. \quad (3.11)$$

Upon factorizing the wave function in the form

$$\Psi(A, F) = e^{iPF} \psi_P(A) \quad (3.12)$$

one obtains

$$(\partial_A^2 + P^2 + 2e^{6A}\lambda)\psi_P(A) = 0. \quad (3.13)$$

It is useful to define $\nu = iP/3$ and $z = \frac{\sqrt{2\lambda}}{3}e^{3A}$, in this way the Hankel functions $H_\nu^{(1)}(z), H_\nu^{(2)}(z)$ are the general solutions

$$\psi_P(A) = c_1 H_\nu^{(1)}(z) + c_2 H_\nu^{(2)}(z), \quad (3.14)$$

with c_1, c_2 arbitrary constants. Let us recall that the Hankel functions can be written in the following integral representation form, for example

$$H_\nu^{(1)}(z) = \frac{e^{-i\pi\nu/2}}{i\pi} \int_{-\infty}^{+\infty} dt e^{iz \cosh t - \nu t}. \quad (3.15)$$

This integral can be evaluated in the large z domain by the saddle point approximation, and the result is

$$H_\nu^{(1)}(z) \sim \sqrt{\frac{2}{\pi z}} \exp \left[i \left(z - \frac{\pi \nu}{2} - \frac{\pi}{4} + \frac{4\nu^2 - 1}{8z} \right) \right], \quad (3.16)$$

To the leading order and in that limit one finds

$$-i\partial_a H_\nu^{(1)}(z) = \sqrt{2\lambda} m_P^3 a^2 H_\nu^{(1)}(z). \quad (3.17)$$

where $\sqrt{2\lambda} m_P^3 a^2 = \pi_a^{\text{cl}}$ corresponds to the classical Friedmann equation and $H = -\sqrt{2\lambda} m_P$, describes a contracting universe. Similarly, the second Hankel function $H_{iP/3}^{(2)}(z)$, can be shown to describe an expanding universe and thus it is the relevant function that is going to be used for inflation. We note that the wave function $e^{iPF} H_{iP/3}^{(2)}(z)$ is a non-normalizable state that describes, for large z , a classical expanding universe with momentum $\pi_\phi = \frac{P}{m_P}$.

3.2.1 Gaussian wave packet solution

A general solution to the homogeneous WdW equation Eq. (3.11), is a superposition of the previous solutions

$$\Psi(A, F) = N \int_{-\infty}^{+\infty} dP e^{iPF} [c_1 f_1(P) H_\nu^{(1)}(z) + c_2 f_2(P) H_\nu^{(2)}(z)]. \quad (3.18)$$

In this model, for every slice of A the wave function is normalizable in the F variable, the normalization integral is

$$\int_{-\infty}^{+\infty} dF |\Psi(A, F)|^2 < +\infty, \quad (3.19)$$

and converges if the functions $f_1(P)$ and $f_2(P)$ are properly chosen. The value of the integral (3.19) depends on A , this means that if we write $\Psi \rightarrow N\Psi = N(A)\Psi$ the wave function is no longer a solution to the WdW equation. Normalization must be properly

used when one calculate the expectation value of some observable $\hat{O}$ as follows

$$\langle \hat{O} \rangle_A = \frac{\int_{-\infty}^{+\infty} dF \Psi_G^*(A, F) \hat{O} \Psi_G(A, F)}{\int_{-\infty}^{+\infty} dF |\Psi_G(A, F)|^2}. \quad (3.20)$$

The wave function describes an expanding universe with a definite momentum P_0 when $f_1(P) = 0$ and $f_2(P) \propto \delta(P - P_0)$. In such a case, for large z , the total wave function behaves as a plane wave. Instead if $f_1 = 0$ and f_2 is a Gaussian packet centered in P_0 one obtains a description which is close to the classical one. Indeed Gaussian states are the quantum states which mimic best the classical evolution. Let us then consider the following Gaussian-weighted superposition of expanding Hankel functions

$$\begin{aligned} \Psi_G(A, F) &= N \int_{-\infty}^{+\infty} dP e^{iP(F-F_0) - \sigma^2(P-P_0)^2} e^{\pi P/6} H_\nu^{(2)}(z) \\ &= -\frac{N}{i\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dP dt e^{iP(F-F_0) - \sigma^2(P-P_0)^2} e^{-iz \cosh t + iPt/3} \\ &= -\frac{N}{i\sqrt{\pi}\sigma^2} \int_{-\infty}^{+\infty} dt e^{-\frac{[t+3(F-F_0)]^2}{36\sigma^2} + \frac{iP_0}{3}[t+3(F-F_0)]} e^{-iz \cosh t}, \end{aligned} \quad (3.21)$$

In the last passage, the Gaussian integral over P is evaluated by completing the square in the exponent. The last integral can be evaluated in two different regimes.

Large z limit

When $z \gg 1$, the previous integral can be evaluated by the saddle-point approximation, the calculations can be followed in the appendix A, the result is

$$\begin{aligned} \Psi_G &= N \frac{6i e^{-i\pi/4}}{\sqrt{-i + 18z\sigma^2}} \\ &\times \exp \left\{ \frac{-2i\sigma^2[P_0^2 + 18(F-F_0)P_0z - 18z^2] + z[2 + 9(F-F_0)^2]}{2i - 36z\sigma^2} + \frac{i}{8z} \right\} \end{aligned} \quad (3.22)$$

and

$$|\Psi_G| = \frac{6|N| \exp \left[-\frac{[P_0 + 9(F - F_0)z]^2 \sigma^2}{1 + 324z^2 \sigma^4} \right]}{(1 + 324z^2 \sigma^4)^{1/4}}. \quad (3.23)$$

The modulus of the wave function is a Gaussian function peaked at

$$F = F_0 - \frac{P_0}{3\sqrt{2\lambda}} e^{-3A} = F_0 - \frac{P_0}{9z}, \quad (3.24)$$

which can be shown to be the large z classical trajectory for an expanding universe. In this limit, we can analytically calculate various expectation values regarding the field variable, the calculations are reported in the appendix C. The expectation value of the field $\hat{F}$ is

$$\langle \hat{F} \rangle_z = F_0 - \frac{P_0}{9z} + \mathcal{O}(z^{-3}), \quad (3.25)$$

with $\langle .. \rangle_z$ evaluated at $A = \frac{1}{3} \log \left(\frac{3z}{\sqrt{2\lambda}} \right)$, it naturally agrees with the maximum of the wave function. The expectation value of $\hat{F}^2$ is

$$\begin{aligned} \langle \hat{F}^2 \rangle_z &= F_0^2 + \sigma^2 - \frac{2F_0 P_0}{9z} \\ &+ \frac{1}{z^2} \left(\frac{P_0^2}{81} + \frac{1}{36} + \frac{1}{324\sigma^2} \right) + \mathcal{O}(z^{-3}). \end{aligned} \quad (3.26)$$

The expectation value of $\hat{\pi}_F$ tends to P_0

$$\langle \hat{\pi}_F \rangle_z = \langle \hat{P} \rangle_z = P_0 - \frac{P_0}{36\sigma^2 z^2} + \mathcal{O}(z^{-4}), \quad (3.27)$$

which confirms that this wave function, in momentum space, is peaked around the classical evolution P_0 and finally

$$\begin{aligned} \langle \hat{\pi}_F^2 \rangle_z &= \langle \hat{P}^2 \rangle_z = P_0^2 + \frac{1}{4\sigma^2} - \frac{P_0^2}{18\sigma^2 z^2} \\ &- \frac{1}{144\sigma^4 z^2} + \mathcal{O}(z^{-4}). \end{aligned} \quad (3.28)$$

The variances are

$$(\Delta F)^2 = \sigma^2 + \frac{1}{36z^2} + \frac{1}{324\sigma^2 z^2} + \mathcal{O}(z^{-4}), \quad (3.29)$$

and

$$(\Delta P)^2 = \frac{1}{4\sigma^2} - \frac{1}{144\sigma^4 z^2} + \mathcal{O}(z^{-4}). \quad (3.30)$$

Finally, the Heisenberg's uncertainty relation holds

$$(\Delta F \Delta P)^2 = \frac{1}{4} + \left(\frac{1}{36\sigma^2 z} \right)^2 + \mathcal{O}(z^{-4}). \quad (3.31)$$

All of these results naturally agree with the strict limit $z \rightarrow \infty$ of the modulus of the normalized wave function

$$\lim_{z \rightarrow \infty} |\Psi_G| = \frac{e^{-\frac{(F-F_0)^2}{4\sigma^2}}}{\sqrt{\sigma}(2\pi)^{1/4}}, \quad (3.32)$$

which highlights the fact that the wave function becomes a Gaussian with a definite width in both variables F and P , and it describes a Gaussian superposition of expanding classical universes.

