Quantum-gravitational effects for inflationary perturbations and the fate of mild singularities in quantum cosmology

I n a u g u r a l - D i s s e r t a t i o n

zur

Erlangung des Doktorgrades

der Mathematisch-Naturwissenschaftlichen Fakultät

der Universität zu Köln

vorgelegt von

Manuel Krämer

aus Hachenburg

Köln 2015

Berichterstatter: Prof. Dr. Claus Kiefer
Prof. Dr. Domenico Giulini

Tag der mündlichen Prüfung: 12. Januar 2015

Abstract

In this dissertation, we investigate cosmological models within the framework of canonical quantum gravity based on the Wheeler–DeWitt equation with regard to whether it is possible to observe effects of quantum gravity in the Cosmic Microwave Background radiation and whether a specific class of mild singularities can be resolved by quantizing classical cosmological models in which they appear.

The first part is motivated by the fact that there are several candidates for a theory of quantum gravity and it is therefore crucial to find tests in order to figure out which theory is closest to the truth. The main problem here is that quantum-gravitational effects are highly suppressed at the energy scales one can nowadays probe in experiments. However, the inflationary phase of the universe takes place at an energy scale where effects of quantum gravity could be sizeable. During inflation one can investigate primordial cosmological perturbations that are thought to be the seed for structure formation in the early universe as well as for primordial gravitational waves. Thus they have left their imprints in the anisotropies and the polarization of the Cosmic Microwave Background radiation, which have been measured by the space observatories COBE, WMAP and Planck. We investigate to which extent quantum-gravitational effects influence these perturbations by canonically quantizing inflationary models, in which a scalar *inflaton* field drives the exponential expansion of the universe. At first, we analyze a simplified model, where we only add perturbations to the scalar field. Secondly, we consider scalar and tensor perturbations in a gauge-invariant way for a de Sitter universe and a generic quasi-de Sitter *slow-roll* model. We perform a semiclassical Born–Oppenheimer type of approximation to the Wheeler–DeWitt equation of each model and recover a Schrödinger equation for the perturbation modes as well as a modified Schrödinger equation with a quantum-gravitational correction term. From the uncorrected Schrödinger equation, we derive the usual slow-roll power spectra. The quantum-gravitational correction term leads to a modification of the power spectra on the largest scales. This effect is, however, too small to be measurable, especially in light of the statistical uncertainty due to cosmic variance, which is most prominent on large scales. We also obtain a quantum-gravitational correction to the tensor-to-scalar ratio, which is, however, much more suppressed than the second-order slow-roll corrections. Finally, we compare our results to other methods in Wheeler–DeWitt quantum cosmology and to findings in other approaches to quantum gravity.

The second part of this dissertation is based on the expectation that a quantum theory of gravity should resolve the singularities appearing in general relativity and in classical cosmology. We will focus on a specific set of cosmological singularities called type IV singularities that are of a mild nature in the sense that only higher derivatives of the Hubble parameter diverge. We model a universe with such a singularity by introducing a perfect fluid described by a generalized *Chaplygin* gas in the form of a scalar field, for which we consider both a standard as well as a phantom field with negative energy. After discussing the classical behavior, we can solve the Wheeler–DeWitt equation of this model analytically for a special case and can draw conclusions for the general case. We use the criterion that a singularity is avoided if the wave function vanishes in the region where the classical singularity is located. However, we obtain as a result that only particular solutions of the Wheeler–DeWitt equation of our model fulfill this criterion and therefore avoid the appearance of a type IV singularity. Lastly, we compare this result to earlier results finding an avoidance of other types of singularities and we discuss singularity resolution in other quantum gravity theories.

Zusammenfassung

In dieser Dissertation untersuchen wir kosmologische Modelle im Rahmen einer kanonischen Quantisierung der Gravitation basierend auf der Wheeler-DeWitt-Gleichung im Hinblick darauf, ob es möglich ist, quantengravitative Effekte in der Strahlung des Kosmischen Mikrowellenhintergrunds zu beobachten, sowie ob eine bestimmte Klasse schwacher Singularitäten durch Quantisierung kosmologischer Modelle, in welchen diese auftreten, beseitigt werden kann.

Der erste Teilaspekt gründet darauf, dass uns mehrere Kandidaten einer Quantentheorie der Gravitation zur Verfügung stehen und es daher notwendig ist, Möglichkeiten zu finden, um zu testen, welche dieser Theorien am ehesten die Natur beschreibt. Das Hauptproblem hierbei ist, dass quantengravitative Effekte bei den Energieskalen, die uns heute experimentell zugänglich sind, stark unterdrückt sind. Die inflationäre Phase des Universums läuft jedoch bei Energien ab, bei denen Effekte der Quantengravitation eine größere Rolle spielen könnten. Es ist möglich, primordiale kosmologische Störungen während dieser Inflationsphase zu untersuchen, welche als Keime der Strukturentwicklung im frühen Universum sowie als Ursprung primordialer Gravitationswellen angesehen werden. Somit sind diese Störungen letztlich für die Anisotropien bzw. die Polarisation der Kosmischen Mikrowellenhintergrundstrahlung verantwortlich, welche von den Raumsonden COBE, WMAP und Planck gemessen wurden. Wir untersuchen, inwieweit quantengravitative Effekte diese Störungen beeinflussen, indem wir Inflationsmodelle, in denen die exponentielle Expansion des Universums durch ein skalares Inflatonfeld hervorgerufen wird, kanonisch quantisieren. Zunächst untersuchen wir

ein vereinfachtes Modell, in welchem wir lediglich zu dem Skalarfeld Störungen hinzufügen. Nachfolgend betrachten wir skalare und tensorielle Störungen in einer eichinvarianten Formulierung sowohl in einem de-Sitter-Universum als auch in einem Quasi-de-Sitter-Universum, welches auch als Slow-Roll-Modell bezeichnet wird. Wir führen eine semiklassische Born-Oppenheimer-ähnliche Näherung der Wheeler-DeWitt-Gleichung der jeweiligen Modelle durch und erhalten eine Schrödingergleichung für die Störungsmoden sowie eine modifizierte Schrödingergleichung mit einem quantengravitativen Korrekturterm. Mit Hilfe der unkorrigierten Schrödingergleichung können wir die bekannten Leistungsspektren der Slow-Roll-Modelle herleiten. Der quantengravitative Korrekturterm führt zu einer Modifizierung der Leistungsspektren auf den größten Längenskalen. Dieser Effekt ist jedoch zu klein um messbar zu sein, insbesondere im Hinblick auf die statistische Unsicherheit aufgrund der Kosmischen Varianz, die auf großen Skalen am dominantesten ist. Wir erhalten ebenfalls eine quantengravitative Korrektur zu dem Verhältnis der tensoriellen zu den skalaren Störungen, welches allerdings im Vergleich zu den Korrekturen der zweiten Ordnung der Slow-Roll-Näherung stark unterdrückt ist. Zuletzt vergleichen wir unsere Ergebnisse mit anderen Methoden innerhalb der Wheeler-DeWitt-Quantenkosmologie sowie mit anderen Zugängen zur Quantengravitation.

Der zweite Teil der Dissertation basiert auf der Erwartung, dass eine Quantentheorie der Gravitation die Singularitäten beseitigen sollte, die in der Allgemeinen Relativitätstheorie und in der klassischen Kosmologie auftreten. Wir konzentrieren uns auf eine bestimmte Art kosmologischer Singularitäten, welche als Typ-IV-Singularitäten bezeichnet werden und die als schwach bezeichnet werden können, da hier nur höhere Ableitungen des Hubble-Parameters divergieren. Wir modellieren Universen mit einer solchen Singularität, indem wir eine ideale Flüssigkeit, die durch ein *Chaplygin*-Gas beschrieben wird, in der Form eines Skalarfeldes einführen, wobei wir sowohl ein Standard-Skalarfeld als auch ein Phantom-Feld mit negativer Energie betrachten. Nachdem wir das klassische Verhalten untersucht haben, können wir die Wheeler-DeWitt-Gleichung dieses Modells für einen Spezialfall analytisch lösen und hierdurch Rückschlüsse auf den allgemeinen Fall ziehen. Wir verwenden das Kriterium, dass eine Singularität vermieden wird, wenn die Wellenfunktion in der Region, in der die klassische Singularität auftritt, verschwindet. Allerdings erhalten wir als Ergebnis, dass nur bestimmte Lösungen der Wheeler-DeWitt-Gleichung unseres Modells dieses Kriterium erfüllen und somit die Typ-IV-Singularität vermeiden. Abschließend vergleichen wir dieses Ergebnis mit Resultaten aus vorherigen Untersuchungen, in denen eine Vermeidung von Singularitäten anderer Arten auftritt, und diskutieren Singularitätsvermeidung in anderen Quantengravitationstheorien.

Notation

Unless explicitly stated, we set the velocity of light $c \equiv 1$ throughout this thesis. The same holds for the reduced Planck constant $\hbar$ starting from chapter 5.

The gravitational constant G will appear most of the time in the form of the Planck mass $\mathfrak{M}_{\mathrm{P}}$, which in its original form is defined as

$$\mathfrak{M}_{\mathrm{P}} := \sqrt{\frac{\hbar c}{G}} \simeq 1.22 \times 10^{19}\,\mathrm{GeV}/c^2\,.$$

However, in order to avoid the appearance of numerical factors, we use either the reduced Planck mass

$$M_{\mathrm{P}} := \frac{1}{\sqrt{8\pi}}\mathfrak{M}_{\mathrm{P}} = \sqrt{\frac{\hbar c}{8\pi G}} \simeq 2.435 \times 10^{18}\,\mathrm{GeV}/c^2$$

or for the semiclassical approximation in chapter 5 and following, a rescaled Planck mass

$$m_{\mathrm{P}} := \sqrt{\frac{3\pi}{2}}\mathfrak{M}_{\mathrm{P}} = \sqrt{\frac{3\pi\,\hbar c}{2G}} \simeq 2.65 \times 10^{19}\,\mathrm{GeV}/c^2\,.$$

The latter two definitions can appear together in one expression.
Additionally, in chapter 8, the gravitational constant G appears in the definition

$$\kappa := \sqrt{8\pi\,G} = \frac{1}{M_{\mathrm{P}}}\,.$$

In chapter 5, we define the wave number k corresponding to a length L as

$$k := \frac{2\pi}{L}\,.$$

In chapter 6, we skip the appearing factor of 2π and define

$$k := \frac{1}{L}\,.$$

For the signature of a spacetime metric g, we use the spacelike (or "east-coast" or "mostly plus") convention:

$$\mathrm{sign}(g) = (-,+,+,+)\,.$$

In this context, Greek indices run from 0 to 3, while Latin indices range from 1 to 3. For repeatedly appearing indices, the Einstein summation convention is used.

Contents

1

Introduction

About ninety-nine years before these lines were written, on November 25, 1915, Albert Einstein presented the final version of his theory of general relativity. The theory introduced a completely new notion of space and time and explained a couple of deviations from Newtonian gravity, for instance, for light deflection around the Sun or the perihelion shift of Mercury, which were testable already at that time. Nowadays, general relativity has been tested to an incredibly high precision, notably by the measurement of binary pulsars.

Yet we know that the theory is unlikely to be the final answer of how we should understand the concept of space and time. In fact, the theory's problems lie deep within itself. Even the simplest solutions to the central equations of general relativity include a singularity, a point at which the theory breaks down and spacetime in some sense comes to an end. In the case of black hole solutions, these singularities are in most cases hidden behind a horizon, through which no information can reach us. However, in cosmological scenarios a singularity means that quantities like the energy density or pressure of the matter inside the universe diverge, which would have drastic consequences in the case of a singularity that happens later in the evolution of the universe – one could speak of a doomsday event. In the case of the cosmological model describing our universe best, there is a singularity of infinite energy density and pressure at the beginning of the evolution of the universe, the *Big Bang*, which is unavoidable in the classical theory.

In the decade that followed the discovery of general relativity, quantum mechanics, the other cornerstone of our current understanding of Nature, was developed. Today in physics there is often the dichotomy that quantum mechanics and quantum field theory are used to describe Nature on microscopic scales from atoms to nuclei and beyond, while general relativity is applied to describe macroscopic scales from the movement of satellites in the gravitational field of the Earth, planets in our solar system, and so forth up to cosmology.

This dichotomy works practically in most cases, mainly because the energy scale where quantum effects of gravity would become sizeable is thought to be at the Planck scale, which can be characterized by the Planck mass $\mathfrak{M}_\text{P}$ that is defined in terms of the reduced Planck constant $\hbar$, the velocity of light c and the gravitational constant G as

$$\mathfrak{M}_\text{P} = \sqrt{\frac{\hbar c}{G}} \simeq 1.22 \times 10^{19}\,\text{GeV}/c^2 \,.$$

This corresponds to an extremely high energy. An accelerator probing this energy scale built with current technology would have to be the size of the solar system. However, simply accepting this dichotomy and moving on is not satisfying for several reasons. First of all, gravity as an interaction couples to all kinds of matter that is generally quantized. Describing gravity as a classical interaction can therefore be regarded as inconsistent. Furthermore, without quantizing gravity, the singularities appearing in general relativity that have been described above would necessarily remain. One expects that these singularities disappear in a theory of quantum gravity, which might lead to a new notion of spacetime.

Thus, the search for a theory of quantum gravity has been ongoing for more than eighty years.

The most ambitious attempt is, of course, to unify all forces in Nature. For this approach, the most elaborate candidate theory is *string theory*, which can only be formulated consistently in 10, 11 or 26 spacetime dimensions. In order to describe our apparent four-dimensional reality, the additional dimensions have to be compactified, which is an intricate procedure that is non-unique and leads to an enormous amount of solutions called string vacua. This is one of the reasons why string theory has not yet led to testable predictions. Additionally, most parts of string theory are only formulated perturbatively on a fixed background like in quantum field theory. A fundamentally background-independent formulation of string theory has not yet been achieved.

A more humble approach is to restrict oneself to just quantizing gravity, that is to find a quantum theory of spacetime that leads to general relativity in the low-energy limit. This approach can be divided further into two parts: *covariant* and *canonical* quantum gravity.

In covariant quantum gravity, one tries to quantize general relativity using perturbation theory or path-integral methods, but since general relativity has turned out to be non-renormalizable, one had to find new methods in order to make sense of covariant quantum gravity, for instance, by considering *Asymptotic Safety* [94] or by discretizing spacetime using *Causal Dynamical Triangulation* [8].

Canonical quantum gravity is, as the name implies, based on a direct canonical quantization of a Hamiltonian formulation of general relativity. This approach is further split, because one can either use the usual three-metric as canonical variable, which leads to *Quantum Geometrodynamics* [43, 110], or one introduces new variables that, for example, lead to a loop-like structure, which gave the name for *Loop Quantum Gravity* [10, 11, 97].

We see that there are a number of candidates for a theory of quantum gravity, so we are faced with the problem to decide which of these theories is closest to the truth. One could be satisfied with mathematical consistency, but in the end it should always be the experiment that decides the validity of a theory.

However, as we have mentioned above, the energy scale where effects of quantum gravity are expected to become sizeable is extremely high.

Situations where such energies are present could probably occur in black holes, but these objects are not particularly suited for observations. Another situation is the very early universe and here we luckily are capable of seeing the relicts of physics that happened at very high energies in the anisotropies of the Cosmic Microwave Background. These can be related to quantum fluctuations that were in a sense enhanced to macroscopic scales during a very early period of exponential expansion of the universe called *inflation*, which happened at energy scales of up to 10^{15} GeV, which is only four orders of magnitude below the Planck scale.

The aim of this dissertation is first of all to use canonical quantum gravity based on the Wheeler–DeWitt equation as a conservative approach to quantum gravity in order to investigate whether quantum-gravitational effects can be measurable in the anisotropies of the Cosmic Microwave Background. We use a particular feature of the Wheeler–DeWitt equation, which is that one can use a systematic semiclassical approximation to recover quantum field theory in curved spacetime in the form of a functional Schrödinger equation and in a further step quantum-gravitational corrections to it, which allows us to calculate corrections to known quantities like the power spectra of inflationary perturbations.

Furthermore, we also tackle the question whether singularities appearing in cosmological models are resolved by quantizing these models. We focus on cosmological models containing a dark-energy-like fluid and additionally consider a type of mild singularities that has not yet been investigated in the context of Wheeler–DeWitt quantum cosmology.

This dissertation is organized in the following way. In chapter 2, we will give an introduction into classical cosmology and its problems, the theory of inflation to solve these problems, as well as the physics of the Cosmic Microwave Background. Chapter 3 is then devoted to Quantum Geometrodynamics, the direct canonical quantization of general relativity. Here we will present the derivation of the Wheeler–DeWitt equation for both the full theory of general relativity as well as for a symmetry-reduced model describing our universe. In chapter 4, we shall present semiclassical approximation schemes in quantum mechanics and how they can be used for the Wheeler–DeWitt equation. In chapter 5, we then present the Wheeler–DeWitt equation of a model of an inflationary universe with perturbations of a scalar field and use a semiclassical approximation to derive the Schrödinger equation for the perturbation modes with a quantum-gravitational correction term, from which we can deduce how the power spectrum of these perturbations is modified due to this correction term. Chapter 6 extends this analysis to gauge-invariant scalar and tensor perturbations which allows us to also include primordial gravitational waves. In chapter 7, we will discuss whether these corrections are actually measurable in the CMB and we will compare our results with similar calculations in other approaches to quantum gravity. The topic of chapter 8 is the question whether type IV singularities are resolved in quantum cosmology and we conclude with a summary and outlook in chapter 9.

2

Cosmology, inflation and the Cosmic Microwave Background

In this chapter, we will present all the aspects of the present state of cosmology that are relevant for our discussion on quantum-cosmological applications in the following chapters. We start with a short description of homogeneous Friedmann cosmology and its problems, followed by an introduction to the theory of inflation and close with a short description of the Cosmic Microwave Background. We base our description here on several standard textbooks on cosmology [45, 77, 92, 99] as well as [17, 34, 78, 107].

2.1 The homogeneous universe

Cosmology studies the physics of the universe on scales of typically more than 1 Mpc up to the largest observable scales. From observations performed by the 2-degree Field Galaxy Redshift Survey (2dFGRS) and the Sloan Digital Sky Survey (SDSS) we know that the large-scale matter distribution in our universe is homogeneous and isotropic on scales above about 200 kpc, i. e. the scale of galaxy clusters, to a good approximation. On larger scales, this observation is even more apparent, since the Cosmic Microwave Background (CMB) fills the universe with a background radiation that is homogeneous and isotropic up to one part over 10^5. [56, 4] The tiny deviations from the isotropy of the CMB are nevertheless extremely important in order to understand the formation of structure in the universe as we will see in chapter 5 and following but we shall neglect them at first.

Homogeneity means that a certain property is the same at every point of observation and isotropy means that a property is independent of the direction of observation. In light of the above-mentioned empirical observations, we can establish the so-called *cosmological principle* which states that on large scales the universe looks the same for all observers, it does not possess a privileged point or direction and it is therefore homogeneous and isotropic with respect to all locations.

A further observation that arises from measuring the redshift of galaxies is that these galaxies seem to move away from us. This apparent movement is due to the expansion of the universe itself. In our local universe, the apparent velocity v can be described by Hubble's law

$$v = H_0 D \,, \tag{2.1}$$

where D is the proper distance of the observed object and H_0 is the Hubble constant that according to recent measurements of the Planck satellite [4] has the value:

$$H_0 = 67.80 \pm 0.77 \frac{\mathrm{km}}{\mathrm{s\,Mpc}} \,. \tag{2.2}$$

There is, however, an observed deviation from the linear Hubble law for objects that are farther away from us. The objects whose redshift is observable best at large distances are the Type Ia supernovae due to the fact that they are bright standard candles. Measurement of these supernovae have shown that the expansion of the universe accelerates, which leads to the problem of Dark Energy, which we will discuss in chapter 8.

2.1.1 The Friedmann–Lemaître–Robertson–Walker metric

We now want to describe our expanding homogeneous and isotropic universe within the framework of general relativity. In order to do this, we assume that our spacetime is a four-dimensional globally hyperbolic Lorentzian manifold $(\mathcal{M}, g)$ with metric g, such that we can foliate it into spatial hypersurfaces along a suitable time axis. The most general ansatz for such a metric can be obtained by using the ADM method named after Richard Arnowitt, Stanley Deser and Charles W. Misner [9] and looks as follows

$$\mathrm{d}s^2 = \left[-N^2(\mathbf{x},t) + N_i(\mathbf{x},t) N^i(\mathbf{x},t)\right] \mathrm{d}t^2 + 2 N_i(\mathbf{x},t)\,\mathrm{d}t\,\mathrm{d}x^i + h_{ij}(\mathbf{x},t)\,\mathrm{d}x^i\,\mathrm{d}x^j \,, \tag{2.3}$$

where $N(\mathbf{x},t)$ is the lapse function, $N^i(\mathbf{x},t)$ the shift vector and $h_{ij}(\mathbf{x},t)$ is the three-metric on the spatial hypersurface. Assuming spatial homogeneity and isotropy as the symmetries of our spacetime translates into invariance under translations and rotations. The former implies that $N(\mathbf{x},t)$ and $N^i(\mathbf{x},t)$ are independent of $\mathbf{x}$ and the latter demands that the shift vector $N^i(t)$ be equal to zero. Furthermore, we can write the spatial part of the metric as

$$h_{ij}(\mathbf{x},t)\,\mathrm{d}x^i\,\mathrm{d}x^j = a^2(t)\,\mathrm{d}\Omega^2_{3,\mathcal{K}} \,, \tag{2.4}$$

where $a(t)$ is called *scale factor* and $\mathrm{d}\Omega^2_{3,\mathcal{K}}$ can be written with the radial coordinate $r \in [0, \infty)$ and angular coordinates $\vartheta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$ as

$$\mathrm{d}\Omega^2_{3,\mathcal{K}} = \frac{\mathrm{d}r^2}{1 - \mathcal{K}\, r^2} + r^2 \left(\mathrm{d}\vartheta^2 + \sin^2(\vartheta)\, \mathrm{d}\varphi^2\right). \tag{2.5}$$

The parameter $\mathcal{K}$ can take the values $\mathcal{K} = -1, 0, 1$, which correspond to the cases of an open, flat or closed universe, in which the spatial slice takes the form of a hyperboloid, cube or sphere, respectively.

In the end, we are left with the metric

$$\mathrm{d}s^2 = -N^2(t)\, \mathrm{d}t^2 + a^2(t)\, \mathrm{d}\Omega^2_{3,\mathcal{K}}, \tag{2.6}$$

which is most generally called *Friedmann–Lemaître–Robertson–Walker metric*, where the name *Lemaître* is often and both *Friedmann* and *Lemaître* are occasionally dropped. We will refer to it as *FLRW metric* from now on.

We see that due to spatial homogeneity and isotropy, the ten degrees of freedom of the metric tensor have been reduced to the lapse function $N(t)$ and the scale factor $a(t)$. But in fact, because of the time reparametrization invariance of general relativity, the former is just part of the gauge freedom and, hence, not a dynamical degree of freedom, such that we are left with just one physically meaningful degree of freedom, the scale factor $a(t)$.

An alternative, often convenient choice of time is the *conformal time* η defined by

$$\mathrm{d}\eta = \frac{\mathrm{d}t}{a(t)}, \tag{2.7}$$

which can be incorporated into the FLRW metric by setting the lapse function equal to the scale factor, $N(t) = a(t)$. In the following, we will set $N(t) \equiv 1$ and refer to the different choices of time by using t for cosmic and η for conformal time.

The spatial coordinates we have introduced here are in fact *comoving*, which means that they are not influenced by the cosmic expansion that is encoded in the scale factor $a(t)$. Therefore, in order to describe the proper physical distance Δx_{prop} at a time t, we have to scale the comoving distance Δx_{com} set at a special point in time $t = t_0$ with $a(t)$:

$$\Delta x_{\mathrm{prop}}(t) = a(t)\, \Delta x_{\mathrm{com}}. \tag{2.8}$$

One usually chooses t_0 to be today, which implies that the scale factor is set to $a(t_0) = 1$ at present time.

Note that the scale factor here is a dimensionless quantity. Later, when we canonically quantize models of the universe, we redefine the scale factor to have the dimension of a length.

An alternative form of the spatial part of the FLRW metric (2.6) can be found by introducing a new radial coordinate $\chi \in [0, \infty)$ that is related to the previous coordinate r in (2.5) by means of the function $r = f_{\mathcal{K}}(\chi)$. The function $f_{\mathcal{K}}(\chi)$ depends on the parameter $\mathcal{K}$ describing the curvature of the universe – which in this case is not restricted to the values -1, 0 and 1 – and is defined as

$$f_{\mathcal{K}}(\chi) = \begin{cases} \frac{1}{\sqrt{\mathcal{K}}} \sin\left(\sqrt{\mathcal{K}}\,\chi\right) & \text{for } \mathcal{K} > 0\,, \\ \chi & \text{for } \mathcal{K} = 0\,, \\ \frac{1}{\sqrt{-\mathcal{K}}} \sinh\left(\sqrt{-\mathcal{K}}\,\chi\right) & \text{for } \mathcal{K} < 0\,. \end{cases} \tag{2.9}$$

Using this, the spatial part $\mathrm{d}\Omega^2_{3,\mathcal{K}}$ of the FLRW metric can be written as

$$\mathrm{d}\Omega^2_{3,\mathcal{K}} = \mathrm{d}\chi^2 + f^2_{\mathcal{K}}(\chi)\left(\mathrm{d}\vartheta^2 + \sin^2(\vartheta)\,\mathrm{d}\varphi^2\right). \tag{2.10}$$

We can thus write out the FLRW metric as

$$\mathrm{d}s^2 = -\,\mathrm{d}t^2 + a^2(t)\left[\mathrm{d}\chi^2 + f^2_{\mathcal{K}}(\chi)\left(\mathrm{d}\vartheta^2 + \sin^2(\vartheta)\,\mathrm{d}\varphi^2\right)\right] \tag{2.11}$$

and, for later convenience, we define

$$\gamma_{\mu\nu} := a^2(t)\,\mathrm{diag}\left(0,\, 1,\, f^2_{\mathcal{K}}(\chi),\, f^2_{\mathcal{K}}(\chi)\,\sin^2(\vartheta)\right). \tag{2.12}$$

The function $f_{\mathcal{K}}(\chi)$ is also used to define the angular diameter distance.

2.1.2 The Friedmann equations

Up to now, we have only discussed the kinematics of the homogeneous universe. In general relativity, the dynamics of spacetime are described by the Einstein equations. Therefore, in order to describe the dynamics of the homogeneous universe characterized by the evolution of the scale factor $a(t)$, we have to write out and then analyze the equations of motion arising from the Einstein equations for the FLRW metric (2.6).

The Einstein equations with cosmological constant Λ and energy–momentum tensor $T_{\mu\nu}$ are given by

$$G_{\mu\nu} + \Lambda\, g_{\mu\nu} = 8\pi G\, T_{\mu\nu}\,, \tag{2.13}$$

where $G_{\mu\nu}$ is the Einstein tensor,

$$G_{\mu\nu} := R_{\mu\nu} - \frac{1}{2}\, g_{\mu\nu}\, R\,, \tag{2.14}$$

whose components we have to compute for the FLRW metric. This calculation is, for instance, presented in [92]. By defining the Hubble parameter H as

$$H := \frac{\dot{a}}{a}\,, \tag{2.15}$$

we can write out the components of the Einstein tensor as follows:

$$G_{00} = 3\left(H^2 + \frac{\mathcal{K}}{a^2}\right)\,, \quad G_{ij} = -\left(H^2 + \frac{2\ddot{a}}{a} + \frac{\mathcal{K}}{a^2}\right)\gamma_{ij}\,, \tag{2.16}$$

where γ_{ij} is given by (2.12).

We now want to define an energy–momentum tensor for our universe. In order to do so, we have to introduce a set of observers whose world lines are tangent to the four-velocity

$$u^\mu = \frac{\mathrm{d}x^\mu}{\mathrm{d}\tau}\,, \qquad g_{\mu\nu}u^\mu u^\nu = -1\,, \tag{2.17}$$

where τ is the proper time of the observers. We can therefore write the metric of the spatial sections orthogonal to u^μ as

$$\hat{\gamma}_{\mu\nu} \equiv g_{\mu\nu} + u_\mu u_\nu\,. \tag{2.18}$$

The most general form of the energy–momentum tensor of an (im)perfect fluid then takes the form

$$T_{\mu\nu} = \rho\, u_\mu u_\nu + P\,\hat{\gamma}_{\mu\nu} + 2\,q_{(\mu}u_{\nu)} + \Sigma_{\mu\nu}\,, \tag{2.19}$$

where ρ is the energy density and P is the isotropic pressure, which are given by

$$\rho = T_{\mu\nu}u^\mu u^\nu \quad \text{and} \quad P = \frac{1}{3}T_{\mu\nu}\hat{\gamma}^{\mu\nu}\,. \tag{2.20}$$

Furthermore, q_μ is the energy-flux vector defined as

$$q_\mu = -\,\hat{\gamma}_\mu{}^\alpha T_{\alpha\beta}u^\beta\,, \tag{2.21}$$

and $\Sigma_{\mu\nu}$ is the symmetric and trace-free anisotropic stress tensor that is given by

$$\Sigma_{\mu\nu} = \hat{\gamma}^{\;\alpha}_{[\mu}\hat{\gamma}^{\;\beta}_{\nu]}\,T_{\alpha\beta}\,. \tag{2.22}$$

Since one can assume that galaxies are freely streaming through space, it is reasonable to consider a perfect fluid for the energy–momentum tensor of our universe and for this case, one can find a unique four-velocity such that both q_μ and $\Sigma_{\mu\nu}$ vanish. If we furthermore consider a frame that is comoving with the fluid, we can set $u_\mu = (1,0,0,0)$, such that $\hat{\gamma}_{ij} = \gamma_{ij}$ as defined in (2.12), and we finally arrive at an energy–momentum tensor of the form

$$T_{\mu\nu} = \rho\, u_\mu u_\nu + P\,\gamma_{\mu\nu}\,. \tag{2.23}$$

Hence, we can write out $T_{\mu\nu}$ as follows

$$T_{\mu\nu} = \mathrm{diag}\Big(\rho,\, P\,a^2,\, P\,a^2 f_{\mathcal{K}}^2(\chi),\, P\,a^2 f_{\mathcal{K}}^2(\chi)\,\sin^2(\vartheta)\Big)\,. \tag{2.24}$$

Going back to the Einstein equations (2.13), we can now insert our results for $G_{\mu\nu}$ and $T_{\mu\nu}$. For the $(0,0)$-component of the Einstein equations we get

$$H^2 = \left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\,\rho - \frac{\mathcal{K}}{a^2} + \frac{\Lambda}{3}\,, \tag{2.25}$$

while for the (i,j)-components, we obtain after inserting the previous equation

$$\frac{\ddot{a}}{a} = -\,\frac{4\pi G}{3}\,\big(\rho + 3P\big) + \frac{\Lambda}{3}\,. \tag{2.26}$$

These two equations are called *Friedmann equations*.

Since the energy–momentum tensor is covariantly conserved,

$$T^{\mu\nu}{}_{;\mu} = 0\,, \tag{2.27}$$

we furthermore find a continuity equation

$$\dot{\rho} + 3H\,\big(\rho + P\big) = 0\,, \tag{2.28}$$

which one can also derive directly by combining the two Friedmann equations. This is due to the fact that the three equations (2.25), (2.26) and (2.28) are not independent of one another.

2.1.3 Matter constituents and epochs of the universe

The two independent Friedmann equations determine the time evolution of three independent variables, the scale factor a, the energy density ρ and the pressure P. Therefore, we need another relation between the variables to find a solution to this system of differential equations. This additional information is given by the equation of state that relates ρ and P. In the most simple form, one introduces a constant parameter w called barotropic index that depends on the nature of the matter. The equation of state is then given by

$$P = w\,\rho\,, \tag{2.29}$$

such that w takes the following values for the forms of matter usually considered in cosmology:

$$w = \begin{cases} 0 & \text{for pressureless matter (dust),} \\ \frac{1}{3} & \text{for radiation,} \\ -1 & \text{for a cosmological constant.} \end{cases} \tag{2.30}$$

In fact, the barotropic index can also be time-dependent as it is, for example, the case in more complicated equations of state such as the one for a *Chaplygin gas*

$$P = -\frac{A}{\rho}, \quad A = \text{const.} > 0\,, \tag{2.31}$$

which exhibits dust-like behavior at early times and behaves like a cosmological constant at late times. This type of matter will be studied further in chapter 8.

But sticking at first to the simple form (2.29), equation (2.28) takes the form

$$\frac{\partial \rho}{\partial t} + 3H\rho\,(1+w) = 0 \quad \Leftrightarrow \quad \frac{\partial \rho}{\partial a} + \frac{3}{a}\rho\,(1+w) = 0\,, \tag{2.32}$$

such that we can easily find a solution for $\rho(a)$ with the ansatz $\rho(a) \propto a^n$, which is then given by

$$\rho(a) \propto a^{-3(1+w)}\,. \tag{2.33}$$

We can also define dimensionless density parameters for matter and radiation using the critical density, which corresponds to the density of an exactly flat universe at the present epoch and is given by

$$\rho_{\text{crit}} := \frac{3H_0^2}{8\pi G}\,, \tag{2.34}$$

where $H_0 := H(t_0)$ is the Hubble constant at the present time. The dimensionless density parameters then read

$$\Omega_{\text{m}}(a) := \frac{\rho_{\text{m}}(a)}{\rho_{\text{crit}}}, \quad \Omega_{\text{m,0}} := \frac{\rho_{\text{m,0}}}{\rho_{\text{crit}}}, \quad \Omega_{\text{r}}(a) := \frac{\rho_{\text{r}}(a)}{\rho_{\text{crit}}}, \quad \Omega_{\text{r,0}} := \frac{\rho_{\text{r,0}}}{\rho_{\text{crit}}}\,, \tag{2.35}$$

where we have used the index 0 to denote the densities at the present epoch t_0. Additionally, the cosmological constant leads to the density parameter

$$\Omega_\Lambda := \frac{\rho_\Lambda}{\rho_{\text{crit}}} = \frac{\Lambda}{3H_0^2}\,. \tag{2.36}$$

We can also introduce total density parameters, which are the sum of the matter constituents of the universe. They are given by

$$\Omega_{\text{tot}}(a) := \Omega_{\text{m}}(a) + \Omega_{\text{r}}(a) + \Omega_\Lambda\,, \tag{2.37}$$

$$\Omega_0 := \Omega_{\text{m,0}} + \Omega_{\text{r,0}} + \Omega_\Lambda\,. \tag{2.38}$$

With these definitions, we can rewrite the first Friedmann equation (2.25) in the following way

$$H^2 = H_0^2\left(\frac{\Omega_{\text{r,0}}}{a^4} + \frac{\Omega_{\text{m,0}}}{a^3} - \frac{\mathcal{K}}{a^2 H_0^2} + \Omega_\Lambda\right). \tag{2.39}$$

Given that the curvature parameter $\mathcal{K}$ can be written as

$$\mathcal{K} = H_0^2 \left(\Omega_0 - 1\right), \tag{2.40}$$

equation (2.39) can be expressed as

$$H^2 = H_0^2 \left(\frac{\Omega_{\mathrm{r},0}}{a^4} + \frac{\Omega_{\mathrm{m},0}}{a^3} + \frac{1 - \Omega_0}{a^2} + \Omega_\Lambda \right). \tag{2.41}$$

This equation immediately allows us to determine, which matter type dominates at which epoch. Radiation dominated at very early times, after which a period of ordinary matter (dust) domination followed. Then the curvature term took over and at late times, the cosmological constant will be the only contributor driving the expansion of the universe.

2.2 Problems of the cosmological standard model

The standard model of cosmology as outlined above has been widely successful to describe a large set observations in the universe using only a minimal set of parameters. However, several problems have been identified, which have made it clear that the model needs to be extended in some way.

The flatness problem

The first problem arises from the apparent flatness of the universe. From recent measurements of the Planck satellite [4], it was deduced that the universe is spatially flat to a very high precision, at a confidence level of 95 %, the limits of the total density parameter at the current epoch are within

$$0.993 < \Omega_0 < 1.006 .$$

This flatness, however, leads to a problem of finetuning, because as we will show below, the universe must have been much flatter, i.e. finetuned to $\Omega_0 = 1$, in order to obtain the present-day approximate flatness.

In order to see this, we rewrite the total density parameter $\Omega_{\mathrm{tot}}(a)$ as given in (2.37) in terms of the present-time density parameters by using equation (2.41):

$$\Omega_{\mathrm{tot}}(a) - 1 = \frac{\Omega_0 - 1}{\Omega_{\mathrm{r},0}\, a^{-2} + \Omega_{\mathrm{m},0}\, a^{-1} + \left(1 - \Omega_0\right) + a^2 \Omega_\Lambda} . \tag{2.42}$$

In the limit $a \ll 1$, we thus obtain

$$\Omega_{\mathrm{tot}}(a) - 1 = a^2 \, \frac{\Omega_0 - 1}{\Omega_{\mathrm{r},0}} . \tag{2.43}$$

We see that at early times, $\Omega_{\rm tot}(a) - 1$ approaches zero no matter what the values of the current density parameters are. This also means that in order for the Ω_0 to be close to unity today, it had to be several orders of magnitude closer to unity at earlier times. Hence, the universe must have been finetuned to be flat to a very large degree at early times, which calls for an explanation.

The horizon problem

As we have mentioned before, we can infer from the observation of the Cosmic Microwave Background (CMB) radiation, whose anisotropies are of the order 10^{-5}, that the universe is largely isotropic. However, as we will now show such a large isotropy cannot be explained within the cosmological standard model.