Small σ limit

In the small- σ limit, the dominant contribution to the integral comes from the neighborhood of $t = -3(F - F_0)$. The calculations can be followed in the appendix B, on defining $y \equiv F - F_0$, one obtains

$$\begin{aligned} \Psi_G = & \frac{6Ne^{i\pi/4}}{\sqrt{-i + 18z\sigma^2 \cosh(3y)}} \\ & \times \exp \left\{ \frac{2i\sigma^2 [P_0^2 + 6P_0 z \sinh(3y) - \frac{9}{2}z^2(3 + \cosh(6y))] - 2z \cosh(3y)}{-2i + 36z\sigma^2 \cosh(3y)} \right\}. \end{aligned} \quad (3.33)$$

and

$$|\Psi_G| = \frac{6|N| \exp \left[-\frac{[P_0 + 3z \sinh 3(F - F_0)]^2 \sigma^2}{1 + 324z^2 \sigma^4 \cosh^2 3(F - F_0)} \right]}{[1 + 324z^2 \sigma^4 \cosh^2 3(F - F_0)]^{1/4}}. \quad (3.34)$$

The shape of the packet is no longer purely Gaussian. Its peak can be estimated calculating the minimum of the argument of the exponent, which is

$$F = F_0 - \frac{1}{3} \operatorname{arcsinh} \left(\frac{P_0}{3z} \right). \quad (3.35)$$

We note that the corresponding trajectory deviates from the classical one, but for large z , when this approximation is no longer valid, the wave function becomes the previous one (3.23), and the two peaks coincide. Moreover, the moduli of the two wave functions (3.23, 3.34) coincide for small values of $F - F_0$, where $\cosh 3(F - F_0) \simeq 1$ and $\sinh 3(F - F_0) \simeq 3(F - F_0)$. The figure below shows the evolution of a small σ wave function $|\Psi_G|$, one can observe how the two approximations (3.34, 3.23) are reliable in their domains.

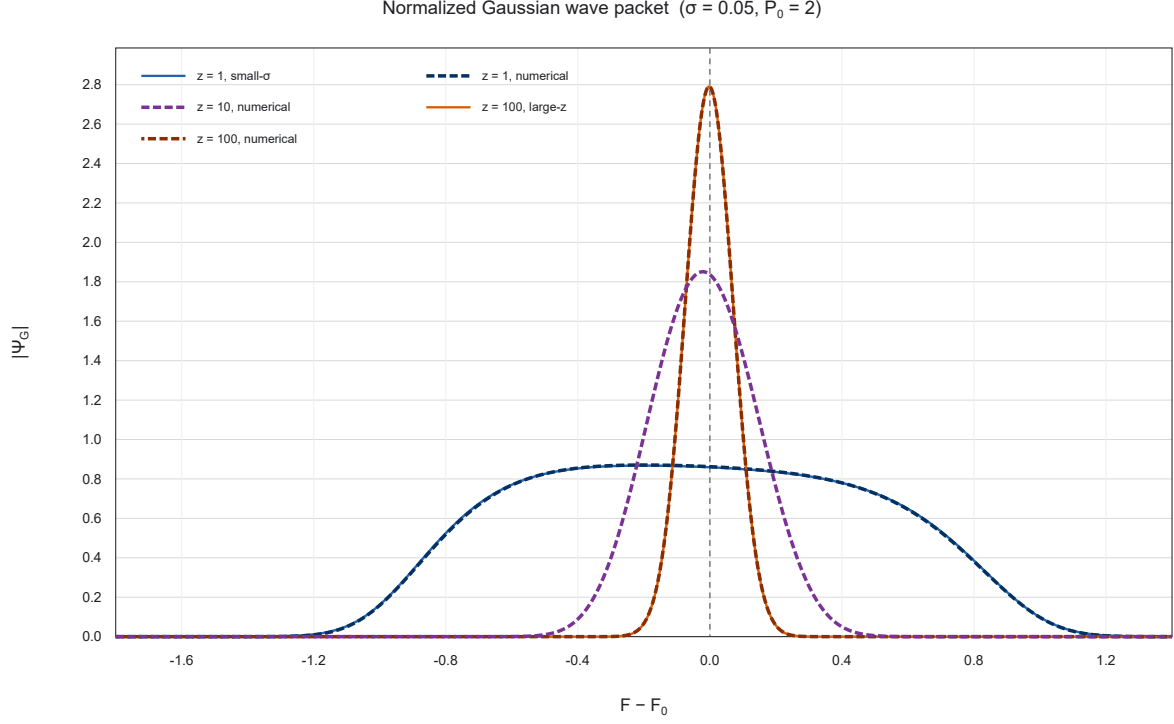


Figure 3.1: Modulus of the wave function for $P_0 = 2$ and $\sigma = 1/20$. The blue lines are the numerical result (dashed) and the small σ approximation for $z = 1$, the dashed purple line is the numerical result for $z = 10$ and the red lines are the numerical result (dashed) and the large z approximation for $z = 100$. Note that the blue lines have not an exact Gaussian shape

3.3 Inflationary perturbations

The previous calculations illustrated in the chapter 2 can be now followed to canonically quantise both the homogeneous and perturbations variables. The WdW equation can be written in the compact form

$$\left[\eta^{IJ} \partial_I \partial_J + 2e^{6A} \lambda + e^{2A} (\hat{\pi}_k^2 + \omega_k^2 \hat{v}_k^2) \right] \bar{\Psi}(A, F, v_k) = 0, \quad (3.36)$$

where $I, J = 1, 2$ correspond, respectively, to A, F , and $\eta^{IJ} = \text{diag}\{1, -1\}$; the operators $\hat{v}_k$ and $\hat{\pi}_k$ describe the Mukhanov-Sasaki variable and $\omega_k^2 = k^2 - \frac{z_{MS}''}{z_{MS}}$ is the usual frequency

that classically depends on the homogeneous variables (a, ϕ) . The frequency ω_k is here considered fully classical, this is an approximation that is equivalent to neglecting the quantum fluctuations of the homogeneous variables on the evolution of the perturbations. It is a reasonable assumption since we are interested in the power spectrum, and in the semiclassical approach $\langle 0|v_k^2|0\rangle \propto \hbar$, while the inclusion of such fluctuations would lead to a correction of order $\mathcal{O}(\hbar^2)$. We consider a single perturbation mode, since the same procedure and identical results are obtained when all k modes are taken into account. The factorised solutions are now

$$|\bar{\Psi}(A, F, v_k)\rangle = \tilde{\Psi}(A, F)|\tilde{\chi}_k(A, F, v_k)\rangle \quad (3.37)$$

where $|\tilde{\chi}_k(A, F, v_k)\rangle$ is the properly normalised wave function for v_k . The WdW equation becomes

$$\begin{aligned} \eta^{IJ} [(\partial_I \partial_J \tilde{\Psi})|\tilde{\chi}_k\rangle + 2(\partial_I \tilde{\Psi})\partial_J |\tilde{\chi}_k\rangle + \tilde{\Psi}\partial_I \partial_J |\tilde{\chi}_k\rangle] \\ + 2e^{6A}\lambda \tilde{\Psi}|\tilde{\chi}_k\rangle + e^{2A}\tilde{\Psi}(\hat{\pi}_k^2 + \omega_k^2 \hat{v}_k^2)|\tilde{\chi}_k\rangle = 0, \end{aligned} \quad (3.38)$$

and, upon contracting this equation with $\langle \tilde{\chi}_k|$, one obtains the equation for the wave function of the homogeneous degrees of freedom

$$\left\{ \eta^{IJ} \left[\partial_I \partial_J + 2\langle \tilde{\partial}_J \rangle_k \partial_I + \langle \tilde{\partial}_I \tilde{\partial}_J \rangle_k \right] + 2e^{6A}\lambda + 2e^{2A}\langle \tilde{H}_k \rangle_k \right\} \tilde{\Psi} = 0. \quad (3.39)$$

where $\langle \tilde{O} \rangle_k \equiv \langle \tilde{\chi}_k | \hat{O} | \tilde{\chi}_k \rangle$. The multiplication of Eq. (3.39) by $|\tilde{\chi}_k\rangle$ and the subtraction of the resulting equation from Eq. (3.38), leads to the equation for the wave function of v_k

$$\begin{aligned} \eta^{IJ} \left[2(\partial_I \tilde{\Psi})\tilde{\Psi}^{-1} \left(\partial_J - \langle \tilde{\partial}_J \rangle_k \right) |\tilde{\chi}_k\rangle + \left(\partial_I \partial_J - \langle \tilde{\partial}_I \tilde{\partial}_J \rangle_k \right) |\tilde{\chi}_k\rangle \right] \\ + 2e^{2A} \left(\hat{H}_k - \langle \tilde{H}_k \rangle_k \right) |\tilde{\chi}_k\rangle = 0. \end{aligned} \quad (3.40)$$

The above derivation corresponds to the standard Born–Oppenheimer decomposition of the WdW equation. One can now redefine $\tilde{\Psi}$ and $|\tilde{\chi}_k\rangle$ having opposite phases

$$\tilde{\Psi} = e^{i\theta}\Psi, \quad |\tilde{\chi}_k\rangle = e^{-i\theta}|\chi_k\rangle \quad (3.41)$$

with $\theta = \theta(A, F)$, thus obtaining

$$\partial_I |\tilde{\chi}_k\rangle = e^{-i\theta} [(\partial_I |\chi_k\rangle) - i(\partial_I \theta) |\chi_k\rangle], \quad (3.42)$$

$$\partial_I^2 |\tilde{\chi}_k\rangle = e^{-i\theta} \{(\partial_I^2 |\chi_k\rangle) - 2i(\partial_I \theta)(\partial_I |\chi_k\rangle) - [i(\partial_I^2 \theta) + (\partial_I \theta)^2] |\chi_k\rangle\} \quad (3.43)$$

and

$$\partial_I \tilde{\Psi} = e^{i\theta} [(\partial_I \Psi) + i(\partial_I \theta) \Psi], \quad (3.44)$$

$$\partial_I^2 \tilde{\Psi} = e^{i\theta} \{(\partial_I^2 \Psi) + 2i(\partial_I \theta)(\partial_I \Psi) + [i(\partial_I^2 \theta) - (\partial_I \theta)^2] \Psi\}. \quad (3.45)$$