Let us follow [99] and consider two points of space in the universe. In order for these to have been in causal contact since the beginning of the universe, both must lie within a horizon called Hubble radius that can be expressed as a comoving quantity as

$$r_{\rm hor,com}(a) = \int_0^t \frac{\mathrm{d}\tilde{t}}{a(\tilde{t})} = \frac{1}{H_0}\int_0^a \frac{\mathrm{d}\tilde{a}}{\tilde{a}^2 H(\tilde{a})}\,. \tag{2.44}$$

As we will discuss in section 2.4, the CMB was formed during an epoch where the universe was matter-dominated. Thus for our purposes here, we can evaluate the above expression by inserting the corresponding matter part of (2.41):

$$r_{\rm hor,com}(a) = \frac{1}{H_0}\int_0^a \frac{\mathrm{d}\tilde{a}}{\sqrt{\tilde{a}\,\Omega_{\rm m,0}}} = \frac{2}{H_0}\sqrt{\frac{a}{\Omega_{\rm m,0}}}\,. \tag{2.45}$$

We also easily obtain the proper horizon length during matter domination:

$$r_{\rm hor,prop}(a) = a\, r_{\rm hor,com}(a) = \frac{2}{H_0}\frac{a^{3/2}}{\sqrt{\Omega_{\rm m,0}}}\,. \tag{2.46}$$

In order to relate the proper horizon length to an angle on the sky, we need to find an expression for the angular diameter distance $D_{\sphericalangle}$ of a source located at a certain redshift z, where z can is related to a by

$$a = \frac{1}{1+z}\,. \tag{2.47}$$

Using the comoving distance χ and the function $f_{\mathcal{K}}$ defined in (2.9), we can express $D_{\sphericalangle}$ as

$$D_{\sphericalangle}(z) = a(z)\, f_{\mathcal{K}}(\chi(z))\,. \tag{2.48}$$

There is an analytic expression available for the angular diameter distance in a matter-dominated universe, which is the *Mattig relation*:

$$D_{\measuredangle}(z) = \frac{1}{H_0} \frac{2}{\Omega_{\mathrm{m},0}^2 (1+z)^2} \left[\Omega_{\mathrm{m},0} z + \left(\Omega_{\mathrm{m},0} - 2 \right) \left(\sqrt{1 + \Omega_{\mathrm{m},0} z} - 1 \right) \right] . \tag{2.49}$$

We want to calculate the angular diameter distance from today to the redshift, where the CMB was formed, which happened at about $z_{\mathrm{CMB}} \simeq 1000$. Therefore, we can simplify the above relation to:

$$D_{\measuredangle}(z_{\mathrm{CMB}}) \simeq \frac{1}{H_0} \frac{2}{\Omega_{\mathrm{m},0} \, z_{\mathrm{CMB}}} . \tag{2.50}$$

The angle on the sky corresponding to the horizon scale at the time the CMB was created can thus be calculated as:

$$\vartheta_{\mathrm{hor,CMB}} = \frac{r_{\mathrm{hor,prop}}(z_{\mathrm{CMB}})}{D_{\measuredangle}(z_{\mathrm{CMB}})} \simeq \sqrt{\frac{\Omega_{\mathrm{m},0}}{z_{\mathrm{CMB}}}} \simeq \frac{\sqrt{\Omega_{\mathrm{m},0}}}{30} \simeq 2^\circ \sqrt{\Omega_{\mathrm{m},0}} . \tag{2.51}$$

Hence, we see that parts of the sky that are seperated by more than 2° should never have been in causal contact according to the cosmological standard model, which clearly contradicts the observed near isotropy of the CMB.

2.3 Inflation

Cosmologist have developed a framework called *inflation* in order to tackle the above-mentioned problems of the standard model of cosmology. The main assumption of inflationary models is that the universe underwent a phase of rapid accelerated expansion at the very first instances after the Big Bang. Alan Guth [52] and Andrei D. Linde [84] worked out such models in 1981, after Alexei A. Starobinsky had used a similar idea two years before [103]. In the meantime, inflation has become regarded as a very successful theory, especially because it gives an explanation for the origin of structure in the universe as quantum fluctuations of spacetime that become macroscopic due to inflation, which we will discuss in more detail in chapters 5 to 7.

But let us first give a brief overview of the main ideas of inflation using one of the simplest possible models. We base this presentation on [78, 82, 83, 92].

Inflationary models

The easiest way to obtain an inflationary phase in the evolution of the universe is to introduce a scalar field ϕ, whose energy density and pressure are given by:

$$\rho_\phi = \frac{1}{2} \dot{\phi}^2 + \mathcal{V}(\phi) , \qquad P_\phi = \frac{1}{2} \dot{\phi}^2 - \mathcal{V}(\phi) . \tag{2.52}$$

We have to demand that the following condition be fulfilled

$$\rho_\phi + 3 P_\phi < 0 \,, \tag{2.53}$$

in order to achieve an accelerated expansion. The potential $\mathcal{V}(\phi)$ can, for instance, be chosen to have the simple form used in the *chaotic inflation* model [85] with a mass m:

$$\mathcal{V}(\phi) = \frac{1}{2} m^2 \phi^2 \,. \tag{2.54}$$

The Friedmann equations (2.25) and (2.26) then yield:

$$H^2 = \frac{8\pi G}{3} \left(\frac{1}{2} \dot{\phi}^2 + \mathcal{V}(\phi) \right) , \tag{2.55}$$

$$\ddot{\phi}(t) + 3H\,\dot{\phi}(t) + \mathcal{V}'(\phi) = 0 \,. \tag{2.56}$$

The slow-roll approximation

An approximation that is often used, because it is in good agreement with observations, is the so-called *slow-roll approximation*. It assumes that the scalar field ϕ stays approximately constant during inflation, which simplifies the equations of motion outlined above significantly:

$$H^2 \simeq \frac{8\pi G}{3} \mathcal{V}(\phi) , \qquad 3H\dot{\phi}(t) \simeq -\mathcal{V}'(\phi) \,. \tag{2.57}$$

We can also define the slow-roll parameters ϵ_V and η_V in terms of the potential $\mathcal{V}$ as follows

$$\epsilon_V = \frac{1}{16\pi G} \left(\frac{\mathcal{V}'}{\mathcal{V}} \right)^2 , \quad \eta_V = \frac{1}{8\pi G} \frac{\mathcal{V}''}{\mathcal{V}} , \tag{2.58}$$

where we have used a prime to indicate a derivative with respect to ϕ. Using these parameters, the conditions for slow-roll inflation can be written as

$$\epsilon_V \ll 1 , \quad |\eta_V| \ll 1 \,. \tag{2.59}$$

An estimate of the magnitude of the expansion occurring during inflation can be given by the number of e-foldings defined as

$$N := \ln \left[\frac{a(t_{\text{end}})}{a(t_{\text{initial}})} \right] = \int_{t_{\text{initial}}}^{t_{\text{end}}} \mathrm{d}t\, H(t) \simeq -8\pi G \int_{\phi_{\text{intial}}}^{\phi_{\text{end}}} \frac{\mathrm{d}\phi\, \mathcal{V}'}{\mathcal{V}} \,. \tag{2.60}$$

About 70 e-foldings, which implies an expansion by a factor of about 10^{30}, are necessary in order to flatten spacetime sufficiently during inflation such that the flatness problem described above can be regarded as solved [82].

Considering the slow-roll approximation in the chaotic inflation model with the potential $\mathcal{V}(\phi)$ defined in equation (2.54), we can write the Friedmann equations as

$$H^2 = \frac{4\pi G}{3}\, m^2 \phi^2\,, \qquad 3H\,\dot{\phi} + m^2\phi = 0\,, \tag{2.61}$$

while the slow-roll parameters are given by

$$\epsilon_V = \eta_V = \frac{1}{4\pi G\,\phi^2}\,. \tag{2.62}$$

This allows us to solve equations (2.61) as well as (2.60) analytically and we obtain:

$$\phi(t) = \phi_{\text{init}} - \frac{m}{\sqrt{12\pi G}}\, t\,, \tag{2.63}$$

$$a(t) = a_{\text{init}}\, \exp\left[\sqrt{\frac{4\pi G}{3}}\, m \left(\phi_{\text{init}}\, t - \frac{m}{\sqrt{48\pi G}}\, t^2\right)\right], \tag{2.64}$$

$$N = 2\pi G\,\phi_{\text{init}}^2 - \frac{1}{2}\,, \tag{2.65}$$

where a_{init} and ϕ_{init} are the values at the start of inflation.

A very special case of inflation is to take a constant scalar field $\phi(t) \equiv \phi_0$, such that the scalar field acts as a "supercharged" cosmological constant. We can immediately solve the Friedmann equation

$$H^2 = \frac{4\pi G}{3}\, m^2\phi_0^2 = \text{const.} \tag{2.66}$$

in this case and arrive at

$$a(t) = a_{\text{init}}\, \mathrm{e}^{Ht} = a_{\text{init}}\, \exp\left[\sqrt{\frac{4\pi G}{3}}\, m\,\phi_0\, t\right]. \tag{2.67}$$

The spacetime that is generated by this type of inflation is the *de Sitter spacetime*, which can be represented as the embedding of the four-dimensional hyperboloid described by

$$-z_0^2 + z_1^2 + z_2^2 + z_3^2 + z_4^2 = \frac{1}{H^2} \tag{2.68}$$

within a five-dimensional Lorentzian manifold.

Depending on what kind of slicing of the five-dimensional manifold one uses, different representations of the de Sitter spacetime emerge. A Euclidean slicing leads to the flat de Sitter spacetime described above, whose metric reads

$$ds^2 = -\,dt^2 + e^{2Ht}\,d\Omega^2_{3,\mathcal{K}=0}\,. \tag{2.69}$$

Using a spherical slicing yields a closed de Sitter spacetime, for which the metric is given by

$$ds^2 = -\,dt^2 + \frac{\cosh^2(Ht)}{H^2}\,d\Omega^2_{3,\mathcal{K}=1}\,. \tag{2.70}$$

In this case, the scale factor takes the form

$$a(t) \propto \cosh(Ht)\,. \tag{2.71}$$

2.4 The Cosmic Microwave Background

In the following, we will give a short overview of the physical processes that lead to the emergence of the Cosmic Microwave Background. Its radiation originated during a phase in the thermal history of the universe called *recombination*. For this reason, we will focus on describing this phase in the following. A more detailed description of the thermal history of the universe as a whole can be found, for instance, in [77].

Recombination and the origin of the CMB

We consider the epoch after the lightest elements have already been created by primordial nucleosynthesis and after the universe has transitioned from radiation to matter domination. In this era the temperature of the universe continues to decrease until it reaches the temperature that allows free electrons to combine with nuclei for the first time and thus form neutral atoms. Although the universe has always been ionized before, the name *re*combination is used for this process.

The binding energy of a hydrogen atom is approximately 13.6 eV $\approx 10^5$ K, but due to the fact that there are photons that have a higher energy than this binding energy in the Wien tail of the energy distribution and that can therefore reionize the newly formed hydrogen atoms, recombination only effectively starts when the universe has reached a temperature of about 3000 K. Additionally, one has to take into account that each recombination process creates a photon with an energy high enough to ionize another neutral atom and the cross section for this process is sufficiently high to occur frequently. Therefore, the actual process leading to recombination goes via a more complicated process, the two-photon decay.

Nevertheless, as soon as the process of recombination starts at the redshift of about $z \sim 1000$, it is so effective that the universe transitions from being almost entirely ionized to being almost completely neutral in a relatively short timespan of around $\Delta z \sim 60$.

However, one also has to take into account the expansion rate of the universe, which for small enough ionizations is larger than the recombination rate, such that the process of recombination is not completely finished, because there are nuclei left that do not encounter an electron to combine with fast enough, which causes a remaining a net ionization of about 10^{-4}. Nevertheless, the remaining electrons do not obstruct the propagation of photons entirely, since the optical depth of Thomson scattering caused by these elections is small for photons whose wavelength is larger than 1216 Å [99]. This allows photons from that epoch, also called last scattering, to still be around in the universe today without having experienced an interaction with matter. At the time of last scattering, the energy distribution of these photons corresponded to a Planck spectrum and therefore it should be possible to observe a background of photons having such a spectrum today, but due to the expansion of the universe, these photos should be redshifted into the microwave regime.

Exactly this is the Cosmic Microwave Background (CMB) that was discovered by Arno Penzias and Robert Wilson in 1965 [91]. In fact, the existence of the CMB was already predicted by George Gamov in 1946 [49]. Measuring the spectrum of the CMB revealed the most precise Planck spectrum ever encountered, but the temperature anisotropies being only of order 10^{-5} have turned out to be one of the most important measurements for cosmology.

Anisotropies in the CMB

During the era described above, there were already inhomogeneities present in the universe, such that the CMB exhibits anisotropies in its temperature that originate from the structure at the time the photons forming the CMB decoupled from matter. More precisely, these *primary* anisotropies are due to the gravitational redshifting of those photons that originate from regions with a higher matter density, which is the so-called *Sachs–Wolfe effect*. Additionally, the energy of photons in regions of higher density is also changed by the Doppler effect caused by the peculiar velocity of the matter they interact with. These effects producing anisotropies in the CMB are counteracted on smaller scales due to *Silk damping*, which is a process that is caused by the decoupling of photons and baryons on small scales.

The CMB photons are furthermore influenced by *secondary anisotropies* on their propagation through the universe until the present day. One process is the Thomson scattering of photons with matter that has been reionized. Another change of energy called *integrated Sachs–Wolfe effect* arises, when photons propagate through a gravitational potential that changes in time. Furthermore, photons are gravitationally deflected by the structure of matter on their way and are scattered by hot gas in galaxy clusters, which is called the *Sunyaev–Zel'dovich effect*.

Description of the CMB anisotropies

The anisotropies of the CMB temperature T can be described by the quantity

$$\mathcal{T}(\mathbf{n}) = \frac{T(\mathbf{n}) - \overline{T}}{\overline{T}}\,, \tag{2.72}$$

where $\mathbf{n}$ is a normal unit vector on the 2-sphere and $\overline{T}$ denotes the mean temperature of the CMB.

In order to average over all pairs of directions $\mathbf{n}$ and $\mathbf{n}'$ that are separated by a given angle ϑ, one introduces the correlation function:

$$C(\vartheta) = \left\langle \mathcal{T}(\mathbf{n})\,\mathcal{T}(\mathbf{n}')\right\rangle\,, \tag{2.73}$$

We can also define the power spectrum of the temperature anisotropies by using a decomposition of the above-defined correlation function in terms of spherical harmonics on the 2-sphere. The coefficients of the power spectrum are then given by $\ell(\ell+1)C_\ell$ using the quantity ℓ that is related to the angle ϑ by

$$\vartheta \simeq \frac{\pi}{\ell}\,, \tag{2.74}$$

such that $\ell = 1$ corresponds to the dipole, $\ell = 2$ the quadrupole of the temperature anisotropies and so forth, cf. for instance, [58] for more details.

Features of the CMB power spectrum

Looking at the form of the CMB power spectrum measured by WMAP [56] and Planck [4], one immediately notices a large number of so-called *acoustic peaks* for multipoles above $\ell \gtrsim 100$, which are caused by oscillations of the baryon–photon fluid. Temperature fluctuations originate from these oscillation because of the Doppler effect and adiabatic compression. The acoustic peaks contain several pieces of information about cosmological parameters. In particular, it is possible to derive the curvature of the universe from the exact position of the first peak at around $\ell \sim 200$, because the position of this peak, i.e. the angular size of the most prominent features of the CMB anisotropies, is determined by the physical length of the horizon during recombination, which can then be compared to each other by means of a relation depending on the curvature of the universe, such that it is possible to determine the curvature.

For larger multipoles the amplitude of the anisotropies decreases because of Silk damping. On the other hand, for lower multipoles, i.e. larger scales, the Sachs–Wolfe effect is the main contributor for the anisotropies and thus the power spectrum of the primordial cosmological perturbations is directly imprinted in the CMB on these scales. However, on large scales, the *integrated* Sachs–Wolfe effect also has to be taken into account. In the presence of a cosmological constant becoming more dominant at present times, the gravitational potentials of structures the photons propagate through change in time and thus modify the energy of the CMB photons, such that the power of the anisotropies is increased at large scales depending on the magnitude of the cosmological constant.

3

The Wheeler–DeWitt equation

In this chapter, we will present the procedure to canonically quantize gravity described by general relativity, which leads to the Wheeler–DeWitt equation. We shall first discuss the general case and then move to a symmetry-reduced model that describes a homogeneous and isotropic universe. This chapter is based on [54, 69, 73, 78].

3.1 The 3+1-decomposition of general relativity

In order to apply a canonical quantization scheme to general relativity, one has to reformulate the theory such that it obtains a Hamiltonian structure. Such a reformulation was developed by Richard Arnowitt, Stanley Deser and Charles W. Misner [9] and it is therefore referred to as ADM formalism.

The Hamiltonian structure of general relativity is obtained by a foliation of a spacetime $\mathcal{M}$ with a metric $g_{\mu\nu}$ into space-like hypersurfaces Σ_t. This procedure does not break the covariance of general relativity, because one takes into account all possible foliations of spacetime. We thus introduce a time function t and a vector field t^μ, which obey

$$t^\mu \nabla_\mu t = 1\,. \tag{3.1}$$

We assign a normal unit vector n^μ, $n^\mu n_\mu = -1$, to each hypersurface Σ_t and can thus decompose t^μ into a normal and tangential component with respect to Σ_t in the subsequent way

$$t^\mu = N n^\mu + N^\mu\,, \tag{3.2}$$

where we have introduced the *lapse function* N as well as the *shift vector* N^μ.

Furthermore, we can then write the three-metric $h_{\mu\nu}$ that is induced by $g_{\mu\nu}$ on each hypersurface as

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

We now define the *extrinsic curvature* $K_{\mu\nu}$ describing the embedding curvature of Σ_t into $\mathcal{M}$ in terms of a Lie derivative along the normal vector field n^μ as follows

$$K_{\mu\nu} = \frac{1}{2}\,\mathfrak{L}_{\mathbf{n}} h_{\mu\nu} = h_\mu^{\ \sigma}\,\nabla_\sigma n_\nu \,. \tag{3.4}$$

The spatial part of the extrinsic curvature can be expressed in terms of the lapse function and shift vector in the following way

$$K_{ij} = \frac{1}{2N}\left(\dot{h}_{ij} - D_i N_j - D_j N_i\right). \tag{3.5}$$

Here D_i stands for the spatial covariant derivative. We can use this quantity and its contraction to rewrite the Einstein–Hilbert action as

$$S_{\mathrm{EH}} = \frac{1}{16\pi G}\int_{\mathcal{M}} \mathrm{d}t\,\mathrm{d}^3\mathbf{x}\; N\sqrt{h}\left(K_{ij}K^{ij} - K^2 + {}^{(3)}\!R - 2\Lambda\right), \tag{3.6}$$

where ${}^{(3)}\!R$ denotes the three-dimensional Ricci scalar, h stands for the determinant of h_{ij} and Λ is the cosmological constant. We can simplify the notation slightly by introducing the so-called *DeWitt metric*, which is defined by

$$G_{ijkl} = \frac{1}{2\sqrt{h}}\left(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}\right), \tag{3.7}$$

such that the Einstein–Hilbert action takes the form

$$S_{\mathrm{EH}} = \frac{1}{16\pi G}\int_{\mathcal{M}} \mathrm{d}t\,\mathrm{d}^3\mathbf{x}\; N\left(G^{ijkl}K_{ij}K_{kl} + \sqrt{h}\left[{}^{(3)}\!R - 2\Lambda\right]\right). \tag{3.8}$$

Using the Lagrange density

$$\mathcal{L}^{\mathrm{g}} := N\left(G^{ijkl}K_{ij}K_{kl} + \sqrt{h}\left[{}^{(3)}\!R - 2\Lambda\right]\right), \tag{3.9}$$

the conjugate momenta of the lapse function N and shift vector N^i read:

$$p_N = \frac{\partial \mathcal{L}^{\mathrm{g}}}{\partial \dot{N}} = 0\,, \quad p_i^{\mathrm{g}} = \frac{\partial \mathcal{L}^{\mathrm{g}}}{\partial \dot{N}^i} = 0\,. \tag{3.10}$$

The fact that both expressions vanish is because they act as Lagrange multipliers instead of being dynamical variables.

For the conjugate momenta to the three-metric h_{ij}, we obtain:

$$p^{ij} = \frac{\partial \mathcal{L}^{\mathrm{g}}}{\partial \dot{h}_{ij}} = \frac{1}{16\pi G} G^{ijkl} K_{kl} = \frac{\sqrt{h}}{16\pi G} \left(K^{ij} - K h^{ij} \right) . \tag{3.11}$$

The Hamiltonian density $\mathcal{H}^{\mathrm{g}}$ is therefore given by the Legendre transform

$$\mathcal{H}^{\mathrm{g}} = p^{ij} \dot{h}_{ij} - \mathcal{L}^{\mathrm{g}} \tag{3.12}$$

and we can express $\dot{h}_{ij}$ in terms of the momenta p_{ij} as

$$\dot{h}_{ij} = \frac{32\pi G N}{\sqrt{h}} \left(p_{ij} - \frac{1}{2} p\, h_{ij} \right) + D_i N_j + D_j N_i \, , \tag{3.13}$$

where we have defined

$$p := p^{ij} h_{ij} \, . \tag{3.14}$$

The Hamiltonian density (3.12) thus reads

$$\mathcal{H}^{\mathrm{g}} = 16\pi G N\, G_{ijkl}\, p^{ij} p^{kl} - N \frac{\sqrt{h}}{16\pi G} \left({}^{(3)}R - 2\Lambda \right) - 2 N_j \left(D_i p^{ij} \right) \tag{3.15}$$

and we immediately obtain the full Hamiltonian H^{g} by the following integration:

$$H^{\mathrm{g}} = \int \mathrm{d}^3\mathbf{x}\; \mathcal{H}^{\mathrm{g}} = \int \mathrm{d}^3\mathbf{x} \left(N\, \mathcal{H}^{\mathrm{g}}_{\perp} + N^i\, \mathcal{H}^{\mathrm{g}}_i \right) , \tag{3.16}$$

where we have introduced

$$\mathcal{H}^{\mathrm{g}}_{\perp} := 16\pi G\, G_{ijkl}\, p^{ij} p^{kl} - \frac{\sqrt{h}}{16\pi G} \left({}^{(3)}R - 2\Lambda \right) , \tag{3.17}$$

$$\mathcal{H}^{\mathrm{g}}_i := -2\, D_j p_i{}^j \, . \tag{3.18}$$

Finally, we can therefore rewrite the Einstein–Hilbert action (3.6) as

$$S_{\mathrm{EH}} = \frac{1}{16\pi G} \int_{\mathcal{M}} \mathrm{d}t\, \mathrm{d}^3\mathbf{x} \left(p^{ij} \dot{h}_{ij} - N\, \mathcal{H}^{\mathrm{g}}_{\perp} - N^i\, \mathcal{H}^{\mathrm{g}}_i \right) . \tag{3.19}$$

Varying this action with respect to N and N^i then leads to the following two constraints:

$$\mathcal{H}^{\mathrm{g}}_{\perp} \approx 0 \, , \tag{3.20}$$

$$\mathcal{H}^{\mathrm{g}}_i \approx 0 \, , \tag{3.21}$$

where the first constraint is the *Hamiltonian constraint* and the second one the *diffeomorphism constraint*. The approximation sign is used here to denote a weak equality as defined by Dirac [44], which means that one first has to evaluate the corresponding Poisson brackets before setting the constraint equal to zero.

3.2 Quantum Geometrodynamics

Now that we have obtained a Hamiltonian form for general relativity, we can directly quantize the theory canonically. This form of canonical quantum gravity is usually called *Quantum Geometrodynamics*. Our canonical variables are thus the three-metric h_{ij} and its conjugate momenta p^{ij}. We promote both variables to quantum operators $\hat{h}_{ij}$ and $\hat{p}^{ij}$, which obey the following commutation relations:

$$\left[\hat{h}_{ij}(\mathbf{x}), \hat{p}^{kl}(\mathbf{y})\right] = \mathrm{i}\hbar\, \delta^{k}_{(i}\delta^{l}_{j)}\, \delta(\mathbf{x},\mathbf{y})\,, \tag{3.22}$$

where we have indicated a symmetrization of indices by parentheses.

These operators then act on a wave functional Ψ, which is defined in the space of all three-geometries called *superspace*, in the following way

$$\hat{h}_{ij}(\mathbf{x})\,\Psi\left[h_{ab}(\mathbf{x})\right] = h_{ij}(\mathbf{x})\,\Psi\left[h_{ab}(\mathbf{x})\right]\,, \tag{3.23}$$

$$\hat{p}^{ij}(\mathbf{x})\,\Psi\left[h_{ab}(\mathbf{x})\right] = -\,\mathrm{i}\hbar\,\frac{\delta}{\delta h_{ij}(\mathbf{x})}\,\Psi\left[h_{ab}(\mathbf{x})\right]. \tag{3.24}$$

Using these relations, we can convert the classical constraints (3.20) and (3.21) to quantum operators, let them act on a wave functional Ψ and set these expressions equal to zero. From the Hamiltonian constraint we then obtain the *Wheeler–DeWitt equation*

$$\hat{\mathcal{H}}^{g}_{\perp}\Psi\left[h_{ab}(\mathbf{x})\right] = \left[-\,16\pi G\,\hbar^2\,G_{ijkl}\,\frac{\delta^2}{\delta h_{ij}\delta h_{kl}} - \frac{\sqrt{h}}{16\pi G}\left({}^{(3)}\!R - 2\,\Lambda\right)\right]\Psi\left[h_{ab}(\mathbf{x})\right] = 0\,, \tag{3.25}$$

which is the central equation of Quantum Geometrodynamics. The diffeomorphism constraint leads to

$$\hat{\mathcal{H}}^{g}_{i}\,\Psi\left[h_{ab}(\mathbf{x})\right] = -\,2\,D_j h_{ik}\,\frac{\hbar}{\mathrm{i}}\,\frac{\delta}{\delta h_{jk}}\,\Psi\left[h_{ab}(\mathbf{x})\right] = 0\,. \tag{3.26}$$

We can see that the Wheeler–DeWitt equation (3.25) does not contain any dependence on time, it is entirely *timeless*. It is, however, possible to recover a notion of time within a semiclassical approximation scheme, as we shall see in the next chapter.

One also has to remark that it is problematic to define equation (3.25) in a strict mathematical sense because of the appearance of *second* functional derivatives, which lead to indefinite expressions. In the following we will apply the quantization scheme presented here to a symmetry-reduced model of the universe, where the problem related to the functional derivatives does not appear.

3.3 Minisuperspace

Now we will focus our attention to the quantization of cosmological models. The large symmetry inherent in these models implies that the quantization procedure simplifies drastically.

We take a homogeneous and isotropic universe that is described by the Friedmann–Lemaître–Robertson–Walker metric (2.6) with lapse function $N(t)$

$$\mathrm{d}s^2 = -N^2(t)\,\mathrm{d}t^2 + a^2(t)\,\mathrm{d}\Omega^2_{3,\mathcal{K}}\,, \tag{3.27}$$

where $\mathrm{d}\Omega^2_{3,\mathcal{K}}$ is defined in (2.9) and (2.10) for $\mathcal{K} = 0, \pm 1$. Due to the maximal symmetry of the spatial part, the shift vector N^i does not appear here. Furthermore, we add a massive scalar field ϕ as matter. Hence, the infinitely many degrees of freedom of the full superspace are reduced to a set of two, which are the scale factor a and the scalar field ϕ. They thus form the so-called *minisuperspace*.

From the form of the FLRW metric, the 3+1-decomposition of spacetime is immediately apparent and we can write out induced spatial metric $h_{ij}(t)$ on the space-like hypersurfaces as

$$h_{ij}(t) = a^2(t)\,\mathrm{diag}\Big(1, f^2_{\mathcal{K}}(\chi), f^2_{\mathcal{K}}(\chi)\sin^2(\vartheta)\Big) \tag{3.28}$$

and its time derivative reads

$$\dot{h}_{ij} = \dot{a}\,\frac{\partial h_{ij}}{\partial a} = \frac{2\,\dot{a}}{a}\,h_{ij}\,. \tag{3.29}$$

We can thus write the extrinsic curvature (3.5) as

$$K_{ij} = \frac{1}{2N}\,\dot{h}_{ij} = \frac{1}{N}\,\frac{\dot{a}}{a}\,h_{ij} \tag{3.30}$$

and its trace is given by

$$K = K_{ij}h^{ij} = \frac{3}{N}\,\frac{\dot{a}}{a}\,, \tag{3.31}$$

since $h_{ij}h^{ij} = 3$. The Einstein–Hilbert action (3.6) therefore becomes

$$S_{\mathrm{grav}} = \frac{3\pi}{4G}\int \mathrm{d}t\,N\left(-\frac{a\,\dot{a}^2}{N^2} + \mathcal{K}\,a - \frac{\Lambda\,a^3}{3}\right), \tag{3.32}$$

where the integration over the spatial part was carried out assigning the volume of a three-sphere to it, which is $2\pi^2$.

On top of that we need the action S_{mat} for the scalar field ϕ with potential $\mathcal{V}(\phi)$, which is given by

$$S_{\mathrm{mat}} = \pi^2 \int \mathrm{d}t\, N a^3 \left(\frac{\dot{\phi}^2}{N^2} - 2\,\mathcal{V}(\phi) \right). \tag{3.33}$$

Here we have also integrated over the spatial part and assigned the value $2\pi^2$ to it.

Therefore we arrive at the following minisuperspace action

$$S = S_{\mathrm{grav}} + S_{\mathrm{mat}} = \int L(a, \phi, \dot{a}, \dot{\phi})\,\mathrm{d}t\,, \tag{3.34}$$

where the Lagrangian $L(a, \phi, \dot{a}, \dot{\phi})$ takes the form

$$L(a,\phi,\dot{a},\dot{\phi}) = N \left[-\frac{3\pi}{4G}\frac{a}{N^2}\,\dot{a}^2 + \frac{\pi^2 a^3}{N^2}\,\dot{\phi}^2 - \pi^2 a^3 \left(\frac{\Lambda}{4\pi G} - \frac{3\,\mathcal{K}}{4\pi G}\frac{1}{a^2} + 2\,\mathcal{V}(\phi) \right) \right]. \tag{3.35}$$

We now simplify this expression by introducing a minisuperspace metric. For this purpose, we define a "vector" q^A, whose index runs from from 0 to 1 and to which we assign the variables

$$q^0 := a\,, \quad q^1 := \phi\,. \tag{3.36}$$

Using the subsequent definition of a metric $\mathcal{G}_{AB}$ for the minisuperspace

$$\mathcal{G}_{AB} := \mathrm{diag}\left(-\frac{3\pi}{2G}\,a,\, 2\pi^2 a^3 \right) \tag{3.37}$$

and defining a minisuperspace potential $V(a, \phi)$ as

$$V(a,\phi) := -\frac{3\pi\mathcal{K}}{4G}\,a + \pi^2 a^3 \left(2\,\mathcal{V}(\phi) + \frac{\Lambda}{4\pi G} \right), \tag{3.38}$$

we can rewrite the Lagrangian (3.35) in the following way

$$L(q^J, \dot{q}^J) = N \left(\frac{1}{2N^2}\,\mathcal{G}_{AB}\,\dot{q}^A \dot{q}^B - V(q^J) \right). \tag{3.39}$$

The canonical momentum for the lapse function N again vanishes

$$p_{(N)} = \frac{\partial L}{\partial \dot{N}} = 0\,, \tag{3.40}$$

whereas we obtain for the scale factor a and the scalar field ϕ:

$$p_{(a)} = \frac{\partial L}{\partial \dot{a}} = -\frac{3\pi}{2G}\frac{a}{N}\,\dot{a}\,, \quad p_{(\phi)} = \frac{\partial L}{\partial \dot{\phi}} = \frac{2\pi^2 a^3}{N}\,\dot{\phi}\,. \tag{3.41}$$

In order to arrive at the Hamiltonian, we use the Legendre transform

$$H = p_{(a)}\dot{a} + p_{(\phi)}\dot{\phi} - L\,, \tag{3.42}$$

which leads to:

$$H = N\left(-\frac{G}{3\pi a}\,p_{(a)}^2 + \frac{1}{4\pi^2 a^3}\,p_{(\phi)}^2 + V(a,\phi)\right). \tag{3.43}$$

With the minisuperspace metric (3.37) and potential (3.38), this Hamiltonian simplifies to

$$H = N\left(\frac{1}{2}\,\mathcal{G}^{AB}\,p_A\,p_B + V(q^J)\right). \tag{3.44}$$

3.4 Quantum Cosmology

In order to canonically quantize the minisuperspace Hamiltonian, we proceed as for the general case of the full superspace and promote a and ϕ as well as their canonical momenta to quantum operators. The operators for the momenta are then replaced by partial derivatives with respect to the corresponding minisuperspace variable.

However, in the product $\hat{\mathcal{G}}^{AB}\,\hat{p}_A\,\hat{p}_B$ appearing in the quantum operator version of (3.44), we face an ambiguity in the factor ordering. In order to specify a certain ordering, we take the method from [69], where the factor ordering is chosen in that way that the invariance of the kinetic term under transformations in configuration space is kept, which leads to the so-called *Laplace–Beltrami* factor ordering. It uses the covariant generalization of the Laplace operator, the *Laplace–Beltrami operator* $\triangle_{\text{LB}}$, that is defined for a metric $g_{\mu\nu}$ with determinant g as

$$\triangle_{\text{LB}} := \frac{1}{\sqrt{-g}}\,\partial_\mu\left(\sqrt{-g}\,g^{\mu\nu}\,\partial_\nu\right). \tag{3.45}$$

The quantum operator product $\hat{\mathcal{G}}^{AB}\,\hat{p}_A\,\hat{p}_B$ is thus replaced by

$$\hat{\mathcal{G}}^{AB}\,\hat{p}_A\,\hat{p}_B \to -\frac{\hbar}{\sqrt{-\mathcal{G}}}\,\frac{\partial}{\partial q_A}\left(\sqrt{-\mathcal{G}}\,\mathcal{G}^{AB}\,\frac{\partial}{\partial q_B}\right), \tag{3.46}$$

where we have used the determinant $\mathcal{G}$ of $\mathcal{G}_{AB}$, which can be written out as

$$\mathcal{G} = -\frac{3\pi^2}{G}\,a^4\,. \tag{3.47}$$

The expression (3.46) then explicitly takes the form

$$-\frac{\hbar}{\sqrt{-\mathcal{G}}}\frac{\partial}{\partial q_a}\left(\sqrt{-\mathcal{G}}\,\mathcal{G}^{ab}\frac{\partial}{\partial q_b}\right)=\frac{2\hbar^2 G}{3\pi}\left(\frac{1}{a}\frac{\partial}{\partial a}+\frac{1}{a^2}\frac{\partial^2}{\partial a^2}\right)-\frac{\hbar}{2\pi^2}\frac{1}{a^3}\frac{\partial^2}{\partial\phi^2}$$
$$=\frac{2\hbar^2 G}{3\pi}\frac{1}{a^3}\frac{\partial}{\partial a}\left(a\frac{\partial}{\partial a}\right)-\frac{\hbar}{2\pi^2}\frac{1}{a^3}\frac{\partial^2}{\partial\phi^2}. \quad (3.48)$$

Letting the quantum Hamiltonian $\hat{H}$ derived from (3.44) with $N \equiv 1$ act on the minisuperspace wave function $\Psi(a,\phi)$ leads to the Wheeler–DeWitt equation

$$\hat{H}\Psi(a,\phi)=0\,, \quad (3.49)$$

which using (3.48) explicitly reads:

$$\left[\frac{\hbar^2 G}{3\pi a^2}\frac{\partial}{\partial a}\left(a\frac{\partial}{\partial a}\right)-\frac{\hbar^2}{4\pi^2 a^3}\frac{\partial^2}{\partial\phi^2}\right.$$
$$\left.-\frac{3\pi\mathcal{K}}{4G}\,a+a^3\pi^2\left(2\,\mathcal{V}(\phi)+\frac{\Lambda}{4\pi G}\right)\right]\Psi(a,\phi)=0\,. \quad (3.50)$$

4

The semiclassical approximation to the Wheeler–DeWitt equation

This chapter is devoted to the semiclassical approximation of canonical quantum gravity leading to the Wheeler–DeWitt equation. In general, any theory of quantum gravity has to recover classical spacetime in some appropriate limit and for the Wheeler–DeWitt equation this can be achieved by using a Born–Oppenheimer type of expansion in terms of the gravitational constant, which we will describe below. From this expansion one recovers general relativity in the form of a Hamilton–Jacobi equation and subsequently quantum field theory on curved spacetime as a functional Schrödinger equation. Furthermore, this approximation scheme allows us to derive quantum-gravitational corrections terms to this Schrödinger equation and we will use this in the following chapters to calculate the effects arising from these corrections terms to the power spectra of inflationary perturbations.

We will present here a summary of the semiclassical approximation scheme for the full Wheeler–DeWitt equation based on [69, 75, 78]. The calculation for a cosmological model will be derived in detail in the next chapter.

4.1 The classical limit in quantum mechanics

Before focussing on canonical quantum gravity, let us briefly recap how the semiclassical limit is obtained in ordinary quantum mechanics. Considering the Schrödinger equation for a wave function $\psi(\mathbf{x}, t)$ with potential $V(\mathbf{x})$,

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = \left[-\frac{\hbar}{2m} \nabla + V(\mathbf{x}) \right] \psi(\mathbf{x}, t) \, , \tag{4.1}$$

one makes the following ansatz with the function $S(\mathbf{x},t)$

$$\psi(\mathbf{x},t) = \mathrm{e}^{\mathrm{i}S(\mathbf{x},t)/\hbar}, \tag{4.2}$$

that is also used in the WKB approximation. Hence, one obtains

$$-\frac{\partial S}{\partial t} = \frac{1}{2m}(\nabla S)^2 - \frac{\mathrm{i}\hbar}{2m}(\nabla S^2) + V(\mathbf{x}). \tag{4.3}$$

The semiclassical approximation is then performed by taking the limit $\hbar \to 0$, for which the second term on the right-hand side vanishes and we recover the classical Hamilton–Jacobi equation.

4.2 The Born–Oppenheimer type of approximation

For the semiclassical approximation of the Wheeler–DeWitt equation (3.25) we use a similar ansatz as (4.2), but combine it with a Born–Oppenheimer type of approximation that establishes a hierarchy between the gravitational part and a matter part, for which we introduce a scalar field ϕ with potential $\mathcal{U}$ and matter Hamiltonian $\mathcal{H}_{\mathrm{m}}$ that is given by

$$\mathcal{H}_{\mathrm{m}}\left[h_{ij}(\mathbf{x}), \phi(\mathbf{x})\right] = -\frac{\hbar^2}{2\sqrt{h}}\frac{\delta^2}{\delta\phi^2} + \mathcal{U}\left[h_{ij}, \phi, \phi_{,i}\right]. \tag{4.4}$$

Thus our Wheeler–DeWitt equation reads

$$\left[-16\pi G\hbar^2 G_{ijkl}\frac{\delta^2}{\delta h_{ij}\delta h_{kl}} - \frac{\sqrt{h}\,{}^{(3)}\!R}{16\pi G} - \frac{\hbar^2}{2\sqrt{h}}\frac{\delta^2}{\delta\phi^2} + \mathcal{U}\left[h_{mn}, \phi, \phi_{,m}\right]\right]\Psi\left[h_{mn}, \phi\right] = 0, \tag{4.5}$$

where we have also set the cosmological constant Λ equal to zero.

The smallness of the gravitational constant that appears as a factor in front of the first term and in the denominator of the second term implies that the dynamics of the gravitational part are negligible compared to matter field. In the language of atomic and molecular physics, where the Born–Oppenheimer approximation is usually used, the gravitational background thus corresponds to a heavy nucleus, whereas the matter field plays the role of a light electron.

Before we continue with our derivation, let us follow [75] and first simplify equation (4.5) by combining indices that only appear in pairs in the following way

$$h_{ij} \to h_a, \quad G_{ijkl} \to G_{ab}, \quad \frac{\delta}{\delta h_{ij}} \to \frac{\delta}{\delta h_a}. \tag{4.6}$$

and by defining the gravitational potential

$$V[h_a(\mathbf{x})] := -2\sqrt{h}\,{}^{(3)}\!R\,. \tag{4.7}$$

For later convenience, we also introduce a parameter M

$$M := \frac{1}{32\pi G} \tag{4.8}$$

with respect to which we will carry out the semiclassical expansion. Hence, equation (4.5) finally reads:

$$\left[-\frac{\hbar^2}{2M}G_{ab}\frac{\delta^2}{\delta h_a \delta h_b} + M\,V[h_a] - \frac{\hbar^2}{2\sqrt{h}}\frac{\delta^2}{\delta\phi^2} + \mathcal{U}[h_a,\phi,\phi_{,a}]\right]\Psi[h_a,\phi] = 0\,. \tag{4.9}$$

We then implement the Born–Oppenheimer type of approximation as in [75] by using the following WKB-type ansatz for the wave functional $\Psi[h_a,\phi]$

$$\Psi[h_a,\phi] = \exp\left(\frac{\mathrm{i}}{\hbar}S[h_a,\phi]\right), \tag{4.10}$$

where we expand the functional $S[h_a,\phi]$ in terms of the parameter M in the following way:

$$S = M^1 S_0 + M^0 S_1 + M^{-1} S_2 + \dots \tag{4.11}$$

We plug the ansatz (4.10) with the above expansion into equation (4.9) and *formally* treat the appearing functional derivatives as ordinary partial derivatives. In the resulting equation we collect all the terms containing a factor of a certain power of M and set the collection of these terms equal to zero for each power of M individually.