On contracting (3.42,3.43) with $\langle \tilde{\chi}_k| = e^{i\theta} \langle \chi_k|$, one obtains

$$\langle \tilde{\partial}_I \rangle_k = \langle \partial_I \rangle_k - i\partial_I \theta, \quad (3.46)$$

$$\langle \tilde{\partial}_I^2 \rangle_k = \langle \partial_I^2 \rangle_k - 2i(\partial_I \theta) \langle \partial_I \rangle_k - [i(\partial_I^2 \theta) + (\partial_I \theta)^2]. \quad (3.47)$$

If one chooses θ in such a way that $\langle \partial_I \rangle_k = 0$ and

$$\langle \partial_I \chi_k | \partial_I \chi_k \rangle + \langle \chi_k | \partial_I^2 \chi_k \rangle = 0, \quad (3.48)$$

then the equations for the homogeneous inflaton-gravity system (3.39) and for the perturbations (3.40) simplify to

$$\eta^{IJ} \partial_I \partial_J \Psi + 2e^{6A} \lambda \Psi = -2e^{2A} \Psi \langle \hat{H}_k \rangle_k - \eta^{IJ} \Psi \langle \partial_I \partial_J \rangle_k, \quad (3.49)$$

$$\eta^{IJ} \frac{\partial_I \Psi}{\Psi} \partial_J |\chi_k\rangle + e^{2A} \left(\hat{H}_k - \langle \hat{H}_k \rangle_k \right) |\chi_k\rangle = \frac{\eta^{IJ}}{2} (\langle \partial_I \partial_J \rangle_k - \partial_I \partial_J) |\chi_k\rangle. \quad (3.50)$$

The right-hand sides (RHS) of these equations can be neglected. Indeed, the RHS of Eq. (3.49) describes the back-reaction of the perturbations on the homogeneous inflaton-gravity system, likewise the RHS of Eq. (3.50) contains the non-adiabatic corrections to the evolution of v_k (terms neglected also in Eq. (2.37)). These corrections are always present within the Born–Oppenheimer treatment, and are typically tiny, being of order $\sim (\hbar/m_P)^2$. The final resulting approximate system of equations is therefore

$$\begin{cases} (\eta^{IJ} \partial_I \partial_J + 2e^{6A} \lambda) \Psi = 0, \\ \eta^{IJ} \frac{\partial_I \Psi}{\Psi} \partial_J |\chi_k\rangle + e^{2A} \left(\hat{H}_k - \langle \hat{H}_k \rangle_k \right) |\chi_k\rangle = 0 \end{cases} \quad (3.51)$$

where the first equation coincides with the homogeneous WdW Eq. (3.11), and the second equation is equivalent to the Mukhanov–Sasaki equation when time is introduced.

3.3.1 Emergence of time

Starting from the solution to the first equation

$$\Psi = N e^{iPF} H_\nu^{(2)}(z), \quad (3.52)$$

the first term in the equation for the perturbation can be calculated. To the leading order for z large, one has

$$\eta^{IJ} \frac{\partial_I \Psi}{\Psi} \partial_J |\chi_k\rangle = -i \left(\sqrt{2\lambda} e^{3A} \partial_A + P \partial_F \right) |\chi_k\rangle \quad (3.53)$$

where $\sqrt{2\lambda} e^A = A'_{\text{cl}}$ and $e^{-2A} P = F'_{\text{cl}}$. Thus

$$\eta^{IJ} \frac{\partial_I \Psi}{\Psi} \partial_J |\chi_k\rangle = -ie^{2A} [A'_{\text{cl}}(\eta) \partial_A + F'_{\text{cl}}(\eta) \partial_F] |\chi_k\rangle = -ie^{2A} \frac{d}{d\eta} |\chi_k\rangle \quad (3.54)$$

is the total (conformal) time derivative along the classical trajectory. The second Eq. (3.51) can then be rewritten as

$$i \frac{d}{d\eta} |\chi_k\rangle_s = \hat{H}_k(\eta) |\chi_k\rangle_s \quad (3.55)$$

where

$$|\chi_k\rangle_s = |\chi_k\rangle e^{-i \int^\eta d\eta' \langle \hat{H}_k(\eta') \rangle_k} \quad (3.56)$$

which is the Schrödinger equation (or Schwinger–Tomonaga equation) corresponding to the MS equation. Let us now note that the cancellations leading to Eqs. (3.51) are a consequence of a suitable phase redefinition yielding $\langle \partial_I \rangle_k = 0$, or equivalently,

$$\partial_A \theta = i \langle \widetilde{\partial_A} \rangle_k, \quad \partial_F \theta = i \langle \widetilde{\partial_F} \rangle_k. \quad (3.57)$$

Such a suitable phase θ exists only if

$$\partial_F \langle \widetilde{\partial_A} \rangle_k = \partial_A \langle \widetilde{\partial_F} \rangle_k \iff \text{Im} \langle \partial_F \widetilde{\chi}_k | \partial_A \widetilde{\chi}_k \rangle = 0. \quad (3.58)$$

Since the quantum fluctuations are neglected, F is evaluated along the classical trajectory. One therefore has $F = F_{\text{cl}}(A)$ and $\partial_F = (dF_{\text{cl}}/dA)^{-1} \partial_A$. The condition (3.58) is then automatically satisfied

$$\langle \partial_F \widetilde{\chi}_k | \partial_A \widetilde{\chi}_k \rangle = (dF_{\text{cl}}/dA)^{-1} \| |\partial_A \widetilde{\chi}_k\rangle \|^2. \quad (3.59)$$

The resulting solution of the WdW Eq. (3.36) is

$$\bar{\Psi} = \Psi(A, F) |\chi(A, v_k)\rangle = \Psi(A, F) |\chi(A, v_k)\rangle_s e^{i \int^\eta d\eta' \langle \hat{H}_k(\eta') \rangle_k}. \quad (3.60)$$

The linearity of the WdW equation guarantees that any superposition of the approximate solutions is a solution to the same order of approximation. Thus

$$\bar{\Psi} = \sum_i c_i \Psi_i(A, F) |\chi_i(A, v_k)\rangle \quad (3.61)$$

and, in particular, for the Gaussian wave-packet solution (3.21), $i \rightarrow P$ and

$$|\bar{\Psi}(A, F, v_k)\rangle = N \int_{-\infty}^{+\infty} dP e^{iP(F-F_0) - \sigma^2(P-P_0)^2} e^{\pi P/6} H_\nu^{(2)}(z) |\chi_P(A, v_k)\rangle. \quad (3.62)$$

In this context, time is introduced along each classical trajectory, labelled by P .

3.4 Power Spectrum

Let us now calculate the spectrum of the MS variable, $\langle \hat{v}_k^2 \rangle$. In the standard semiclassical approach there is a single classical solution describing the homogeneous background

$$P_v(k; P_0) \equiv \langle \hat{v}_k^2 \rangle_A = \langle \chi_{P_0}(A, v_k) | \hat{v}_k^2 | \chi_{P_0}(A, v_k) \rangle \equiv \int_{-\infty}^{+\infty} dv_k |\chi_{P_0}|^2 v_k^2 \quad (3.63)$$

where P_0 labels the particular classical trajectory and A plays the role of the time variable. It can be shown that $P_v(k; P_0)$ is related to the power spectrum of curvature perturbations $P_{\mathcal{R}}(k; P_0)$ as

$$P_{\mathcal{R}}(k; P_0) = \frac{k^3}{2\pi^2} \frac{P_v(k; P_0)}{z_{MS}^2} \Big|_{A_{end}}, \quad (3.64)$$

where A_{end} is the value of A at the end of inflation (this model does not predict the end of inflation, we need an external mechanism). In the fully quantised description, the homogeneous inflaton field is instead described by a wave function with a Gaussian distribution peaked around P_0 . If $A = \frac{1}{3} \log \left(\frac{3z}{\sqrt{2\lambda}} \right)$ is used to parametrize the time

evolution, one has

$$\langle \hat{v}_k^2 \rangle_A = \langle \bar{\Psi}(A, F, v_k) | \hat{v}_k^2 | \bar{\Psi}(A, F, v_k) \rangle \equiv \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dv_k dF |\bar{\Psi}|^2 v_k^2 \quad (3.65)$$

and the inflationary power spectrum is obtained after integrating also over the homogeneous degree of freedom F . More explicitly, for the solution (3.62) one finds

$$\begin{aligned} \langle \hat{v}_k^2 \rangle_A = N^2 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dF dP d\bar{P} e^{i(P-\bar{P})(F-F_0)-\sigma^2(\bar{P}-P_0)^2-\sigma^2(P-P_0)^2} e^{\pi(\bar{P}+P)/6} \\ \times \left(H_{i\bar{P}/3}^{(2)}(z) \right)^* H_{iP/3}^{(2)}(z) \langle \chi_{\bar{P}}(A, v_k) | \hat{v}_k^2 | \chi_P(A, v_k) \rangle \end{aligned} \quad (3.66)$$

where the integration over F produces the Dirac delta distribution $2\pi\delta(P-\bar{P})$. We observe that, once time has been introduced and the tiny quantum corrections are neglected, one recovers the semiclassical MS equation, in which the dependence on F is replaced by its corresponding P -dependent classical trajectory $F_{\text{cl}}(A; P)$. Performing also the integration over $\bar{P}$, one obtains

$$\begin{aligned} \langle \hat{v}_k^2 \rangle_A = 2\pi N^2 \int_{-\infty}^{+\infty} dP e^{-2\sigma^2(P-P_0)^2} e^{\pi P/3} \left(H_{\nu}^{(2)}(z) \right)^* H_{\nu}^{(2)}(z) \langle \chi_P(A, v_k) | \hat{v}_k^2 | \chi_P(A, v_k) \rangle \\ = 2\pi N^2 \int_{-\infty}^{+\infty} dP e^{-2\sigma^2(P-P_0)^2} e^{\pi P/3} |H_{\nu}^{(2)}(z)|^2 P_v(k; P). \end{aligned} \quad (3.67)$$

As expected, different background trajectories do not interfere because the MS equation is solved along each classical background trajectory independently. Nevertheless, describing the homogeneous inflaton by a Gaussian wave packet has non-trivial consequences for the resulting power spectrum. The above expression can be further simplified in the large- a limit (and using the saddle point approximation). Indeed, starting from the integral representation of the Hankel functions, Eq. (3.15), one finds

$$|H_{\nu}^{(2)}(z)|^2 = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{dt d\bar{t}}{\pi^2} e^{-\pi P/3} e^{iP(t-\bar{t})/3 - iz(\cosh t - \cosh \bar{t})} \simeq \frac{2}{z\pi} e^{-\pi P/3} \quad (3.68)$$

and Eq. (3.67) reduces to

$$\langle \hat{v}_k^2 \rangle_A = \frac{4}{z} \left(\frac{\sqrt{8\pi}}{z\sigma} \right)^{-1} \int_{-\infty}^{+\infty} dP e^{-2\sigma^2(P-P_0)^2} P_v(k; P) \quad (3.69)$$

where the proper normalisation factor has been calculated for large a accordingly. Notice that in the limit $\sigma \rightarrow \infty$ we recover the standard semiclassical limit in the P_0 trajectory

$$\lim_{\sigma \rightarrow \infty} \langle \hat{v}_k^2 \rangle_A = \int_{-\infty}^{+\infty} dP \delta(P - P_0) P_v(k; P) = P_v(k; P_0), \quad (3.70)$$

which again shows that this procedure is a generalisation of the standard semiclassical approach. Following the analysis presented in the appendix D, the power spectrum can be expanded as

$$P_v(k; P) \simeq c_k^{(0)} + c_k^{(2)} P^2 \quad (3.71)$$

where $c_k^{(0)}$ is the deSitter spectrum and $c_k^{(2)} P^2$ the correction coming from the transient evolution of the background. The power spectrum in our context is then

$$\begin{aligned} \langle \hat{v}_k^2 \rangle_A &= \sqrt{\frac{2\sigma^2}{\pi}} \int_{-\infty}^{+\infty} dP e^{-2\sigma^2(P-P_0)^2} \left(c_k^{(0)} + c_k^{(2)} P^2 \right) \\ &= c_k^{(0)} + c_k^{(2)} \frac{1 + 4\sigma^2 P_0^2}{4\sigma^2}. \end{aligned} \quad (3.72)$$

As σ decreases, the additional P_0 -independent term $c_k^{(2)}/(4\sigma^2)$ grows, whereas the P_0 -dependent term $c_k^{(2)} P_0^2$ is unchanged. We further note that the k -dependence of $c_k^{(0)}$ and $c_k^{(2)}$ differ, leading to changes in both the spectrum normalisation and the spectral index. In this way, we have found that the quantum cosmology approach, given the exact homogeneous wave function, gives a relevant contribution to the inflationary power spectrum. The term $\frac{c_k^{(2)}}{4\sigma^2}$ is the quantum cosmological effect of this model.

3.4.1 A formal generalisation of the Gaussian wave packet

In the previous section we supposed that the superposition was exactly Gaussian, however, we can consider a generic superposition $f(P)$ of expanding Hankel function

$$|\Psi(A, F, v_k)\rangle^{[f]} = N \int_{-\infty}^{+\infty} dP e^{iP(F-F_0)} f(P) e^{\pi P/6} H_\nu^{(2)}(z) |\chi_P(A, v_k)\rangle. \quad (3.73)$$

If the spectrum for a given value of P can be written as

$$P_v(k; P) \simeq c_k^{(0)} + c_k^{(2)} P^2, \quad (3.74)$$

the general result is

$$\left\langle \Psi | \hat{v}_k^2 | \Psi \right\rangle_A^{[f]} = \left\langle \hat{v}_k^2 \right\rangle_A^{[f]} \simeq c_k^{(0)} + c_k^{(2)} \left\langle \Psi | P^2 | \Psi \right\rangle_A^{[f]}. \quad (3.75)$$

In particular, for large z , and if we keep an extra term in the Hankel function expansion we obtain

$$e^{\pi P/3} |H_{iP/3}^{(2)}(z)|^2 = \frac{2}{\pi z} \left[1 - \frac{1}{z^2} u(P) + O(z^{-4}) \right], \quad (3.76)$$

where $u(P) = \frac{1}{8} + \frac{P^2}{18}$. Following the previous calculations, we find

$$\left\langle \hat{v}_k^2 \right\rangle_A^{[f]} = \frac{\left\langle P_v(k; P) \left[1 - \frac{u(P)}{z^2} \right] \right\rangle_f}{\left\langle 1 - \frac{u(P)}{z^2} \right\rangle_f} + O(z^{-4}). \quad (3.77)$$

where

$$\langle X(P) \rangle_f \equiv \frac{1}{I_0} \int_{-\infty}^{+\infty} dP |f(P)|^2 X(P), \quad I_0 \equiv \int_{-\infty}^{+\infty} dP |f(P)|^2. \quad (3.78)$$

The resulting expectation value is then

$$\langle \hat{v}_k^2 \rangle_A^{[f]} = c_k^{(0)} + c_k^{(2)} \left[\langle P^2 \rangle_f - \frac{\langle P^4 \rangle_f - \langle P^2 \rangle_f^2}{18z^2} \right] + O(z^{-4}). \quad (3.79)$$

To leading order, for a general superposition amplitude $f(P)$, the term $\langle P^2 \rangle_f$ is equal to the expectation value of P^2 for a Gaussian distribution with the same mean and variance of $\frac{|f(P)|^2}{I_0}$. This means that, to leading order, if $\langle P \rangle_f = P_0$ and $\langle \Delta P^2 \rangle_f = \frac{1}{4\sigma^2}$ the result $\langle \hat{v}_k^2 \rangle_A^{[f]}$ is indistinguishable from $\langle \hat{v}_k^2 \rangle_A^{[Gaussian]}$, with the previous Gaussian superposition $e^{-\sigma^2(P-P_0)^2}$.

The difference arises when the contributions proportional to $1/z^2$ are non-negligible. Indeed, for a Gaussian we have

$$\langle \hat{v}_k^2 \rangle_A^{[Gaussian]} = c_k^{(0)} + c_k^{(2)} \left[P_0^2 + \frac{1}{4\sigma^2} - \frac{P_0^2}{18\sigma^2 z^2} - \frac{1}{144\sigma^4 z^2} + O(z^{-4}) \right], \quad (3.80)$$

while, for a general superposition $f(P)$

$$\langle \hat{v}_k^2 \rangle_A^{[f]} = c_k^{(0)} + c_k^{(2)} \left[P_0^2 + \frac{1}{4\sigma^2} - \frac{\langle P^4 \rangle_f - \langle P^2 \rangle_f^2}{18z^2} + O(z^{-4}) \right], \quad (3.81)$$

where $\langle P^4 \rangle_f$, which must be finite, is not uniquely determined by the mean and variance, and may therefore differ from the corresponding Gaussian counterpart.