4.3 The gravitational background

We find that the highest order of M that appears in the expansion is M^2 and the differential equation at this order is given by:

$$\frac{1}{2\sqrt{h}}\left(\frac{\delta S_0[h_a,\phi]}{\delta\phi}\right)^2 = 0\,. \tag{4.12}$$

This simply implies that S_0 is independent of the matter field ϕ, $S_0[h_a,\phi] \equiv S_0[h_a]$, and thus S_0 represents purely the gravitational background.

The next order, which is M^1, then leads to the subsequent equation

$$\frac{1}{2}G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_0}{\delta h_b} + V[h_a] = 0\,, \tag{4.13}$$

which is the Hamilton–Jacobi equation of the gravitational background. This equation is equivalent to the Einstein equations [50]. Hence, we have recovered general relativity from canonical quantum gravity with the Wheeler–DeWitt equation.

4.4 The functional Schrödinger equation

At the subsequent order M^0, we obtain an equation where additionally S_1 appears:

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_1}{\delta h_b}-\frac{\mathrm{i}\hbar}{2}G_{ab}\frac{\delta^2 S_0}{\delta h_a\delta h_b}+\frac{1}{2\sqrt{h}}\left(\frac{\delta S_1}{\delta\phi}\right)^2-\frac{\mathrm{i}\hbar}{2\sqrt{h}}\frac{\delta^2 S_1}{\delta\phi^2}+\mathcal{U}[h_a,\phi,\phi_{,a}]=0\,. \tag{4.14}$$

It is possible to rewrite this equation with respect to a wave functional

$$\psi^{(0)}[h_a,\phi]:=\gamma[h_a]\,\mathrm{e}^{\mathrm{i}S_1[h_a,\phi]/\hbar}\,, \tag{4.15}$$

where we have introduced a prefactor $\gamma[h_a]$, onto which we can impose a condition, such that it disappears in the following, cf. [75]. The resulting equation takes the form

$$\mathcal{H}_\mathrm{m}\,\psi^{(0)}=\mathrm{i}\hbar\,G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta\psi^{(0)}}{\delta h_b} \tag{4.16}$$

and it allows us to define a *WKB time* τ as

$$\frac{\delta}{\delta\tau}:=G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta}{\delta h_b}\,, \tag{4.17}$$

such that we can rewrite (4.16) as a functional Schrödinger equation:

$$\mathrm{i}\hbar\frac{\delta\psi^{(0)}}{\delta\tau}=\mathcal{H}_\mathrm{m}\,\psi^{(0)}\,. \tag{4.18}$$

Hence, we see that from the Wheeler–DeWitt equation, one can also recover quantum field theory on a curved spacetime in the form of a functional Schrödinger equation for matter fields acting on a background that is described by the Hamilton–Jacobi equation (4.13).

4.5 The quantum-gravitationally corrected functional Schrödinger equation

Up to now we have recovered known physics, but the next order M^{-1} takes us into the quantum gravity regime and we can derive quantum-gravitational correction terms to the functional Schrödinger equation (4.18) obtained above. The respective equation from the expansion of (3.25) thus incorporates S_2 and takes the form

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_2}{\delta h_b}+\frac{1}{2}G_{ab}\frac{\delta S_1}{\delta h_a}\frac{\delta S_1}{\delta h_b}-\frac{\mathrm{i}\hbar}{2}G_{ab}\frac{\delta^2 S_1}{\delta h_a\delta h_b}+\frac{1}{\sqrt{h}}\frac{\delta S_1}{\delta\phi}\frac{\delta S_2}{\delta\phi}-\frac{\mathrm{i}\hbar}{2\sqrt{h}}\frac{\delta^2 S_2}{\delta\phi^2}=0\,. \tag{4.19}$$

We split the function S_2 into a part $\varsigma[h_a]$ that only depends on the background and a part $\eta[h_a, \phi]$ that additionally depends on the matter field

$$S_2[h_a, \phi] = \varsigma[h_a] + \eta[h_a, \phi] \,. \tag{4.20}$$

Since we can impose a condition on the background part $\varsigma[h_a]$ as for the WKB prefactor $\gamma[h_a]$ in order to remove it from the subsequent equations (cf. [75] or section 5.2.4 for details), we can define a corrected wave functional $\psi^{(1)}$ using $\psi^{(0)}$ from (4.15) and additionally only $\eta[h_a, \phi]$ in the following way

$$\psi^{(1)}[h_a, \phi] := \psi^{(0)}[h_a, \phi]\, \mathrm{e}^{\mathrm{i} M^{-1}\, \eta[h_a, \phi]/\hbar} \,. \tag{4.21}$$

From (4.19), we can deduce that this corrected wave functional obeys the equation

$$\mathrm{i}\hbar\, \frac{\delta \psi^{(1)}}{\delta \tau} = \mathcal{H}_\mathrm{m}\, \psi^{(1)} + \frac{\hbar^2}{2M\, \psi^{(0)}} \left(\frac{2}{\gamma}\, G_{ab}\, \frac{\delta \psi^{(0)}}{\delta h_a} \frac{\delta \gamma}{\delta h_b} - G_{ab}\, \frac{\delta^2 \psi^{(0)}}{\delta h_a \delta h_b} \right) \psi^{(1)} \,, \tag{4.22}$$

which already has the form of a Schrödinger equation with a quantum-gravitational correction term that is suppressed by M. We can rewrite the correction term in terms of the matter Hamiltonian $\mathcal{H}_\mathrm{m}$ using a decomposition of $\delta\psi^{(0)}/\delta h_a$ into a normal and tangential part with respect to the hypersurfaces given by $S_0 = \text{const.}$, see [75] and section 5.2.4 for the detailed derivation.

In the end, we arrive at the following form for the quantum-gravitationally corrected functional Schrödinger equation:

$$\mathrm{i}\hbar\, \frac{\delta \psi^{(1)}}{\delta \tau} = \mathcal{H}_\mathrm{m}\, \psi^{(1)} + \frac{4\pi G}{\sqrt{h}\,{}^{(3)}\!R} \left[\mathcal{H}_\mathrm{m}^2 + \mathrm{i}\hbar \left(\frac{\delta \mathcal{H}_\mathrm{m}}{\delta \tau} - \frac{1}{\sqrt{h}\,{}^{(3)}\!R}\, \frac{\delta(\sqrt{h}\,{}^{(3)}\!R)}{\delta \tau}\, \mathcal{H}_\mathrm{m} \right) \right] \psi^{(1)} \,. \tag{4.23}$$

5

Quantum-gravitational effects on scalar-field perturbations during inflation

In this and the following two chapters, we will discuss how canonical quantum gravity based on the Wheeler–DeWitt equation influences cosmological perturbations during inflation and whether such a quantum-gravitational effect can be seen in the anisotropies of the Cosmic Microwave Background (CMB).

In the present chapter we shall focus on the simplest model in which such an investigation can be performed, which is a homogeneous and isotropic universe that contains a scalar field, which acts as an inflaton and thus drives the exponential expansion of the universe, but also contains fluctuations in space that we will regard in this simplified model as the seed for structure formation.

We will quantize this model canonically and perform a semiclassical Born–Oppenheimer type of approximation to the resulting Wheeler–DeWitt equation as presented in the previous chapter in order to obtain the power spectrum of the scalar field perturbations and quantum-gravitational corrections to it. We shall then connect this result with observations and discuss whether such an effect of quantum gravity can be seen in the CMB anisotropies.

Even though this model is largely simplified, it will serve as a initial step to estimate the qualitative features and the magnitude of quantum-gravitational effects. In the subsequent chapter, we will then extend this model in order to be in accordance with the standard methods of cosmological perturbation theory.

The present chapter is based on the two articles [71] and [22] as well as the essay [70], where the first article is partly based on the diploma thesis of the author of this dissertation [78], which also partially serves as a source of this chapter.

5.1 Derivation of the Wheeler–DeWitt equation

We consider a flat Friedmann–Lemaître universe, for which the Robertson–Walker line element is given by

$$ds^2 = -N^2(t)\,dt^2 + a^2(t)\,d\mathbf{x}^2\,. \tag{5.1}$$

We work with cosmic time t, which is why we can set the lapse function $N(t)$ equal to one. Furthermore, we introduce a scalar field ϕ that acts as an inflaton, which means that it is approximately constant in space and time and leads to an accelerated expansion of the universe. The choice of the potential $\mathcal{V}(\phi)$ does not influence our result as long as a slow-roll condition of the form

$$\dot{\phi}^2 \ll |\mathcal{V}(\phi)| \tag{5.2}$$

holds at the classical level, but for definiteness we choose

$$\mathcal{V}(\phi) = \frac{1}{2}\,m^2\phi^2\,, \tag{5.3}$$

which is the simplest potential in chaotic inflation [85].

As we have derived in the chapter 3, we can immediately write down the Wheeler–DeWitt equation for the minisuperspace background. We set $\hbar = 1$ and define a rescaled Planck mass

$$m_{\mathrm{P}} := \sqrt{\frac{3\pi}{2G}} \approx 2.65 \times 10^{19}\,\mathrm{GeV}\,. \tag{5.4}$$

Note that we still use the capital letter M_{P} for the reduced Planck mass $M_{\mathrm{P}} = (8\pi G)^{-1/2}$. We introduce the quantity α defined with respect to a reference scale factor a_0, which we will not explicitly write out in the following, as

$$\alpha := \ln\left(\frac{a}{a_0}\right) \tag{5.5}$$

and after furthermore redefining the scalar field

$$\phi \to \frac{1}{\sqrt{2\pi}}\,\phi\,, \tag{5.6}$$

we get the following the Wheeler–DeWitt equation for the background

$$\frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[\frac{1}{m_{\mathrm{P}}^2}\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial\phi^2} + \mathrm{e}^{6\alpha}m^2\phi^2\right]\Psi_0(\alpha,\phi) = 0\,. \tag{5.7}$$

In order to implement the slow-roll approximation (5.2), we assume that the kinetic term of the scalar field is small compared to the potential term

$$\frac{\partial^2 \Psi_0}{\partial \phi^2} \ll e^{6\alpha} m^2 \phi^2 \Psi_0 \tag{5.8}$$

and consequently neglect the ϕ-kinetic term in (5.7).

Furthermore, due to the slow-roll approximation, we can replace the scalar field ϕ by the quasistatic inflationary Hubble parameter H, which in the classical limit obeys $|\dot{H}| \ll H^2$. From the Friedmann equation in the slow-roll limit, we get

$$H^2 \simeq \frac{8\pi G}{3} \mathcal{V}(\phi) \overset{(5.4;5.6)}{=} \frac{1}{m_P^2} m^2 \phi^2 \tag{5.9}$$

and can therefore set

$$m\phi \approx m_P H \approx \text{const.} \tag{5.10}$$

The fact that ϕ is a quantum variable, whereas H is a classical variable does not represent a problem, because in the Born–Oppenheimer approximation that follows, equation (5.7) will describe the classical background, on which the quantum fluctuations of the scalar field propagate. We will therefore omit the variable ϕ in the following. Finally, our Wheeler–DeWitt equation for the minisuperspace background takes the simple form

$$\mathcal{H}_0 \Psi_0(\alpha) = \frac{1}{2} e^{-3\alpha} \left[\frac{1}{m_P^2} \frac{\partial^2}{\partial \alpha^2} + e^{6\alpha} m_P^2 H^2 \right] \Psi_0(\alpha) = 0 \,. \tag{5.11}$$

Effectively, we are dealing now with a pure de Sitter background, since we regard H as being constant in the subsequent calculations.

We now want to add perturbations to the inflaton field ϕ, which in our simplified picture then become the source of structure in the universe. We therefore add fluctuations of an inhomogeneous inflaton field on top of its homogeneous part in the following way

$$\phi \to \phi(t) + \delta\phi(\mathbf{x}, t) \,. \tag{5.12}$$

We then decompose these fluctuations into Fourier modes $f_k(t)$ with wave vector $\mathbf{k}$, $k := |\mathbf{k}|$,

$$\delta\phi(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} f_{\mathbf{k}}(t)\, e^{i\mathbf{k}\cdot\mathbf{x}} \,. \tag{5.13}$$

From the action of a scalar field in a FLRW metric, we get

$$S = \frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \int dt\; a^3 \left(-\left|\dot{f}_{\mathbf{k}}\right|^2 + \frac{k^2}{a^2} \left|f_{\mathbf{k}}\right|^2 + m^2 \left|f_{\mathbf{k}}\right|^2 \right) \tag{5.14}$$

and we can therefore write out the Hamiltonian density for each fluctuation mode

$$\mathcal{H}_k = \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[-\frac{\partial^2}{\partial f_k^2} + \left(k^2\,\mathrm{e}^{4\alpha} + m^2\,\mathrm{e}^{6\alpha}\right) f_k^2\right]. \qquad (5.15)$$

For simplicity, we now assume that the universe is compact and that therefore the spectrum for **k** is discrete. This, of course, implies that there is a maximum scale $\mathcal{L}$ and we have to take this into consideration later when we want to discuss observable quantities. We can thus replace the integral by a sum using the relation [90]

$$\int \mathrm{d}^3\mathbf{k}\left\{\cdots\right\} \quad \rightarrow \quad \left(\frac{2\pi}{\mathcal{L}}\right)^3 \sum_{k\neq 0}^{\infty}\left\{\cdots\right\} \qquad (5.16)$$

and we obtain

$$\delta\phi(\mathbf{x},t) = \frac{1}{\mathcal{L}^3}\sum_k f_k(t)\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \qquad (5.17)$$

Consequently, our Wheeler–DeWitt equation for the full wave function $\Psi\left(\alpha, \{f_k\}_{k=1}^{\infty}\right)$ including the fluctuation modes reads [55]

$$\left[\mathcal{H}_0 + \frac{1}{\mathcal{L}^3}\sum_{k=1}^{\infty}\mathcal{H}_k\right]\Psi\left(\alpha, \{f_k\}_{k=1}^{\infty}\right) = 0\,. \qquad (5.18)$$

We can eliminate the length scale $\mathcal{L}$ appearing here by making the following replacements:

$$k \rightarrow \frac{k}{k_0} = \frac{k}{2\pi}\,\mathcal{L}\,, \quad \mathrm{e}^{\alpha} \rightarrow \mathrm{e}^{\alpha}\,\mathcal{L}\,. \qquad (5.19)$$

This means that we have to regard k as a dimensionless variable, while the quantity e^{α} has to be understood as having the dimension of a length when we want to replace it with α.

Since we deal with small fluctuations, we can neglect their self-interaction, and can therefore make the following product ansatz for the full wave function:

$$\Psi\left(\alpha, \{f_k\}_{k=1}^{\infty}\right) = \Psi_0(\alpha)\prod_{k=1}^{\infty}\widetilde{\Psi}_k(\alpha, f_k)\,.$$

If we define the wave functions

$$\Psi_k(\alpha, f_k) := \Psi_0(\alpha)\,\widetilde{\Psi}_k(\alpha, f_k)\,, \qquad (5.20)$$

we immediately see that each wave function $\Psi_k(\alpha, f_k)$ obeys the following Wheeler–DeWitt equation [55, 65]

$$\frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[\frac{1}{m_\mathrm{P}^2}\frac{\partial^2}{\partial\alpha^2} + \mathrm{e}^{6\alpha}\,m_\mathrm{P}^2 H^2 - \frac{\partial^2}{\partial f_k^2} + W_k(\alpha)\,f_k^2\right]\Psi_k(\alpha, f_k) = 0\,, \qquad (5.21)$$

where we have used the definition

$$W_k(\alpha) := k^2\, e^{4\alpha} + m^2\, e^{6\alpha}\,. \tag{5.22}$$

Equation (5.21) is our master equation that we use as the starting point for the subsequent semiclassical Born–Oppenheimer type of approximation.

5.2 Semiclassical approximation

We now want to perform a semiclassical approximation to equation (5.21) that is of a Born–Oppenheimer type in the sense that we treat the background represented by the logarithmic scale factor α and the quasi-constant inflaton field ϕ as the "heavy" variable, while the scalar field perturbations are treated as the "light" variable.

We take advantage of the fact that the appearing factors of the rescaled Planck mass m_{P} act as a weighting factor that on the one hand, suppresses the derivative of the background variable α, such that its influence on the dynamics of the scalar field perturbations is negligible, and on the other hand, enhances the minisuperspace potential given by the inflationary Hubble parameter.

As presented in chapter 4 as well as partly in [78], we follow the procedure taken in [75] and start with the WKB-like ansatz

$$\Psi_k(\alpha, f_k) = e^{\mathrm{i}S(\alpha, f_k)}\,. \tag{5.23}$$

Note that we do not include a prefactor at this point as in the usual WKB approximation; such a prefactor will however appear later.

The Born–Oppenheimer approximation is implemented by expanding $S(\alpha, f_k)$ in terms of powers of m_{P}^2

$$S(\alpha, f_k) = m_{\mathrm{P}}^2\, S_0 + m_{\mathrm{P}}^0\, S_1 + m_{\mathrm{P}}^{-2}\, S_2 + \dots \tag{5.24}$$

and inserting the ansatz (5.23) with this expansion into (5.21). The resulting equation has the form

$$\sum_{n=0}^{\infty} A_n\, m_{\mathrm{P}}^{4-2n} = 0 \tag{5.25}$$

and we set the coefficients A_n equal to zero individually.

5.2.1 $\mathcal{O}(m_{\mathrm{P}}^4)$: The background condition

At the highest order, $n = 0$, which corresponds to the terms including a factor of m_{P}^4, we obtain the subsequent equation

$$\frac{\partial}{\partial f_k} S_0(\alpha, f_k) = 0\,. \tag{5.26}$$

It immediately implies that S_0 is independent of the perturbation variable f_k and only depends on the background variable α, such that we can set $S_0(\alpha, f_k) \equiv S_0(\alpha)$. Therefore the background of our universe – i.e. the “heavy” part of our system – is entirely described by the wave function $\mathrm{e}^{\mathrm{i}\, m_{\mathrm{P}}^2 S_0}$ and we can thus write

$$\Psi_0(\alpha) = \mathrm{e}^{\mathrm{i}\, m_{\mathrm{P}}^2 S_0(\alpha)}\,. \tag{5.27}$$

5.2.2 $\mathcal{O}(m_{\mathrm{P}}^2)$: The Hamilton–Jacobi equation for the background

The next order, i.e. terms with a factor of m_{P}^2, leads to the following differential equation

$$\left(\frac{\partial S_0}{\partial \alpha}\right)^2 - \mathrm{e}^{6\alpha} H^2 = 0\,, \tag{5.28}$$

which is the Hamilton–Jacobi equation for the classical minisuperspace background. It is solved by

$$S_0(\alpha) = \pm \frac{1}{3}\, \mathrm{e}^{3\alpha} H\,, \tag{5.29}$$

such that the background wave function $\Psi_0(\alpha)$ takes the form

$$\Psi_0(\alpha) = \exp\left(\pm \frac{\mathrm{i}}{3}\, m_{\mathrm{P}}^2\, \mathrm{e}^{3\alpha} H\right)\,. \tag{5.30}$$

5.2.3 $\mathcal{O}(m_{\mathrm{P}}^0)$: The Schrödinger equation for the perturbation modes

At the next order m_{P}^0, we obtain the following expression, which for the first time contains terms with $S_1(\alpha, f_k)$ and $W_k(\alpha)$ that depend on f_k:

$$-2\,\frac{\partial S_0}{\partial \alpha}\frac{\partial S_1}{\partial \alpha} + \mathrm{i}\,\frac{\partial^2 S_0}{\partial \alpha^2} + \left(\frac{\partial S_1}{\partial f_k}\right)^2 - \mathrm{i}\,\frac{\partial^2 S_1}{\partial f_k^2} + W_k(\alpha) f_k^2 = 0\,. \tag{5.31}$$

We shall now show how we can derive a Schrödinger equation from this expression. In order to do so, we introduce a wave function $\psi_k^{(0)}(\alpha, f_k)$ that is defined as

$$\psi_k^{(0)}(\alpha, f_k) := \gamma(\alpha)\, \mathrm{e}^{\mathrm{i} S_1(\alpha, f_k)}\,, \tag{5.32}$$

where we have introduced a function $\gamma(\alpha)$ that represents the inverse of the WKB prefactor we have omitted in our ansatz (5.23). We demand that γ fulfill the following condition

$$\frac{\partial}{\partial\alpha}\left(\frac{1}{2\gamma^2}\frac{\partial S_0}{\partial\alpha}\right)=0 \quad\Leftrightarrow\quad \frac{1}{\gamma}\frac{\partial S_0}{\partial\alpha}\frac{\partial\gamma}{\partial\alpha}-\frac{1}{2}\frac{\partial^2 S_0}{\partial\alpha^2}=0\,. \tag{5.33}$$

We now apply the Hamiltonian density $\mathcal{H}_k$ of the perturbation modes to the wave function $\psi_k^{(0)}(\alpha,f_k)$ and manipulate it using the above expressions

$$\begin{aligned}
\mathcal{H}_k\psi_k^{(0)} &= \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[-\frac{\partial^2}{\partial f_k^2}+W_k(\alpha)\,f_k^2\right]\psi_k^{(0)}\\
&\overset{(5.32)}{=} \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[-\frac{\partial^2}{\partial f_k^2}+W_k(\alpha)\,f_k^2\right]\gamma(\alpha)\,\mathrm{e}^{\mathrm{i}S_1(\alpha,f_k)}\\
&= \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[\left(\frac{\partial S_1}{\partial f_k}\right)^2-\mathrm{i}\,\frac{\partial^2 S_1}{\partial f_k^2}+W_k(\alpha)\,f_k^2\right]\psi_k^{(0)}\\
&\overset{(5.31)}{=} \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[-\mathrm{i}\,\frac{\partial^2 S_0}{\partial\alpha^2}+2\,\frac{\partial S_0}{\partial\alpha}\,\frac{\partial S_1}{\partial\alpha}\right]\psi_k^{(0)}\\
&\overset{(5.33)}{=} \mathrm{e}^{-3\alpha}\left[-\frac{\mathrm{i}}{\gamma}\,\frac{\partial S_0}{\partial\alpha}\,\frac{\partial\gamma}{\partial\alpha}+\frac{\partial S_0}{\partial\alpha}\,\frac{\partial S_1}{\partial\alpha}\right]\psi_k^{(0)}\\
&= -\mathrm{i}\,\mathrm{e}^{-3\alpha}\,\frac{\partial S_0}{\partial\alpha}\,\frac{\partial}{\partial\alpha}\left[\gamma(\alpha)\,\mathrm{e}^{\mathrm{i}S_1(\alpha,f_k)}\right]=-\mathrm{i}\,\mathrm{e}^{-3\alpha}\,\frac{\partial S_0}{\partial\alpha}\,\frac{\partial\psi_k^{(0)}}{\partial\alpha}\,.
\end{aligned} \tag{5.34}$$

We can now define the WKB time

$$\frac{\partial}{\partial t}:=-\,\mathrm{e}^{-3\alpha}\,\frac{\partial S_0}{\partial\alpha}\,\frac{\partial}{\partial\alpha}\,, \tag{5.35}$$

which allows us to rewrite (5.34) as a Schrödinger equation for each mode $\psi_k^{(0)}$:

$$\boxed{\mathrm{i}\,\frac{\partial}{\partial t}\,\psi_k^{(0)}=\mathcal{H}_k\psi_k^{(0)}\,.} \tag{5.36}$$

We will use this equation to derive the power spectrum of the scalar field perturbations later. It is also possible to derive this Schrödinger equation using a less systematic semiclassical approximation, see e.g. [55] and [65]. For our purposes, the scheme presented here is favorable, because it enables us to continue in a rather straightforward way and calculate quantum-gravitational corrections to this Schrödinger equation, which we shall do in the following.

5.2.4 $\mathcal{O}(m_{\rm P}^{-2})$: Quantum-gravitational corrections to the Schrödinger equation

At the order $m_{\rm P}^{-2}$, we leave the regime of quantum theory on a classical background and enter the regime where quantum gravity comes into play. The expression we obtain at this order looks as follows and contains S_2 for the first time:

$$-\frac{\partial S_0}{\partial \alpha}\frac{\partial S_2}{\partial \alpha}-\frac{1}{2}\left(\frac{\partial S_1}{\partial \alpha}\right)^2+\frac{\rm i}{2}\frac{\partial^2 S_1}{\partial \alpha^2}+\frac{\partial S_1}{\partial f_k}\frac{\partial S_2}{\partial f_k}-\frac{\rm i}{2}\frac{\partial^2 S_2}{\partial f_k^2}=0\,. \tag{5.37}$$

In order to obtain correction terms to the Schrödinger equation (5.36), we follow [75, 78] and decompose S_2 into a part ς that depends only on the logarithmic scale factor α and a part η, which also includes the scalar field perturbations f_k:

$$S_2(\alpha, f_k)\equiv \varsigma(\alpha)+\eta(\alpha, f_k)\,. \tag{5.38}$$

In order to calculate the derivatives appearing in (5.37), we write out S_1 in terms of γ and $\psi_k^{(0)}$ using the definition (5.32)

$$S_1(\alpha, f_k)=-{\rm i}\ln\left(\frac{1}{\gamma(\alpha)}\,\psi_k^{(0)}(\alpha, f_k)\right)\,. \tag{5.39}$$

The respective derivatives of S_1 then read as follows:

$$\frac{\partial}{\partial \alpha}S_1(\alpha, f_k)={\rm i}\left(\frac{1}{\gamma}\frac{\partial \gamma}{\partial \alpha}-\frac{1}{\psi_k^{(0)}}\frac{\partial \psi_k^{(0)}}{\partial \alpha}\right),$$
$$\frac{\partial^2}{\partial \alpha^2}S_1(\alpha, f_k)={\rm i}\left[-\frac{1}{\gamma^2}\left(\frac{\partial \gamma}{\partial \alpha}\right)^2+\frac{1}{\gamma}\frac{\partial^2 \gamma}{\partial \alpha^2}+\frac{1}{(\psi_k^{(0)})^2}\left(\frac{\partial \psi_k^{(0)}}{\partial \alpha}\right)^2-\frac{1}{\psi_k^{(0)}}\frac{\partial^2 \psi_k^{(0)}}{\partial \alpha^2}\right],$$
$$\frac{\partial}{\partial f_k}S_1(\alpha, f_k)=-\frac{\rm i}{\psi_k^{(0)}}\frac{\partial \psi_k^{(0)}}{\partial f_k}\,.$$

Plugging these expressions together with the derivatives of S_2 into equation (5.37), we obtain

$$\begin{aligned}&-\frac{\partial S_0}{\partial \alpha}\left(\frac{\partial \varsigma}{\partial \alpha}+\frac{\partial \eta}{\partial \alpha}\right)+\frac{1}{2}\left(\frac{1}{\gamma}\frac{\partial \gamma}{\partial \alpha}-\frac{1}{\psi_k^{(0)}}\frac{\partial \psi_k^{(0)}}{\partial \alpha}\right)^2\\&-\frac{1}{2}\left[-\frac{1}{\gamma^2}\left(\frac{\partial \gamma}{\partial \alpha}\right)^2+\frac{1}{\gamma}\frac{\partial^2 \gamma}{\partial \alpha^2}+\frac{1}{(\psi_k^{(0)})^2}\left(\frac{\partial \psi_k^{(0)}}{\partial \alpha}\right)^2-\frac{1}{\psi_k^{(0)}}\frac{\partial^2 \psi_\alpha^{(0)}}{\partial \alpha^2}\right]\\&-\frac{\rm i}{\psi_k^{(0)}}\frac{\partial \psi_k^{(0)}}{\partial f_k}\frac{\partial \eta}{\partial f_k}-\frac{\rm i}{2}\frac{\partial^2 \eta}{\partial f_k^2}=0\,.\end{aligned} \tag{5.40}$$

After performing a couple of straightforward manipulations of this expression, we collect all the terms containing $\psi_k^{(0)}$ and put them on one side of the equation:

$$\begin{aligned}&-\frac{\partial S_0}{\partial\alpha}\frac{\partial\varsigma}{\partial\alpha}-\frac{\partial S_0}{\partial\alpha}\frac{\partial\eta}{\partial\alpha}+\frac{1}{\gamma^2}\left(\frac{\partial\gamma}{\partial\alpha}\right)^2-\frac{1}{2\gamma}\frac{\partial^2\gamma}{\partial\alpha^2}\\&=\frac{1}{\gamma\psi_k^{(0)}}\frac{\partial\psi_k^{(0)}}{\partial\alpha}\frac{\partial\gamma}{\partial\alpha}-\frac{1}{2\psi_k^{(0)}}\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}+\frac{\mathrm{i}}{\psi_k^{(0)}}\frac{\partial\psi_k^{(0)}}{\partial f_k}\frac{\partial\eta}{\partial f_k}+\frac{\mathrm{i}}{2}\frac{\partial^2\eta}{\partial f_k^2}\,.\end{aligned}\tag{5.41}$$

At this point, we demand that $\varsigma(\alpha)$ be the standard second-order WKB correction of the background part of the wave function $\Psi(\alpha, f_k)$, which translates into the following condition on $\varsigma(\alpha)$:

$$-\frac{\partial S_0}{\partial\alpha}\frac{\partial\varsigma}{\partial\alpha}+\frac{1}{\gamma^2}\left(\frac{\partial\gamma}{\partial\alpha}\right)^2-\frac{1}{2\gamma}\frac{\partial^2\gamma}{\partial\alpha^2}=0\,.\tag{5.42}$$

Using the WKB time (5.35) this condition reads

$$\frac{\partial\varsigma}{\partial t}=\mathrm{e}^{-3\alpha}\left[\frac{1}{\gamma^2}\left(\frac{\partial\gamma}{\partial\alpha}\right)^2-\frac{1}{2\gamma}\frac{\partial^2\gamma}{\partial\alpha^2}\right].\tag{5.43}$$

Due to this condition, equation (5.41) simplifies significantly, in particular, all terms including ς are eliminated and we obtain

$$-\frac{\partial S_0}{\partial\alpha}\frac{\partial\eta}{\partial\alpha}=\frac{1}{\gamma\psi_k^{(0)}}\frac{\partial\psi_k^{(0)}}{\partial\alpha}\frac{\partial\gamma}{\partial\alpha}-\frac{1}{2\psi_k^{(0)}}\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}+\frac{\mathrm{i}}{\psi_k^{(0)}}\frac{\partial\psi_k^{(0)}}{\partial f_k}\frac{\partial\eta}{\partial f_k}+\frac{\mathrm{i}}{2}\frac{\partial^2\eta}{\partial f_k^2}\,.\tag{5.44}$$

We can again use the WKB time (5.35) to rewrite this equation:

$$\frac{\partial\eta}{\partial t}=\frac{\mathrm{e}^{-3\alpha}}{\psi_k^{(0)}}\left(\frac{1}{\gamma}\frac{\partial\psi_k^{(0)}}{\partial\alpha}\frac{\partial\gamma}{\partial\alpha}-\frac{1}{2}\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}+\mathrm{i}\frac{\partial\psi_k^{(0)}}{\partial f_k}\frac{\partial\eta}{\partial f_k}+\frac{\mathrm{i}\psi_k^{(0)}}{2}\frac{\partial^2\eta}{\partial f_k^2}\right).\tag{5.45}$$

Now we define the wave functions

$$\psi_k^{(1)}(\alpha,f_k):=\psi_k^{(0)}(\alpha,f_k)\,\mathrm{e}^{\mathrm{i}m_{\mathrm{P}}^{-2}\eta(\alpha,f_k)}\,,\tag{5.46}$$

which – as we shall see – are the functions that obey the quantum-gravitationally corrected Schrödinger equation we are about to derive.

Analogously to the calculation at order m_{P}^0, we let the Hamiltonian density of the perturbation modes $\mathcal{H}_k$ act on $\psi_k^{(1)}(\alpha, f_k)$, which leads to

$$\begin{aligned}&\mathcal{H}_k\psi_k^{(1)}(\alpha,f_k)\\&=\frac{1}{2}\mathrm{e}^{-3\alpha}\left[-\frac{\partial^2}{\partial f_k^2}+W_k f_k^2\right]\psi_k^{(1)}\\&=\frac{1}{2}\mathrm{e}^{-3\alpha}\left[-\frac{\partial^2}{\partial f_k^2}\left(\psi_k^{(0)}\,e^{\mathrm{i}m_{\mathrm{P}}^{-2}\eta}\right)+W_k f_k^2\,\psi_k^{(0)}\,\mathrm{e}^{\mathrm{i}m_{\mathrm{P}}^{-2}\eta}\right]\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[-\frac{\partial^2\psi_k^{(0)}}{\partial f_k^2}\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta} - 2\,\frac{\partial\psi_k^{(0)}}{\partial f_k}\,\frac{\partial\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}}{\partial f_k} - \psi_k^{(0)}\,\frac{\partial^2\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}}{\partial f_k^2} + W_k f_k^2\,\psi_k^{(0)}\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\right]\\
&= \frac{\mathrm{e}^{-3\alpha}}{2}\left[-\frac{\partial^2\psi_k^{(0)}}{\partial f_k^2} + W_k f_k^2\,\psi_k^{(0)}\right]\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta} - \frac{\mathrm{e}^{-3\alpha}}{2}\left[2\,\frac{\partial\psi_k^{(0)}}{\partial f_k}\,\frac{\partial\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}}{\partial f_k} + \psi_k^{(0)}\,\frac{\partial^2\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}}{\partial f_k^2}\right]\\
&= \left[\mathcal{H}_k\psi_k^{(0)}\right]\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta} - \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[\frac{2\,\mathrm{i}}{m_\mathrm{P}^2}\,\frac{\partial\psi_k^{(0)}}{\partial f_k}\,\frac{\partial\eta}{\partial f_k}\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\right.\\
&\qquad\qquad\left. + \frac{\mathrm{i}\,\psi_k^{(0)}}{m_\mathrm{P}^2}\,\frac{\partial^2\eta}{\partial f_k^2}\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta} - \underbrace{\frac{\psi_k^{(0)}}{m_\mathrm{P}^4}\left(\frac{\partial\eta}{\partial f_k}\right)^2}_{\mathcal{O}(m_\mathrm{P}^{-4})}\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\right]\\
&\overset{(5.36)}{=} \left[\mathrm{i}\,\frac{\partial}{\partial t}\,\psi_k^{(0)}\right]\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta} - \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2}\left[\mathrm{i}\,\frac{\partial\psi_k^{(0)}}{\partial f_k}\,\frac{\partial\eta}{\partial f_k} + \frac{\mathrm{i}\,\psi_k^{(0)}}{2}\,\frac{\partial^2\eta}{\partial f_k^2}\right]\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\,. \qquad (5.47)
\end{aligned}
$$

In the second-to-last line we neglected the term proportional to m_P^{-4}, since we truncate our approximation at the order m_P^{-2}.