As an example, let us consider the generalised Gaussian distributions. We define

$$f_\beta(P) = \left[\frac{\beta}{2\lambda_\beta \Gamma(1/\beta)} \right]^{1/2} \exp \left[-\frac{1}{2} \left(\frac{|P - P_0|}{\lambda_\beta} \right)^\beta \right], \quad (3.82)$$

where

$$\lambda_\beta = \frac{1}{2\sigma} \left[\frac{\Gamma(1/\beta)}{\Gamma(3/\beta)} \right]^{1/2}. \quad (3.83)$$

The corresponding normalised distribution is therefore

$$|f_\beta(P)|^2 = \frac{\beta}{2\lambda_\beta\Gamma(1/\beta)} \exp\left[-\left(\frac{|P-P_0|}{\lambda_\beta}\right)^\beta\right], \quad \int_{-\infty}^{+\infty} dP |f_\beta(P)|^2 = 1. \quad (3.84)$$

With the choice in Eq. (3.83), all values of β have the same mean and variance,

$$\langle P \rangle_{f_\beta} = P_0, \quad \langle \Delta P^2 \rangle_{f_\beta} = \frac{1}{4\sigma^2}. \quad (3.85)$$

The following result can then be obtained

$$\langle P^4 \rangle_{f_\beta} = P_0^4 + \frac{3P_0^2}{2\sigma^2} + \frac{1}{16\sigma^4} \frac{\Gamma(1/\beta)\Gamma(5/\beta)}{\Gamma(3/\beta)^2}. \quad (3.86)$$

It follows that the power spectrum, for the generalised Gaussian distribution is

$$\langle v_k^2 \rangle_A^{[f_\beta]} = c_k^{(0)} + c_k^{(2)} \left[P_0^2 + \frac{1}{4\sigma^2} - \frac{P_0^2}{18\sigma^2 z^2} - \frac{1}{288\sigma^4 z^2} \left(\frac{\Gamma(1/\beta)\Gamma(5/\beta)}{\Gamma(3/\beta)^2} - 1 \right) + O(z^{-4}) \right]. \quad (3.87)$$

Therefore, to the leading-order, the spectrum is independent of β , while the finite- z correction probes the shape of the distribution through its fourth moment.

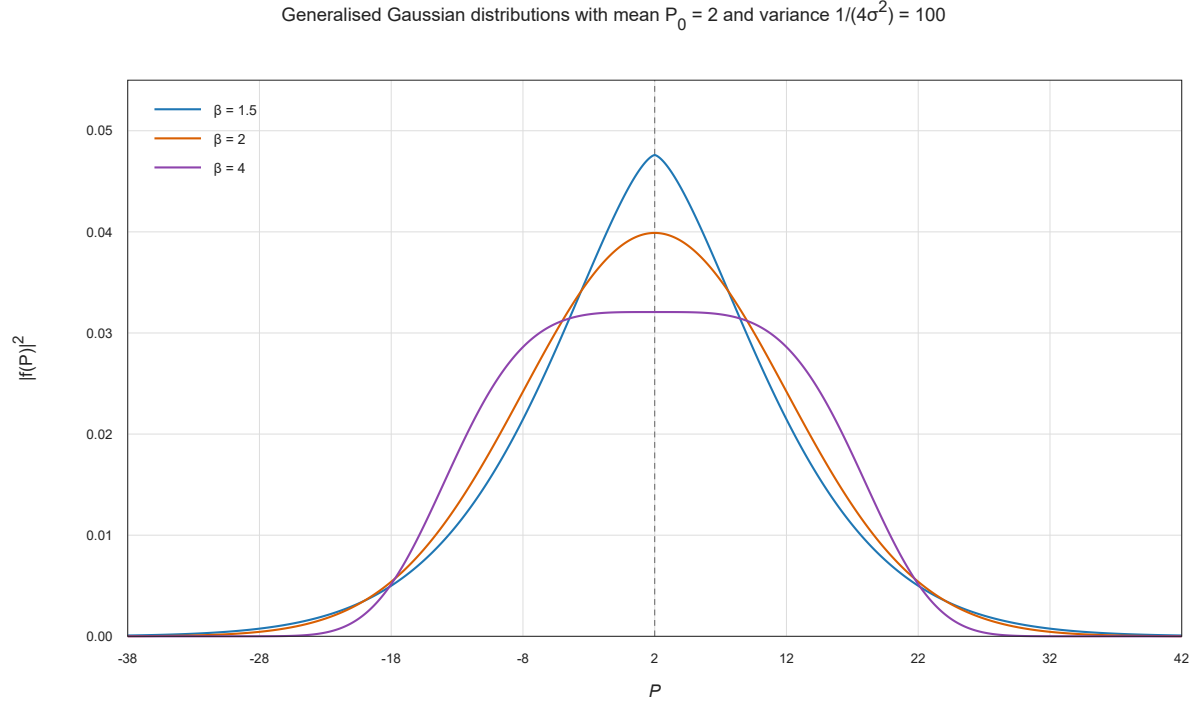


Figure 3.2: Generalised Gaussian distributions with $P_0 = 2$ and $\sigma = 1/20$. The blue, red and purple lines correspond, respectively, to $\beta = 1.5, 2, 4$

For $\beta = 1.5$, for example, one has

$$\langle v_k^2 \rangle_A^{[f_{1.5}]} = c_k^{(0)} + c_k^{(2)} \left[P_0^2 + \frac{1}{4\sigma^2} - \frac{P_0^2}{18\sigma^2 z^2} - \frac{1}{288\sigma^4 z^2} \left(\frac{56\pi}{27\sqrt{3}} - 1 \right) + O(z^{-4}) \right], \quad (3.88)$$

and for $\beta = 4$

$$\langle v_k^2 \rangle_A^{[f_4]} = c_k^{(0)} + c_k^{(2)} \left[P_0^2 + \frac{1}{4\sigma^2} - \frac{P_0^2}{18\sigma^2 z^2} - \frac{1}{288\sigma^4 z^2} \left(\frac{\Gamma(1/4)^2}{4\Gamma(3/4)^2} - 1 \right) + O(z^{-4}) \right]. \quad (3.89)$$

The difference between the two power spectrum (3.89) and (3.88) is therefore

$$\langle v_k^2 \rangle_A^{[f_4]} - \langle v_k^2 \rangle_A^{[f_{1.5}]} = c_k^{(2)} \frac{1.57351}{288\sigma^4 z^2} + O(z^{-4}), \quad (3.90)$$

thus vanishing for $z \rightarrow \infty$.

To the leading order, the Gaussian superposition of expanding universes completely determines the quantum cosmological corrections in the power spectrum.

Conclusions

The standard approach in inflationary models treats the homogeneous variables classically (the scale factor and the homogeneous part of the inflaton field), while the perturbations quantum mechanically. We ultimately expect all variables to be governed by quantum mechanics, in this regard, this thesis focused on the canonical quantisation of the inflaton-gravity system, which quantises also the homogeneous variables. The original part of this thesis is about a minimally coupled inflaton scalar field with constant potential. This model was used mostly because of its exact solution to the homogeneous WdW equation, but nonetheless has also some physical interest. A Gaussian superposition of these solutions with definite momenta conjugate to the field was chosen as the quantum wave function that most closely reproduces the classical evolution.

The resulting perturbation spectrum, which is the observable of interest, was therefore obtained by “averaging” over different semiclassical trajectories, and the spectrum derived in this way is indeed found to be modified. Additional effects are expected because of the explicit dependence of the Mukhanov–Sasaki variable on the homogeneous inflaton and scale factor. Such effects were neglected since they are expected to be smaller with respect to the effects we have obtained, being of order m_P^{-2} .

Moreover, during the early stage of inflation, we have found that the Gaussian wave packets may slightly deviate from the corresponding classical trajectories, which are recovered only at later times. This is an interesting result that deserves further investigation in future work.

Finally, we have also relaxed the hypothesis of a Gaussian superposition and found that, to the leading order and under certain conditions, the power spectrum is equal to the one obtained previously. For this reason, the Gaussian superposition, with its two parameters, completely determines the general imprint of the gravitational wave function on the result and thus governs the quantum cosmological corrections to the inflationary spectrum.

The original part of this thesis is presented in a manuscript and is currently under review in a scientific journal [18].

In the context of quantum cosmology, we expect that similar results could be obtained when considering a realistic inflationary model with a nearly flat potential and a slow roll evolution. However this study is left for future work.

Appendix A

Large- z approximation of the wave function

We start from the exact integral representation of the Gaussian wave packet,

$$\Psi_G(A, F) = -\frac{N}{i\sqrt{\pi\sigma^2}} \int_{-\infty}^{+\infty} dt e^{S(t)}, \quad (\text{A.1})$$

where

$$S(t) = -\frac{[t + 3(F - F_0)]^2}{36\sigma^2} + \frac{iP_0}{3}[t + 3(F - F_0)] - iz \cosh t. \quad (\text{A.2})$$

For convenience, we define

$$y = F - F_0. \quad (\text{A.3})$$

Saddle-point

The saddle point t_s is determined by

$$S'(t_s) = 0. \quad (\text{A.4})$$

Since

$$S'(t) = -\frac{t + 3y}{18\sigma^2} + \frac{iP_0}{3} - iz \sinh t, \quad (\text{A.5})$$

the saddle-point equation is

$$t_s + 18iz\sigma^2 \sinh t_s = -3y + 6i\sigma^2 P_0. \quad (\text{A.6})$$

In the large- z regime, $t_s = \mathcal{O}(z^{-1})$. Expanding $\sinh t_s = t_s + \mathcal{O}(t_s^3)$, one obtains

$$t_s = \frac{-3y + 6i\sigma^2 P_0}{1 + 18iz\sigma^2} + \mathcal{O}(z^{-3}). \quad (\text{A.7})$$

Expansion of $S(t)$, up to the fourth derivative

The derivatives of $S(t)$ are

$$S''(t) = -\frac{1}{18\sigma^2} - iz \cosh t, \quad (\text{A.8})$$

$$S'''(t) = -iz \sinh t, \quad (\text{A.9})$$

$$S^{(4)}(t) = -iz \cosh t. \quad (\text{A.10})$$

We introduce the notation

$$S_s = S(t_s), \quad S_n = S^{(n)}(t_s). \quad (\text{A.11})$$

Expanding around the saddle, $t = t_s + \tau$, gives

$$S(t_s + \tau) = S_s + \frac{S_2}{2}\tau^2 + \frac{S_3}{6}\tau^3 + \frac{S_4}{24}\tau^4 + \mathcal{O}(\tau^5). \quad (\text{A.12})$$