Now we want to take a look at the other side of the Schrödinger equation that contains the time derivative of $\psi_k^{(1)}(\alpha, f_k)$:

$$
\begin{aligned}
&\mathrm{i}\,\frac{\partial}{\partial t}\,\psi_k^{(1)}\\
&= \mathrm{i}\,\frac{\partial}{\partial t}\left[\psi_k^{(0)}\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\right]\\
&= \left[\mathrm{i}\,\frac{\partial}{\partial t}\,\psi_k^{(0)}\right]\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta} - \frac{\psi_k^{(0)}}{m_\mathrm{P}^2}\,\frac{\partial\eta}{\partial t}\,\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\\
&\overset{(5.45)}{=} \left[\mathrm{i}\,\frac{\partial}{\partial t}\,\psi_k^{(0)}\right]\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta} - \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2}\left(\frac{1}{\gamma}\,\frac{\partial\psi_k^{(0)}}{\partial\alpha}\,\frac{\partial\gamma}{\partial\alpha} - \frac{1}{2}\,\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}\right.\\
&\qquad\qquad\left. + \mathrm{i}\,\frac{\partial\psi_k^{(0)}}{\partial f_k}\,\frac{\partial\eta}{\partial f_k} + \frac{\mathrm{i}\,\psi_k^{(0)}}{2}\,\frac{\partial^2\eta}{\partial f_k^2}\right)\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\\
&\overset{(5.47)}{=} \mathcal{H}_k\psi_k^{(1)} + \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2}\left(\mathrm{i}\,\frac{\partial\psi_k^{(0)}}{\partial f_k}\,\frac{\partial\eta}{\partial f_k} + \frac{\mathrm{i}\,\psi_k^{(0)}}{2}\,\frac{\partial^2\eta}{\partial f_k^2}\right)\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\\
&\qquad - \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2}\left(\frac{1}{\gamma}\,\frac{\partial\psi_k^{(0)}}{\partial\alpha}\,\frac{\partial\gamma}{\partial\alpha} - \frac{1}{2}\,\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2} + \mathrm{i}\,\frac{\partial\psi_k^{(0)}}{\partial f_k}\,\frac{\partial\eta}{\partial f_k} + \frac{\mathrm{i}\,\psi_k^{(0)}}{2}\,\frac{\partial^2\eta}{\partial f_k^2}\right)\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\\
&= \mathcal{H}_k\psi_k^{(1)} + \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2}\left(\frac{1}{\gamma}\,\frac{\partial\psi_k^{(0)}}{\partial\alpha}\,\frac{\partial\gamma}{\partial\alpha} - \frac{1}{2}\,\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}\right)\mathrm{e}^{\mathrm{i}m_\mathrm{P}^{-2}\eta}\\
&= \mathcal{H}_k\psi_k^{(1)} + \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2\,\psi_k^{(0)}}\left(-\frac{1}{\gamma}\,\frac{\partial\psi_k^{(0)}}{\partial\alpha}\,\frac{\partial\gamma}{\partial\alpha} + \frac{1}{2}\,\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}\right)\psi_k^{(1)}\,. \qquad (5.48)
\end{aligned}
$$

Already at this point, we can regard the final expression in (5.48) as the corrected Schrödinger equation of order m_P^{-2} for the wave function $\psi_k^{(1)}$:

$$\mathrm{i}\frac{\partial}{\partial t}\psi_k^{(1)} = \mathcal{H}_k\psi_k^{(1)} + \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2\psi_k^{(0)}}\left(-\frac{1}{\gamma}\frac{\partial\psi_k^{(0)}}{\partial\alpha}\frac{\partial\gamma}{\partial\alpha} + \frac{1}{2}\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}\right)\psi_k^{(1)}\,. \tag{5.49}$$

However, in the following, we want to express the two terms appearing in this expression in terms of the Hamiltonian of the perturbation modes. For notational simplicity we define

$$V(\alpha) := \mathrm{e}^{6\alpha}H^2\,, \tag{5.50}$$

such that the Hamilton–Jacobi equation (5.28) of the background reads

$$\left(\frac{\partial S_0}{\partial\alpha}\right)^2 = V(\alpha) > 0\,. \tag{5.51}$$

Therefore we have

$$\frac{\partial S_0}{\partial\alpha} = \sqrt{V(\alpha)} \tag{5.52}$$

and we can rewrite the derivative of $\psi_k^{(0)}$ with respect to α as follows

$$\begin{aligned}\frac{\partial\psi_k^{(0)}}{\partial\alpha} &= -\,\mathrm{i}\,\mathrm{e}^{3\alpha}\left(\frac{\partial S_0}{\partial\alpha}\right)^{-1}\mathrm{i}\,\mathrm{e}^{-3\alpha}\frac{\partial S_0}{\partial\alpha}\frac{\partial\psi_k^{(0)}}{\partial\alpha}\\ &\overset{(5.35)}{=} \mathrm{i}\,\mathrm{e}^{3\alpha}\left(\frac{\partial S_0}{\partial\alpha}\right)^{-1}\mathrm{i}\frac{\partial}{\partial t}\psi_k^{(0)}\\ &\overset{(5.36)}{=} \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{\sqrt{V}}\mathcal{H}_k\psi_k^{(0)}\,.\end{aligned} \tag{5.53}$$

For the second derivative we then obtain

$$\begin{aligned}\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2} &= \frac{3\,\mathrm{i}\,\mathrm{e}^{3\alpha}}{\sqrt{V}}\mathcal{H}_k\psi_k^{(0)} - \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{2V^{3/2}}\frac{\partial V}{\partial\alpha}\mathcal{H}_k\psi_k^{(0)} + \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{\sqrt{V}}\frac{\partial\mathcal{H}_k}{\partial\alpha}\psi_k^{(0)} + \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{\sqrt{V}}\mathcal{H}_k\frac{\partial\psi_k^{(0)}}{\partial\alpha}\\ &\overset{(5.53)}{=} \frac{3\,\mathrm{i}\,\mathrm{e}^{3\alpha}}{\sqrt{V}}\mathcal{H}_k\psi_k^{(0)} - \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{2V^{3/2}}\frac{\partial V}{\partial\alpha}\mathcal{H}_k\psi_k^{(0)} + \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{\sqrt{V}}\frac{\partial\mathcal{H}_k}{\partial\alpha}\psi_k^{(0)} - \frac{\mathrm{e}^{6\alpha}}{V}\left(\mathcal{H}_k\right)^2\psi_k^{(0)}\,.\end{aligned} \tag{5.54}$$

We also need to use the condition we imposed on γ in (5.33)

$$0 = \frac{1}{\gamma}\frac{\partial S_0}{\partial\alpha}\frac{\partial\gamma}{\partial\alpha} - \frac{1}{2}\frac{\partial^2 S_0}{\partial\alpha^2} = \frac{\sqrt{V}}{\gamma}\frac{\partial\gamma}{\partial\alpha} - \frac{1}{2}\frac{\partial}{\partial\alpha}\left(\sqrt{V}\right) = \frac{\sqrt{V}}{\gamma}\frac{\partial\gamma}{\partial\alpha} - \frac{1}{4\sqrt{V}}\frac{\partial V}{\partial\alpha}\,, \tag{5.55}$$

such that we end up with

$$\frac{1}{\gamma}\frac{\partial\gamma}{\partial\alpha} = \frac{1}{4V}\frac{\partial V}{\partial\alpha}\,. \tag{5.56}$$

Inserting the expressions (5.53) and (5.54) into the quantum-gravitationally corrected Schrödinger equation (5.48) then leads to

$$
\begin{aligned}
\mathrm{i}\frac{\partial}{\partial t}\psi_k^{(1)} &= \mathcal{H}_k\psi_k^{(1)} + \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2\psi_k^{(0)}}\left(-\frac{1}{\gamma}\frac{\partial\psi_k^{(0)}}{\partial\alpha}\frac{\partial\gamma}{\partial\alpha} + \frac{1}{2}\frac{\partial^2\psi_k^{(0)}}{\partial\alpha^2}\right)\psi_k^{(1)} \qquad (5.57)\\
&= \mathcal{H}_k\psi_k^{(1)} + \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2\psi_k^{(0)}}\left(-\frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{\sqrt{V}}\frac{1}{\gamma}\frac{\partial\gamma}{\partial\alpha}\mathcal{H}_k\psi_k^{(0)} + \frac{3\,\mathrm{i}\,\mathrm{e}^{3\alpha}}{2\sqrt{V}}\mathcal{H}_k\psi_k^{(0)}\right.\\
&\qquad\left. - \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{4V^{3/2}}\frac{\partial V}{\partial\alpha}\mathcal{H}_k\psi_k^{(0)} + \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{2\sqrt{V}}\frac{\partial\mathcal{H}_k}{\partial\alpha}\psi_k^{(0)} - \frac{\mathrm{e}^{6\alpha}}{2V}\left(\mathcal{H}_k\right)^2\psi_k^{(0)}\right)\psi_k^{(1)}\\
&= \mathcal{H}_k\psi_k^{(1)} + \frac{\mathrm{e}^{-3\alpha}}{m_\mathrm{P}^2\psi_k^{(0)}}\left(\frac{3\,\mathrm{i}\,\mathrm{e}^{3\alpha}}{2\sqrt{V}}\mathcal{H}_k\psi_k^{(0)} - \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{2V^{3/2}}\frac{\partial V}{\partial\alpha}\mathcal{H}_k\psi_k^{(0)}\right.\\
&\qquad\left. + \frac{\mathrm{i}\,\mathrm{e}^{3\alpha}}{2\sqrt{V}}\frac{\partial\mathcal{H}_k}{\partial\alpha}\psi_k^{(0)} - \frac{\mathrm{e}^{6\alpha}}{2V}\left(\mathcal{H}_k\right)^2\psi_k^{(0)}\right)\psi_k^{(1)}\\
&= \mathcal{H}_k\psi_k^{(1)} + \frac{1}{2m_\mathrm{P}^2\psi_k^{(0)}}\left(\mathrm{i}\,\mathrm{e}^{-3\alpha}\sqrt{V}\frac{\partial}{\partial\alpha}\left(\frac{\mathrm{e}^{3\alpha}\mathcal{H}_k}{V}\right)\psi_k^{(0)} - \frac{\mathrm{e}^{3\alpha}}{V}\left(\mathcal{H}_k\right)^2\psi_k^{(0)}\right)\psi_k^{(1)}\\
&= \mathcal{H}_k\psi_k^{(1)} + \frac{1}{2m_\mathrm{P}^2\psi_k^{(0)}}\left(-\mathrm{i}\frac{\partial}{\partial t}\left(\frac{\mathrm{e}^{3\alpha}\mathcal{H}_k}{V}\right)\psi_k^{(0)} - \frac{\mathrm{e}^{3\alpha}}{V}\left(\mathcal{H}_k\right)^2\psi_k^{(0)}\right)\psi_k^{(1)}
\end{aligned}
$$

and finally we obtain:

$$
\boxed{\mathrm{i}\frac{\partial}{\partial t}\psi_k^{(1)} = \mathcal{H}_k\psi_k^{(1)} - \frac{\psi_k^{(1)}}{2m_\mathrm{P}^2\psi_k^{(0)}}\left(\frac{\mathrm{e}^{3\alpha}}{V}\left(\mathcal{H}_k\right)^2\psi_k^{(0)} + \mathrm{i}\frac{\partial}{\partial t}\left(\frac{\mathrm{e}^{3\alpha}\mathcal{H}_k}{V}\right)\psi_k^{(0)}\right).} \qquad (5.58)
$$

In principle, we could follow [75] further and eliminate the appearing wave functions $\psi_k^{(0)}$ using the following argument. We can decompose derivatives of $\psi_k^{(1)}$ with respect to $q \in \{\alpha, f_k\}$ and neglect all the terms of order m_P^{-2}, since these terms would translate to terms of order m_P^{-4} in the correction term of the Schrödinger equation (5.58). Doing this for the first and higher derivatives iteratively leads to [78]

$$
\begin{aligned}
\frac{\partial\psi_k^{(1)}(q)}{\partial q} &= \frac{\partial}{\partial q}\left(\psi_k^{(0)}(q)\,e^{\mathrm{i}m_\mathrm{P}^{-2}\eta(q)}\right) = \frac{1}{\psi_k^{(0)}}\frac{\partial\psi_k^{(0)}}{\partial q}\psi_k^{(1)} + \underbrace{\cancel{\frac{\mathrm{i}}{m_\mathrm{P}^2}\frac{\partial\eta}{\partial q}}}_{\mathcal{O}(m_\mathrm{P}^{-2})}\psi_k^{(1)}\\
\frac{\partial^2\psi_k^{(1)}(q)}{\partial q^2} &= \frac{1}{\psi_k^{(0)}}\frac{\partial^2\psi_k^{(0)}}{\partial q^2}\psi_k^{(1)} + \underbrace{\cancel{\frac{1}{m_\mathrm{P}^2}\frac{2\mathrm{i}}{\psi_k^{(0)}}\frac{\partial\psi_k^{(0)}}{\partial q}\frac{\partial\eta}{\partial f_k}}}_{\mathcal{O}(m_\mathrm{P}^{-2})}\psi_k^{(1)} + \mathcal{O}(m_\mathrm{P}^{-4})\\
\ldots \quad \Rightarrow \quad \frac{\partial^n\psi_k^{(1)}(q)}{\partial q^n} &= \frac{1}{\psi_k^{(0)}}\frac{\partial^n\psi_k^{(0)}}{\partial q^n}\psi_k^{(1)} + \mathcal{O}(m_\mathrm{P}^{-2})\,. \qquad (5.59)
\end{aligned}
$$

Hence, we end up with the subsequent corrected Schrödinger equation, which corresponds to the final result in [75]:

$$\mathrm{i}\,\frac{\partial}{\partial t}\,\psi_k^{(1)} = \mathcal{H}_k\psi_k^{(1)} - \frac{1}{2\,m_{\mathrm{P}}^2}\left(\frac{\mathrm{e}^{3\alpha}}{V}\,(\mathcal{H}_k)^2\,\psi_k^{(1)} + \mathrm{i}\,\frac{\partial}{\partial t}\left(\frac{\mathrm{e}^{3\alpha}\,\mathcal{H}_k}{V}\right)\psi_k^{(1)}\right). \tag{5.60}$$

However, finding a solution for $\psi_k^{(1)}$ using (5.60) is much harder than for the previous equation (5.58), because in the latter equation the correction term translates into an additional factor that does not contain derivates of $\psi_k^{(1)}$ unlike in (5.60). Therefore we will skip the last step and use (5.58) as our quantum-gravitationally corrected Schrödinger equation in the following.

The second term in the correction term of (5.58), which is proportional to the imaginary unit i, induces a small violation of unitarity. A consistent definition of unitarity in the full theory of Wheeler–DeWitt quantum gravity has not been found, since the Hilbert space structure of the theory is unknown. However, the states ψ_k corresponding to f_k obey an approximate Schrödinger equation and therefore we can define unitarity here with respect to the standard $\mathcal{L}^2$-inner product for the modes f_k. [71]

We can interpret this term by noting that the Wheeler–DeWitt equation corresponds to a Klein–Gordon type of equation, instead of a Schrödinger type. If one expands the conserved Klein–Gordon-type current in powers of m_{P}^{-2}, one obtains an exact conservation of the Schrödinger current at order m_{P}^{0}, but going to the order m_{P}^{-2} then leads to a violation of this conservation due to a term corresponding to the unitarity-violating term in (5.58). [22]

It can be shown that this unitarity-violating term is subdominant compared to the term containing the square of the Hamiltonian in most situations [75]. Note in this context that this term would have to be multiplied by $\hbar$ when reinstating the natural constants. Using this argument we will neglect the unitarity-violating term from now on. An alternative method would be to use an appropriate redefinition of the wave function in order to restore unitarity at order m_{P}^{-2}. This procedure was shown for the general case in [20] and also applied in the context of the quantum-mechanical Klein–Gordon equation in an external gravitational field in [80].

Neglecting the unitarity-violating term, we arrive at the following corrected Schrödinger equation

$$\mathrm{i}\,\frac{\partial}{\partial t}\,\psi_k^{(1)} = \mathcal{H}_k\psi_k^{(1)} - \frac{\mathrm{e}^{3\alpha}}{2\,m_{\mathrm{P}}^2\,V\,\psi_k^{(0)}}\left[(\mathcal{H}_k)^2\,\psi_k^{(0)}\right]\psi_k^{(1)}. \tag{5.61}$$

5.3 Derivation of the power spectrum

In order to derive the power spectrum of the scalar-field perturbations, we have to solve the uncorrected Schrödinger equation (5.36). Since perturbations during inflation are assumed to remain in the ground state, we make the Gaussian ansatz

$$\psi_k^{(0)}(t,f_k) = \mathcal{N}_k^{(0)}(t)\,\mathrm{e}^{-\frac{1}{2}\Omega_k^{(0)}(t)f_k^2}\,. \tag{5.62}$$

Here, we use the WKB time defined via (5.35), which allows us also to set $\alpha = Ht$. Inserting this ansatz into (5.36), we find the following coupled set of nonlinear differential equations for $\mathcal{N}_k^{(0)}$ and $\Omega_k^{(0)}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{N}_k^{(0)}(t) = -\frac{\mathrm{i}}{2}\,\mathrm{e}^{-3Ht}\mathcal{N}_k^{(0)}(t)\,\Omega_k^{(0)}(t)\,, \tag{5.63}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Omega_k^{(0)}(t) = \mathrm{i}\,\mathrm{e}^{-3Ht}\left[-\left(\Omega_k^{(0)}(t)\right)^2 + k^2\mathrm{e}^{4Ht} + m^2\mathrm{e}^{6Ht}\right]. \tag{5.64}$$

We can immediately find a solution for $\mathcal{N}_n^{(0)}(t)$ by considering the usual normalization condition of the wave function $\psi_k^{(0)}$, which reads

$$\left|\psi_k^{(0)}\right|^2 = \left\langle\psi_k^{(0)}\middle|\psi_k^{(0)}\right\rangle = \int_{-\infty}^{\infty}\psi_k^{*(0)}\psi_k^{(0)}\,\mathrm{d}f_k \overset{!}{=} 1\,. \tag{5.65}$$

Therefore we have

$$\begin{aligned}\left|\psi_k^{(0)}\right|^2 &= \left|\mathcal{N}_k^{(0)}(t)\right|^2\int_{-\infty}^{\infty}\mathrm{e}^{-\frac{1}{2}\left[\Omega_k^{*(0)}(t)+\Omega_k^{(0)}(t)\right]f_k^2}\,\mathrm{d}f_k \\ &= \left|\mathcal{N}_k^{(0)}(t)\right|^2\int_{-\infty}^{\infty}\mathrm{e}^{-\mathfrak{Re}\,\Omega_k^{(0)}(\eta)f_k^2}\,\mathrm{d}f_k = \left|\mathcal{N}_k^{(0)}(t)\right|^2\frac{\sqrt{\pi}}{\sqrt{\mathfrak{Re}\,\Omega_k^{(0)}(t)}} \overset{!}{=} 1\,,\end{aligned} \tag{5.66}$$

which leads to

$$\left|\mathcal{N}_k^{(0)}(t)\right|^2 = \sqrt{\frac{\mathfrak{Re}\,\Omega_k^{(0)}(t)}{\pi}}\,. \tag{5.67}$$

If we insert this solution into (5.63), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathfrak{Re}\,\Omega_k^{(0)}(t) = 2\,\mathfrak{Re}\,\Omega_k^{(0)}(t)\,\mathfrak{Im}\,\Omega_k^{(0)}(t)\,. \tag{5.68}$$

We get the same expression when taking the real part of equation (5.64).

In order to solve equation (5.64), which corresponds to a Riccati equation that is widely applied in physics [100], we introduce the dimensionless variable

$$\xi(t) := \frac{k}{Ha(t)}\,, \tag{5.69}$$

such that we can write for the time derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} = -\,\xi H\,\frac{\mathrm{d}}{\mathrm{d}\xi}\,. \tag{5.70}$$

Equation (5.64) therefore takes the form

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\Omega_k^{(0)}(\xi) = \mathrm{i}\left[\frac{H^2\xi^2}{k^3}\left(\Omega_k^{(0)}(\xi)\right)^2 - \frac{k^3}{H^2\xi^2}\left(1-\frac{m^2}{H^2\xi^2}\right)\right]. \tag{5.71}$$

In [71], the last term proportional to m^2/H^2 is neglected using the argument that the mass m of the inflaton has to be much smaller than the Hubble parameter in chaotic inflation [85], which is used here as our model. Furthermore, it is assumed that for large wave numbers $k \to \infty$, the state (5.62) approaches the free Minkowski vacuum. This translates to the condition that for $\xi \to \infty$, the function $\Omega_k^{(0)}$ approaches

$$\Omega_k^{(0)}(\xi) \approx \frac{k^3}{H^2\xi^2} = k\,a^2\,, \tag{5.72}$$

which in the massive case corresponds to the Bunch–Davies vacuum [33]. Neglecting the mass term and choosing the above-mentioned boundary condition then immediately leads to the solution

$$\Omega_k^{(0)} = \frac{k^3}{H^2}\frac{1}{\xi(\xi-\mathrm{i})}\,. \tag{5.73}$$

In [22], equation (5.71) including the mass term is solved. Following these calculations, we define the dimensionless quantity

$$\mu := \frac{m}{H}\,. \tag{5.74}$$

The resulting solution can then be written in terms of an unknown parameter U_1 as well as the Bessel functions J_ν and Y_ν at order

$$\nu := \frac{1}{2}\sqrt{9-4\mu^2}\,. \tag{5.75}$$

As we have mentioned before, in scenarios of inflation, and especially in chaotic inflation, one assumes that $m < H$. Because of this, ν is a real parameter. The explicit form of the solution thus reads

$$\begin{aligned}\Omega_k^{(0)}(\xi) = \frac{k^3}{H^2}\,\frac{1}{\xi^2\left(U_1 Y_\nu(\xi)+J_\nu(\xi)\right)}\Bigg\{ -\,\mathrm{i}\,U_1 Y_{\nu+1}(\xi) + \frac{\mathrm{i}}{2\xi}\Big[&(3U_1+2U_1\nu)\,Y_\nu(\xi) \\ &-\,2\xi\,J_{\nu+1}(\xi)+(3+2\nu)\,J_\nu(\xi)\Big]\Bigg\}.\end{aligned} \tag{5.76}$$

Solving the Klein–Gordon equation for a massive scalar field in de Sitter space leads to a similar solution, cf. e.g. [53], or equation (51) of [16], or section 8.3.2 in [92].

Considering now the massless case $\mu = 0$, the coefficient ν of the Bessel functions takes the value $\nu = 3/2$ and using standard relations between the Bessel functions of half-odd order [1], we find the following general solution

$$\begin{aligned}\Omega_k^{(0)}(\xi) &= \frac{k^3}{H^2}\,\frac{\mathrm{i}\left(U_1\cos\xi - \sin\xi\right)}{\xi\left[(U_1+\xi)\cos\xi + (U_1\xi - 1)\sin\xi\right]}\\ &= \frac{k^3}{H^2}\,\frac{\mathrm{i}\left(J_{1/2} - U_1 J_{-1/2}\right)}{\xi\left[(1-\xi U_1)J_{1/2} - (U_1+\xi)J_{-1/2}\right]}\,. \end{aligned} \tag{5.77}$$

From this equation we obtain the previous solution (5.73), by setting $U_1 = -\mathrm{i}$. In order to investigate the general solution (5.77) further, we write U_1 in terms of two variables ζ and β as follows

$$U_1 = \zeta \mathrm{e}^{\mathrm{i}\beta}\,. \tag{5.78}$$

This allows us to re-express (5.77) in the following form

$$\Omega_k^{(0)}(\xi) = \frac{k^3}{H^2}\,\frac{\mathrm{i}}{\xi}\,\frac{AB^*}{|B|^2}\,, \tag{5.79}$$

where A and B are given by

$$A := \rho + \mathrm{i}\sigma\,, \quad B := \gamma + \mathrm{i}\delta \tag{5.80}$$

and we used the definitions

$$\begin{aligned}\rho &:= \zeta\left[\cos(\beta+\xi) + \cos(\beta-\xi)\right] - 2\sin\xi = 2\left(\zeta\cos\beta\cos\xi - \sin\xi\right),\\ \sigma &:= \zeta\left[\sin(\beta+\xi) + \sin(\beta-\xi)\right] = 2\zeta\sin\beta\cos\xi\,,\\ \gamma &:= \zeta\left\{\left[\cos(\beta+\xi)+\cos(\beta-\xi)\right] + \xi\left[\sin(\beta+\xi) - \sin(\beta-\xi)\right]\right\} + 2(\xi\cos\xi - \sin\xi)\\ &= 2\zeta\left[\cos\beta\,(\cos\xi + \xi\sin\xi) - (\sin\xi - \xi\cos\xi)\right],\\ \delta &:= \zeta\left\{\left[\sin(\beta+\xi)+\sin(\beta-\xi)\right] - \xi\left[\cos(\beta+\xi) - \cos(\beta-\xi)\right]\right\}\\ &= 2\zeta\sin\beta\,(\cos\xi + \sin\xi)\,. \end{aligned} \tag{5.81}$$

We now want to derive an expression for the power spectrum of the scalar-field perturbations. We follow the description in [89], and start with the energy density ρ of the scalar field $\phi(\mathbf{x}, t)$, which is classically given by

$$\rho \simeq \frac{1}{2}\dot{\phi}^2\,. \tag{5.82}$$

The energy density of small perturbations of $\phi(\mathbf{x}, t)$ can therefore be written up to the first order as

$$\delta\rho(\mathbf{x}, t) = \rho(\mathbf{x}, t) - \overline{\rho}(t) = \frac{1}{2}\left(\dot{\phi}(t) + \delta\dot{\phi}(\mathbf{x}, t)\right)^2 - \frac{1}{2}\dot{\phi}^2(t)$$
$$= \dot{\phi}(t)\,\delta\dot{\phi}(\mathbf{x}, t) + \frac{1}{2}\,\delta\dot{\phi}^2(\mathbf{x}, t) \simeq \dot{\phi}(t)\,\delta\dot{\phi}(\mathbf{x}, t)\,. \quad (5.83)$$

Going into momentum space, we can write

$$\delta\rho_k(t) = \dot{\phi}(t)\,\dot{\sigma}_k(t)\,, \quad (5.84)$$

where $\sigma_k(t)$ is the classical quantity related to the quantum-mechanical quantity f_k. Establishing this relation is in principle a highly non-trivial task that requires the consideration of the decoherence of the quantum fluctuations of the scalar field ϕ, see e.g. [72, 73, 74]. Here we take a simplified approach like in [89] and define the $\sigma_k(t)$ by taking the expectation value of f_k for a Gaussian state, which leads to

$$\sigma_k^2(t) := \left\langle \psi_k | f_k^2 | \psi_k \right\rangle = \sqrt{\frac{\Re\mathfrak{e}\,\Omega_k}{\pi}} \int_{-\infty}^{\infty} f_k^2\, \mathrm{e}^{-\frac{1}{2}\left[\Omega_k^*(t)+\Omega_k(t)\right] f_k^2}\, \mathrm{d}f_k = \frac{1}{2\,\Re\mathfrak{e}\,\Omega_k(t)}\,. \quad (5.85)$$

Assuming that the average energy density during inflation is dominated by the quasi-constant inflaton potential $\mathcal{V}(\phi) \simeq \mathcal{V}_0 = \text{const.}$, we can write the density contrast of the scalar-field perturbations as

$$\delta_k(t) = \frac{\dot{\phi}(t)\,\dot{\sigma}_k(t)}{\mathcal{V}_0}\,. \quad (5.86)$$

We have to evaluate $\delta_k(t)$ for each mode individually at the time t_{enter} when it reenters the Hubble radius during the radiation-dominated phase. At this point the relation

$$\frac{k}{Ha} = 2\pi \quad (5.87)$$

holds. Following [89], we can derive a relation between the density contrast of a mode at the time t_{exit} when it leaves the Hubble radius during the inflationary phase and the time t_{enter} when it reenters it. For modes outside of the Hubble radius, we have the following relation of pressure P and energy density ρ

$$\delta_k(t) \propto 1 + \frac{P(t)}{\rho(t)}\,. \quad (5.88)$$

This can be translated to the subsequent relation

$$\frac{\delta_n(t_{\text{exit}})}{1 + \frac{P(t_{\text{exit}})}{\rho(t_{\text{exit}})}} = \frac{\delta_n(t_{\text{enter}})}{1 + \frac{P(t_{\text{enter}})}{\rho(t_{\text{enter}})}}\,. \quad (5.89)$$

During inflation, we have

$$1+\frac{P(t)}{\rho(t)}\simeq\frac{\dot{\phi}^2}{\mathcal{V}_0}\,. \tag{5.90}$$

In the radiation-dominated phase, we find by using the relation (2.30)

$$1+\frac{P(t)}{\rho(t)}=1+w=\frac{4}{3}\,. \tag{5.91}$$

Putting all this together therefore leads to the following relation

$$\delta_k(t_{\text{enter}})=\frac{4}{3}\,\frac{\mathcal{V}_0}{\dot{\phi}^2}\,\delta_k(t_{\text{exit}}) \tag{5.92}$$

and finally using equation (5.86), we end up with

$$\delta_k(t_{\text{enter}})=\frac{4}{3}\,\frac{\dot{\sigma}_k(t)}{\dot{\phi}(t)}\bigg|_{t=t_{\text{exit}}}\,. \tag{5.93}$$

In the case considered here, we can write σ_k at the level of approximation of $\psi_k^{(0)}$ as

$$\sigma_k^{(0)}(t)=\frac{1}{\sqrt{2}}\left[\mathfrak{Re}\,\Omega_k^{(0)}(t)\right]^{-\frac{1}{2}}. \tag{5.94}$$

The derivative of σ_k appearing in (5.93) reads in terms of ξ

$$\left|\dot{\sigma}_k^{(0)}(t)\right|=\left|\frac{H\xi}{\sqrt{2}}\,\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\mathfrak{Re}\,\Omega_k^{(0)}(\xi)\right]^{-\frac{1}{2}}\right|. \tag{5.95}$$

Inserting our general solution for the massless case (5.79) then leads to

$$\begin{aligned}\left|\dot{\sigma}_k^{(0)}(t)\right|_{t_{\text{exit}}}&=\frac{H^2}{2\sqrt{2}\,k^{\frac{3}{2}}}\left|\xi\left[\frac{(\rho\delta-\gamma\sigma)}{\xi\,(\gamma^2+\delta^2)}\right]^{-\frac{3}{2}}\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\frac{(\rho\delta-\gamma\sigma)}{\xi\,(\gamma^2+\delta^2)}\right]\right|_{\xi=2\pi}\\&=\frac{2\sqrt{2}\pi^2H^2}{k^{\frac{3}{2}}}\left|\frac{\sqrt{\zeta}\,(\zeta+2\pi\cos\beta)}{\sqrt{\sin\beta}\sqrt{\zeta^2+4\pi\cos\beta+4\pi^2}}\right|.\end{aligned} \tag{5.96}$$

In the last step, we have used the condition $\xi(t_{\text{exit}})=k/(Ha)=2\pi$ at Hubble-scale crossing. We define the function $f(\zeta,\beta)$ as

$$f(\zeta,\beta):=\frac{\sqrt{\zeta}\,(\zeta+2\pi\cos\beta)}{\sqrt{\sin\beta}\sqrt{\zeta^2+4\pi\cos\beta+4\pi^2}}\,, \tag{5.97}$$

and plot this function in Figure 5.1. We see that $f(\zeta,\beta)$ shows no relative minima or maxima, and therefore one cannot determine specific preferred values of ζ and

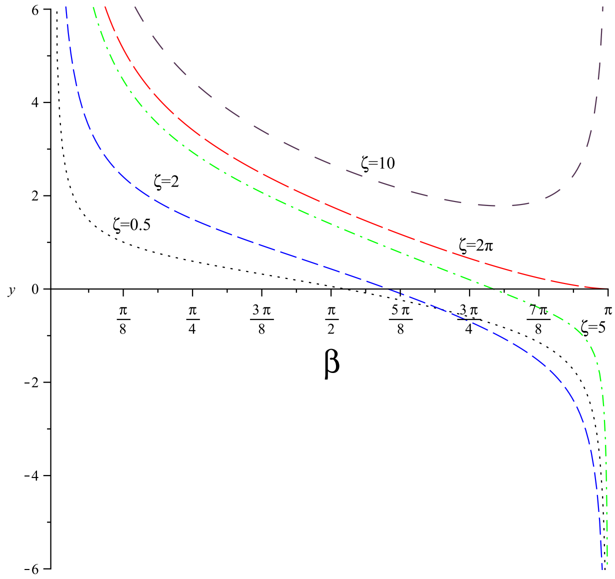

Figure 5.1: The function $f(\zeta,\beta)$ defined in equation (5.97) plotted for the values $\zeta \in \{0.5, 2, 5, 2\pi, 10\}$, from [22].

β from a mathematical point of view. For the case considered in [71], i.e. setting $\zeta = 1$, $\beta = \frac{3}{2}\pi$, $\mu = 0$, we get

$$\left|\dot{\sigma}_k^{(0)}(t)\right|_{t=t_{\text{exit}}} = \frac{\xi^2}{\sqrt{2(\xi^2+1)}} \frac{H^2}{k^{\frac{3}{2}}}\bigg|_{t=t_{\text{exit}}} = \frac{2\sqrt{2}\,\pi^2}{\sqrt{4\pi^2+1}} \frac{H^2}{k^{\frac{3}{2}}} . \tag{5.98}$$

The power spectrum of the scalar-field perturbations can be directly inferred from (5.93) and is given by

$$\mathcal{P}_\phi^{(0)}(k) := \frac{k^3}{2\pi^2} \left|\delta_k(t_{\text{enter}})\right|^2 . \tag{5.99}$$

Inserting our solution (5.96), we get

$$\mathcal{P}_\phi^{(0)}(k) = \frac{64}{9}\pi^2 \left|f(\zeta,\beta)\right|^2 \frac{H^4}{\left|\dot{\phi}(t)\right|^2_{t_{\text{exit}}}} . \tag{5.100}$$

Using the definition of the slow-roll parameter ϵ

$$\epsilon := -\frac{\dot{H}}{H^2} = \frac{4\pi G \left|\dot{\phi}(t)\right|^2_{t_{\text{exit}}}}{H^2} , \tag{5.101}$$

and defining

$$M_{\text{P}} := \sqrt{\frac{1}{8\pi G}} \tag{5.102}$$

we can rewrite (5.100) as

$$\mathcal{P}_{\phi}^{(0)}(k) = \frac{32}{9}\,\pi^2 \left|f(\zeta,\beta)\right|^2 \frac{H^2}{M_{\mathrm{P}}^2\,\epsilon}\,. \tag{5.103}$$

5.4 Quantum-gravitational corrections

We now want to calculate quantum-gravitational corrections to the power spectrum (5.103) by using the corrected Schrödinger equation (5.61) without the unitarity-violating term. For convenience, we write out this equation together with the definition of the relevant quantities once again:

$$\mathrm{i}\frac{\partial}{\partial t}\psi_k^{(1)} = \mathcal{H}_k\psi_k^{(1)} - \frac{\mathrm{e}^{3\alpha}}{2m_{\mathrm{P}}^2\psi_k^{(0)}}\left[\frac{(\mathcal{H}_k)^2}{V}\psi_k^{(0)}\right]\psi_k^{(1)}\,, \tag{5.104}$$

where

$$V := \mathrm{e}^{6\alpha}H^2,\quad \mathcal{H}_k := \frac{1}{2}\,\mathrm{e}^{-3\alpha}\left[-\frac{\partial^2}{\partial f_k^2} + W_k f_k^2\right] \text{ and } W_k := k^2\mathrm{e}^{4\alpha} + m^2\mathrm{e}^{6\alpha}\,. \tag{5.105}$$

Following [71] and [22], we assume that the corrected wave functions $\psi_k^{(1)}$ can be described by the following Gaussian ansatz, where we included corrections of $\mathcal{N}_k$ and Ω_k, which are suppressed by the factor m_{P}^{-2}

$$\psi_k^{(1)} = \left(\mathcal{N}_k^{(0)}(t) + m_{\mathrm{P}}^{-2}\,\mathcal{N}_k^{(1)}(t)\right)\exp\left[-\frac{1}{2}\left(\Omega_k^{(0)}(t) + m_{\mathrm{P}}^{-2}\,\Omega_k^{(1)}(t)\right)f_k^2(t)\right]. \tag{5.106}$$

After plugging this ansatz into the corrected Schrödinger equation (5.104), we obtain the following differential equation

$$\begin{aligned}
&\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\log\left(N_k^{(0)} + \frac{N_k^{(1)}}{m_{\mathrm{P}}^2}\right) - \frac{\mathrm{i}}{2}\left(\dot{\Omega}_k^{(0)} + \frac{\dot{\Omega}_k^{(1)}}{m_{\mathrm{P}}^2}\right)f_k^2 \\
&= \frac{1}{2}\,\mathrm{e}^{-3\alpha}\Bigg\{\Omega_k^{(0)} + \frac{1}{m_{\mathrm{P}}^2}\left[\Omega_k^{(1)} - \frac{3}{4V}\left(\left(\Omega_k^{(0)}\right)^2 - \frac{2}{3}W_k\right)\right] \\
&\quad + \left[W_k - \left(\Omega_k^{(0)} + \frac{\Omega_k^{(1)}}{m_{\mathrm{P}}^2}\right)^2 - \frac{3\Omega_k^{(0)}(W_k - (\Omega_k^{(0)})^2)}{2V m_{\mathrm{P}}^2}\right]f_k^2 + \mathcal{O}\left(f_k^4\right)\Bigg\}.
\end{aligned} \tag{5.107}$$

This equation can be written in the form

$$\sum_{l=0}^{2} A_{2l}\, f_k^{2l} = 0 \tag{5.108}$$

where the A_{2l} are time-dependent coefficients. The differential equation we have to solve in order to find a solution for $\Omega_k^{(1)}$ is obtained by setting the coefficient A_2 to zero and it reads

$$\dot{\Omega}_k^{(1)}(t) = -2\mathrm{i}\,\mathrm{e}^{-3\alpha}\,\Omega_k^{(0)}(t)\left(\Omega_k^{(1)}(t) - \frac{3}{4V(t)}\left[\left(\Omega_k^{(0)}(t)\right)^2 - W_k(t)\right]\right). \quad (5.109)$$

Converting this equation to the variable ξ, where $\mathrm{e}^{-\alpha} = H\xi/k$, and inserting our solution (5.79), this equation takes the following form

$$\frac{\mathrm{d}\Omega_k^{(1)}}{\mathrm{d}\xi} = \frac{2\mathrm{i}\xi}{(\gamma^2+\delta^2)}(C+\mathrm{i}D)\left[\Omega_k^{(1)} + \frac{3}{4}\left(\mu^2 + \xi^2 - \xi^4\frac{(C^2 - D^2 + 2\mathrm{i}CD)}{(\gamma^2+\delta^2)^2}\right)\right], \quad (5.110)$$

where we have used the definitions

$$C := \rho\delta - \gamma\sigma\,, \qquad D := \rho\gamma + \sigma\delta\,. \quad (5.111)$$

Now we have to choose a suitable boundary condition for $\Omega_k^{(1)}$. The choice made in [71] and [22] is to demand that the quantum-gravitational corrections vanish for late times, which is consistent and in agreement with observations. The relation between ξ and t is given by

$$\xi(t) = \mathrm{e}^{-Ht}\,\frac{k}{H}\,. \quad (5.112)$$

Therefore our chosen boundary condition $\Omega_k^{(1)}(t) \to 0$ for $t \to \infty$ translates to

$$\Omega_k^{(1)}(\xi) \to 0 \quad \text{for} \quad \xi \to 0\,. \quad (5.113)$$

We start as in [71] by considering the choice that the initial state of the perturbations is the Bunch–Davies vacuum. This means that we set $\zeta = 1$ and $\beta = \frac{3}{2}\pi$. Furthermore, we neglect the mass term μ. Consequently, equation (5.110) simplifies considerably to

$$\frac{\mathrm{d}\Omega_k^{(1)}}{\mathrm{d}\xi} = \frac{2\mathrm{i}\xi}{(\xi-\mathrm{i})}\,\Omega_k^{(1)} + \frac{3}{2}\,\xi^3\,\frac{(2\xi-\mathrm{i})}{(\xi-\mathrm{i})^3}\,. \quad (5.114)$$

With the boundary condition (5.113), we then find the exact solution given in [22]

$$\Omega_k^{(1)}(\xi) = -\frac{3}{8}\,\mathrm{e}^{2\mathrm{i}\xi}\,\frac{[1+\mathrm{Ei}(1,2)\mathrm{e}^2]}{(1+\mathrm{i}\xi)^2} + \Omega_k^{(1,\mathrm{part})}(\xi)\,, \quad (5.115)$$

where

$$\Omega_k^{(1,\mathrm{part})}(\xi) = \frac{3}{8}\,\frac{\left[-5 + 6(1+\mathrm{i}\xi) + 4\mathrm{Ei}\left(1, 2(1+\mathrm{i}\xi)\right)\mathrm{e}^{2(1+i\xi)} - 4\xi^2(1+\mathrm{i}\xi)\right]}{(1+\mathrm{i}\xi)^2}\,. \quad (5.116)$$

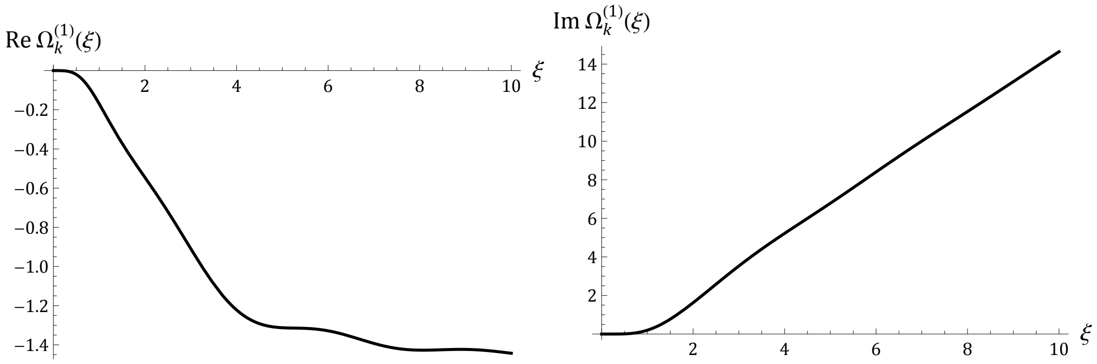

Figure 5.2: Plot of the real and imaginary part of $\Omega_k^{(1)}(\xi)$ using $E_1(z)$.

$\mathrm{Ei}(a,z)$ denotes the exponential integral that is defined by

$$\mathrm{Ei}(a,z) := \int_1^\infty \frac{\mathrm{e}^{-tz}}{t^a}\mathrm{d}t\,. \tag{5.117}$$

In the present case the function appearing in (5.115) and (5.116) is $\mathrm{Ei}(1,z)$, which can be rewritten as (cf. [1], Sec. 5.1.)

$$\mathrm{Ei}(1,z) \equiv \Gamma(0,z) \equiv E_1(z)\,. \tag{5.118}$$

We present a plot of the real and imaginary part of $\Omega_k^{(1)}(\xi)$ in figure 5.2.