Therefore,

$$e^{S(t_s+\tau)} \simeq e^{S_s} e^{S_2 \tau^2/2} \left[1 + \frac{S_3}{6} \tau^3 + \frac{S_4}{24} \tau^4 + \frac{S_3^2}{72} \tau^6 + \dots \right]. \quad (\text{A.13})$$

The term proportional to τ^3 is odd and does not contribute. The required Gaussian integrals are

$$\int_C d\tau e^{S_2 \tau^2/2} = \sqrt{\frac{2\pi}{-S_2}}, \quad (\text{A.14})$$

$$\int_C d\tau \tau^4 e^{S_2 \tau^2/2} = \frac{3}{S_2^2} \sqrt{\frac{2\pi}{-S_2}}, \quad (\text{A.15})$$

and

$$\int_C d\tau \tau^6 e^{S_2 \tau^2/2} = -\frac{15}{S_2^3} \sqrt{\frac{2\pi}{-S_2}}. \quad (\text{A.16})$$

It follows that

$$\int_C d\tau e^{S(t_s+\tau)} \simeq e^{S_s} \sqrt{\frac{2\pi}{-S_2}} \left[1 + \frac{S_4}{8S_2^2} - \frac{5S_3^2}{24S_2^3} \right]. \quad (\text{A.17})$$

Consequently, the fourth-order saddle-point approximation is

$$\Psi_G \simeq -\frac{N}{i\sqrt{\pi\sigma^2}} e^{S_s} \sqrt{\frac{2\pi}{-S_2}} \left[1 + \frac{S_4}{8S_2^2} - \frac{5S_3^2}{24S_2^3} \right]. \quad (\text{A.18})$$

In the large- z regime, using $t_s = \mathcal{O}(z^{-1})$,

$$S_2 = -iz - \frac{1}{18\sigma^2} + \mathcal{O}(z^{-1}), \quad (\text{A.19})$$

$$S_3 = -iz \sinh t_s = \mathcal{O}(1), \quad (\text{A.20})$$

$$S_4 = -iz \cosh t_s = -iz + \mathcal{O}(z^{-1}). \quad (\text{A.21})$$

Thus,

$$\frac{S_4}{8S_2^2} = \frac{i}{8z} + \mathcal{O}(z^{-2}), \quad (\text{A.22})$$

whereas

$$\frac{S_3^2}{S_2^3} = \mathcal{O}(z^{-3}). \quad (\text{A.23})$$

The fourth-order correction is therefore

$$1 + \frac{S_4}{8S_2^2} - \frac{5S_3^2}{24S_2^3} = 1 + \frac{i}{8z} + \mathcal{O}(z^{-2}). \quad (\text{A.24})$$

we obtain the correct result, which is

$$\begin{aligned} \Psi_G(F, z) &\simeq \frac{6Ne^{-i\pi/4}}{\sqrt{-i + 18z\sigma^2}} \\ &\times \exp \left[\frac{-2i\sigma^2 [P_0^2 + 18(F - F_0)P_0z - 18z^2] + z [2 + 9(F - F_0)^2]}{2i - 36z\sigma^2} + \frac{i}{8z} \right] \end{aligned} \quad (\text{A.25})$$

Appendix B

Small- σ approximation of the wave function

We define

$$x = 3(F - F_0), \quad B = \frac{P_0}{3} + z \sinh x, \quad (\text{B.1})$$

for small σ , the saddle is close to $-x$. Expanding the saddle equation gives

$$t_s = -x + 18i\sigma^2 B + 324\sigma^4 z \cosh x B + \mathcal{O}(\sigma^6). \quad (\text{B.2})$$

The exponent evaluated at the saddle, can be shown to be

$$S(t_s) = -iz \cosh x - 9\sigma^2 B^2 + 162i\sigma^4 z \cosh x B^2 + \mathcal{O}(\sigma^6). \quad (\text{B.3})$$

Expansion through the fourth derivative

Set

$$t = t_s + \eta. \quad (\text{B.4})$$

Since $S'(t_s) = 0$,

$$S(t_s + \eta) = S(t_s) + \frac{S''(t_s)}{2}\eta^2 + \frac{S^{(3)}(t_s)}{6}\eta^3 + \frac{S^{(4)}(t_s)}{24}\eta^4 + \mathcal{O}(\eta^5). \quad (\text{B.5})$$

Therefore

$$\begin{aligned} \int dt e^{S(t)} &\simeq e^{S(t_s)} \int d\eta \exp \left[-\frac{1}{2} \left(\frac{1}{18\sigma^2} + iz \cosh t_s \right) \eta^2 \right] \\ &\times \left[1 + \frac{S^{(3)}(t_s)}{6}\eta^3 + \frac{S^{(4)}(t_s)}{24}\eta^4 + \frac{S^{(3)}(t_s)^2}{72}\eta^6 + \dots \right]. \end{aligned} \quad (\text{B.6})$$

The odd term proportional to η^3 integrates to zero. Using

$$\langle f(\eta) \rangle = \frac{\int d\eta e^{\frac{1}{2}S''(t_s)\eta^2} f(\eta)}{\int d\eta e^{\frac{1}{2}S''(t_s)\eta^2}} \quad (\text{B.7})$$

we have

$$\langle \eta^4 \rangle = \frac{3}{\left(\frac{1}{18\sigma^2} + iz \cosh t_s \right)^2}, \quad (\text{B.8})$$

$$\langle \eta^6 \rangle = \frac{15}{\left(\frac{1}{18\sigma^2} + iz \cosh t_s \right)^3}, \quad (\text{B.9})$$

one obtains

$$\begin{aligned} \int dt e^{S(t)} &\simeq e^{S(t_s)} \sqrt{\frac{2\pi}{\frac{1}{18\sigma^2} + iz \cosh t_s}} \\ &\times \left[1 + \frac{S^{(4)}(t_s)}{8 \left(\frac{1}{18\sigma^2} + iz \cosh t_s \right)^2} + \frac{5S^{(3)}(t_s)^2}{24 \left(\frac{1}{18\sigma^2} + iz \cosh t_s \right)^3} + \dots \right]. \end{aligned} \quad (\text{B.10})$$

Since

$$\frac{1}{18\sigma^2} + iz \cosh t_s = \mathcal{O}(\sigma^{-2}), \quad (\text{B.11})$$

the term containing $S^{(4)}$ is of order σ^4 , whereas the term containing $S^{(3)2}$ is of order σ^6 . Thus, we obtain

$$\begin{aligned} \Psi_G(F, z) &\simeq \frac{Ni}{\sqrt{\pi}\sigma} \sqrt{\frac{2\pi}{\frac{1}{18\sigma^2} + iz \cosh t_s}} e^{S(t_s)} \\ &\times \left[1 - \frac{iz \cosh t_s}{8 \left(\frac{1}{18\sigma^2} + iz \cosh t_s \right)^2} + \mathcal{O}(\sigma^6) \right]. \end{aligned} \quad (\text{B.12})$$

and explicitly, after some calculations,

$$\begin{aligned} \Psi_G(F, z) &\simeq \frac{6Ne^{i\pi/4}}{\sqrt{-i + 18z\sigma^2 \cosh[3(F - F_0)]}} \\ &\times \exp \left\{ \frac{2i\sigma^2 [P_0^2 + 6P_0z \sinh[3(F - F_0)] - \frac{27}{2}z^2 - \frac{9}{2}z^2 \cosh[6(F - F_0)]]}{-2i + 36z\sigma^2 \cosh[3(F - F_0)]} \right. \\ &\quad \left. - \frac{2z \cosh[3(F - F_0)]}{-2i + 36z\sigma^2 \cosh[3(F - F_0)]} \right\} \\ &\times \left[1 + \mathcal{O}(\sigma^4) \right]. \end{aligned} \quad (\text{B.13})$$

Appendix C

Expectation values in the large- z approximation

We consider the Gaussian wave packet

$$\Psi_G(A, F) = \int_{-\infty}^{+\infty} dP e^{iP(F-F_0) - \sigma^2(P-P_0)^2} e^{\pi P/6} H_{iP/3}^{(2)}(z), \quad (\text{C.1})$$

with normalized expectation values

$$\langle F^n \rangle_A = \frac{\int_{-\infty}^{+\infty} dF F^n |\Psi_G(A, F)|^2}{\int_{-\infty}^{+\infty} dF |\Psi_G(A, F)|^2}. \quad (\text{C.2})$$

Large- z expansion

For $z \gg 1$, the Hankel function admits the expansion

$$e^{\pi P/6} H_{iP/3}^{(2)}(z) = \mathcal{C}(z) \left[1 + \frac{iu(P)}{z} + \frac{v(P)}{z^2} + \mathcal{O}(z^{-3}) \right], \quad (\text{C.3})$$

where

$$\mathcal{C}(z) = \sqrt{\frac{2}{\pi z}} e^{-iz+i\pi/4}, \quad (\text{C.4})$$

and

$$u(P) = \frac{1}{8} + \frac{P^2}{18}, \quad v(P) = -\frac{9}{128} - \frac{5P^2}{144} - \frac{P^4}{648}. \quad (\text{C.5})$$

Defining

$$B(P, z) = 1 + \frac{iu(P)}{z} + \frac{v(P)}{z^2} + \mathcal{O}(z^{-3}), \quad (\text{C.6})$$

the packet becomes

$$\Psi_G(A, F) \simeq \mathcal{C}(z) \int_{-\infty}^{+\infty} dP e^{iP(F-F_0)-\sigma^2(P-P_0)^2} B(P, z). \quad (\text{C.7})$$

Let

$$y = F - F_0. \quad (\text{C.8})$$

The leading Fourier transform is

$$G(y) = \int_{-\infty}^{+\infty} dP e^{-\sigma^2(P-P_0)^2+iPy} = \frac{\sqrt{\pi}}{\sigma} e^{-y^2/(4\sigma^2)+iP_0y}, \quad (\text{C.9})$$

while powers of P are generated through

$$\int_{-\infty}^{+\infty} dP P^n e^{-\sigma^2(P-P_0)^2+iPy} = (-i\partial_y)^n G(y). \quad (\text{C.10})$$

It follows that

$$\begin{aligned} \Psi_G(F, z) \simeq \mathcal{C}(z) & \left[G(y) + \frac{i}{z} \left(\frac{1}{8} G(y) - \frac{1}{18} G''(y) \right) \right. \\ & \left. + \frac{1}{z^2} \left(-\frac{9}{128} G(y) + \frac{5}{144} G'''(y) - \frac{1}{648} G^{(4)}(y) \right) \right]. \end{aligned} \quad (\text{C.11})$$

The corresponding probability density can be written as

$$|\Psi_G(F, z)|^2 = \mathcal{K}(z) e^{-y^2/(2\sigma^2)} \left[1 + \frac{R_1(y)}{z} + \frac{R_2(y)}{z^2} + \mathcal{O}(z^{-3}) \right], \quad (\text{C.12})$$

where $\mathcal{K}(z)$ is independent of F and cancels from normalized expectation values. The first-order correction is

$$R_1(y) = -\frac{P_0 y}{9\sigma^2}. \quad (\text{C.13})$$

Introducing the leading Gaussian average

$$\langle f(y) \rangle_0 = \frac{\int_{-\infty}^{+\infty} dy f(y) e^{-y^2/(2\sigma^2)}}{\int_{-\infty}^{+\infty} dy e^{-y^2/(2\sigma^2)}}, \quad (\text{C.14})$$

the relevant contractions are

$$\langle y \rangle_0 = 0, \quad \langle y^2 \rangle_0 = \sigma^2, \quad \langle y^4 \rangle_0 = 3\sigma^4, \quad (\text{C.15})$$

together with

$$\langle R_1 \rangle_0 = 0, \quad \langle y R_1 \rangle_0 = -\frac{P_0}{9}, \quad \langle y^2 R_1 \rangle_0 = 0. \quad (\text{C.16})$$

At second order, only the following combinations are needed:

$$\langle R_2 \rangle_0 = -\frac{1}{8} - \frac{P_0^2}{18} - \frac{1}{72\sigma^2}, \quad \langle y R_2 \rangle_0 = 0, \quad (\text{C.17})$$

and

$$\langle y^2 R_2 \rangle_0 - \sigma^2 \langle R_2 \rangle_0 = \frac{1}{36} + \frac{P_0^2}{81} + \frac{1}{324\sigma^2}. \quad (\text{C.18})$$

Field expectation values

Using Eq. (C.12), the first moment is

$$\langle F \rangle_z = F_0 - \frac{P_0}{9z} + \mathcal{O}(z^{-3}). \quad (\text{C.19})$$

Similarly,

$$\langle y^2 \rangle_z = \sigma^2 + \frac{1}{z^2} \left(\frac{1}{36} + \frac{P_0^2}{81} + \frac{1}{324\sigma^2} \right) + \mathcal{O}(z^{-4}). \quad (\text{C.20})$$

Since $F = F_0 + y$, one obtains

$$\begin{aligned} \langle F^2 \rangle_z &= F_0^2 + \sigma^2 - \frac{2F_0P_0}{9z} \\ &+ \frac{1}{z^2} \left(\frac{P_0^2}{81} + \frac{1}{36} + \frac{1}{324\sigma^2} \right) + \mathcal{O}(z^{-3}). \end{aligned} \quad (\text{C.21})$$

Therefore,

$$\Delta y^2 = \Delta F^2 = \sigma^2 + \frac{1}{36z^2} + \frac{1}{324\sigma^2 z^2} + \mathcal{O}(z^{-4}). \quad (\text{C.22})$$

Momentum expectation values

The momentum conjugate to F is

$$\widehat{\pi}_F = -i \frac{\partial}{\partial F}. \quad (\text{C.23})$$

Since the Hankel functions are independent of F ,

$$\widehat{\pi}_F^n \Psi_G = \mathcal{C}(z) \int_{-\infty}^{+\infty} dP P^n e^{iP(F-F_0) - \sigma^2(P-P_0)^2} B(P, z) = \hat{P}^n \Psi_G. \quad (\text{C.24})$$

The integration over F produces

$$\int_{-\infty}^{+\infty} dF e^{i(P-P')(F-F_0)} = 2\pi\delta(P - P'), \quad (\text{C.25})$$

so that

$$\langle \pi_F^n \rangle_z = \frac{\int_{-\infty}^{+\infty} dP P^n e^{-2\sigma^2(P-P_0)^2} |B(P, z)|^2}{\int_{-\infty}^{+\infty} dP e^{-2\sigma^2(P-P_0)^2} |B(P, z)|^2}. \quad (\text{C.26})$$

Since

$$|B(P, z)|^2 = 1 - \frac{u(P)}{z^2} + \mathcal{O}(z^{-4}), \quad (\text{C.27})$$

we have

$$\langle \pi_F^n \rangle_z = \frac{\int dP P^n e^{-2\sigma^2(P-P_0)^2} \left[1 - \frac{u(P)}{z^2} \right]}{\int dP e^{-2\sigma^2(P-P_0)^2} \left[1 - \frac{u(P)}{z^2} \right]} + \mathcal{O}(z^{-4}). \quad (\text{C.28})$$

For the leading momentum Gaussian,

$$\langle P \rangle_0 = P_0, \quad \langle P^2 \rangle_0 = P_0^2 + \frac{1}{4\sigma^2}, \quad (\text{C.29})$$

$$\langle P^3 \rangle_0 = P_0^3 + \frac{3P_0}{4\sigma^2}, \quad \langle P^4 \rangle_0 = P_0^4 + \frac{3P_0^2}{2\sigma^2} + \frac{3}{16\sigma^4}. \quad (\text{C.30})$$

Equation (C.28) then gives

$$\langle \pi_F \rangle_z = P_0 - \frac{P_0}{36\sigma^2 z^2} + \mathcal{O}(z^{-4}), \quad (\text{C.31})$$

and

$$\langle \pi_F^2 \rangle_z = P_0^2 + \frac{1}{4\sigma^2} - \frac{P_0^2}{18\sigma^2 z^2} - \frac{1}{144\sigma^4 z^2} + \mathcal{O}(z^{-4}). \quad (\text{C.32})$$

Consequently,

$$(\Delta \pi_F)^2 = \frac{1}{4\sigma^2} - \frac{1}{144\sigma^4 z^2} + \mathcal{O}(z^{-4}). \quad (\text{C.33})$$

and

$$\Delta F^2 \Delta \pi_F^2 = \frac{1}{4} + \left(\frac{1}{36\sigma^2 z} \right)^2 + \mathcal{O}(z^{-4}). \quad (\text{C.34})$$

Appendix D

Solution of the MS equation in a specific background P

In both cosmic and conformal time, the Mukhanov-Sasaki equation is not analytically solvable, consequently we prefer to use conformal time, consistently with all of the other calculations. The Mukhanov-Sasaki equation in conformal time (eq.1.140) reads

$$v_k'' + \left(k^2 - \frac{z_{MS}''}{z_{MS}} \right) v_k = 0. \quad (\text{D.1})$$

The background variables are governed by

$$\dot{\phi} = \frac{\pi_{\phi}}{a^3}, \quad H = \frac{1}{\sqrt{3}M_P} \sqrt{\frac{\pi_{\phi}^2}{2a^6} + V_0}. \quad (\text{D.2})$$

Given that

$$z_{MS} = a \sqrt{-\frac{H'}{4\pi G a H^2}} \quad (\text{D.3})$$

APPENDIX D. SOLUTION OF THE MS EQUATION IN A SPECIFIC BACKGROUND P

after some calculation, where the second derivative of a are obtained by the derivative of the Friedmann equation, the following holds

$$z_{MS} = \sqrt{\frac{3}{2}} a \sqrt{\frac{\pi_\phi^2}{4\pi G a^6 \left(\frac{\pi_\phi^2}{2a^6} + V_0 \right)}} \quad (\text{D.4})$$

and then

$$\frac{z_{MS}''}{z_{MS}} = -\frac{\pi_\phi^4 + 34a^6\pi_\phi^2V_0 - 8a^{12}V_0^2}{6a^4(\pi_\phi^2 + 2a^6V_0)M_P^2}. \quad (\text{D.5})$$

The Mukhanov–Sasaki equation we need to solve is then

$$\frac{d^2v_k}{d\eta^2} + \left[k^2 + \frac{\pi_\phi^4 + 34\pi_\phi^2V_0 a(\eta)^6 - 8V_0^2 a(\eta)^{12}}{6a(\eta)^4 M_P^2 (\pi_\phi^2 + 2V_0 a(\eta)^6)} \right] v_k = 0, \quad (\text{D.6})$$

with $a(\eta)$ satisfying

$$\frac{da(\eta)}{d\eta} = \frac{a(\eta)^2}{\sqrt{3} M_P} \sqrt{\frac{\pi_\phi^2}{2a(\eta)^6} + V_0}. \quad (\text{D.7})$$

We are interested in the large a domain, specifically when

$$\frac{\pi_\phi^2}{a^6} \ll V_0 \iff \frac{P^2}{(m_P a)^6} \ll \lambda, \quad (\text{D.8})$$

we then study the 0-th and first order solution of both equations in this limit.