A further investigation of the differential equation (5.114) can be found in the appendix. We can also use our solution (5.115) for the special case $\zeta = 1$, $\beta = \frac{3}{2}\pi$, $\mu = 0$ in order to look for a solution of the general equation (5.110) when considering a linearization around $\zeta = 1$ and $\beta = \frac{3}{2}\pi$, while keeping $\mu = 0$. This means to look for solutions of the form

$$\Omega_k^{(1)}(\xi) = \widetilde{\Omega}_k^{(1)}(\xi) + (\zeta - 1)\,\Omega_k^{(1)a}(\xi) + \left(\beta - \frac{3}{2}\pi\right)\Omega_k^{(1)b}(\xi)\,, \tag{5.119}$$

where $\widetilde{\Omega}_k^{(1)}$ denotes the special solution (5.115). Inserting (5.119) into (5.110) leads to the following set of equations:

$$\begin{aligned}\frac{\mathrm{d}\Omega_k^{(1)a}}{\mathrm{d}\xi} &= -\frac{2\mathrm{i}\xi}{(\mathrm{i}-\xi)}\,\Omega_k^{(1)a} - \frac{1}{4}\,\frac{\mathrm{i}\,\xi\left(\mathrm{i}\sin\xi - 2\cos\xi - 2\mathrm{i}\cos^2\xi\sin\xi + 2\cos^3\xi\right)}{\left(\mathrm{i}\sin\xi - 3\cos\xi - 4\mathrm{i}\cos^2\xi\sin\xi + \cos^3\xi\right)(i-\xi)^3}\,\mathcal{A}(\xi)\,,\\ \frac{\mathrm{d}\Omega_k^{(1)b}}{\mathrm{d}\xi} &= -\frac{2\mathrm{i}\xi}{(\mathrm{i}-\xi)}\,\Omega_k^{(1)b} + \frac{\xi^2\left(2\cos^2\xi - 1 + 2\mathrm{i}\cos\xi\sin\xi\right)}{4(\mathrm{i}-\xi)^4}\,\mathcal{A}(\xi)\,,\end{aligned} \tag{5.120}$$

where $\mathcal{A}(\xi)$ is defined as

$$\mathcal{A}(\xi) = 12\xi^4 - 6\xi^2 + 18\mathrm{i}\xi + 3 + 8\mathrm{e}^{2\mathrm{i}\xi}P_1 + 12\,\mathrm{Ei}(1, 2(1+\mathrm{i}\xi))\,\mathrm{e}^{2(1+\mathrm{i}\xi)}\,, \tag{5.121}$$

and P_1 stands for

$$P_1 = -\frac{3}{8} - \frac{3}{2}\,\mathrm{e}^2\,\mathrm{Ei}(1,2)\,. \tag{5.122}$$

These differential equations can only be studied numerically, which could be useful to investigate what kind of influence the choice of a different vacuum for the initial state would have. However, such an investigation is beyond the scope of this work and we shall therefore focus in the following on the special case $\zeta = 1$, $\beta = \frac{3}{2}\pi$, $\mu = 0$ with the solution (5.115).

In order to calculate the quantum-gravitationally corrected power spectrum, we have to insert the real parts of (5.73) and (5.114) into the following equation that represents the quantum-gravity correction to (5.95)

$$\left|\dot{\sigma}_k^{(1)}(t)\right| = \left|\frac{H\xi}{\sqrt{2}}\frac{\mathrm{d}}{\mathrm{d}\xi}\left[\left(\mathfrak{Re}\,\Omega_k^{(0)}(\xi) + m_{\mathrm{P}}^{-2}\mathfrak{Re}\,\Omega_k^{(1)}(\xi)\right)^{-\frac{1}{2}}\right]\right|. \tag{5.123}$$

This leads to

$$\left|\dot{\sigma}_k^{(1)}(t)\right| = \left|\frac{\xi^2}{\sqrt{2(\xi^2+1)}}\frac{H^2}{k^{\frac{3}{2}}}\left(1 + \frac{\xi^2+1}{k^3}\,\mathfrak{Re}\,\Omega_k^{(1)}(\xi)\,\frac{H^2}{m_{\mathrm{P}}^2}\right)^{-\frac{3}{2}} \times\left(1 - \frac{(\xi^2+1)^2}{2\xi\,k^3}\,\mathfrak{Re}\left[\frac{\mathrm{d}}{\mathrm{d}\xi}\,\Omega_k^{(1)}(\xi)\right]\frac{H^2}{m_{\mathrm{P}}^2}\right)\right|. \tag{5.124}$$

Comparing this with (5.98), we see that we can combine the two terms in brackets into one correction function C_k defined as

$$C_k := \left(1 + \frac{\xi^2+1}{k^3}\,\mathfrak{Re}\,\Omega_k^{(1)}(\xi)\,\frac{H^2}{m_{\mathrm{P}}^2}\right)^{-\frac{3}{2}}\left(1 - \frac{(\xi^2+1)^2}{2\xi\,k^3}\,\mathfrak{Re}\left[\frac{\mathrm{d}}{\mathrm{d}\xi}\,\Omega_k^{(1)}(\xi)\right]\frac{H^2}{m_{\mathrm{P}}^2}\right) \tag{5.125}$$

and consequently, we get

$$\left|\dot{\sigma}_k^{(1)}(t)\right| = |C_k|\left|\dot{\sigma}_k^{(0)}(t)\right|. \tag{5.126}$$

Therefore, all that is left to do in order to obtain the power spectrum is to evaluate (5.125) at the point of horizon crossing, $\xi = 2\pi$. For the function $\Omega_k^{(1)}$, we obtain the following numerical values from (5.115)

$$\mathfrak{Re}\,\Omega_k^{(1)}(\xi = 2\pi) \simeq -1.343 \quad \text{and} \quad \mathfrak{Re}\left[\frac{\mathrm{d}}{\mathrm{d}\xi}\Omega_k^{(1)}(\xi)\right]_{\xi=2\pi} \simeq -0.061\,. \tag{5.127}$$

Hence, we get the following expression for (5.125)

$$C_k \simeq \left(1 - \frac{54.37}{k^3}\frac{H^2}{m_P^2}\right)^{-\frac{3}{2}}\left(1 + \frac{7.98}{k^3}\frac{H^2}{m_P^2}\right). \tag{5.128}$$

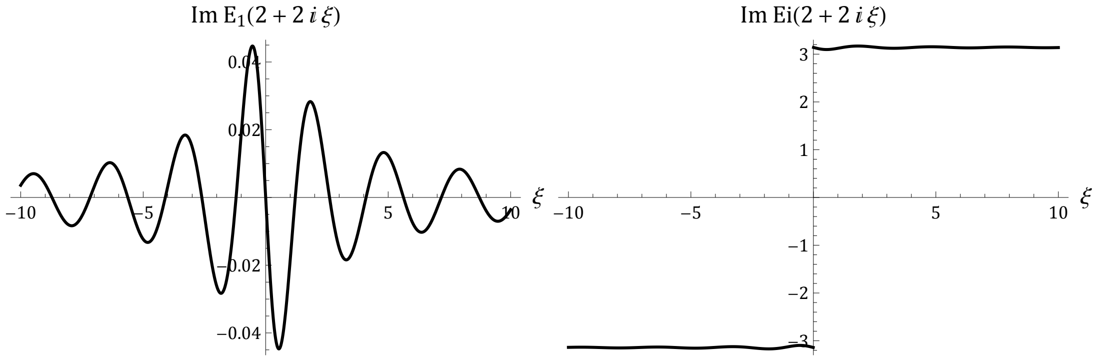

Figure 5.3: Plot of the imaginary part of $E_1(2\mathrm{i}\xi+2)$ and $\mathrm{Ei}(2i\xi+2)$.

The corrected power spectrum $\mathcal{P}^{(1)}(k)$ can therefore be written as

$$\mathcal{P}^{(1)}(k) = \mathcal{P}^{(0)}(k)\, C_k^2 \simeq \mathcal{P}^{(0)}(k) \left[1 + \frac{89.54}{k^3}\frac{H^2}{m_P^2} + \frac{1}{k^6}\,\mathcal{O}\left(\frac{H^4}{m_P^4}\right)\right]^2$$
$$\simeq \mathcal{P}^{(0)}(k) \left[1 + \frac{179.09}{k^3}\frac{H^2}{m_P^2} + \frac{1}{k^6}\,\mathcal{O}\left(\frac{H^4}{m_P^4}\right)\right]. \qquad (5.129)$$

Thus, the quantum-gravitational correction leads to an *enhancement* of power on the largest scales.

In the original article [71], a different exact solution of (5.114) is used, which is of the same form as (5.115), but the exponential integral $\mathrm{Ei}(1,z)$ is replaced – instead of $E_1(z)$ – by the following exponential integral

$$\mathrm{Ei}(z) := -\int_{-z}^{\infty} \frac{\mathrm{e}^{-t}}{t}\,\mathrm{d}t\,. \qquad (5.130)$$

While both solutions $\mathrm{Ei}(z)$ and $E_1(z)$ are defined to assume the value zero for $\xi = 0$, the solution $E_1(z)$ approaches this value continuously, whereas the function $\mathrm{Ei}(z)$ makes a jump of size π in its imaginary part according to the relation [1]

$$E_1(-x \pm \mathrm{i}\,0) = -\,\mathrm{Ei}(x) \mp \mathrm{i}\,\pi\,, \qquad (5.131)$$

where E_1 is defined as given above

$$E_1(z) := \int_{z}^{\infty} \frac{\mathrm{e}^{-t}}{t}\,\mathrm{d}t \quad \text{for} \quad |\arg z| < \pi\,. \qquad (5.132)$$

This behavior is illustrated in figure 5.3. The additional $\mathrm{i}\pi$ causes an oscillatory behavior of the solution $\Omega_k^{(1)}$ as it is shown in figure 5.4.

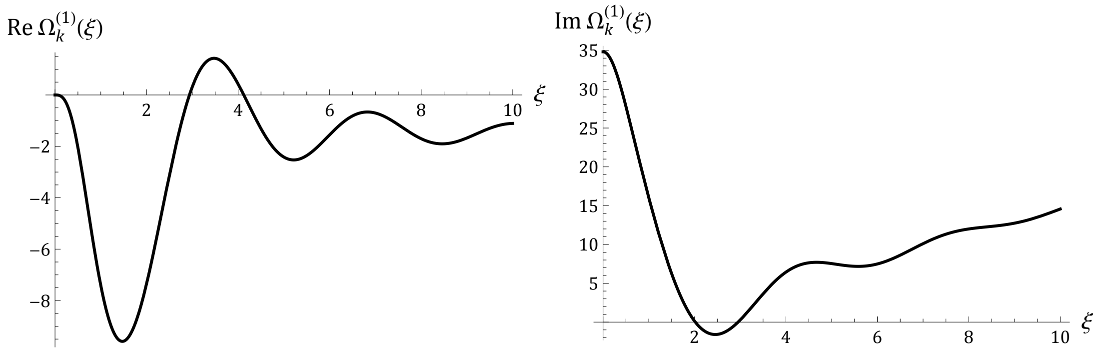

Figure 5.4: Plot of the real and imaginary part of $\Omega_k^{(1)}(\xi)$ using Ei(z).

Hence, if we want to impose the continuity of our solution as a selection criterion, we would have to disregard the second solution defined with $\mathrm{Ei}(x)$. However, one could also argue in the following way: This discontinuity only happens for the imaginary part of $\Omega_k^{(1)}$ and the relevant quantity $\dot{\sigma}_k^{(1)}$ to calculate the power spectrum only contains the real part of $\Omega_k^{(1)}$, which goes to zero for $\xi \to 0$. Therefore independently of which value the imaginary part takes, $\dot{\sigma}_k^{(1)}$ goes to $\dot{\sigma}_k^{(0)}$ for $\xi \to 0$. Therefore, it is in accordance with our requirement that the quantum-gravitational correction should vanish for late times.

Evaluating $\Omega_k^{(1)}(\xi)$ and its derivative at $\xi = 2\pi$ with the $\mathrm{Ei}(x)$ solution gives the values of [71]

$$\mathfrak{Re}\,\Omega_k^{(1)}(\xi = 2\pi) \simeq -1.076 \quad \text{and} \quad \mathfrak{Re}\left[\frac{\mathrm{d}}{\mathrm{d}\xi}\Omega_k^{(1)}(\xi)\right]_{\xi=2\pi} \simeq 1.451\,. \tag{5.133}$$

Note that the derivative has changed the sign compared to (5.127). Inserting these values into (5.125) and setting $\xi = 2\pi$ then leads to

$$C_k \simeq \left(1 - \frac{43.56}{k^3}\frac{H^2}{m_P^2}\right)^{-\frac{3}{2}} \left(1 - \frac{189.18}{k^3}\frac{H^2}{m_P^2}\right). \tag{5.134}$$

For the corrected power spectrum we then get a *suppression* of power on large scales in contrast to (5.129)

$$\begin{aligned}\mathcal{P}^{(1)}(k) = \mathcal{P}^{(0)}(k)\,C_k^2 &\simeq \mathcal{P}^{(0)}(k)\left[1 - \frac{123.83}{k^3}\frac{H^2}{m_P^2} + \frac{1}{k^6}\,\mathcal{O}\!\left(\frac{H^4}{m_P^4}\right)\right]^2 \\ &\simeq \mathcal{P}^{(0)}(k)\left[1 - \frac{247.68}{k^3}\frac{H^2}{m_P^2} + \frac{1}{k^6}\,\mathcal{O}\!\left(\frac{H^4}{m_P^4}\right)\right].\end{aligned} \tag{5.135}$$

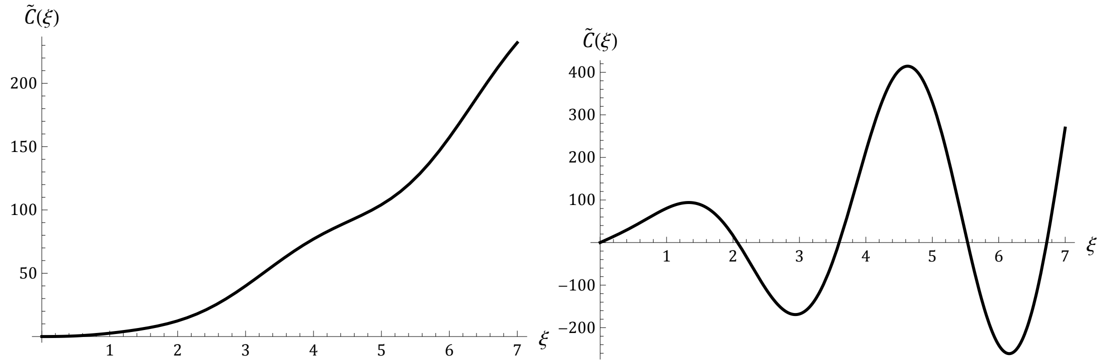

Figure 5.5: Plot of $\widetilde{C}(\xi)$ using $E_1(z)$ (left) and $\mathrm{Ei}(z)$ (right).

In order to investigate this issue further, we can plot the function $\widetilde{C}(\xi)$, which is defined via

$$C_k^2 \simeq 1 + \frac{\widetilde{C}(\xi)}{k^3}\frac{H^2}{m_P^2} + \frac{1}{k^6}\mathcal{O}\left(\frac{H^4}{m_P^4}\right) \tag{5.136}$$

and describes which value the correction term is multiplied with depending on which value of ξ the quantity $\dot{\sigma}_k^{(1)}$ is evaluated at. Figure 5.5 shows that using the continuous function $E_1(z)$ always leads to an enhancement of the power spectrum, no matter at which value ξ we evaluate the perturbations. However, when using $\mathrm{Ei}(z)$, the function $\widetilde{C}(\xi)$ oscillates and the result whether one has an enhancement or suppression of the power depends on the value of ξ at which we evaluate the power spectrum. Our choice $\xi = 2\pi$ leads to a suppression.

Furthermore, we see that both functions go to zero for $\xi \to 0$ and therefore fulfill the requirement we have chosen to set the boundary condition, namely that the quantum-gravitational corrections vanish for late times.

We can also evaluate $\widetilde{C}(\xi)$ at the value $\xi = 1$ in order to find out, how the correction term behaves, if we use the definition $k = L^{-1}$ for the wave number. This leads to the value

$$\widetilde{C}(\xi = 1) \simeq 2.6387 \tag{5.137}$$

for the choice $E_1(z)$ and

$$\widetilde{C}(\xi = 1) \simeq 80.4527 \tag{5.138}$$

if we use the function $\mathrm{Ei}(z)$. Hence, we see that we have an enhancement in both cases, which is, however, more prominent if we use the function $E_1(z)$.

For later purposes, we can also write the corrected power spectrum in the form

$$\mathcal{P}_{\phi}^{(1)}(k) = \mathcal{P}_{\phi}^{(0)}(k)\left[1 + \Delta_{\phi}^{\mathrm{WDW}}(k) + \mathcal{O}\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right], \tag{5.139}$$

where the correction function is given by

$$\Delta_{\phi}^{\mathrm{WDW}}(k) = \frac{H^2}{m_{\mathrm{P}}^2}\frac{\widetilde{C}(\xi)}{k^3}\,. \tag{5.140}$$

In the next chapter, we shall extend the analysis of perturbations during inflation to gauge-invariant scalar and tensor perturbations. In chapter 7, we will then discuss whether the quantum-gravity correction discussed in this and the subsequent chapter can in principle be observable in the Cosmic Microwave Background.

6

Quantum-gravitational effects on gauge-invariant scalar and tensor perturbations during inflation

In this chapter, we are going to extend the analysis on quantum-gravitational corrections to the power spectrum of primordial perturbations presented in the previous chapter. We use gauge-invariant variables for scalar perturbations to make our work more comparable with the standard procedure in cosmological perturbation theory and also include tensor perturbations to see how quantum gravity influences the power spectrum of primordial gravitational waves. We perform our calculations both in a pure de Sitter universe as well as for a generic model of slow-roll inflation.

6.1 Derivation of the Wheeler–DeWitt equation

6.1.1 The background

We start with formulating the Wheeler–DeWitt equation for our background universe in terms of the conformal time η, for which we recall its definition in terms of the cosmic time t and scale factor a

$$\frac{\mathrm{d}\eta}{\mathrm{d}t} = \frac{1}{a}\,. \tag{6.1}$$

The Robertson–Walker line element then takes the following form

$$\mathrm{d}s^2 = a^2(\eta)\left(-\,\mathrm{d}\eta^2 + \mathrm{d}\mathbf{x}^2\right), \tag{6.2}$$

such that by comparison with the standard form,

$$\mathrm{d}s^2 = -\,N^2(t)\,\mathrm{d}t^2 + a^2(t)\,\mathrm{d}\Omega^2_{3,\mathcal{K}}\,, \tag{6.3}$$

we set the lapse function N equal to a, such that the action for a flat FLRW universe without cosmological constant and including a massive scalar field ϕ with potential $\mathcal{V}(\phi)$, which we have derived in the chapter 3 as

$$S = \frac{1}{2}\int \mathrm{d}t\,\mathfrak{L}^3 N\,a^3 \left(-\frac{3\pi}{2G}\frac{1}{N^2}\frac{\dot{a}^2}{a^2} + \frac{\dot{\phi}^2}{N^2} - 2\,\mathcal{V}(\phi)\right), \tag{6.4}$$

becomes

$$S = \frac{1}{2}\int \mathrm{d}\eta\,\mathfrak{L}^3 \left(-\frac{3\pi}{2G}\,a'^2 + a^2\,\phi'^2 - 2\,a^4\,\mathcal{V}(\phi)\right) \equiv \int \mathrm{d}\eta\,L\,, \tag{6.5}$$

where we denote derivatives with respect to η as primes and have introduced an arbitrary length scale $\mathfrak{L}$ that enters here due to the former integration over the volume. Since we do not want to denote this length scale explicitly in the subsequent calculations, we follow [64] and make the replacements

$$a_{\text{new}} = a_{\text{old}}\,\mathfrak{L}\,, \qquad \eta_{\text{new}} = \frac{\eta_{\text{old}}}{\mathfrak{L}}\,. \tag{6.6}$$

In doing so, the scale factor a has the dimension of a length and η is dimensionless. The length scale $\mathfrak{L}$ appearing in (6.5) is then effectively set to one. We have to remember to restore $\mathfrak{L}$ explicitly in all respective quantities when discussing observational consequences of our calculations.

After performing this replacement, the Lagrangian itself takes the form

$$L = -\frac{3\pi}{4G}\,a'^2 + \frac{a^2}{2}\,\phi'^2 - a^4\,\mathcal{V}(\phi)\,. \tag{6.7}$$

The canonical momenta then read

$$\pi_a = \frac{\partial L}{\partial a'} = -\frac{3\pi}{2G}\,a'\,, \qquad \pi_\phi = \frac{\partial L}{\partial \phi'} = a^2\phi'\,, \tag{6.8}$$

such that by using the Legendre transform

$$H = \pi_a\,a' + \pi_\phi\,\phi' - L\,, \tag{6.9}$$

we obtain the following Hamiltonian

$$H = -\frac{G}{3\pi}\,\pi_a^2 + \frac{1}{2a^2}\,\pi_\phi^2 + a^4\,\mathcal{V}(\phi)\,. \tag{6.10}$$

Before we proceed to quantization, let us introduce the minisuperspace metric $\mathcal{G}_{AB}$, whose indices run from 0 to 1, in the following way

$$\mathcal{G}_{AB} = \mathrm{diag}\left(-\frac{3\pi}{2G}, a^2\right), \qquad \mathcal{G} = -\frac{3\pi}{2G}\,a^2 \tag{6.11}$$

such that by defining $q^0 := a$ and $q^1 := \phi$, we can write

$$L(q^A, q'^A) = \frac{1}{2}\,\mathcal{G}_{AB}\, q'^A q'^B - V(q^A)\,, \tag{6.12}$$

and

$$H = \frac{1}{2}\,\mathcal{G}^{AB}\, p_A p_B + V(q^A)\,, \tag{6.13}$$

where $V(q^A) = a^4\,\mathcal{V}(\phi)$.

For quantization we use the Laplace–Beltrami factor ordering, which means that we perform the following replacement

$$\mathcal{G}^{AB}\, p_A p_B \to -\frac{\hbar^2}{\sqrt{-\mathcal{G}}}\frac{\partial}{\partial q_A}\left(\sqrt{-\mathcal{G}}\,\mathcal{G}^{AB}\frac{\partial}{\partial q_B}\right). \tag{6.14}$$

In our case, this leads to

$$-\frac{\hbar^2}{\sqrt{-\mathcal{G}}}\frac{\partial}{\partial q_A}\left(\sqrt{-\mathcal{G}}\,\mathcal{G}^{AB}\frac{\partial}{\partial q_B}\right) = \frac{2\hbar^2 G}{3\pi a}\frac{\partial}{\partial a}\left(a\,\frac{\partial}{\partial a}\right) - \frac{\hbar^2}{a^2}\frac{\partial^2}{\partial\phi^2}\,. \tag{6.15}$$

Our choice is motivated by the fact that the Laplace–Beltrami factor ordering ensures that the kinetic term is invariant under transformations in configuration space. Different choices for the factor ordering, which in this case only affect the term containing derivatives of a, can be parametrized by introducing a parameter s in the following way

$$a^{-s}\,\frac{\partial}{\partial a}\left(a^s\,\frac{\partial}{\partial a}\right). \tag{6.16}$$

For the Laplace–Beltrami factor ordering, $s = 1$. We will later see that the factor ordering does not influence our results, since the affected term will only appear in the definition of the WKB time and can therefore be incorporated into this definition.

Finally, we can write out the Wheeler–DeWitt equation for our background universe

$$\left[\frac{\hbar^2 G}{3\pi a}\frac{\partial}{\partial a}\left(a\,\frac{\partial}{\partial a}\right) - \frac{\hbar^2}{2a^2}\frac{\partial^2}{\partial\phi^2} + a^4\,\mathcal{V}(\phi)\right]\Psi_0(a,\phi) = 0\,. \tag{6.17}$$

A common simplification of this equation is to introduce the quantity α, defined in terms of a reference scale factor a_0 as

$$\alpha := \ln\left(\frac{a}{a_0}\right). \tag{6.18}$$

We will refrain from writing out a_0 explicitly in the following. Our Wheeler–DeWitt equation then reads

$$\left[\frac{\hbar^2 G}{3\pi}\,\mathrm{e}^{-2\alpha}\,\frac{\partial^2}{\partial\alpha^2} - \frac{\hbar^2}{2}\,\mathrm{e}^{-2\alpha}\,\frac{\partial^2}{\partial\phi^2} + \mathrm{e}^{6\alpha}\,\mathcal{V}(\phi)\right]\Psi_0(\alpha,\phi) = 0\,. \tag{6.19}$$

If we now set $\hbar \equiv 1$ and define for convenience

$$m_{\mathrm{P}}^2 := \frac{3\pi}{2G}\,, \tag{6.20}$$

we finally arrive at

$$\frac{1}{2}\,\mathrm{e}^{-2\alpha}\left[\frac{1}{m_{\mathrm{P}}^2}\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial\phi^2} + 2\,\mathrm{e}^{6\alpha}\,\mathcal{V}(\phi)\right]\Psi_0(\alpha,\phi) = 0\,. \tag{6.21}$$

6.1.2 Scalar perturbations

The next step is to introduce scalar perturbations to the background metric that can be parametrized by the four scalar functions A, B, ψ and E, which are functions of space and time, as follows

$$\mathrm{d}s^2 = a^2(\eta)\left\{-(1-2A)\,\mathrm{d}\eta^2 + 2\left(\partial_i B\right)\mathrm{d}x^i\mathrm{d}\eta + \left[\left(1-2\psi\right)\delta_{ij} + 2\partial_i\partial_j E\right]\mathrm{d}x^i\mathrm{d}x^j\right\}. \tag{6.22}$$

This parametrization still contains three unphysical degrees of freedom, because gauge transformations have not been taken into account up to now. In order to remove these additional degrees of freedom, we consider infinitesimal coordinate transformations of the form

$$x^\mu \to \tilde{x}^\mu = x^\mu + \xi^\mu\,, \tag{6.23}$$

where the generator ξ^μ can be decomposed into a temporal as well as a spatial part, and the latter can be further decomposed into a transversal and a longitudinal part

$$\xi^\mu = \delta^\mu_0\,\xi^0 + \delta^\mu_i\left(\xi^i_{\mathrm{T}} + \delta^{ij}\xi_{,j}\right). \tag{6.24}$$

The spatial transversal part ξ^i_{T} only influences vector perturbations. Hence, we are left with the following two coordinate transformations for our four scalar degrees of freedom

$$\eta \to \tilde{\eta} = \eta + \xi^0\,, \quad x^i \to \tilde{x}^i = x^i + \delta^{ij}\,\partial_j\xi\,. \tag{6.25}$$

Consequently, the scalar functions A, B, ψ and E transform in the subsequent way

$$A \to \tilde{A} = A + \mathcal{H}\,\xi^0 + \left(\xi^0\right)'\,, \quad B \to \tilde{B} = B + \xi^0 - \xi'\,, \tag{6.26}$$

$$\psi \to \tilde{\psi} = \psi + \mathcal{H}\,\xi^0\,, \qquad E \to \tilde{E} = E + \xi\,, \tag{6.27}$$

where $\mathcal{H} := a'/a$ as before. From this, one can construct two gauge-invariant quantities that characterize the *physical* scalar metric perturbations. These quantities are called the *Bardeen potentials* Φ_{B} and Ψ_{B} and are defined as

$$\Phi_{\mathrm{B}}(\eta,\mathbf{x}) := A + \frac{1}{a}\left[a\left(B - E'\right)\right]'\,, \quad \Psi_{\mathrm{B}}(\eta,\mathbf{x}) := \psi - \mathcal{H}\left(B + E'\right). \tag{6.28}$$

Apart from the metric perturbations, the scalar sector also includes fluctuations $\delta\phi(\eta,\mathbf{x})$ of the scalar inflaton field $\phi(\eta)$. These fluctuations can be expressed in a gauge-invariant way as follows

$$\delta\phi^{(\mathrm{gi})}(\eta,\mathbf{x}) = \delta\phi + \phi'\left(B - E'\right) . \tag{6.29}$$

Finally, as it was shown e.g. in [87], we can combine the quantities Φ_B and $\delta\phi^{(\mathrm{gi})}$ to a single gauge-invariant quantity, the so-called *Mukhanov–Sasaki variable* v, that fully describes the scalar sector of the perturbations:

$$v(\eta,\mathbf{x}) = a\left[\delta\phi^{(\mathrm{gi})} + \phi'\frac{\Phi_\mathrm{B}}{\mathcal{H}}\right] . \tag{6.30}$$

From an expansion of the Einstein–Hilbert action plus the scalar field action around a FLRW background up to the second order in the perturbations, one obtains the following action for the variable v [87]

$$^{(2)}\delta S = \frac{1}{2}\int \mathrm{d}\eta\,\mathrm{d}^3\mathbf{x}\left[\left(v'\right)^2 - \delta^{ij}\,\partial_i v\,\partial_j v + \frac{z''}{z}\,v^2\right] , \tag{6.31}$$

where z is given by

$$z = \frac{\phi'}{H} = \frac{a}{\mathcal{H}}\,\phi' , \tag{6.32}$$

such that z''/z in the general case becomes a highly intricate expression containing first and second η-derivatives of ϕ and a. However, in the de Sitter and slow-roll cases we will discuss later, we can significantly simplify the respective expressions.

Given that we deal with a linear theory, we can assume that all modes of the perturbations evolve independently and, hence, perform a Fourier transform of the variable v:

$$v\left(\eta,\mathbf{x}\right) = \int_{\mathbb{R}^3}\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}}\,v_\mathbf{k}(\eta)\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} . \tag{6.33}$$

Note that in this chapter, we relate the wave vector $\mathbf{k}$ and its modulus $k = |\mathbf{k}|$ to a length *without* including the factor 2π, i. e. we have the following relation for the wave length L corresponding to k

$$k = L^{-1} . \tag{6.34}$$

Since v is real, the relation $v_{-\mathbf{k}} = v^*_\mathbf{k}$ holds. Inserting the Fourier transform into eq. (6.31) then leads to

$$^{(2)}\delta S = \int \mathrm{d}\eta\int \mathrm{d}^3\mathbf{k}\left\{v'_\mathbf{k}v^{*\prime}_\mathbf{k} + v_\mathbf{k}v^*_\mathbf{k}\left[\frac{z''}{z} - k^2\right]\right\} , \tag{6.35}$$

where we have taken the integral over the spatial volume. Note that the **k**-integral here is understood to be taken only over half of the Fourier space.

For later convenience, we now want to replace the integral over **k** by a sum over $k := |\mathbf{k}|$. In order to do so, we have to introduce an arbitrary length scale $\mathcal{L}$ like for the background in the previous section, cf. [90],

$$\int \mathrm{d}^3\mathbf{k} \left\{ \cdots \right\} \quad \to \quad \frac{1}{\mathfrak{L}^3} \sum_{k\neq 0}^{\infty} \left\{ \cdots \right\}. \tag{6.36}$$

We thus obtain

$$^{(2)}\delta S = \int \mathrm{d}\eta \, \frac{1}{\mathfrak{L}^3} \sum_{k\neq 0}^{\infty} \left\{ v'_{\mathbf{k}} v^{*\prime}_{\mathbf{k}} + v_{\mathbf{k}} v^*_{\mathbf{k}} \left[\frac{z''}{z} - k^2 \right] \right\}. \tag{6.37}$$

Again following [64], we can eliminate $\mathfrak{L}$ by performing the replacements (6.6) done in the previous section in addition to two replacements for v and k:

$$a_{\mathrm{new}} = a_{\mathrm{old}} \, \mathfrak{L}, \quad \eta_{\mathrm{new}} = \frac{\eta_{\mathrm{old}}}{\mathfrak{L}}, \quad v_{\mathrm{new}} = \frac{v_{\mathrm{old}}}{\mathfrak{L}^2}, \quad k_{\mathrm{new}} = k_{\mathrm{old}} \, \mathfrak{L}, \tag{6.38}$$

which means that the wave vector k is now regarded as a dimensionless quantity and we have to introduce a reference scale later when comparing our result to observations. For our action we end up with

$$^{(2)}\delta S = \int \mathrm{d}\eta \sum_{k\neq 0}^{\infty} \left\{ v'_{\mathbf{k}} v^{*\prime}_{\mathbf{k}} + v_{\mathbf{k}} v^*_{\mathbf{k}} \left[\frac{z''}{z} - k^2 \right] \right\}. \tag{6.39}$$

Defining the canonical momentum as

$$p_{\mathbf{k}} = \frac{\partial \mathcal{L}}{\partial v^{*\prime}_{\mathbf{k}}} = v'_{\mathbf{k}}, \tag{6.40}$$

we can write out the Hamiltonian as follows

$$H = \sum_{k\neq 0}^{\infty} \left\{ p_{\mathbf{k}} p^*_{\mathbf{k}} + v_{\mathbf{k}} v^*_{\mathbf{k}} \left[k^2 - \frac{z''}{z} \right] \right\}. \tag{6.41}$$

In principle, in order to perform a complete quantization that includes the background variables a and ϕ, we also have to replace the η-derivatives of a and ϕ appearing in z''/z by their canonical momenta like it is, for example, done in [81]. This would complicate the quantization procedure significantly and since we will later only consider the de Sitter and slow-roll cases, in which the derivatives contained in z''/z are approximated by parameters determined at the classical level, we shall keep z''/z unquantized.

For convenience, we define the quantity

$$ {}^{\mathrm{S}}\omega_{\mathbf{k}}^2(\eta) = k^2 - \frac{z''}{z}\,, \tag{6.42} $$

which can be regarded as a time-dependent frequency of the parametric harmonic oscillator described by the Hamiltonian (6.41). The Mukhanov–Sasaki variable consequently obeys the following equation of motion at the classical level:

$$ v_{\mathbf{k}}'' + {}^{\mathrm{S}}\omega_{\mathbf{k}}^2(\eta)\, v_{\mathbf{k}} = 0\,. \tag{6.43} $$

Before quantization, we make the subsequent definitions in order to be able to work with real variables:

$$ v_{\mathbf{k}} \equiv \frac{1}{\sqrt{2}}\left(v_{\mathbf{k}}^{\mathrm{R}} + \mathrm{i}\, v_{\mathbf{k}}^{\mathrm{I}}\right)\,, \quad p_{\mathbf{k}} \equiv \frac{1}{\sqrt{2}}\left(p_{\mathbf{k}}^{\mathrm{R}} + \mathrm{i}\, p_{\mathbf{k}}^{\mathrm{I}}\right)\,. \tag{6.44} $$

Note that the resulting wave functional can be factorized as follows:

$$ \Psi\left[v(\eta,\mathbf{x})\right] = \prod_{\mathbf{k}} \Psi_{\mathbf{k}}\left(v_{\mathbf{k}}^{\mathrm{R}}, v_{\mathbf{k}}^{\mathrm{I}}\right) = \prod_{\mathbf{k}} \Psi_{\mathbf{k}}^{\mathrm{R}}\left(v_{\mathbf{k}}^{\mathrm{R}}\right) \Psi_{\mathbf{k}}^{\mathrm{I}}\left(v_{\mathbf{k}}^{\mathrm{I}}\right). \tag{6.45} $$

We now promote $v_{\mathbf{k}}$ and $p_{\mathbf{k}}$ to quantum operators $\hat{v}_{\mathbf{k}}$ and $\hat{p}_{\mathbf{k}}$ that obey the following commutation relations

$$ \left[\hat{v}_{\mathbf{k}}^{\mathrm{R}}, \hat{p}_{\mathbf{q}}^{\mathrm{R}}\right] = \mathrm{i}\,\delta\left(\mathbf{k}-\mathbf{q}\right)\,, \quad \left[\hat{v}_{\mathbf{k}}^{\mathrm{I}}, \hat{p}_{\mathbf{q}}^{\mathrm{I}}\right] = \mathrm{i}\,\delta\left(\mathbf{k}-\mathbf{q}\right)\,, \tag{6.46} $$

such that we can represent $\hat{v}_{\mathbf{k}}$ and $\hat{p}_{\mathbf{k}}$ in the subsequent way

$$ \hat{v}_{\mathbf{k}}^{\mathrm{R,I}}\Psi = v_{\mathbf{k}}^{\mathrm{R,I}}\Psi\,, \quad \hat{p}_{\mathbf{k}}^{\mathrm{R,I}}\Psi = -\mathrm{i}\,\frac{\partial \Psi}{\partial v_{\mathbf{k}}^{\mathrm{R,I}}}\,. \tag{6.47} $$

The total quantum Hamiltonian for the scalar perturbations then reads

$$ {}^{\mathrm{S}}\hat{\mathcal{H}} = \sum_{k\neq 0}^{\infty}\left({}^{\mathrm{S}}\hat{\mathcal{H}}_{\mathbf{k}}^{\mathrm{R}} + {}^{\mathrm{S}}\hat{\mathcal{H}}_{\mathbf{k}}^{\mathrm{I}}\right)\,, \tag{6.48} $$

where the Hamiltonians for the individual modes are given by

$$ {}^{\mathrm{S}}\hat{\mathcal{H}}_{\mathbf{k}}^{\mathrm{R,I}} = -\frac{1}{2}\frac{\partial^2}{\partial\left(v_{\mathbf{k}}^{\mathrm{R,I}}\right)^2} + \frac{1}{2}\,{}^{\mathrm{S}}\omega_{\mathbf{k}}^2(\eta)\left(v_{\mathbf{k}}^{\mathrm{R,I}}\right)^2. \tag{6.49} $$

For notational simplicity we now omit the labels R and I as well as the circumflex to denote the quantum-operator nature of $\mathcal{H}$, such that the Hamiltonian of the scalar fluctuations finally takes the form:

$$ {}^{\mathrm{S}}\mathcal{H} = \sum_{k\neq 0}^{\infty} {}^{\mathrm{S}}\mathcal{H}_{\mathbf{k}} = \sum_{\mathbf{k}}\left\{-\frac{1}{2}\frac{\partial^2}{\partial v_{\mathbf{k}}^2} + \frac{1}{2}\,{}^{\mathrm{S}}\omega_{\mathbf{k}}^2(\eta)\, v_{\mathbf{k}}^2\right\}. \tag{6.50} $$

6.1.3 Tensor perturbations

Apart from the scalar perturbations we also introduce tensor perturbations that would lead to primordial gravitational waves. In the CMB radiation, these would be detectable especially as B-mode polarization.

We introduce tensor perturbations as a symmetric, traceless and divergenceless tensor h_{ij} as follows

$$\mathrm{d}s^2 = a^2(\eta)\left[-\mathrm{d}\eta^2 + \left(\delta_{ij} + h_{ij}\right)\mathrm{d}x^i\mathrm{d}x^j\right]. \tag{6.51}$$

These perturbations are already gauge-invariant by construction. The six independent components of the symmetric tensor $h_{ij} = h_{ji}$ are reduced by three due to its divergencelessness $\partial^i h_{ij} = 0$ and by one due to its tracelessness $\delta^{ij}h_{ij} = 0$, such that two degrees of freedom remain that correspond to two polarizations, $h^{(+)}$ and $h^{(\times)}$. If we define

$$v_{\mathbf{k}}^{(\lambda),\mathrm{R}} := \frac{aM_{\mathrm{P}}}{\sqrt{2}}\mathfrak{Re}\left(h_{\mathbf{k}}\right), \qquad v_{\mathbf{k}}^{(\lambda),\mathrm{I}} := \frac{aM_{\mathrm{P}}}{\sqrt{2}}\mathfrak{Im}\left(h_{\mathbf{k}}\right), \tag{6.52}$$

we can write out the total Hamiltonian for the tensor perturbations in the following way

$${}^{\mathrm{T}}\hat{\mathcal{H}} = \sum_{\lambda=+,\times}\int \mathrm{d}^3\mathbf{k}\left({}^{\mathrm{T}}\hat{\mathcal{H}}_{\mathbf{k}}^{(\lambda),\mathrm{R}} + {}^{\mathrm{T}}\hat{\mathcal{H}}_{\mathbf{k}}^{(\lambda),\mathrm{I}}\right), \tag{6.53}$$

where the Hamiltonians for the respective polarization modes are given by

$${}^{\mathrm{T}}\hat{\mathcal{H}}_{\mathbf{k}}^{(\lambda);\mathrm{R,I}} = -\frac{1}{2}\frac{\partial^2}{\partial\left(v_{\mathbf{k}}^{(\lambda);\mathrm{R,I}}\right)^2} + \frac{1}{2}\,{}^{\mathrm{T}}\omega_{\mathbf{k}}^2(\eta)\left({v_{\mathbf{k}}}^{(\lambda);\mathrm{R,I}}\right)^2. \tag{6.54}$$

The crucial difference to the scalar perturbations apart from the two polarizations lies in the time-dependent frequency, which is now given by

$${}^{\mathrm{T}}\omega_{\mathbf{k}}^2(\eta) = k^2 - \frac{a''}{a}. \tag{6.55}$$

We can replace the integral in (6.53) by a sum using the procedure presented in (6.36) and (6.38), which leads to

$${}^{\mathrm{T}}\hat{\mathcal{H}} = \sum_{\lambda=+,\times}\sum_{k\neq 0}^{\infty}\left(\hat{\mathcal{H}}_{\mathbf{k}}^{(\lambda),\mathrm{R}} + {}^{\mathrm{T}}\hat{\mathcal{H}}_{\mathbf{k}}^{(\lambda),\mathrm{I}}\right). \tag{6.56}$$

Again, omitting the labels R and I as well as the circumflex leads to the following Hamiltonian for the tensor perturbations:

$${}^{\mathrm{T}}\mathcal{H} = \sum_{k\neq 0}^{\infty}{}^{\mathrm{T}}\mathcal{H}_{\mathbf{k}} = \sum_{k\neq 0}^{\infty}\left\{-\frac{1}{2}\frac{\partial^2}{\partial v_{\mathbf{k}}^2} + \frac{1}{2}\,{}^{\mathrm{T}}\omega_{\mathbf{k}}^2(\eta)\,v_{\mathbf{k}}^2\right\}, \tag{6.57}$$

i. e. the Hamiltonian has the same form as for the scalar perturbations, which allows us to treat both cases in the same manner.

6.1.4 Master Wheeler–DeWitt equation

In the end, our master Wheeler–DeWitt equation for both scalar and tensor perturbations reads:

$$\frac{1}{2}\left\{\mathrm{e}^{-2\alpha}\left[\frac{1}{m_\mathrm{P}^2}\frac{\partial^2}{\partial\alpha^2}-\frac{\partial^2}{\partial\phi^2}+2\,\mathrm{e}^{6\alpha}\,\mathcal{V}(\phi)\right]+\sum_{\mathbf{k};\mathrm{S,T}}\left[-\frac{\partial^2}{\partial v_\mathbf{k}^2}+{}^{\mathrm{S,T}}\omega_\mathbf{k}^2(\eta)\,v_\mathbf{k}^2\right]\right\}\Psi(\alpha,\phi,\{v_\mathbf{k}\})=0\,. \tag{6.58}$$

For notational simplicity, we shall skip the superscripts S and T as well as the hat to denote operators from now on and we therefore use the following Hamiltonian density for both scalar and tensor perturbations

$$\mathcal{H}_\mathbf{k}=-\frac{\partial^2}{\partial v_\mathbf{k}^2}+\omega_\mathbf{k}^2(\eta)\,v_\mathbf{k}^2\,. \tag{6.59}$$

Assuming that we can neglect the self-interaction of the perturbation modes, we can use a product ansatz for the wave function of the form

$$\Psi\big(\alpha,\phi,\{v_\mathbf{k}\}_{k=1}^{\infty}\big)=\Psi_0(\alpha,\phi)\prod_{k=1}^{\infty}\widetilde{\Psi}_\mathbf{k}(\alpha,\phi,v_\mathbf{k}) \tag{6.60}$$

and find that each of the wave functions

$$\Psi_\mathbf{k}(\alpha,\phi,v_\mathbf{k}):=\Psi_0(\alpha,\phi)\widetilde{\Psi}_\mathbf{k}(\alpha,\phi,v_\mathbf{k}) \tag{6.61}$$

fulfills the following Wheeler–DeWitt equation

$$\frac{1}{2}\left\{\mathrm{e}^{-2\alpha}\left[\frac{1}{m_\mathrm{P}^2}\frac{\partial^2}{\partial\alpha^2}-\frac{\partial^2}{\partial\phi^2}+2\,\mathrm{e}^{6\alpha}\,\mathcal{V}(\phi)\right]-\frac{\partial^2}{\partial v_\mathbf{k}^2}+\omega_\mathbf{k}^2(\eta)\,v_\mathbf{k}^2\right\}\Psi_\mathbf{k}(\alpha,\phi,v_\mathbf{k})=0\,. \tag{6.62}$$

We now want to streamline the notation by introducing a minisuperspace metric. In order to do so, we rescale the scalar field ϕ with the inversely squared Planck mass

$$\tilde{\phi}:=m_\mathrm{P}^{-1}\phi \tag{6.63}$$

and introduce the minisuperspace variable q^A, whose index can take either the value 0 or 1. We set

$$q^0:=\alpha\quad\text{and}\quad q^1:=\tilde{\phi}\,. \tag{6.64}$$

Defining a minisuperspace metric $\mathcal{G}_{AB}$ as

$$\mathcal{G}_{AB}:=\mathrm{diag}\Big(-\mathrm{e}^{-2\alpha},\mathrm{e}^{-2\alpha}\Big)\,, \tag{6.65}$$

and using the definition

$$V(q^A):=\frac{2}{m_\mathrm{P}^2}\,\mathrm{e}^{4\alpha}\,\mathcal{V}(\phi)=2\,\mathrm{e}^{4\alpha}\,\mathcal{V}(\tilde{\phi})\,, \tag{6.66}$$

we can finally write

$$\frac{1}{2}\left\{-\frac{1}{m_\mathrm{P}^2}\,\mathcal{G}_{AB}\,\frac{\partial^2}{\partial q_A\partial q_B}+m_\mathrm{P}^2\,V(q^A)-\frac{\partial^2}{\partial v_\mathbf{k}^2}+\omega_\mathbf{k}^2(\eta)\,v_\mathbf{k}^2\right\}\Psi_\mathbf{k}(\alpha,\phi,v_\mathbf{k})=0\,. \tag{6.67}$$

6.2 Semiclassical approximation

In order to calculate the power spectrum and quantum-gravitational corrections to it, we now want to perform the semiclassical approximation that was introduced in the previous chapter. The calculation in the present case is largely analogous to the former one, the only difference is the use of the conformal time instead of cosmic time, as well as the inclusion of the kinetic term of the scalar field in the background. However, by using the minisuperspace metric (6.65), the equations become formally equivalent to just using the scale factor as background and therefore we shall only present the main steps of the semiclassical approximation in the following.

As before, we start with the WKB ansatz

$$\Psi_{\mathbf{k}}(q^A, v_{\mathbf{k}}) = \mathrm{e}^{\mathrm{i}\,S(q^A, v_{\mathbf{k}})} \tag{6.68}$$

and expand $S(q^A, v_{\mathbf{k}})$ in terms of powers of m_{P}^2

$$S(q^A, v_{\mathbf{k}}) = m_{\mathrm{P}}^2 S_0 + m_{\mathrm{P}}^0 S_1 + m_{\mathrm{P}}^{-2} S_2 + \dots\,. \tag{6.69}$$

We again insert this ansatz into (6.67), collect terms with a certain power of m_{P} and set the sum of terms with a specific power of m_{P} equal to zero. The highest order appearing is m_{P}^4 and from this we obtain the background condition

$$\frac{\partial}{\partial v_{\mathbf{k}}} S_0(q^A, v_{\mathbf{k}}) = 0\,, \tag{6.70}$$

which implies that S_0 does not depend on the $v_{\mathbf{k}}$.

At order m_{P}^2, our approximation leads to the Hamilton–Jacobi equation of the background

$$\mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial S_0}{\partial q_B} + V(q^A) = 0\,, \tag{6.71}$$

which is equivalent to the Friedmann equation. We will solve this equation in the de Sitter and slow-roll case later.

The next order corresponds to m_{P}^0. Here we get the following equation:

$$2\,\mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial S_1}{\partial q_B} - \mathrm{i}\,\mathcal{G}_{AB}\,\frac{\partial^2 S_0}{\partial q_A \partial q_B} + \left(\frac{\partial S_1}{\partial v_{\mathbf{k}}}\right)^2 - \mathrm{i}\,\frac{\partial^2 S_1}{\partial v_{\mathbf{k}}^2} + \omega_{\mathbf{k}}^2\, v_{\mathbf{k}}^2 = 0\,. \tag{6.72}$$

In this case, we go through the derivation of the Schrödinger equation in more detail, because we now want to use conformal time and need to make sure that the resulting Schrödinger equation with conformal time is consistent. We again define the following wave function that will obey the Schrödinger equation we are about to derive:

$$\psi^{(0)}_{\mathbf{k}}(q^A, v_{\mathbf{k}}) := \gamma(q^A)\,\mathrm{e}^{\mathrm{i}S_1(q^A, v_{\mathbf{k}})}\,. \tag{6.73}$$

The prefactor γ is again the WKB prefactor we actually omitted in the WKB ansatz (6.68) we used. We impose the following condition on γ:

$$\mathcal{G}_{AB}\,\frac{\partial}{\partial q_A}\left[\frac{1}{2\gamma^2}\,\frac{\partial S_0}{\partial q_B}\right] = 0 \quad\Leftrightarrow\quad \frac{1}{\gamma}\,\mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial \gamma}{\partial q_B} - \frac{1}{2}\,\mathcal{G}_{AB}\,\frac{\partial^2 S_0}{\partial q_A \partial q_B} = 0\,. \tag{6.74}$$

If we furthermore define the conformal WKB time to be

$$\frac{\partial}{\partial \eta} := \mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial}{\partial q_B} = \mathrm{e}^{-2\alpha}\left[-\frac{\partial S_0}{\partial \alpha}\,\frac{\partial}{\partial \alpha} + \frac{\partial S_0}{\partial \tilde{\phi}}\,\frac{\partial}{\partial \tilde{\phi}}\right], \tag{6.75}$$

we can make the following manipulations to the Hamiltonian densities of the scalar (6.49) and tensor (6.54) modes

$$\begin{aligned}
\mathcal{H}_{\mathbf{k}}\psi^{(0)}_{\mathbf{k}} &= \left[-\frac{1}{2}\,\frac{\partial^2}{\partial v_{\mathbf{k}}^2} + \frac{1}{2}\,\omega^2_{\mathbf{k}}(\eta)\,v^2_{\mathbf{k}}\right]\psi^{(0)}_{\mathbf{k}} \\
&= \left[-\frac{1}{2}\,\frac{\partial^2}{\partial v_{\mathbf{k}}^2} + \frac{1}{2}\,\omega^2_{\mathbf{k}}(\eta)\,v^2_{\mathbf{k}}\right]\gamma(q_a)\,\mathrm{e}^{\mathrm{i}S_1(q_a, f_n)} \\
&= \frac{1}{2}\left[\left(\frac{\partial S_1}{\partial v_{\mathbf{k}}}\right)^2 - \mathrm{i}\,\frac{\partial^2 S_1}{\partial v^2_{\mathbf{k}}} + \omega^2_{\mathbf{k}}(\eta) v^2_{\mathbf{k}}\right]\psi^{(0)}_{\mathbf{k}} \\
&\overset{(6.72)}{=} \left[\frac{\mathrm{i}}{2}\,\mathcal{G}_{AB}\,\frac{\partial^2 S_0}{\partial q_A \partial q_B} - \mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial S_1}{\partial q_B}\right]\psi^{(0)}_{\mathbf{k}} \\
&\overset{(6.74)}{=} \left[\frac{\mathrm{i}}{\gamma}\,\mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial \gamma}{\partial q_B} - \mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial S_1}{\partial q_B}\right]\psi^{(0)}_{\mathbf{k}} \\
&= \mathrm{i}\,\mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial}{\partial q_B}\left[\gamma(q^A)\,\mathrm{e}^{\mathrm{i}S_1(q^A, v_{\mathbf{k}})}\right] = \mathrm{i}\,\mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial \psi^{(0)}_{\mathbf{k}}}{\partial q_B} \\
&\overset{(6.75)}{=} \mathrm{i}\,\frac{\partial}{\partial \eta}\,\psi^{(0)}_{\mathbf{k}}\,.
\end{aligned} \tag{6.76}$$

Hence, we finally arrive at the following Schrödinger equation

$$\boxed{\mathrm{i}\,\frac{\partial}{\partial \eta}\,\psi^{(0)}_{\mathbf{k}} = \mathcal{H}_{\mathbf{k}}\psi^{(0)}_{\mathbf{k}}} \tag{6.77}$$

In order to obtain quantum-gravitational correction terms to this equation, we again have to look at the terms of order m_{P}^{-2}, where we get

$$\mathcal{G}_{AB}\,\frac{\partial S_0}{\partial q_A}\,\frac{\partial S_2}{\partial q_B} + \frac{1}{2}\,\mathcal{G}_{AB}\,\frac{\partial S_1}{\partial q_A}\,\frac{\partial S_1}{\partial q_B} - \frac{\mathrm{i}}{2}\,\mathcal{G}_{AB}\,\frac{\partial^2 S_1}{\partial q_A \partial q_B} + \frac{\partial S_1}{\partial v_{\mathbf{k}}}\,\frac{\partial S_2}{\partial v_{\mathbf{k}}} - \frac{\mathrm{i}}{2}\,\frac{\partial^2 S_2}{\partial v^2_{\mathbf{k}}} = 0\,. \tag{6.78}$$

As before, we split S_2 into a part ς depending only on the background variables, and a part ξ containing also the perturbations $v_{\mathbf{k}}$:

$$S_2(q^A, v_{\mathbf{k}}) \equiv \varsigma(q^A) + \xi(q^A, v_{\mathbf{k}})\,. \tag{6.79}$$

This split leads to the following equation for ξ

$$\mathcal{G}_{AB}\frac{\partial S_0}{\partial q_A}\frac{\partial \xi}{\partial q_B} = -\frac{1}{\gamma\psi_{\mathbf{k}}^{(0)}}\mathcal{G}_{AB}\frac{\partial \psi_{\mathbf{k}}^{(0)}}{\partial q_A}\frac{\partial \gamma}{\partial q_B} + \frac{1}{2\psi_{\mathbf{k}}^{(0)}}\mathcal{G}_{AB}\frac{\partial^2 \psi_{\mathbf{k}}^{(0)}}{\partial q_A \partial q_B} + \frac{\mathrm{i}}{\psi_{\mathbf{k}}^{(0)}}\frac{\partial \psi_{\mathbf{k}}^{(0)}}{\partial v_{\mathbf{k}}}\frac{\partial \xi}{\partial v_{\mathbf{k}}} + \frac{\mathrm{i}}{2}\frac{\partial^2 \xi}{\partial v_{\mathbf{k}}^2}\,, \tag{6.80}$$

which can be rewritten using (6.75) as

$$\frac{\partial \xi}{\partial \eta} = \frac{1}{\psi_{\mathbf{k}}^{(0)}}\left(-\frac{1}{\gamma}\mathcal{G}_{AB}\frac{\partial \psi_{\mathbf{k}}^{(0)}}{\partial q_A}\frac{\partial \gamma}{\partial q_B} + \frac{1}{2}\mathcal{G}_{AB}\frac{\partial^2 \psi_{\mathbf{k}}^{(0)}}{\partial q_A \partial q_B} + \mathrm{i}\frac{\partial \psi_{\mathbf{k}}^{(0)}}{\partial v_{\mathbf{k}}}\frac{\partial \xi}{\partial v_{\mathbf{k}}} + \frac{\mathrm{i}\psi_{\mathbf{k}}^{(0)}}{2}\frac{\partial^2 \xi}{\partial v_{\mathbf{k}}^2}\right). \tag{6.81}$$

We define again the quantum-gravitationally corrected wave function $\psi_{\mathbf{k}}^{(1)}(q^A, v_{\mathbf{k}})$ for the perturbation modes as follows

$$\psi_{\mathbf{k}}^{(1)}(q^A, v_{\mathbf{k}}) := \psi_{\mathbf{k}}^{(0)}(q^A, v_{\mathbf{k}})\,\mathrm{e}^{\mathrm{i}\,m_{\mathrm{P}}^{-2}\,\xi(q^A, v_{\mathbf{k}})}\,, \tag{6.82}$$

and after some calculations, which are analogous to the ones presented in the previous chapter, we obtain

$$\mathrm{i}\frac{\partial}{\partial \eta}\psi_{\mathbf{k}}^{(1)} = \mathcal{H}_{\mathbf{k}}\psi_{\mathbf{k}}^{(1)} + \frac{\psi_{\mathbf{k}}^{(1)}}{m_{\mathrm{P}}^2\psi_{\mathbf{k}}^{(0)}}\left(\frac{1}{\gamma}\mathcal{G}_{AB}\frac{\partial \psi_{\mathbf{k}}^{(0)}}{\partial q_A}\frac{\partial \gamma}{\partial q_B} - \frac{1}{2}\mathcal{G}_{AB}\frac{\partial^2 \psi_{\mathbf{k}}^{(0)}}{\partial q_A \partial q_B}\right). \tag{6.83}$$

In the end, this leads to the quantum-gravitationally corrected Schrödinger equation

$$\boxed{\mathrm{i}\frac{\partial}{\partial \eta}\psi_{\mathbf{k}}^{(1)} = \mathcal{H}_{\mathbf{k}}\psi_{\mathbf{k}}^{(1)} - \frac{\psi_{\mathbf{k}}^{(1)}}{2\,m_{\mathrm{P}}^2\psi_{\mathbf{k}}^{(0)}}\left[\frac{\left(\mathcal{H}_{\mathbf{k}}\right)^2}{V}\psi_{\mathbf{k}}^{(0)} + \mathrm{i}\frac{\partial}{\partial \eta}\left(\frac{\mathcal{H}_{\mathbf{k}}}{V}\right)\psi_{\mathbf{k}}^{(0)}\right].} \tag{6.84}$$

6.3 Gaussian ansatz

As in the previous chapter, where we only considered scalar field perturbations, we also assume here that the scalar and tensor perturbations are in the ground state. In order to solve the Schrödinger equation (6.77), we therefore make the following Gaussian ansatz with normalization factor $\mathcal{N}_{\mathbf{k}}^{(0)}(\eta)$ and inverse Gaussian width $\Omega_{\mathbf{k}}^{(0)}(\eta)$

$$\psi_{\mathbf{k}}^{(0)}(\eta, v_{\mathbf{k}}) = \mathcal{N}_{\mathbf{k}}^{(0)}(\eta)\,\mathrm{e}^{-\frac{1}{2}\Omega_{\mathbf{k}}^{(0)}(\eta)\,v_{\mathbf{k}}^2}. \tag{6.85}$$

Inserting this ansatz into equation (6.77), collecting all terms that contain a factor of $v_{\mathbf{k}}^2$ or $v_{\mathbf{k}}^0$ and setting these equal to zero individually, leads to the following two equations

$$\mathrm{i}\mathcal{N}_{\mathbf{k}}^{\prime(0)}(\eta) = -\frac{1}{2}\mathcal{N}_{\mathbf{k}}^{(0)}(\eta)\,\Omega_{\mathbf{k}}^{(0)}(\eta)\,, \tag{6.86}$$

$$\mathrm{i}\,\Omega_{\mathbf{k}}^{\prime(0)}(\eta) = \left(\Omega_{\mathbf{k}}^{(0)}(\eta)\right)^2 - \omega_{\mathbf{k}}^2(\eta)\,. \tag{6.87}$$

We can find a solution to the first one immediately by considering the normalization of the wave function

$$\begin{aligned}\left|\psi_{\mathbf{k}}^{(0)}\right|^2 &= \left|\mathcal{N}_{\mathbf{k}}^{(0)}(\eta)\right|^2 \int\limits_{-\infty}^{\infty} \mathrm{d}v_{\mathbf{k}}\, \mathrm{e}^{-\frac{1}{2}\left[\Omega_{\mathbf{k}}^{*(0)}(\eta)+\Omega_{\mathbf{k}}^{(0)}(\eta)\right]v_{\mathbf{k}}^2} \\ &= \left|\mathcal{N}_{\mathbf{k}}^{(0)}(\eta)\right|^2 \int\limits_{-\infty}^{\infty} \mathrm{d}v_{\mathbf{k}}\, \mathrm{e}^{-\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}(\eta)\,v_{\mathbf{k}}^2} = \left|\mathcal{N}_{\mathbf{k}}^{(0)}(\eta)\right|^2 \frac{\sqrt{\pi}}{\sqrt{\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}(\eta)}} \stackrel{!}{=} 1\,. \end{aligned} \tag{6.88}$$

This leads to

$$|\mathcal{N}_{\mathbf{k}}^{(0)}(\eta)|^2 = \sqrt{\frac{\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}(\eta)}{\pi}}\,. \tag{6.89}$$

Inserting this solution into (6.86) yields

$$\mathfrak{Re}\,\Omega_{\mathbf{k}}^{\prime(0)}(\eta) = 2\,\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}(\eta)\,\mathfrak{Im}\,\Omega_{\mathbf{k}}^{(0)}(\eta)\,, \tag{6.90}$$

which is the same expression as taking the real part of equation (6.87).

For the quantum-gravitationally corrected Schrödinger equation, we make again the following ansatz as motivated in the previous chapter

$$\psi_{\mathbf{k}}^{(1)}(\eta, v_{\mathbf{k}}) = \left(\mathcal{N}_{\mathbf{k}}^{(0)}(\eta) + \frac{1}{m_{\mathrm{P}}^2}\mathcal{N}_{\mathbf{k}}^{(1)}(\eta)\right)\exp\left[-\frac{1}{2}\left(\Omega_{\mathbf{k}}^{(0)}(\eta) + \frac{1}{m_{\mathrm{P}}^2}\Omega_{\mathbf{k}}^{(1)}(\eta)\right)v_{\mathbf{k}}^2\right]. \tag{6.91}$$

Taking into account only the first part of the correction term in (6.84), we get the following differential equation for $\Omega_{\mathbf{k}}^{(1)}$:

$$\mathrm{i}\,\Omega_{\mathbf{k}}^{\prime(1)}(\eta) = 2\,\Omega_{k}^{(0)}(\eta)\left(\Omega_{\mathbf{k}}^{(1)}(\eta) - \frac{3}{4V(\eta)}\left[\left(\Omega_{\mathbf{k}}^{(0)}(\eta)\right)^2 - \omega_{\mathbf{k}}^2(\eta)\right]\right). \tag{6.92}$$

6.4 Derivation of the power spectra

6.4.1 The de Sitter case

In the previous chapter, we did our calculations assuming that our background is a de Sitter universe. Before discussing the more realistic quasi-de Sitter case, we shall consider the pure de Sitter case again due to its computational simplicity.

In order to use a de Sitter universe as our background, we set the scalar field ϕ to a constant value determined by the constant Hubble parameter H during inflation and the mass m of the scalar field

$$\phi = m_{\mathrm{P}}\,\tilde{\phi} = m_{\mathrm{P}}\,\frac{H}{m}\,. \tag{6.93}$$

We therefore have

$$\mathcal{V}(\phi) = \frac{1}{2}\,m^2\phi^2 = \frac{1}{2}\,m_{\mathrm{P}}^2 H^2\,. \tag{6.94}$$

Furthermore we can neglect the derivative with respect to ϕ, such that our master Wheeler–DeWitt equation simplifies to

$$\frac{1}{2}\left\{\mathrm{e}^{-2\alpha}\left[\frac{1}{m_{\mathrm{P}}^2}\,\frac{\partial^2}{\partial\alpha^2} + \mathrm{e}^{6\alpha}\,m_{\mathrm{P}}^2 H^2\right] - \frac{\partial^2}{\partial v_{\mathbf{k}}^2} + \omega_{\mathbf{k}}^2(\eta)\,v_{\mathbf{k}}^2\right\}\Psi(\alpha, v_{\mathbf{k}}) = 0\,. \tag{6.95}$$

The quantity $\omega_{\mathbf{k}}^2(\eta)$ is given for both scalar and tensor perturbations as

$$\omega_{\mathbf{k}}^2(\eta) = k^2 - \frac{2}{\eta^2}\,. \tag{6.96}$$

Hence, we will treat both perturbations at once up to the point where we calculate the power spectra.

The Hamilton–Jacobi equation (6.71) reads

$$\left(\frac{\partial S_0}{\partial\alpha}\right)^2 - \mathrm{e}^{6\alpha}H^2 = 0\,, \tag{6.97}$$

and its solution is given by

$$S_0(\alpha) = \pm\,\frac{1}{3}\,\mathrm{e}^{3\alpha}H\,. \tag{6.98}$$

The definition of the WKB conformal time therefore takes the form

$$\frac{\partial}{\partial\eta} = -\,\mathrm{e}^{-2\alpha}\,\frac{\partial S_0}{\partial\alpha}\,\frac{\partial}{\partial\alpha} = \pm\,\mathrm{e}^{\alpha}H\,\frac{\partial}{\partial\alpha}\,. \tag{6.99}$$

In order to obtain the usual definition of time, we have to choose the minus sign in equation (6.98)

$$S_0(\alpha) = -\,\frac{1}{3}\,\mathrm{e}^{3\alpha}H \quad\Rightarrow\quad \frac{\partial}{\partial\eta} = \mathrm{e}^{\alpha}H\,\frac{\partial}{\partial\alpha}\,. \tag{6.100}$$

The Schrödinger equation (6.77) takes the form

$$\mathrm{i}\,\frac{\partial}{\partial\eta}\,\psi_{\mathbf{k}}^{(0)} = \frac{1}{2}\left[-\frac{\partial^2}{\partial v_{\mathbf{k}}^2} + \left(k^2 - \frac{2}{\eta^2}\right)v_{\mathbf{k}}^2\right]\psi_{\mathbf{k}}^{(0)}\,. \tag{6.101}$$

With the Gaussian ansatz (6.85)

$$\psi_{\mathbf{k}}^{(0)}(\eta, v_{\mathbf{k}}) = \mathcal{N}_{\mathbf{k}}^{(0)}(\eta)\,\mathrm{e}^{-\frac{1}{2}\Omega_{\mathbf{k}}^{(0)}(\eta)\,v_{\mathbf{k}}^2}\,, \tag{6.102}$$

we have to solve the following differential equation

$$\mathrm{i}\,\Omega_{\mathbf{k}}^{\prime(0)}(\eta) = \left(\Omega_{\mathbf{k}}^{(0)}(\eta)\right)^2 - k^2 + \frac{2}{\eta^2}\,. \tag{6.103}$$

The corresponding equation from our previous calculation reads

$$\mathrm{i}\,\dot{\Omega}_{\mathbf{k},\mathrm{old}}^{(0)}(t) = \mathrm{e}^{-3Ht}\left(\Omega_{\mathbf{k},\mathrm{old}}^{(0)}(t)\right)^2 - \mathrm{e}^{Ht}\,k^2\,. \tag{6.104}$$

In order to transform the two equations into each other, one has to perform the following transformation

$$\Omega_{\mathbf{k}}^{(0)}(\eta) = a^2\,\Omega_{\mathbf{k},\mathrm{old}}^{(0)}(t) - \mathrm{i}\,aH \;= \frac{\Omega_{\mathbf{k},\mathrm{old}}^{(0)}(t)}{H^2\eta^2} + \frac{\mathrm{i}}{\eta}\,. \tag{6.105}$$

We see that there is an additional imaginary term i/η. This term appears because in (6.30) we multiplied the perturbation variable with the scale factor before quantization. Such a term is also discussed in [86], where it is shown that it does not influence the classical result. We should, however, not expect that this also holds for the quantum-gravitational corrections. Due to the inclusion of the scale factor, the full quantum theory we are discussing here is different from the one discussed in chapter 5.

While equation (6.103) can be solved directly by integration, a more elegant way to find a solution, which is the one normally taken, is to use the ansatz

$$\Omega_{\mathbf{k}}^{(0)}(\eta) = -\,\mathrm{i}\,\frac{y'(\eta)}{y(\eta)}\,, \tag{6.106}$$

which leads to the following equation for both the scalar and tensor modes

$$y_{\mathbf{k}}''(\eta) + \left(k^2 - \frac{2}{\eta^2}\right)y_{\mathbf{k}}(\eta) = 0\,. \tag{6.107}$$

This equation can be solved by

$$y_{\mathbf{k}}(\eta) = \sqrt{\frac{2}{k\pi}}\left\{c_1\left[\frac{\sin(k\eta)}{k\eta} - \cos(k\eta)\right] + c_2\left[-\frac{\cos(k\eta)}{k\eta} - \sin(k\eta)\right]\right\}. \tag{6.108}$$

In order to obtain the Bunch–Davies vacuum for $\eta \to -\infty$, we have to set

$$c_1 = -1\,, \quad c_2 = -\mathrm{i}\,, \tag{6.109}$$

which leads to

$$y_{\mathbf{k}}(\eta) = \sqrt{\frac{2}{\pi}}\,\frac{1}{\sqrt{k}}\,\mathrm{e}^{\mathrm{i}k\eta}\left(1+\frac{\mathrm{i}}{k\eta}\right) \tag{6.110}$$

and consequently

$$\Omega_{\mathbf{k}}^{(0)}(\eta) = -\,\mathrm{i}\,\frac{y'(\eta)}{y(\eta)} = \frac{k^2\eta}{\mathrm{i}+k\eta} + \frac{\mathrm{i}}{\eta} = \frac{k^2\eta\,(k\eta-\mathrm{i})}{k^2\eta^2+1} + \frac{\mathrm{i}}{\eta}\,. \tag{6.111}$$

For later convenience, we rewrite this result in terms of the dimensionless variable

$$\xi := \frac{k}{Ha} = -\,k\eta\,, \tag{6.112}$$

which leads to

$$\Omega_{\mathbf{k}}^{(0)}(\xi) = \frac{k\,\xi}{\xi-\mathrm{i}} - \frac{\mathrm{i}\,k}{\xi} = \frac{k\,\xi\,(\xi+\mathrm{i})}{\xi^2+1} - \frac{\mathrm{i}\,k}{\xi} = \frac{k\,\xi^2}{\xi^2+1} + \mathrm{i}\left(\frac{k\,\xi}{\xi^2+1} - \frac{k}{\xi}\right). \tag{6.113}$$

Compared to our previous result

$$\Omega_{\mathbf{k},\mathrm{old}}^{(0)}(\eta) = \frac{k^2}{H^2\eta}\,\frac{1}{\mathrm{i}+k\eta} = \frac{k^3}{H^2\xi}\,\frac{1}{\xi-\mathrm{i}}\,, \tag{6.114}$$

we can confirm that the transformation (6.105) yields the new result as well.

Power spectrum of the scalar perturbations

In order to derive the power spectrum of the scalar perturbations in the standard formalism (cf. e. g. [86]), we have to consider the two-point correlation function

$$\left\langle \psi_{\mathbf{k}} \left| \hat{v}(\eta,\mathbf{x})\hat{v}(\eta,\mathbf{x}+\mathbf{r}) \right| \psi_{\mathbf{k}} \right\rangle = \int \prod_{\mathbf{k}} \mathrm{d}v_{\mathbf{k}}^{\mathrm{R}}\mathrm{d}v_{\mathbf{k}}^{\mathrm{I}}\,\psi_{\mathbf{k}}^{*}(v_{\mathbf{k}}^{\mathrm{R}},v_{\mathbf{k}}^{\mathrm{I}})\,v(\eta,\mathbf{x})\,v(\eta,\mathbf{x}+\mathbf{r})\,\psi_{\mathbf{k}}(v_{\mathbf{k}}^{\mathrm{R}},v_{\mathbf{k}}^{\mathrm{I}})\,. \tag{6.115}$$

One can show that this can be simplified to

$$\left\langle \psi_{\mathbf{k}} \left| \hat{v}(\eta,\mathbf{x})\hat{v}(\eta,\mathbf{x}+\mathbf{r}) \right| \psi_{\mathbf{k}} \right\rangle = \frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{p}\,\mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}}\,\frac{1}{2\,\mathfrak{Re}\,\Omega_{\mathbf{p}}^{(0)}}\,. \tag{6.116}$$

$\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}$ can be rewritten as

$$\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)} = -\,\frac{\mathrm{i}}{2}\,\frac{W}{|y_{\mathbf{k}}|^2}\,, \tag{6.117}$$

where

$$W = y'_{\mathbf{k}} y^*_{\mathbf{k}} - y'^*_{\mathbf{k}} y_{\mathbf{k}} \,. \tag{6.118}$$

In the Heisenberg quantization the Wronskian W has to be defined as being equal to i, in the Schrödinger quantization the value is not fixed and also does not influence any observable quantity. We set it to i nevertheless for convenience. Hence, we arrive at

$$\left\langle \psi_{\mathbf{k}} \left| \hat{v}(\eta,\mathbf{x})\hat{v}(\eta,\mathbf{x}+\mathbf{r}) \right| \psi_{\mathbf{k}} \right\rangle = \frac{1}{(2\pi)^3} \int \mathrm{d}\mathbf{p}\, \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}} \frac{\mathrm{i}}{W} |y_{\mathbf{p}}|^2 = \frac{1}{2\pi^2} \int_0^{+\infty} \frac{\mathrm{d}p}{p} \frac{\sin(pr)}{pr} p^3 \, |y_{\mathbf{p}}|^2 \tag{6.119}$$

and we can define the power spectrum as

$$\mathcal{P}_v^{(0)}(k) = \frac{k^3}{2\pi^2} \, |y_{\mathbf{k}}|^2 \,. \tag{6.120}$$

Doing the same calculation in order to obtain the two-point correlation function of the Fourier transformed variable v, we arrive at

$$\left\langle \psi_{\mathbf{k}} \left| \hat{v}_{\mathbf{k}} \hat{v}^*_{\mathbf{p}} \right| \psi_{\mathbf{k}} \right\rangle = \int \prod_{\mathbf{q}} \mathrm{d}v^{\mathrm{R}}_{\mathbf{q}} \, \mathrm{d}v^{\mathrm{I}}_{\mathbf{q}} \psi^*_{\mathbf{q}} \, \hat{v}_{\mathbf{k}} \, \hat{v}^*_{\mathbf{p}} \, \psi_{\mathbf{q}} \,, \tag{6.121}$$

which leads to

$$\left\langle \psi_{\mathbf{k}} \left| \hat{v}_{\mathbf{k}} \hat{v}^*_{\mathbf{p}} \right| \psi_{\mathbf{k}} \right\rangle = \frac{2\pi^2}{k^3} \, \mathcal{P}_v^{(0)}(k) \, \delta(\mathbf{k}-\mathbf{p}) \,. \tag{6.122}$$

The temperature anisotropies of the CMB are directly related to the curvature perturbation ζ defined by

$$\zeta = \frac{2}{3} \frac{\mathcal{H}^{-1}\Phi'_{\mathrm{B}} + \Phi_{\mathrm{B}}}{1+w} + \Phi_{\mathrm{B}} \,, \tag{6.123}$$

where Φ_{B} is the Bardeen potential and w is the barotropic index in the equation of state $P = w\rho$. In the matter-dominated era, during which recombination occurs, and considering only perturbations on large scales, this equation simplifies to

$$\zeta \simeq \frac{5}{3} \, \Phi_{\mathrm{B}} \,. \tag{6.124}$$

In terms of the Mukhanov–Sasaki variable, ζ takes the form

$$\zeta_{\mathbf{k}} = \frac{1}{a\sqrt{2\epsilon}} \frac{v_{\mathbf{k}}}{M_{\mathrm{P}}} \tag{6.125}$$

and the two-point correlation function reads

$$\left\langle \psi_{\mathbf{k}} \left| \hat{\zeta}_{\mathbf{k}} \, \hat{\zeta}^*_{\mathbf{p}} \right| \psi_{\mathbf{k}} \right\rangle = \frac{1}{2a^2 \, M_{\mathrm{P}}^2 \epsilon} \frac{2\pi^2}{k^3} \, \mathcal{P}_v^{(0)}(k) \, \delta\left(\mathbf{k}-\mathbf{p}\right) , \tag{6.126}$$

which we can use to define the power spectrum of the curvature perturbations

$$\mathcal{P}_\zeta^{(0)}(k) = \frac{1}{2a^2 M_\mathrm{P}^2 \epsilon} \mathcal{P}_v^{(0)}(k) = \frac{1}{2a^2 M_\mathrm{P}^2 \epsilon} \frac{k^3}{2\pi^2} |y_\mathbf{k}|^2 = \frac{1}{2a^2 M_\mathrm{P}^2 \epsilon} \frac{k^3}{2\pi^2} \frac{1}{2\mathfrak{Re}\,\Omega_\mathbf{k}^{(0)}} . \tag{6.127}$$

Before we insert the real part of our solution (6.111), we have to take the limit $-k\eta = \xi \to 0$, which is the limit of superhorizon scales. It leads to

$$\mathfrak{Re}\,\Omega_\mathbf{k}^{(0)}(\eta) = \frac{k^3\eta^2}{k^2\eta^2 + 1} \longrightarrow k^3\eta^2 . \tag{6.128}$$

or equivalently

$$\mathfrak{Re}\,\Omega_\mathbf{k}^{(0)}(\xi) = \frac{k\,\xi^2}{\xi^2 + 1} \longrightarrow k\,\xi^2 . \tag{6.129}$$

Inserting this expression into (6.127) together with the relation

$$a = -\frac{1}{H\eta} = \frac{k}{H\xi} \tag{6.130}$$

leads to

$$\mathcal{P}_\zeta^{(0)}(k) = \frac{H^2\eta^2}{2\,M_\mathrm{P}^2\epsilon} \frac{k^3}{2\pi^2} \frac{1}{2k^3\eta^2} = \frac{H^2\xi^2}{2\,M_\mathrm{P}^2\epsilon\,k^2} \frac{k^3}{2\pi^2} \frac{1}{2k\,\xi^2} , \tag{6.131}$$

such that we end up with the following power spectrum for the scalar sector

$$\mathcal{P}_\mathrm{S}^{(0)}(k) = \mathcal{P}_\zeta^{(0)}(k) = \left.\frac{H^2}{8\pi^2 M_\mathrm{P}^2 \epsilon}\right|_{k=Ha} . \tag{6.132}$$

Due to the appearance of the slow-roll parameter ϵ, the final expression has to be evaluated at the point in time, at which a specific mode k reenters the Hubble radius, which is $k = Ha$ (or $\xi = 1$). This makes the power spectrum (6.132) become k-dependent. We thus have obtained a power spectrum that is almost scale-independent, but tilted due to the fact that the ϵ appears and that we evaluate the expression at different points in time for each mode. Hence, even though our calculation was done in the pure de Sitter case, we have obtained a result that describes effectively the quasi-de Sitter case by letting ϵ, which we have considered to be constant in our calculations, vary again.