0-th order solution

The two equations, Eqs. D.6–D.7, simplify enormously:

$$\frac{d^2v_k}{d\eta^2} + \left[k^2 - \frac{2V_0 a(\eta)^2}{3M_P^2} \right] v_k = 0, \quad (\text{D.9})$$

and

$$\frac{da(\eta)}{d\eta} = a(\eta)^2 \sqrt{\frac{V_0}{3M_P^2}}. \quad (\text{D.10})$$

We note that, in this regime, the dependence on π_ϕ disappears. The solution is

$$a(\eta) = -\frac{1}{\sqrt{\frac{V_0}{3M_P^2}} \eta}, \quad (\text{D.11})$$

where we have chosen the integration constant $c_1 = 0$, such that

$$a(\eta \rightarrow -\infty) \rightarrow 0, \quad a(\eta \rightarrow 0^-) \rightarrow \infty. \quad (\text{D.12})$$

With this solution, the Mukhanov–Sasaki equation reduces to

$$\frac{d^2 v_k}{d\eta^2} + \left(k^2 - \frac{2}{\eta^2} \right) v_k = 0, \quad (\text{D.13})$$

which can also be solved analytically

$$v_k(\eta) = A e^{-ik\eta} \left(1 - \frac{i}{k\eta} \right) + B e^{ik\eta} \left(1 + \frac{i}{k\eta} \right) \quad (\text{D.14})$$

which is the standard solution of the MS equation in a deSitter background.

First order solution

We solve analytically the Friedmann equation in the first order after deSitter, retaining all terms up to $\pi_\phi^2/(V_0 a^6)$, we solve

$$\eta = \int da \frac{1}{a^2 H(a)} + C, \quad (\text{D.15})$$

APPENDIX D. SOLUTION OF THE MS EQUATION IN A SPECIFIC BACKGROUND P

which is an hypergeometric function that takes the form

$$\eta(a) = \frac{1}{-\sqrt{\frac{V_0}{3M_P^2}}a} \left(1 - \frac{\pi_\phi^2}{28 V_0 a^6} + O[(\pi_\phi^2/(V_0 a^6))^2]\right), \quad (\text{D.16})$$

with the same constant of integration of the previous solution. We now assume

$$a(\eta) \simeq -\frac{1}{\sqrt{\frac{V_0}{3M_P^2}}\eta} [1 + \delta(\eta)]. \quad (\text{D.17})$$

Putting this ansatz in the previous equation, and keeping only the leading correction, one obtains

$$\delta(\eta) = -\frac{\pi_\phi^2 V_0^2 \eta^6}{756 M_P^6}. \quad (\text{D.18})$$

The scale factor can thus be written as

$$a(\eta) \simeq -\frac{1}{\sqrt{\frac{V_0}{3M_P^2}}\eta} \left(1 - \frac{V_0^2 \pi_\phi^2}{756 M_P^6} \eta^6\right). \quad (\text{D.19})$$

The expansion of $\frac{z_{MS}''}{z_{MS}}$ term leads to

$$\frac{z_{MS}''}{z_{MS}} = a^2 \frac{V_0}{3M_P^2} \left(2 - \frac{19\pi_\phi^2}{2V_0 a^6} + O[(\pi_\phi^2/(V_0 a^6))^2]\right) \quad (\text{D.20})$$

After inserting the first order solution in the scale factor, we can write the approximate first-order Mukhanov–Sasaki equation,

$$\frac{d^2 v_k}{d\eta^2} + \left[k^2 - \frac{2}{\eta^2} + \frac{5\pi_\phi^2 V_0^2}{14M_P^6} \eta^4\right] v_k = 0. \quad (\text{D.21})$$

APPENDIX D. SOLUTION OF THE MS EQUATION IN A SPECIFIC BACKGROUND P

We solve the equation perturbatively by writing

$$v_k(\eta) = v_k^{(0)}(\eta) + \delta v_k(\eta), \quad (\text{D.22})$$

where $v_k^{(0)}$ is the zeroth-order solution given in Eq. (D.14), with integration constants A and B . Substituting this ansatz into Eq. (D.21), we obtain

$$\frac{d^2 \delta v_k}{d\eta^2} + \left(k^2 - \frac{2}{\eta^2}\right) \delta v_k = -\frac{5\pi_\phi^2 V_0^2 \eta^4}{14M_P^6} \left(v_k^{(0)} + \delta v_k\right). \quad (\text{D.23})$$

Assuming

$$|\delta v_k| \ll |v_k^{(0)}|, \quad (\text{D.24})$$

an approximation that is verified a posteriori, the equation reduces to

$$\frac{d^2 \delta v_k}{d\eta^2} + \left(k^2 - \frac{2}{\eta^2}\right) \delta v_k = -\frac{5\pi_\phi^2 V_0^2 \eta^4}{14M_P^6} v_k^{(0)}. \quad (\text{D.25})$$

This inhomogeneous equation can be solved analytically. On using the dimensionless variables $P = m_P \pi_\phi$ and $\lambda = \frac{V_0}{m_P^4}$, we obtain

$$\begin{aligned} v_k(\eta) = & A e^{-ik\eta} + B e^{ik\eta} - \frac{iA e^{-ik\eta}}{k\eta} + \frac{iB e^{ik\eta}}{k\eta} \\ & + P^2 \left[\frac{135A e^{-ik\eta} \lambda^2}{2k^6} + \frac{135B e^{ik\eta} \lambda^2}{2k^6} - \frac{135iA e^{-ik\eta} \lambda^2}{2k^7 \eta} + \frac{135iB e^{ik\eta} \lambda^2}{2k^7 \eta} \right. \\ & + \frac{45A e^{-ik\eta} \eta^2 \lambda^2}{k^4} + \frac{45B e^{ik\eta} \eta^2 \lambda^2}{k^4} + \frac{45iA e^{-ik\eta} \eta^3 \lambda^2}{k^3} - \frac{45iB e^{ik\eta} \eta^3 \lambda^2}{k^3} \\ & \left. - \frac{27A e^{-ik\eta} \eta^4 \lambda^2}{k^2} - \frac{27B e^{ik\eta} \eta^4 \lambda^2}{k^2} - \frac{54iA e^{-ik\eta} \eta^5 \lambda^2}{7k} + \frac{54iB e^{ik\eta} \eta^5 \lambda^2}{7k} \right]. \end{aligned} \quad (\text{D.26})$$

APPENDIX D. SOLUTION OF THE MS EQUATION IN A SPECIFIC BACKGROUND P

Upon redefining $\tilde{A} = A + \frac{135P^2A\lambda^2}{2k^6}$ and $\tilde{B} = B + \frac{135P^2B\lambda^2}{2k^6}$ we obtain

$$\begin{aligned}
 v_k(\eta) = & \tilde{A}e^{-ik\eta} + \tilde{B}e^{ik\eta} - \frac{i\tilde{A}e^{-ik\eta}}{k\eta} + \frac{i\tilde{B}e^{ik\eta}}{k\eta} \\
 & + P^2 \left[\frac{45Ae^{-ik\eta}\eta^2\lambda^2}{k^4} + \frac{45Be^{ik\eta}\eta^2\lambda^2}{k^4} + \frac{45iAe^{-ik\eta}\eta^3\lambda^2}{k^3} - \frac{45iBe^{ik\eta}\eta^3\lambda^2}{k^3} \right. \\
 & \left. - \frac{27Ae^{-ik\eta}\eta^4\lambda^2}{k^2} - \frac{27Be^{ik\eta}\eta^4\lambda^2}{k^2} - \frac{54iAe^{-ik\eta}\eta^5\lambda^2}{7k} + \frac{54iBe^{ik\eta}\eta^5\lambda^2}{7k} \right].
 \end{aligned} \tag{D.27}$$

We note that the perturbation remains much smaller than the deSitter solution as $\eta \rightarrow 0$, thus confirming the hypothesis (D.24). Regardless of the choices of the integration constants, which are connected with the choice of the vacuum in the quantised theory, the power spectrum following from (D.27), can be written in the form

$$P_v(k; P) \simeq c_k^{(0)} + c_k^{(2)}P^2, \quad P^2c_k^{(2)} \ll c_k^{(0)}. \tag{D.28}$$

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