Power spectrum of the tensor perturbations

For the tensor modes, the power spectrum for the Mukhanov–Sasaki variable v is also given by

$$\mathcal{P}_v^{(0)}(k) = \frac{k^3}{2\pi^2}\,|y_{\mathbf{k}}|^2 = \frac{k^3}{2\pi^2}\,\frac{1}{2\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}}\,, \tag{6.133}$$

but the relevant physical variable we have to evaluate reads

$$h_{\mathbf{k}} = \frac{2}{a}\frac{v_{\mathbf{k}}}{M_{\mathrm{P}}}\,, \tag{6.134}$$

such that we have for a single polarization

$$\mathcal{P}_h^{(0)}(k) = \frac{4}{a^2 M_{\mathrm{P}}^2}\mathcal{P}_v^{(0)}(k) = \frac{4}{a^2 M_{\mathrm{P}}^2}\,\frac{k^3}{2\pi^2}\,|y_{\mathbf{k}}|^2 = \frac{4}{a^2 M_{\mathrm{P}}^2}\,\frac{k^3}{2\pi^2}\,\frac{1}{2\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}}\,. \tag{6.135}$$

If we then insert the solution (6.111) we found for $\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}$ and take the superhorizon limit $-k\eta = \xi \to 0$, i.e. equation (6.128), we obtain

$$\mathcal{P}_h^{(0)}(k) = \frac{4H^2\eta^2}{M_{\mathrm{P}}^2}\,\frac{k^3}{2\pi^2}\,\frac{1}{2k^3\eta^2} = \frac{4H^2\xi^2}{M_{\mathrm{P}}^2 k^2}\,\frac{k^3}{2\pi^2}\,\frac{1}{2k\,\xi^2} \tag{6.136}$$

and the power spectrum for one polarization of the tensor perturbations reads

$$\mathcal{P}_h^{(0)}(k) = \frac{H^2}{\pi^2 M_{\mathrm{P}}^2}\,. \tag{6.137}$$

Since we have two polarizations for gravitational waves, we have to multiply the previous expression by two, such that the final power spectrum for tensor perturbations in the de Sitter case is given by

$$\mathcal{P}_{\mathrm{T}}^{(0)}(k) = 2\,\mathcal{P}_h^{(0)}(k) = \frac{2H^2}{\pi^2 M_{\mathrm{P}}^2}\,. \tag{6.138}$$

We thus see that we recover the usual tensor-to-scalar ratio r

$$r^{(0)} = \frac{\mathcal{P}_{\mathrm{T}}^{(0)}(k)}{\mathcal{P}_{\mathrm{S}}^{(0)}(k)} = 16\,\epsilon\,. \tag{6.139}$$

6.4.2 The slow-roll case

Since the pure de Sitter case is often too restrictive to make contact with observations, we shall now regard slow-roll inflation, for which we assume

$$\dot{\phi}^2 \ll \mathcal{V}\,, \quad \ddot{\phi} \ll 3H\dot{\phi}\,. \tag{6.140}$$

The first condition allows us to neglect the ϕ-kinetic term in our Wheeler–DeWitt equation. We use the slow-roll parameters

$$\epsilon = -\frac{\dot{H}}{H^2} = 1 - \frac{\mathcal{H}'}{\mathcal{H}^2} \tag{6.141}$$

and

$$\delta = \epsilon - \frac{\dot{\epsilon}}{2H\epsilon} = -\frac{\ddot{\phi}}{H\dot{\phi}}\,. \tag{6.142}$$

From the relation

$$\frac{\ddot{a}}{a} = H^2\,(1-\epsilon)\,, \tag{6.143}$$

one can see that ϵ must be smaller than 1 in order for inflation to happen, for slow-roll inflation the condition has to be further restricted to $\epsilon \ll 1$ and $\delta \ll 1$. In this case, ϵ and δ can also be expressed in terms of

$$\epsilon_V = \frac{M_{\mathrm{P}}^2}{2\mathcal{V}^2}\left(\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}\phi}\right)^2 \tag{6.144}$$

and

$$\eta_V = \frac{M_{\mathrm{P}}^2}{\mathcal{V}}\left(\frac{\mathrm{d}^2\mathcal{V}}{\mathrm{d}\phi^2}\right) \tag{6.145}$$

as

$$\epsilon = \epsilon_V\,, \qquad \delta = \eta_V - \epsilon_V\,. \tag{6.146}$$

The conformal time can then be expressed as

$$\eta = -\frac{1}{Ha}\left[\frac{1}{1-\epsilon} - 2\epsilon\,(\epsilon-\delta)\right] = -\frac{1}{Ha}\,(1+\epsilon) + \mathcal{O}\Big(2^{\mathrm{nd}}\Big)\,, \tag{6.147}$$

where we have introduced the short-hand notation

$$\mathcal{O}\Big(2^{\mathrm{nd}}\Big) := \mathcal{O}\Big(\epsilon^2, \delta^2, \epsilon\delta\Big)\,. \tag{6.148}$$

This relation means that we have to be careful when replacing η by the dimensionless variable ξ, which we continue to define as

$$\xi = \frac{k}{Ha} = -k\,\eta\,(1+\epsilon) \quad \Leftrightarrow \quad \eta = -\frac{\xi}{k}\,(1-\epsilon)\,. \tag{6.149}$$

We can realize a generic slow-roll model by using the auxiliary potential

$$\mathcal{V}_\epsilon = \frac{1}{2}\, m_\mathrm{P}^2 H^2 (1-\epsilon)^2 \,. \tag{6.150}$$

Neglecting the derivative with respect to ϕ, our master Wheeler–DeWitt equation is given by

$$\frac{1}{2}\left\{ \mathrm{e}^{-2\alpha}\left[\frac{1}{m_\mathrm{P}^2}\frac{\partial^2}{\partial\alpha^2} + \mathrm{e}^{6\alpha}\, m_\mathrm{P}^2 H^2 (1-\epsilon)^2\right] - \frac{\partial^2}{\partial v_\mathbf{k}^2} + \omega_\mathbf{k}^2(\eta)\, v_\mathbf{k}^2 \right\}\Psi(\alpha, v_\mathbf{k}) = 0\,, \tag{6.151}$$

where the quantity $\omega_\mathbf{k}^2(\eta)$ reads for scalar perturbations (see e.g. [92])

$${}^\mathrm{S}\omega_\mathbf{k}^2(\eta) = k^2 - \frac{2+6\epsilon-3\delta}{\eta^2} \tag{6.152}$$

and for tensor perturbations

$${}^\mathrm{T}\omega_\mathbf{k}^2(\eta) = k^2 - \frac{2+3\epsilon}{\eta^2}\,. \tag{6.153}$$

Setting $\delta = \epsilon$ converts the equation for scalar perturbations into the one for tensor perturbations. Therefore we are going to perform all calculations here only for scalar perturbations and afterwards move to tensor perturbations using this relation.

The Hamilton–Jacobi equation (6.71) is given by

$$\left(\frac{\partial S_0}{\partial\alpha}\right)^2 - \mathrm{e}^{6\alpha} H^2 (1-\epsilon)^2 = 0\,, \tag{6.154}$$

such that its solution reads

$$S_0(\alpha) = \pm\frac{1}{3}\,\mathrm{e}^{3\alpha} H (1-\epsilon)\,. \tag{6.155}$$

Using the negative solution, the WKB conformal time is – by construction – consistent with (6.147)

$$\frac{\partial}{\partial\eta} = -\,\mathrm{e}^{-2\alpha}\frac{\partial S_0}{\partial\alpha}\frac{\partial}{\partial\alpha} = \mathrm{e}^{\alpha} H (1-\epsilon)\frac{\partial}{\partial\alpha}\,. \tag{6.156}$$

We can subsequently write out the Schrödinger equation (6.77) for the scalar modes, which is given by

$$\mathrm{i}\,\frac{\partial}{\partial\eta}\,\psi_\mathbf{k}^{(0)} = \frac{1}{2}\left[-\frac{\partial^2}{\partial v_\mathbf{k}^2} + \left(k^2 - \frac{2+6\epsilon-3\delta}{\eta^2}\right) v_\mathbf{k}^2\right]\psi_\mathbf{k}^{(0)}\,. \tag{6.157}$$

As it has been presented, for instance, in [92], such a slow-roll model can be realized by considering a *power-law inflation* model, which is a a particularly elegant way to analyze slow-roll inflation because it leads to analytically solvable models.

Power-law inflation describes inflationary models whose scale factor behaves like

$$a(t) = a_0\, t^p\,, \tag{6.158}$$

where p is a constant, hence the name. This translates with the definition

$$1 + \beta = \frac{p}{1+p} \tag{6.159}$$

to

$$a = a_0\, |\eta|^{1+\beta}\,. \tag{6.160}$$

The slow-roll parameters are constant in this model

$$\epsilon = \delta = \frac{1}{p} \tag{6.161}$$

and the evolution of the universe is therefore exactly given by

$$a(\eta) = -\frac{1}{1-\epsilon}\frac{1}{H\eta} = -\frac{1}{H\eta}(1+\epsilon) + \mathcal{O}\left(2^{\text{nd}}\right). \tag{6.162}$$

We set

$$\beta := -2 - 2\epsilon + \delta\,, \tag{6.163}$$

and require $\beta \lesssim -2$, such that we have

$$\beta(\beta+1) = 2 + 6\epsilon - 3\delta + \mathcal{O}\left(2^{\text{nd}}\right). \tag{6.164}$$

In this way, our Schrödinger equation (6.157) becomes

$$\mathrm{i}\,\frac{\partial}{\partial\eta}\,\psi^{(0)}_{\mathbf{k}} = \frac{1}{2}\left[-\frac{\partial^2}{\partial v_{\mathbf{k}}^2} + \left(k^2 - \frac{\beta(\beta+1)}{\eta^2}\right) v_{\mathbf{k}}^2\right]\psi^{(0)}_{\mathbf{k}} \tag{6.165}$$

and we can follow the analysis presented in [86]. With the Gaussian ansatz (6.85)

$$\psi^{(0)}_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = \mathcal{N}^{(0)}_{\mathbf{k}}(\eta)\,\mathrm{e}^{-\frac{1}{2}\,\Omega^{(0)}_{\mathbf{k}}(\eta)\, v_{\mathbf{k}}^2}\,, \tag{6.166}$$

we find the following differential equation, which we have to solve

$$\mathrm{i}\,\Omega'^{(0)}_{\mathbf{k}}(\eta) = \left(\Omega^{(0)}_{\mathbf{k}}(\eta)\right)^2 - k^2 + \frac{\beta(\beta+1)}{\eta^2}\,. \tag{6.167}$$

Using again the ansatz

$$\Omega_{\mathbf{k}}^{(0)}(\eta) = -\,\mathrm{i}\,\frac{y'(\eta)}{y(\eta)} \tag{6.168}$$

leads to the following equation for the scalar modes

$$y_{\mathbf{k}}''(\eta) + \left(k^2 - \frac{\beta(\beta+1)}{\eta^2}\right) y_{\mathbf{k}}(\eta) = 0\,. \tag{6.169}$$

This equation can be solved in terms of the Bessel functions J_ν as follows [86]

$$y_{\mathbf{k}} = (-k\eta)^{1/2}\left[c_{\mathbf{k},1}\,J_{\beta+1/2}(-k\eta) + c_{\mathbf{k},2}\,J_{-(\beta+1/2)}(-k\eta)\right]. \tag{6.170}$$

In order to obtain the Bunch–Davies vacuum for $\eta \to \infty$, we have to set

$$c_{\mathbf{k},1} = -\,c_{\mathbf{k},2}\,\mathrm{e}^{\mathrm{i}\pi(\beta+1/2)}, \quad c_{\mathbf{k},2} = \frac{\mathrm{i}}{2}\sqrt{\frac{\pi}{k}}\,\frac{\mathrm{e}^{-\mathrm{i}\pi/4-\mathrm{i}\pi(\beta+1/2)/2}}{\sin[\pi(\beta+1/2)]}\,. \tag{6.171}$$

For $\Omega_{\mathbf{k}}^{(0)}(\eta)$, we then get then in the superhorizon limit $-k\eta \to 0$ [86]

$$\begin{aligned}\Omega_{\mathbf{k}}^{(0)}(\eta) = {}& -\frac{\mathrm{i}}{\eta}(1+\beta) - \frac{\mathrm{i}\,k}{2(\beta+3/2)}(-k\eta) - \frac{\mathrm{i}\,k}{\pi}\,2^{2\beta+1}\sin(2\pi\beta)\,\Gamma^2\!\left(\beta+\frac{3}{2}\right)(-k\eta)^{-2\beta-2} \\ &+ \frac{k\,\pi\,2^{2\beta+2}}{\Gamma^2(-\beta-1/2)}(-k\eta)^{-2\beta-2} + \cdots,\end{aligned} \tag{6.172}$$

such that we obtain for the real part of $\Omega_{\mathbf{k}}^{(0)}(\eta)$

$$\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}(\eta) = \frac{k\,\pi\,2^{2\beta+2}}{\Gamma^2(-\beta-1/2)}\,(-k\eta)^{-2\beta-2}\,. \tag{6.173}$$

Expressed in terms of the slow-roll parameters ϵ and δ, this expression reads

$$\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}(\eta) = \frac{k\,\pi\,2^{-2-4\epsilon+2\delta}}{\Gamma^2(3/2+2\epsilon-\delta)}\,(-k\eta)^{4\epsilon-2\delta+2}\,. \tag{6.174}$$

For the inverse that appears in the expression for the power spectrum, we get

$$\frac{1}{\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}(\eta)} = \frac{1}{k\,\pi}\,2^{2+4\epsilon-2\delta}\,\Gamma^2\!\left(\frac{3}{2}+2\epsilon-\delta\right)(-k\eta)^{-4\epsilon+2\delta-2}\,. \tag{6.175}$$

We can expand the appearing Gamma function as follows [1]

$$\Gamma\!\left(\frac{3}{2}+2\epsilon-\delta\right) = \frac{\sqrt{\pi}}{2}\left(1+(2\epsilon-\delta)\,\digamma\!\left(\frac{3}{2}\right)+\mathcal{O}\!\left(2^{\mathrm{nd}}\right)\right), \tag{6.176}$$

where $\digamma$ is the digamma function with

$$\digamma\!\left(\frac{3}{2}\right) = 2-\gamma_{\mathrm{E}}-2\ln(2) \simeq 0.03649\,, \tag{6.177}$$

and $\gamma_{\rm E} \simeq 0.5772$ is the Euler–Mascheroni constant. For $2^{4\epsilon-2\delta}$, we can write

$$2^{4\epsilon-2\delta} = 1 + (2\epsilon - \delta)\, 2\ln(2)\,. \tag{6.178}$$

Hence, neglecting terms of second order in the slow-roll parameters we end up with

$$\begin{aligned}
\frac{1}{\Re\mathfrak{e}\,\Omega_{\mathbf{k}}^{(0)}} &= \frac{4}{k\,\pi}\left[1 + (2\epsilon - \delta)\, 2\ln(2)\right] \frac{\pi}{4}\left[1 + (2\epsilon - \delta)\left(2 - \gamma_{\rm E} - 2\ln(2)\right)\right]^2 (-k\eta)^{-4\epsilon+2\delta-2} \\
&= \frac{1}{k}\left[1 + (2\epsilon - \delta)\, 2\ln(2)\right]\left[1 + 2(2\epsilon - \delta)\left(2 - \gamma_{\rm E} - 2\ln(2)\right)\right](-k\eta)^{-4\epsilon+2\delta-2} \\
&= \frac{1}{k^3\eta^2}\left[1 + (2\epsilon - \delta)\left(4 - 2\gamma_{\rm E} - 2\ln(2)\right)\right](-k\eta)^{-4\epsilon+2\delta}\,.
\end{aligned} \tag{6.179}$$

Using

$$\frac{1}{a^2} = (1-\epsilon)^2 H^2\eta^2 = (1-2\epsilon)H^2\eta^2 + \mathcal{O}\left(2^{\rm nd}\right), \tag{6.180}$$

the power spectrum reads

$$\begin{aligned}
\mathcal{P}_\zeta^{(0)}(k) &= \frac{1}{2a^2 M_{\rm P}^2\epsilon}\mathcal{P}_v^{(0)}(k) = \frac{1}{2a^2 M_{\rm P}^2\epsilon}\,\frac{k^3}{2\pi^2}\,\frac{1}{2\Re\mathfrak{e}\,\Omega_{\mathbf{k}}^{(0)}} \\
&= \frac{H^2}{2M_{\rm P}^2\epsilon}\,\frac{k^3\eta^2}{2\pi^2}\,\frac{1-2\epsilon}{2\Re\mathfrak{e}\,\Omega_{\mathbf{k}}^{(0)}} \\
&= \frac{H^2}{8\pi^2 M_{\rm P}^2\epsilon}(1-2\epsilon)\left[1 + (2\epsilon - \delta)\left(4 - 2\gamma_{\rm E} - 2\ln(2)\right)\right](-k\eta)^{-4\epsilon+2\delta} \\
&= \frac{H^2}{8\pi^2 M_{\rm P}^2\epsilon}\left[1 - 2\epsilon + (2\epsilon - \delta)\left(4 - 2\gamma_{\rm E} - 2\ln(2)\right)\right](-k\eta)^{-4\epsilon+2\delta}\,.
\end{aligned} \tag{6.181}$$

For $(-k\eta)^{-4\epsilon+2\delta}$, we can write

$$\begin{aligned}
(-k\eta)^{-4\epsilon+2\delta} &= \left(\frac{k\,(1+\epsilon)}{aH}\right)^{-4\epsilon+2\delta} \\
&= \left[1 + (-4\epsilon + 2\delta)\epsilon\right]\left[1 + (-4\epsilon + 2\delta)\ln\left(\frac{k}{aH}\right)\right] \\
&= 1 + (-4\epsilon + 2\delta)\ln\left(\frac{k}{aH}\right).
\end{aligned} \tag{6.182}$$

Therefore we can write out the power spectrum of the scalar perturbations as

$$\begin{aligned}
\mathcal{P}_{\rm S}^{(0)}(k) &= \frac{H^2}{8\pi^2 M_{\rm P}^2\epsilon}\left[1 - 2\epsilon + (2\epsilon - \delta)\left(4 - 2\gamma_{\rm E} - 2\ln(2)\right)\right]\left[1 + (-4\epsilon + 2\delta)\ln\left(\frac{k}{aH}\right)\right] \\
&= \frac{H^2}{8\pi^2 M_{\rm P}^2\epsilon}\left[1 - 2\epsilon + (2\epsilon - \delta)\left(4 - 2\gamma_{\rm E} - 2\ln(2)\right) + (-4\epsilon + 2\delta)\ln\left(\frac{k}{aH}\right)\right].
\end{aligned} \tag{6.183}$$

We can use this expression to define the spectral index n_{S} of the scalar perturbations by

$$n_{\mathrm{S}} - 1 := \frac{\mathrm{d}\ln \mathcal{P}_{\mathrm{S}}^{(0)}}{\mathrm{d}\ln k} \simeq -4\epsilon + 2\delta\,. \tag{6.184}$$

Note that we get an equivalent form of the power spectrum by evaluating (6.183) at the point $k = Ha$

$$\mathcal{P}_{\mathrm{S}}^{(0)}(k) = \frac{H^2}{8\pi^2 M_{\mathrm{P}}^2 \epsilon} \left[1 - 2\epsilon + (2\epsilon - \delta)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)\right]\Big|_{k=Ha}\,. \tag{6.185}$$

In order to derive the power spectrum for the tensor modes, we make a shortcut via the relation

$$\mathcal{P}_{\mathrm{T}}^{(0)}(k) = 16\,\epsilon\,\mathcal{P}_{\mathrm{S}}^{(0)}(k)\Big|_{\delta=\epsilon}\,. \tag{6.186}$$

Thus we immediately obtain from (6.183)

$$\mathcal{P}_{\mathrm{T}}^{(0)}(k) = \frac{2H^2}{\pi^2 M_{\mathrm{P}}^2} \left[1 - 2\epsilon + \epsilon\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right) - 2\epsilon\,\ln\left(\frac{k}{aH}\right)\right], \tag{6.187}$$

which we can use to derive the spectral index for the tensor perturbations

$$n_{\mathrm{T}} - 1 := \frac{\mathrm{d}\ln \mathcal{P}_{\mathrm{T}}^{(0)}}{\mathrm{d}\ln k} \simeq -2\epsilon\,. \tag{6.188}$$

Equivalently, we can write

$$\mathcal{P}_{\mathrm{T}}^{(0)}(k) = \frac{2H^2}{\pi^2 M_{\mathrm{P}}^2} \left[1 - 2\epsilon + \epsilon\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)\right]\Big|_{k=Ha}\,. \tag{6.189}$$

6.5 Quantum-gravitational corrections

6.5.1 The de Sitter case

In order to calculate quantum-gravitational corrections to the power spectra found in the previous section, we have to solve the differential equation

$$\mathrm{i}\,\Omega_{\mathbf{k}}^{\prime(1)}(\eta) = 2\,\Omega_{\mathbf{k}}^{(0)}(\eta)\left(\Omega_{\mathbf{k}}^{(1)}(\eta) - \frac{3}{4V(\eta)}\left[\left(\Omega_{\mathbf{k}}^{(0)}(\eta)\right)^2 - \omega_{\mathbf{k}}^2(\eta)\right]\right). \tag{6.190}$$

In the de Sitter case, $V(\eta)$ is given by

$$V(\eta) = \mathrm{e}^{4\alpha} H^2 = \frac{1}{H^2\eta^4}\,. \tag{6.191}$$

Using our result (6.111), we obtain

$$\mathrm{i}\,\Omega_{\mathbf{k}}^{\prime(1)}(\eta) = 2\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right)\left(\Omega_{\mathbf{k}}^{(1)}(\eta)-\frac{3H^2\eta^4}{4}\left[\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right)^2-\left(k^2-\frac{2}{\eta^2}\right)\right]\right). \tag{6.192}$$

Expressed in terms of the dimensionless quantity $\xi = -k\eta$, this leads to

$$\begin{aligned}\frac{\mathrm{d}\Omega_{\mathbf{k}}^{(1)}}{\mathrm{d}\xi} &= \frac{2\,\mathrm{i}}{k}\left(\frac{k\,\xi}{\xi-\mathrm{i}}-\frac{\mathrm{i}\,k}{\xi}\right)\left(\Omega_{\mathbf{k}}^{(1)}(\eta)-\frac{3H^2\xi^4}{4k^4}\left[\left(\frac{k\,\xi}{\xi-\mathrm{i}}-\frac{\mathrm{i}\,k}{\xi}\right)^2-k^2\left(1-\frac{2}{\xi^2}\right)\right]\right)\\ &= 2\,\mathrm{i}\left(\frac{\xi}{\xi-\mathrm{i}}-\frac{\mathrm{i}}{\xi}\right)\left(\Omega_{\mathbf{k}}^{(1)}(\eta)-\frac{3H^2\xi^4}{4k^2}\left[\left(\frac{\xi}{\xi-\mathrm{i}}-\frac{\mathrm{i}}{\xi}\right)^2-\left(1-\frac{2}{\xi^2}\right)\right]\right).\end{aligned} \tag{6.193}$$

This equation is actually analytically solvable, however, we now face a problem with the boundary condition

$$\Omega_{\mathbf{k}}^{(1)}(\xi) \to 0 \quad \text{for} \quad \xi \to 0 \tag{6.194}$$

we have used in the previous chapter, because all solutions to equation (6.193) go to zero for $\xi \to 0$. The general solution reads

$$\Omega_{\mathbf{k}}^{(1)}(\xi) = \frac{3}{2}\frac{H^2}{k^2}\frac{\xi^2}{(1+\mathrm{i}\xi)^2}\left[1+\mathrm{i}\xi+\mathrm{e}^{2\mathrm{i}\xi}\left(\mathrm{e}^2\,\mathrm{Ei}(1,2(1+\mathrm{i}\xi))+\mathrm{Ei}(1,2\mathrm{i}\xi)+A_k\right)\right], \tag{6.195}$$

where the exponential integral $\mathrm{Ei}(a,z)$ is defined as in chapter 5

$$\mathrm{Ei}(a,z) := \int_1^\infty \mathrm{d}t\,\frac{\mathrm{e}^{-tz}}{t^a}. \tag{6.196}$$

We restrict ourselves here to the solution that is continuous on the imaginary axis and therefore have (cf. [1], Sec. 5.1)

$$\mathrm{Ei}(1,z) \equiv \Gamma(0,z) \equiv E_1(z). \tag{6.197}$$

The quantity A_k is given by

$$A_k = \frac{3}{2}\frac{k^2}{H^2}\,C, \tag{6.198}$$

where C is an integration constant. Setting C to an arbitrary real value always leads to a solution that fulfills the boundary condition (6.194), but exhibits an oscillatory behavior if $C \neq 0$. Therefore we make the choice $C = 0$ in order to obtain a non-oscillatory solution.

We define the dimensionless function $\widetilde{\Omega}^{(1)}(\xi)$ via

$$\Omega_{\mathbf{k}}^{(1)}(\xi) = \frac{H^2}{k^2}\,\widetilde{\Omega}^{(1)}(\xi). \tag{6.199}$$

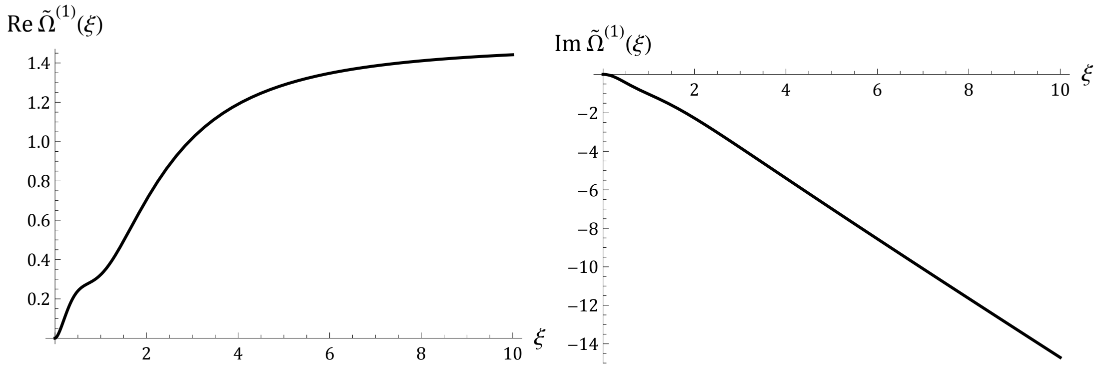

Figure 6.1: Plot of the real and imaginary part of $\widetilde{\Omega}^{(1)}(\xi)$.

In figure 6.1, a plot of the real and imaginary part of this function is shown. We see that this function behaves similarly to the negative of the solution (5.115) (using $E_1(x)$) in the previous chapter, which is plotted in figure 5.2.

For the power spectrum of the scalar perturbations we then get

$$\begin{aligned}\mathcal{P}_{\mathrm{S}}^{(1)}(k) = \mathcal{P}_{\zeta}^{(1)}(k) &= \frac{1}{2a^2 M_{\mathrm{P}}^2 \epsilon}\, \mathcal{P}_{v}^{(1)}(k) \\ &= \frac{1}{2a^2 M_{\mathrm{P}}^2 \epsilon} \frac{k^3}{4\pi^2} \left(\mathfrak{Re}\, \Omega_{\mathbf{k}}^{(0)} + \frac{1}{m_{\mathrm{P}}^2}\, \mathfrak{Re}\, \Omega_{\mathbf{k}}^{(1)} \right)^{-1} \\ &= \frac{1}{2a^2 M_{\mathrm{P}}^2 \epsilon} \frac{k^3}{4\pi^2} \frac{1}{\mathfrak{Re}\, \Omega_{\mathbf{k}}^{(0)}} \left(1 + \frac{1}{m_{\mathrm{P}}^2} \frac{\mathfrak{Re}\, \Omega_{\mathbf{k}}^{(1)}}{\mathfrak{Re}\, \Omega_{\mathbf{k}}^{(0)}} \right)^{-1} \\ &= \frac{\xi^2 H^2}{2k^2 M_{\mathrm{P}}^2 \epsilon} \frac{k^3}{4\pi^2} \frac{1}{k\, \xi^2} \left(1 + \frac{H^2}{m_{\mathrm{P}}^2} \frac{1}{k^3\, \xi^2}\, \mathfrak{Re}\, \tilde{\Omega}^{(1)}(\xi) \right)^{-1} \\ &= \frac{H^2}{8\pi^2 M_{\mathrm{P}}^2 \epsilon} \left[1 - \frac{H^2}{m_{\mathrm{P}}^2} \frac{1}{k^3\, \xi^2}\, \mathfrak{Re}\, \tilde{\Omega}^{(1)}(\xi) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4} \right) \right] . \end{aligned} \tag{6.200}$$

Here we have used the superhorizon limit $\xi \to 0$ for $\mathfrak{Re}\, \Omega_{\mathbf{k}}^{(0)}$ as before. However, for $\mathfrak{Re}\, \Omega_{\mathbf{k}}^{(1)}$, taking this limit conflicts with the boundary condition. Therefore, we evaluate $\mathfrak{Re}\, \Omega_{\mathbf{k}}^{(1)}$ at the point of the horizon reentry of the modes, which is $\xi = 1$, and we obtain

$$\mathfrak{Re}\, \tilde{\Omega}^{(1)}(1) \simeq 0.32347\,, \tag{6.201}$$

such that we end up with

$$\mathcal{P}_{\mathrm{S}}^{(1)}(k) = \frac{H^2}{4\pi^2 M_{\mathrm{P}}^2 \epsilon} \left[1 - \frac{H^2}{m_{\mathrm{P}}^2} \frac{0.32347}{k^3} + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4} \right) \right] . \tag{6.202}$$

For the tensor perturbations, we can analogously infer

$$\begin{aligned}
\mathcal{P}_{\mathrm{T}}^{(1)}(k) &= 2\,\mathcal{P}_{h}^{(1)}(k) = \frac{8}{a^2 M_{\mathrm{P}}^2}\,\mathcal{P}_{v}^{(1)}(k) \\
&= \frac{8}{a^2 M_{\mathrm{P}}^2}\,\frac{k^3}{4\pi^2}\left(\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)} + \frac{1}{m_{\mathrm{P}}^2}\,\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(1)}\right)^{-1} \\
&= \frac{8}{a^2 M_{\mathrm{P}}^2}\,\frac{k^3}{4\pi^2}\,\frac{1}{\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}}\left(1 + \frac{1}{m_{\mathrm{P}}^2}\,\frac{\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(1)}}{\mathfrak{Re}\,\Omega_{\mathbf{k}}^{(0)}}\right)^{-1} \\
&= \frac{8\xi^2 H^2}{k^2 M_{\mathrm{P}}^2}\,\frac{k^3}{4\pi^2}\,\frac{1}{k\,\xi^2}\left(1 + \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{1}{k^3\,\xi^2}\,\mathfrak{Re}\,\tilde{\Omega}^{(1)}(\xi)\right)^{-1} \\
&= \frac{2H^2}{\pi^2 M_{\mathrm{P}}^2}\left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{1}{k^3\,\xi^2}\,\mathfrak{Re}\,\tilde{\Omega}^{(1)}(\xi) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]
\end{aligned} \tag{6.203}$$

Evaluating this expression at $\xi = 1$ then gives

$$\mathcal{P}_{\mathrm{T}}^{(1)}(k) = \frac{2H^2}{\pi^2 M_{\mathrm{P}}^2}\left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{0.32347}{k^3} + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]. \tag{6.204}$$

Thus we immediately see that the tensor-to-scalar ratio is not influenced by quantum-gravitational corrections in the de Sitter case due to the fact that the scalar and tensor perturbations are modified by exactly the same correction term:

$$r^{(1)} = \frac{\mathcal{P}_{\mathrm{T}}^{(1)}(k)}{\mathcal{P}_{\mathrm{S}}^{(1)}(k)} = \frac{\mathcal{P}_{\mathrm{T}}^{(0)}(k)}{\mathcal{P}_{\mathrm{S}}^{(0)}(k)} = r^{(0)} = 16\,\epsilon\,. \tag{6.205}$$

This will no longer be the case in the slow-roll scenario, which we will discuss in the following.

6.5.2 The slow-roll case

In order to consider the slow-roll, quasi-de Sitter case, we should insert the solution (6.170) into equation (6.190) along with the respective expression for $\omega_{\mathbf{k}}^2$. However, this leads to a highly intricate differential equation which is not analytically solvable. We therefore restrict ourselves to the following approximation: For $\omega_{\mathbf{k}}^2$ we use the respective slow-roll expressions (6.152) and (6.153) for the scalar and tensor modes and we also use the slow-roll expressions (6.150) for V and (6.162) for η. However, for $\Omega_{\mathbf{k}}^{(0)}$ we use the de Sitter solution (6.111).

Scalar perturbations

In doing so, we obtain the following differential equation for the scalar modes

$$\mathrm{i}\,\Omega'^{(1)}_{\mathbf{k},\mathrm{S}}(\eta) = 2\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right)\left(\Omega^{(1)}_{\mathbf{k},\mathrm{S}}(\eta) - \frac{3}{4V(\eta)}\left[\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right)^2 - \left(k^2 - \frac{2+6\epsilon-3\delta}{\eta^2}\right)\right]\right). \tag{6.206}$$

Using (6.150) and (6.162), $V(\eta)$ is given by

$$V(\eta) = \frac{2}{m_\mathrm{P}}\,\mathrm{e}^{4\alpha}\mathcal{V}_\epsilon = \mathrm{e}^{4\alpha}H^2(1-\epsilon)^2 = \frac{(1-\epsilon)^2}{H^2\eta^4(1-\epsilon)^4} = \frac{1}{H^2\eta^4(1-2\epsilon)} \tag{6.207}$$

and we get

$$\begin{aligned}\mathrm{i}\,\Omega'^{(1)}_{\mathbf{k},\mathrm{S}}(\eta) &= 2\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right) &(6.208)\\ &\quad\times\left\{\Omega^{(1)}_{\mathbf{k},\mathrm{S}}(\eta) - \frac{3H^2\eta^4(1-2\epsilon)}{4}\left[\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right)^2 - \left(k^2-\frac{2+6\epsilon-3\delta}{\eta^2}\right)\right]\right\}.\end{aligned}$$

This equation is analytically solvable and the result is given by

$$\begin{aligned}\Omega^{(1)}_{\mathbf{k},\mathrm{S}}(\eta) &= \frac{3H^2}{8}\,\frac{(1-2\epsilon)\,\eta^2}{(1-\mathrm{i}k\eta)^2}\Big[4-4\mathrm{i}k\eta+(6\epsilon-3\delta)(7-6\mathrm{i}k\eta+2k^2\eta^2) &(6.209)\\ &\quad + 4\,\mathrm{e}^{-2\mathrm{i}k\eta}\left(\mathrm{e}^2\,\mathrm{Ei}\big(1,2(1-\mathrm{i}k\eta)\big) + (1+6\epsilon-3\delta)\,\mathrm{Ei}(1,-2\mathrm{i}k\eta)\right)\Big].\end{aligned}$$

Using (6.162) and the definition of ξ that we restate here in order to make clear that we define ξ in terms of a and not of η

$$\xi := \frac{k}{Ha}\,, \tag{6.210}$$

we now replace η by

$$\eta = -\frac{\xi}{k(1-\epsilon)} \simeq -\frac{\xi}{k}(1+\epsilon) \tag{6.211}$$

with the intent to set $\xi = 1$. We obtain

$$\begin{aligned}\Omega^{(1)}_{\mathbf{k},\mathrm{S}}(\xi) &= \frac{3}{8}\,\frac{H^2}{k^2}\,\frac{\xi^2(1-2\epsilon)(1+\epsilon)^2}{(1+\mathrm{i}\xi(1+\epsilon))^2} &(6.212)\\ &\quad\times\Big[4+4\mathrm{i}\xi(1+\epsilon)+(6\epsilon-3\delta)(7+6\mathrm{i}\xi(1+\epsilon)-2\xi^2(1+\epsilon)^2)\\ &\quad + 4\,\mathrm{e}^{2\mathrm{i}\xi}\left(\mathrm{e}^2\,\mathrm{Ei}(1,2(1+\mathrm{i}\xi(1+\epsilon))) + (1+6\epsilon-3\delta)\,\mathrm{Ei}(1,2\mathrm{i}\xi(1+\epsilon))\right)\Big].\end{aligned}$$

We have, of course, in principle to expand the terms containing the slow-roll parameters in the above equation and to keep only the terms of first order, but since we will evaluate this equation numerically for $\xi = 1$ anyways, we refrain from writing out the resulting expression. We again define the dimensionless function $\tilde{\Omega}^{(1)}_{\mathrm{S}}(\xi)$ via

$$\Omega^{(1)}_{\mathbf{k},\mathrm{S}}(\xi) = \frac{H^2}{k^2}\,\tilde{\Omega}^{(1)}_{\mathrm{S}}(\xi) \tag{6.213}$$

and can evaluate this function numerically at the point $\xi = 1$. This leads to

$$\mathfrak{Re}\,\tilde{\Omega}^{(1)}_{\mathrm{S}}(1) \simeq 0.32347 + 4.5359\,\epsilon - 2.4772\,\delta\,. \tag{6.214}$$

Before we can determine the power spectrum, we have to express the inverse of $\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k}}$ in terms of ξ

$$\begin{aligned}\frac{1}{\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{S}}} &= \frac{1}{k^3\eta^2}\left[1 + (2\epsilon - \delta)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)\right](-k\eta)^{-4\epsilon+2\delta} \\ &= \frac{1}{k\xi^2}\,(1-2\epsilon)\left[1 + (2\epsilon-\delta)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)\right]\left[1 + (-4\epsilon + 2\delta)\ln(\xi)\right] \\ &= \frac{1}{k\xi^2}\left[1 - 2\epsilon + (2\epsilon-\delta)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right) + (-4\epsilon+2\delta)\ln(\xi)\right].\end{aligned} \tag{6.215}$$

Using the definition

$$C^{\mathrm{S}}_{\epsilon,\delta} := 1 - 2\epsilon + (2\epsilon - \delta)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right), \tag{6.216}$$

we can write

$$\frac{1}{\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{S}}} = \frac{1}{k\xi^2}\left[C^{\mathrm{S}}_{\epsilon,\delta} + (2\delta - 4\epsilon)\ln(\xi)\right]. \tag{6.217}$$

The power spectrum of the scalar perturbations in the slow-roll scenario then reads

$$\begin{aligned}\mathcal{P}^{(1)}_{\mathrm{S}}(k) &= \mathcal{P}^{(1)}_{\zeta}(k) = \frac{1}{2a^2 M_{\mathrm{P}}^2\epsilon}\,\mathcal{P}^{(1)}_{v}(k) \\ &= \frac{1}{2a^2 M_{\mathrm{P}}^2\epsilon}\,\frac{k^3}{4\pi^2}\left(\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{S}} + \frac{1}{m_{\mathrm{P}}^2}\,\mathfrak{Re}\,\Omega^{(1)}_{\mathbf{k},\mathrm{S}}\right)^{-1} \\ &= \frac{1}{2a^2 M_{\mathrm{P}}^2\epsilon}\,\frac{k^3}{4\pi^2}\,\frac{1}{\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{S}}}\left(1 + \frac{1}{m_{\mathrm{P}}^2}\,\frac{\mathfrak{Re}\,\Omega^{(1)}_{\mathbf{k},\mathrm{S}}}{\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{S}}}\right)^{-1} \\ &= \frac{\xi^2 H^2}{2k^2 M_{\mathrm{P}}^2\epsilon}\,\frac{k^3}{4\pi^2}\,\frac{C^{\mathrm{S}}_{\epsilon,\delta} + (2\delta-4\epsilon)\ln(\xi)}{k\,\xi^2} \\ &\qquad\times\left(1 + \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{C^{\mathrm{S}}_{\epsilon,\delta} + (2\delta-4\epsilon)\ln(\xi)}{k^3\,\xi^2}\,\mathfrak{Re}\,\tilde{\Omega}^{(1)}_{\mathrm{S}}(\xi)\right)^{-1} \\ &= \frac{H^2\left[C^{\mathrm{S}}_{\epsilon,\delta} + (2\delta-4\epsilon)\ln(\xi)\right]}{8\pi^2 M_{\mathrm{P}}^2\epsilon}\left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{C^{\mathrm{S}}_{\epsilon,\delta} + (2\delta-4\epsilon)\ln(\xi)}{k^3\,\xi^2}\,\mathfrak{Re}\,\tilde{\Omega}^{(1)}_{\mathrm{S}}(\xi) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right].\end{aligned} \tag{6.218}$$

Now we have to evaluate this expression at the point of the horizon reentry of the modes, $\xi = 1$, and we obtain

$$\mathcal{P}_{\mathrm{S}}^{(1)}(k) = \frac{H^2\, C^{\mathrm{S}}_{\epsilon,\delta}}{8\pi^2 M_{\mathrm{P}}^2 \epsilon} \left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\, \frac{C^{\mathrm{S}}_{\epsilon,\delta}}{k^3}\, \mathfrak{Re}\,\tilde{\Omega}_{\mathrm{S}}^{(1)}(1) + \mathcal{O}\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]\Bigg|_{k=Ha}, \tag{6.219}$$

where $\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{S}}^{(1)}(1)$ is given by (6.214). We also have to evaluate the product of $C^{\mathrm{S}}_{\epsilon,\delta}$ with $\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{S}}^{(1)}(1)$, for which we get

$$\begin{aligned}
&C^{\mathrm{S}}_{\epsilon,\delta}\, \mathfrak{Re}\,\tilde{\Omega}_{\mathrm{S}}^{(1)}(1)\\
&\simeq \left[1 - 2\epsilon + (2\epsilon - \delta)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)\right](0.32347 + 4.5359\,\epsilon - 2.4772\,\delta)\\
&\simeq (1 + 0.9185\,\epsilon - 1.4593\,\delta)(0.32347 + 4.5359\,\epsilon - 2.4772\,\delta)\\
&\simeq 0.32347 + 4.8331\,\epsilon - 2.9492\,\delta + \mathcal{O}\left(2^{\mathrm{nd}}\right).
\end{aligned} \tag{6.220}$$

Consequently, our final result for the quantum-gravitationally corrected power spectrum of the scalar perturbations in slow-roll inflation reads

$$\boxed{\mathcal{P}_{\mathrm{S}}^{(1)}(k) = \frac{H^2\, C^{\mathrm{S}}_{\epsilon,\delta}}{8\pi^2 M_{\mathrm{P}}^2 \epsilon} \left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\, \frac{1}{k^3}\,(0.32347 + 4.8331\,\epsilon - 2.9492\,\delta) + \mathcal{O}\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]\Bigg|_{k=Ha}} \tag{6.221}$$

If we decompose the terms containing the slow-roll parameters as

$$4.8331\,\epsilon - 2.9492\,\delta = -1.0653\,\epsilon + 2.9492\,(2\epsilon - \delta), \tag{6.222}$$

we see that the contribution on ϵ originating from inserting (6.152) into (6.206) is about five times larger than the contribution originating from replacing η by (6.211).

We can write (6.221) using our result (6.185) for the uncorrected power spectrum $\mathcal{P}_{\mathrm{S}}^{(0)}$ as

$$\mathcal{P}_{\mathrm{S}}^{(1)}(k) = \mathcal{P}_{\mathrm{S}}^{(0)}(k)\left[1 + \Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta}(k) + \mathcal{O}\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right], \tag{6.223}$$

where the correction function

$$\Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta}(k) = -\frac{H^2}{m_{\mathrm{P}}^2}\, \frac{1}{k^3}\,(0.32347 + 4.8331\,\epsilon - 2.9492\,\delta)\Big|_{k=Ha} \tag{6.224}$$

has been introduced. The modification of the power spectrum originating from the quantum-gravitational correction term in the Schrödinger equation (6.84) therefore leads to a *suppression* of power on the largest scales.

Tensor perturbations

For the tensor perturbations, we do not need to repeat all these calculations, because we can also set $\delta = \epsilon$ to transform the above expressions from the scalar to the tensor case. The differential equation we have to solve for the tensor perturbations reads

$$\begin{aligned} \mathrm{i}\,\Omega'^{(1)}_{\mathbf{k},\mathrm{T}}(\eta) &= 2\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right) \\ &\times\left\{\Omega^{(1)}_{\mathbf{k},\mathrm{T}}(\eta)-\frac{3H^2\eta^4(1-2\epsilon)}{4}\left[\left(\frac{k^2\eta}{\mathrm{i}+k\eta}+\frac{\mathrm{i}}{\eta}\right)^2-\left(k^2-\frac{2+3\epsilon}{\eta^2}\right)\right]\right\} \end{aligned} \tag{6.225}$$

and it is solved in terms of ξ by

$$\begin{aligned} \Omega^{(1)}_{\mathbf{k},\mathrm{T}}(\xi) &= \frac{3}{8}\frac{H^2}{k^2}\frac{\xi^2(1-2\epsilon)(1+\epsilon)^2}{(1+\mathrm{i}\xi(1+\epsilon))^2} \\ &\times\Big[4+4\mathrm{i}\xi(1+\epsilon)+3\epsilon(7+6\mathrm{i}\xi(1+\epsilon)-2\xi^2(1+\epsilon)^2) \\ &+4\,\mathrm{e}^{2\mathrm{i}\xi}\left(\mathrm{e}^2\,\mathrm{Ei}(1,2(1+\mathrm{i}\xi(1+\epsilon)))+(1+3\epsilon)\,\mathrm{Ei}(1,2\mathrm{i}\xi(1+\epsilon))\right)\Big]. \end{aligned} \tag{6.226}$$

Defining, as in the scalar case, the dimensionless function $\tilde{\Omega}^{(1)}_{\mathrm{T}}(\xi)$ via

$$\Omega^{(1)}_{\mathbf{k},\mathrm{T}}(\xi) = \frac{H^2}{k^2}\,\tilde{\Omega}^{(1)}_{\mathrm{T}}(\xi)\,, \tag{6.227}$$

we perform a numerical evaluation of this function at the point $\xi = 1$ and obtain

$$\mathfrak{Re}\,\tilde{\Omega}^{(1)}_{\mathrm{T}}(1) \simeq 0.32347 + 2.0587\,\epsilon\,. \tag{6.228}$$

The inverse of $\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{T}}$ in terms of ξ is given by

$$\frac{1}{\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{T}}} = \frac{1}{k\xi^2}\left[1-2\epsilon+\epsilon\,\left(4-2\gamma_{\mathrm{E}}-2\ln(2)\right)-2\epsilon\,\ln(\xi)\right], \tag{6.229}$$

such that we can define

$$C^{\mathrm{T}}_{\epsilon} := 1-2\epsilon+\epsilon\,\left(4-2\gamma_{\mathrm{E}}-2\ln(2)\right) \tag{6.230}$$

and express (6.229) as

$$\frac{1}{\mathfrak{Re}\,\Omega^{(0)}_{\mathbf{k},\mathrm{T}}} = \frac{1}{k\xi^2}\left[C^{\mathrm{T}}_{\epsilon}-2\epsilon\,\ln(\xi)\right]. \tag{6.231}$$

For the power spectrum of the tensor perturbations in the slow-roll scenario we subsequently get

$$\begin{aligned}\mathcal{P}_{\mathrm{T}}^{(1)}(k) &= 2\,\mathcal{P}_{h}^{(1)}(k) = \frac{8}{a^2\,M_{\mathrm{P}}^2}\,\mathcal{P}_{v}^{(1)}(k) \\
&= \frac{8}{a^2\,M_{\mathrm{P}}^2}\,\frac{k^3}{4\pi^2}\left(\mathfrak{Re}\,\Omega_{\mathbf{k},\mathrm{T}}^{(0)} + \frac{1}{m_{\mathrm{P}}^2}\,\mathfrak{Re}\,\Omega_{\mathbf{k},\mathrm{T}}^{(1)}\right)^{-1} \\
&= \frac{8}{a^2\,M_{\mathrm{P}}^2}\,\frac{k^3}{4\pi^2}\,\frac{1}{\mathfrak{Re}\,\Omega_{\mathbf{k},\mathrm{T}}^{(0)}}\left(1 + \frac{1}{m_{\mathrm{P}}^2}\,\frac{\mathfrak{Re}\,\Omega_{\mathbf{k},\mathrm{T}}^{(1)}}{\mathfrak{Re}\,\Omega_{\mathbf{k},\mathrm{T}}^{(0)}}\right)^{-1} \\
&= \frac{8\xi^2\,H^2}{k^2\,M_{\mathrm{P}}^2}\,\frac{k^3}{4\pi^2}\,\frac{C_{\epsilon}^{\mathrm{T}} - 2\epsilon\,\ln(\xi)}{k\,\xi^2}\left(1 + \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{C_{\epsilon}^{\mathrm{T}} - 2\epsilon\,\ln(\xi)}{k^3\,\xi^2}\,\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{T}}^{(1)}(\xi)\right)^{-1} \\
&= \frac{2H^2\left[C_{\epsilon}^{\mathrm{T}} - 2\epsilon\,\ln(\xi)\right]}{\pi^2\,M_{\mathrm{P}}^2}\left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{C_{\epsilon}^{\mathrm{T}} - 2\epsilon\,\ln(\xi)}{k^3\,\xi^2}\,\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{T}}^{(1)}(\xi) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right].\end{aligned} \tag{6.232}$$

Evaluating this expression at the point of the horizon re-entry of the modes, $\xi = 1$, yields

$$\mathcal{P}_{\mathrm{T}}^{(1)}(k) = \frac{2H^2\,C_{\epsilon}^{\mathrm{T}}}{\pi^2\,M_{\mathrm{P}}^2}\left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{C_{\epsilon}^{\mathrm{T}}}{k^3}\,\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{T}}^{(1)}(1) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]\Bigg|_{k=Ha}, \tag{6.233}$$

where $\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{T}}^{(1)}(1)$ has been given in (6.214). For the product of $C_{\epsilon}^{\mathrm{T}}$ with $\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{T}}^{(1)}(1)$, we then get

$$\begin{aligned}C_{\epsilon}^{\mathrm{T}}\,\mathfrak{Re}\,\tilde{\Omega}_{\mathrm{T}}^{(1)}(1) &\simeq \left[1 - 2\epsilon + \epsilon\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)\right](0.32347 + 2.0587\,\epsilon) \\
&\simeq (1 - 0.5407\,\epsilon)(0.32347 + 2.0587\,\epsilon) \\
&\simeq 0.32347 + 1.8838\,\epsilon + \mathcal{O}\!\left(2^{\mathrm{nd}}\right).\end{aligned} \tag{6.234}$$

Hence, we can write out our final result for the quantum-gravitationally corrected power spectrum of the tensor perturbations in slow-roll inflation

$$\boxed{\mathcal{P}_{\mathrm{T}}^{(1)}(k) = \frac{2H^2\,C_{\epsilon}^{\mathrm{T}}}{\pi^2\,M_{\mathrm{P}}^2}\left[1 - \frac{H^2}{m_{\mathrm{P}}^2}\,\frac{1}{k^3}\,(0.32347 + 1.8838\,\epsilon) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]\Bigg|_{k=Ha}} \tag{6.235}$$

Setting $\epsilon = \delta$ in (6.221) leads to the same result. Using the uncorrected power spectrum $\mathcal{P}_{\mathrm{T}}^{(0)}$ as given in (6.189), we obtain

$$\mathcal{P}_{\mathrm{T}}^{(1)}(k) = \mathcal{P}_{\mathrm{T}}^{(0)}(k)\left[1 + \Delta_{\mathrm{T};\epsilon}^{\mathrm{WDW}}(k) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right], \tag{6.236}$$

where we have introduced the correction function

$$\Delta^{\mathrm{WDW}}_{\mathrm{T};\epsilon}(k) = -\left.\frac{H^2}{m_{\mathrm{P}}^2}\,\frac{1}{k^3}\,(0.32347 + 1.8838\,\epsilon)\right|_{k=Ha} . \tag{6.237}$$

We thus see that also for the power spectrum of the tensor perturbations, the quantum-gravitational correction term in the Schrödinger equation (6.84) causes a *suppression* of power on the largest scales.

Finally, we can calculate the quantum-gravitationally corrected tensor-to-scalar ratio $r^{(1)}$

$$\begin{aligned} r^{(1)} = \frac{\mathcal{P}^{(1)}_{\mathrm{T}}(k)}{\mathcal{P}^{(1)}_{\mathrm{S}}(k)} &= 16\,\epsilon\,\frac{C^{\mathrm{T}}_{\epsilon}}{C^{\mathrm{S}}_{\epsilon,\delta}}\left[1 + \Delta^{\mathrm{WDW}}_{\mathrm{T};\epsilon}(k) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]\left[1 + \Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta}(k) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right]^{-1} \\ &= 16\,\epsilon\,\frac{C^{\mathrm{T}}_{\epsilon}}{C^{\mathrm{S}}_{\epsilon,\delta}}\left[1 + \left(\Delta^{\mathrm{WDW}}_{\mathrm{T};\epsilon}(k) - \Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta}(k)\right) + \mathcal{O}\!\left(\frac{H^4}{m_{\mathrm{P}}^4}\right)\right] . \end{aligned} \tag{6.238}$$

The quotient $C^{\mathrm{T}}_{\epsilon}/C^{\mathrm{S}}_{\epsilon,\delta}$ can be written up to the first order in the slow-roll parameters as

$$\begin{aligned} \frac{C^{\mathrm{T}}_{\epsilon}}{C^{\mathrm{S}}_{\epsilon,\delta}} &= \frac{1 - 2\epsilon + \epsilon\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)}{1 - 2\epsilon + (2\epsilon - \delta)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right)} \\ &\simeq 1 + (\delta - \epsilon)\left(4 - 2\gamma_{\mathrm{E}} - 2\ln(2)\right) + \mathcal{O}\!\left(2^{\mathrm{nd}}\right) \\ &\simeq 1 + 1.4593\,(\delta - \epsilon) + \mathcal{O}\!\left(2^{\mathrm{nd}}\right) . \end{aligned} \tag{6.239}$$

For the quantum-gravitational part we get

$$\begin{aligned} \Delta^{\mathrm{WDW}}_{\mathrm{T};\epsilon}(k) - \Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta}(k) &= -\frac{H^2}{m_{\mathrm{P}}^2}\,\frac{1}{k^3}\,(1.8838\,\epsilon - 4.8331\,\epsilon + 2.9492\,\delta) \\ &= -\frac{H^2}{m_{\mathrm{P}}^2}\,\frac{1}{k^3}\,2.9492\,(\delta - \epsilon) . \end{aligned} \tag{6.240}$$

Hence, we obtain for the tensor-to-scalar ratio

$$\boxed{r^{(1)} \simeq 16\,\epsilon\left[1 + (\delta - \epsilon)\left(1.4593 - 2.9492\,\frac{H^2}{m_{\mathrm{P}}^2}\,\frac{1}{k^3}\right)\right] .} \tag{6.241}$$

Since the uncorrected tensor-to-scalar ratio already contains a slow-roll parameter, the correction term is, of course, of second order in the slow-roll parameters.

In the next chapter, we shall discuss whether the quantum-gravitational corrections we have calculated in this chapter for the scalar and tensor perturbations could be in principle measurable in the Cosmic Microwave Background.

7

Observability of the quantum-gravitational corrections and comparison with other approaches

7.1 Observability of the corrections

We can combine the quantum-gravitationally corrected power spectra we found in the previous chapters in the following form

$$\mathcal{P}^{(1)}(k) = \mathcal{P}^{(0)}(k) \left[1 + \Delta^{\mathrm{WDW}}_{\phi,\mathrm{S},\mathrm{T}}(k) + \mathcal{O}\left(\frac{H^4}{m_\mathrm{P}^4} \right) \right] . \tag{7.1}$$

For the scalar-field perturbations, the correction function $\Delta^{\mathrm{WDW}}_{\phi,\mathrm{S},\mathrm{T}}(k)$ is given by

$$\Delta^{\mathrm{WDW}}_{\phi}(k) = \frac{H^2}{m_\mathrm{P}^2} \frac{\widetilde{C}(\xi)}{k^3} , \tag{7.2}$$

where we choose the value $\widetilde{C}(\xi = 1) = 2.6387$ from the continuous solution. We set $\xi = 1$ here in order to make the result from chapter 5 compatible with chapter 6, where we have used the convention $k = L^{-1}$. For the gauge-invariant scalar perturbations, we have

$$\Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta}(k) = -\frac{H^2}{m_\mathrm{P}^2} \frac{1}{k^3} \left(0.32347 + 4.8331\,\epsilon - 2.9492\,\delta\right)\Big|_{k=Ha} \tag{7.3}$$

and finally for the tensor perturbations the correction term reads

$$\Delta^{\mathrm{WDW}}_{\mathrm{T};\epsilon}(k) = -\frac{H^2}{m_\mathrm{P}^2} \frac{1}{k^3} \left(0.32347 + 1.8838\,\epsilon\right)\Big|_{k=Ha} . \tag{7.4}$$

Scalar perturbations

We assume that we can treat the scalar-field perturbations on the same footing as the gauge-invariant scalar perturbations and thus present both here at once. Following [35], we can include the corrections given above in the expression for the spectral index n_S. Using the approximate formula

$$\frac{\mathrm{d}}{\mathrm{d}\log k} \approx \frac{1}{H}\frac{\mathrm{d}}{\mathrm{d}t}\,, \tag{7.5}$$

we can write

$$n_\mathrm{S} - 1 := \frac{\mathrm{d}\log \mathcal{P}_\mathrm{S}}{\mathrm{d}\log k} \approx 2\delta - 4\epsilon - 3\Delta^{\mathrm{WDW}}_{\mathrm{S},\phi}(k)\,. \tag{7.6}$$

Furthermore, we can introduce the running of the spectral index, which is of the second order in the slow-roll parameters, as

$$\alpha_\mathrm{S} := \frac{\mathrm{d}n_\mathrm{S}}{\mathrm{d}\log k} \approx 2(5\epsilon\delta - 4\epsilon^2 - \Xi^2) + 9\Delta^{\mathrm{WDW}}_{\mathrm{S},\phi}(k)\,, \tag{7.7}$$

where the second-order slow-roll parameter Ξ has been used, which is defined as

$$\Xi^2 := \frac{1}{H^2}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\ddot{\phi}}{\dot{\phi}}\,. \tag{7.8}$$

In order to give an estimate for the correction term, we have to reinsert a reference wave number k_0 that corresponds to the length scale $\mathfrak{L}$ we have neglected in the previous two chapters. We thus have to replace

$$k \to \frac{k}{k_0}\,. \tag{7.9}$$

As reference wave number we can either use the largest observable scale, which is [35]

$$k_\mathrm{min} \sim 1.4 \times 10^{-4}\,\mathrm{Mpc}^{-1}\,, \tag{7.10}$$

or one of the pivot scales used in the analysis of the CMB spectra. For WMAP this scale has been chosen as [56]

$$k_0 = 2 \times 10^{-3}\,\mathrm{Mpc}^{-1}\,. \tag{7.11}$$

We can also give an upper bound on the ratio H/m_P based on the relation [18]

$$V^{1/4} \sim \left(\frac{r}{0.01}\right)^{1/4} 10^{16}\,\mathrm{GeV}\,, \tag{7.12}$$

which implies that

$$\frac{H}{m_\mathrm{P}} \lesssim 3.5 \times 10^{-6} \tag{7.13}$$

given that the observational bound on the tensor-to-scalar ratio has been measured by Planck to be $r \lesssim 0.11$ [4]. The BICEP2 result of $r \sim 0.2$ [3] would, of course, enhance this bound, however the validity of the BICEP2 result is not yet clear [2].

Hence, we find that for $k \to k/k_0$ the absolute value of the quantum-gravitational correction is limited by

$$\left|\Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta=0}(k_0)\right| \lesssim 4.0 \times 10^{-12}\,, \qquad \left|\Delta^{\mathrm{WDW}}_{\phi}(k)\right| \lesssim 3.2 \times 10^{-11}\,. \tag{7.14}$$

Using k_{min} instead of k_0 as reference wave number, these limits are reduced by

$$\left(\frac{k_{\mathrm{min}}}{k_0}\right)^3 \simeq 3.4 \times 10^{-4} \tag{7.15}$$

and we obtain

$$\left|\Delta^{\mathrm{WDW}}_{\mathrm{S};\epsilon,\delta=0}(k_0)\right| \lesssim 1.3 \times 10^{-15}, \qquad \left|\Delta^{\mathrm{WDW}}_{\phi}(k_0)\right| \lesssim 1.1 \times 10^{-14}. \tag{7.16}$$

If we compare these limits with the values of the spectral index n_{S} and its running α_{S} determined from the WMAP9 data, which are given by [56]

$$n_{\mathrm{S}} = 0.9608 \pm 0.0080 \quad \text{and} \quad \alpha_{\mathrm{S}} = -0.023 \pm 0.011\,, \tag{7.17}$$

where the WMAP9+eCMB+BAO+H_0 dataset was used in both cases, as well as with the 2013 results of the Planck mission, whose values (using WMAP polarization data) read [4]

$$n_{\mathrm{S}} = 0.9603 \pm 0.0073 \quad \text{and} \quad \alpha_{\mathrm{S}} = -0.013 \pm 0.009\,, \tag{7.18}$$

we can conclude that the corrections we calculated are completely drowned out by the statistical uncertainty in the WMAP and Planck data.

Cosmic Variance, which is the main source of statistical uncertainty on large scales, implies that on the largest scales, there will not be any further improvements of the statistics of the data by Planck and future satellite missions to measure the CMB anisotropies. Therefore it is unlikely that one will ever be able to observe effects of the magnitude we have obtained in the CMB anisotropies.

There is also a way to derive an upper bound on the energy scale of inflation given by H from our corrections. If we assume that

$$\left|\Delta^{\mathrm{WDW}}_{\phi,\mathrm{S}}(k_0)\right| < 0.05\,, \tag{7.19}$$

which reflects the fact that the power spectrum should deviate less than about 5 % from scale invariance, we obtain from the gauge-invariant scalar perturbations the very weak limit

$$H \lesssim 0.4\, m_{\mathrm{P}} \approx 1.06 \times 10^{19}\,\mathrm{GeV} \tag{7.20}$$

and from the scalar-field perturbations

$$H \lesssim 0.14\, m_{\mathrm{P}} \approx 3.71 \times 10^{18}\,\mathrm{GeV}. \tag{7.21}$$

These constraints are, of course, much weaker than the observational limit of about $H \lesssim 10^{15}\,\mathrm{GeV}$ from the tensor-to-scalar ratio, but at least we can be reassured that the approach presented here is consistent with this limit.

Tensor perturbations

For the tensor perturbations, we have obtained

$$\mathcal{P}_{\mathrm{T}}^{(1)}(k) = \mathcal{P}_{\mathrm{T}}^{(0)}(k) \left[1 + \Delta_{\mathrm{T};\epsilon}^{\mathrm{WDW}}(k) + \mathcal{O}\left(\frac{H^4}{m_{\mathrm{P}}^4} \right) \right], \tag{7.22}$$

with

$$\Delta_{\mathrm{T};\epsilon}^{\mathrm{WDW}}(k) = -\frac{H^2}{m_{\mathrm{P}}^2} \frac{1}{k^3} \left(0.32347 + 1.8838\,\epsilon\right)\Big|_{k=Ha}. \tag{7.23}$$

Analogously to the presentation above, we can write

$$n_{\mathrm{T}} := \frac{\mathrm{d}\ln \mathcal{P}_{\mathrm{T}}^{(0)}}{\mathrm{d}\ln k} \simeq -2\epsilon - 3\Delta_{\mathrm{T};\epsilon}^{\mathrm{WDW}}(k). \tag{7.24}$$

Given that the contribution of the slow-roll parameter ϵ can be neglected, we obtain the same contraints as for the scalar perturbations, that is for the reference wave vector k_0

$$\left|\Delta_{\mathrm{T};\epsilon=0}^{\mathrm{WDW}}(k_0)\right| \lesssim 4.0 \times 10^{-12}, \tag{7.25}$$

while using k_{min} as reference we get

$$\left|\Delta_{\mathrm{T};\epsilon=0}^{\mathrm{WDW}}(k_0)\right| \lesssim 1.3 \times 10^{-15}. \tag{7.26}$$

Since gravitational waves have not yet been unambiguously detected [2] and, hence, n_{T} is unknown, we cannot give an definite answer on the measurability of the corrections, but the tiny magnitude indicates that the chances of detectability are extremely low.

7.2 Comparison with other approaches

Quantum-gravitational effects for primordial perturbations have also been investigated in other approaches or using other methods. The study which is also based on the Wheeler–DeWitt equation and that is most similar to our method was presented in [59, 64]. Here, the authors use the semiclassical approximation method presented in [20]. The difference to our approach has been explained in the appendix of [22]. The authors define the two-point function of the perturbations as

$$p_k(\eta) := \ _s\langle 0|\hat{v}_k^2|0\rangle_s = \langle \hat{v}_k^2\rangle_0 \tag{7.27}$$

and find that scalar perturbations are modified in the following way

$$p \simeq \frac{1}{2k}(-k\eta)^{-2(1+2\epsilon-\delta)}\left[1+\frac{H^2}{M_\mathrm{P}^2\,k^3}\,\frac{1}{18}\left(25-7(-k\eta)^{-2(\epsilon-\delta)}\right)\right], \tag{7.28}$$

while for the tensor perturbations the following modification was found

$$p \simeq \frac{1}{2k}(-k\eta)^{-2(1+\epsilon)}\left[1+\frac{H^2}{M_\mathrm{P}^2\,k^3}\right]. \tag{7.29}$$

The result differs in some aspects from our findings, but the interesting similarity is the common prefactor of

$$\frac{H^2}{M_\mathrm{P}^2\,k^3}\,. \tag{7.30}$$

One should investigate the origin of this k-dependence further, because it seems to be a general feature.

In [96], the semiclassical approximation scheme of [75] was used to calculate some form of the power spectrum of primordial gravitational waves. The result also depends on the energy scale during inflation denoted here as λ and the correction is of the form

$$\epsilon = 1-2\,\frac{\lambda}{M_P^2}\left\{\cdots\right\}, \tag{7.31}$$

where the term in the brackets contains an complicated dependence on the frequency of the gravitational waves.

In loop quantum cosmology, there are several types of corrections possible due to the structure of the theory. Based on the discreteness of the theory, there are inverse-volume correction that lead to an enhancement on large scales that can, in principle, be measurable [23, 24].

In considerations that take into account a loop-quantum-gravity-induced super-inflation phase [109] or pre-inflationary phase [5, 6, 7], there also seems to be an enhancement.

Certain non-quantum-gravitational inflationary models can also induce an enhancement [105]. A suppression is found in from considering a self-interacting scalar field [79], a model of “just-enough inflation” [93], or if one takes into account non-commutative geometry [108].

8

The fate of type IV singularities in quantum cosmology

In this chapter we investigate cosmological models that at the classical level include a specific type of singularity called type IV within the framework of quantum cosmology based on the Wheeler–DeWitt equation. Our aim is to see whether these singularities can be avoided by quantization.

Type IV singularities are singularities that can appear in cosmological models with a dark-energy-like matter component. They are of a mild nature in the sense that at the singularity only higher derivatives of the Hubble parameter diverge and that geodesics can be extended through the singularity. In this regard, they are different than the singularities whose fate in quantum cosmology has been investigated before. We shall see that this mild nature is reflected in how these singularities are resolved after quantization.

This chapter is largely based on [30].

8.1 Singularities in dark-energy models

We know from the observation of light curves of distant supernovae of type IA that the expansion of our universe is currently accelerating. In order to account for such an acceleration, one can introduce a new type of matter, usually called *Dark Energy*, whose barotropic index w in the equation of state

$$P = w\,\rho \tag{8.1}$$

takes the value

$$w < -\frac{1}{3}\,. \tag{8.2}$$

When investigating models of universes where such a type of matter is introduced, for instance, as an ideal fluid or in the form of a scalar field, it was found that some resulting models contain singularities of the form that one or more quantities diverge at a certain time during the evolution of the universe.

In [88] a classification of the occurring singularities is given. We present this classification here together with references where these singularities have been discussed, see also [47, 38, 46, 40] and references therein:

- Type I – "Big Rip": for $t \to t_{\rm sing}$: $a \to \infty$, $\rho \to \infty$, $|P| \to \infty$. [36, 106, 37]
- Type II – "Big Brake", "sudden singularity" or "Big Démarrage": for $t \to t_{\rm sing}$: $a \to a_{\rm sing}$, $\rho \to \rho_{\rm sing}$, $|P| \to \infty$. [14, 15, 51]
- Type III – "Big Freeze": for $t \to t_{\rm sing}$: $a \to a_{\rm sing}$, $\rho \to \infty$, $|P| \to \infty$. [88, 28, 27]
- Type IV – "Big Separation": for $t \to t_{\rm sing}$: $a \to a_{\rm sing}$, $\rho \to \rho_{\rm sing}$, $|P| \to P_{\rm sing}$, but the second and higher derivatives of the Hubble parameter H diverge. [88, 12]

Additionally, one can define singularities, where the barotropic index w diverges, as type V [39].

We see that the type IV singularity, which is also sometimes called "Big Separation" [40], is one of the mildest among these singularities. Here, at a finite scale factor $a_{\rm sing}$ and at a finite cosmic time $t_{\rm sing}$, the second and higher derivatives of the Hubble rate H diverge, while H and $\dot{H}$ stay finite at the singularity. Furthermore, the singularity only appears in derivatives of curvature invariants, not in the invariants themselves. Geodesics can be extended through the singularity, such that it is not a singularity in the sense of the standard definition used in general relativity.

8.2 Singularity avoidance in quantum cosmology

As we have discussed in the introduction, it is generally expected that a theory of quantum gravity should resolve singularities appearing in general relativity and, hence, in cosmological models.

We focus here on canonical quantum cosmology with the Wheeler–DeWitt equation as central equation. Since Wheeler–DeWitt quantum cosmology does not resolve singularities in general, we have to specify and analyze a concrete model in order to see what is the fate of singularities in this model. For the Wheeler–DeWitt equation, this means to specify the form of the potential. This situation is similar to quantum mechanics, where classical singularities are also only resolved for specific potentials like the Coulomb potential. There are, in fact, many other singular potentials, whose singularities are not cured in the quantum theory [48]. The fact that physically relevant potentials are singularity-free in quantum mechanics might be carried over to quantum cosmology.

In Wheeler–DeWitt quantum cosmology, the general procedure to analyze the fate of singularities is as follows. One considers a universe filled with an ideal fluid with a certain equation of state

$$P = f(\rho)\,, \tag{8.3}$$

which instead of the traditional form $P = w\,\rho$ mostly takes a more complicated form like, for instance, that of a Chaplygin gas $P = -A/\rho$. Then one converts the fluid to a minimally coupled scalar field ϕ with potential $V(\phi)$ using the relations

$$\rho \stackrel{!}{=} \frac{1}{2}\dot{\phi}^2 + V(\phi)\,, \quad P \stackrel{!}{=} \frac{1}{2}\dot{\phi}^2 - V(\phi)\,. \tag{8.4}$$

The resulting potential $V(\phi)$ is then inserted into the Wheeler–DeWitt equation of a Friedmann–Lemaître–Robertson–Walker model, which for a flat universe is given by

$$\frac{\hbar^2}{2}\left(\frac{\kappa^2}{6}\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial\phi^2}\right)\Psi(\alpha,\phi) + a_0^6\,\mathrm{e}^{6\alpha}\,V(\phi)\,\Psi(\alpha,\phi) = 0 \tag{8.5}$$

and we have used the definition

$$\kappa^2 := 8\pi G\,. \tag{8.6}$$

In order to solve this differential equation, one uses a Born–Oppenheimer approximation in the form of the assumption that one can decompose the wave function $\Psi(\alpha,\phi)$ as follows

$$\Psi(\alpha,\phi) = \varphi(\alpha,\phi)\,C(\alpha)\,. \tag{8.7}$$

One then requires the matter part described by $\varphi(\alpha,\phi)$ to obey

$$-\frac{\hbar^2}{2}\frac{\partial^2\varphi}{\partial\phi^2} + a_0^6\,\mathrm{e}^{6\alpha}V(\phi)\,\varphi = E(\alpha)\,\varphi\,, \tag{8.8}$$

where $E(\alpha)$ is an energy function. The gravitational part described by $C(\alpha)$ then obeys

$$\dot{C}\dot{\varphi} + C\ddot{\varphi} + \left(\frac{\kappa^2}{6}\,\ddot{C} + 2E(\alpha)\,C\right)\varphi = 0\,, \tag{8.9}$$

where the terms containing derivatives of φ are neglected. Now one has to find a solution for $\varphi(\alpha,\phi)$ as well as for $C(\alpha)$ and analyze it in the region where at the classical level the singularity is located. As a sufficient – but not necessary – criterion for singularity avoidance, one can use the vanishing of the wave function at this point, as it was already suggested by DeWitt in [43]. Another criterion would be the breakdown of the semiclassical approximation, such that the wave packets disperse.

We shall illustrate this procedure by two examples. In [61], the Big Brake, i.e. type II singularity, is analyzed. It is found that this singularity can be described by an anti-Chaplygin gas with equation of state

$$P = \frac{A}{\rho}, \tag{8.10}$$

where A is a positive constant. This type of matter is realized as a scalar field ϕ with potential

$$V(\phi) \propto \left[\sinh\left(\sqrt{3}\kappa|\phi|\right) - \sinh^{-1}\left(\sqrt{3}\kappa|\phi|\right)\right]. \tag{8.11}$$

In the proximity of the classical singularity this potential can be approximated by

$$V(\phi) \propto \frac{1}{|\phi|}, \tag{8.12}$$

which leads to the Wheeler–DeWitt equation

$$\frac{\hbar^2}{2}\left(\frac{\kappa^2}{6}\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial\phi^2}\right)\Psi(\alpha,\phi) - \frac{\tilde{V}_0}{|\phi|}\,\mathrm{e}^{6\alpha}\,\Psi(\alpha,\phi) = 0\,. \tag{8.13}$$

This equation is actually analytically solvable after using the Born–Oppenheimer approximation and one finds that all normalizable solutions vanish at the Big Brake singularity *and* additionally at the initial Big Bang singularity. Thus both singularities are avoided.

An example, where the second criterion for singularity avoidance is used, is [41]. Here, one considers a universe filled with phantom matter, that is matter with a negative energy density violating the null energy condition $\rho + P > 0$. The motivation to study such an exotic type of matter is that if one wants to describe the observed acceleration of the expansion of the universe by Dark Energy with an equation of state $P = w\rho$, observationally even $w \lesssim -1$ cannot be excluded.

Such a phantom field leads to a Big Rip singularity at late times. The resulting Wheeler–DeWitt equation of this model becomes elliptic because the sign in front of the ϕ-kinetic terms is positive if ϕ is a phantom field. Including a cosmological constant Λ, we get the following Wheeler–DeWitt equation

$$\frac{\hbar^2}{2}\left(\frac{\kappa^2}{6}\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial\phi^2}\right)\Psi(\alpha,\phi) + \mathrm{e}^{6\alpha}\left(V_0\cosh^2\left(\frac{\phi}{F}\right) + \frac{\Lambda}{6}\right)\Psi(\alpha,\phi) = 0\,, \tag{8.14}$$

where F is a constant. One finds that the wave-packet solutions of this equation disperse at the classical Big Rip singularity. Thus, the semiclassical approximation breaks down at this point; time and the classical evolution come to an end and one is left with a stationary quantum state. The classical Big Rip singularity is therefore avoided.

To summarize, singularity avoidance in Wheeler–DeWitt quantum cosmology was shown for models with a singularity of type I (Big Rip) [41, 13], type II (Big Brake or Big Démarrage) [61, 31], and type III (Big Freeze) [31]. Reviews are given in [67, 68] and [60]. We now turn to the analysis of type IV singularities in quantum cosmology.

8.3 Classical model with a type IV singularity

In order to model a universe with a type IV singularity, we use a *generalized Chaplygin gas* (GCG), which is a perfect fluid with the equation of state [63, 19]

$$P = -\frac{A}{\rho^{\beta}}, \tag{8.15}$$

where A and β are positive or negative constants. The original definition of the Chaplygin gas reads [63]

$$P = -\frac{A}{\rho}, \quad A > 0. \tag{8.16}$$

The Chaplygin gas and its generalized form can be applied for various scenarios [63, 21, 19, 29, 26, 25], such as to describe and unify different matter contents in the universe.

In [27], it was shown that a GCG can model universes with almost all kinds of singularities, in particular, also universes with a type IV singularity.

We use the conservation of the energy–momentum tensor of such a kind of fluid leading to the equation

$$\dot{\rho} + 3H\left(\rho + p\right) = 0, \tag{8.17}$$

which we can immediately solve after inserting (8.15) and obtain

$$\rho = \left(A + \frac{B}{a^{3(1+\beta)}}\right)^{\frac{1}{1+\beta}}, \tag{8.18}$$

where B is an arbitrary real constant.

8.3.1 Standard generalized Chaplygin gas

First of all, we consider a standard GCG that fulfills the null, strong and weak energy conditions. As shown in [27], it can induce a type IV singularity in the future in the following cases

$$A < 0\,, \quad B > 0\,, \quad \text{and} \quad -\frac{1}{2} < \beta < 0\,, \quad \text{where} \quad \beta \neq \frac{1}{2p} - \frac{1}{2}\,, \tag{8.19}$$

and p is a positive integer. We can then express the energy density (8.18) and pressure in the form

$$\rho = |A|^{\frac{1}{1+\beta}} \left[\left(\frac{a_{\max}}{a} \right)^{3(1+\beta)} - 1 \right]^{\frac{1}{1+\beta}}, \quad P = |A|^{\frac{1}{1+\beta}} \left[\left(\frac{a_{\max}}{a} \right)^{3(1+\beta)} - 1 \right]^{-\frac{\beta}{1+\beta}}, \tag{8.20}$$

where we have introduced the maximum scale factor $a_{\max}$, which is given by

$$a_{\max} := \left| \frac{B}{A} \right|^{\frac{1}{3(1+\beta)}}. \tag{8.21}$$

From (8.20) we see that both the energy density and pressure go to zero for $a \to a_{\max}$. In spite of this, the universe described here faces a type IV singularity at $a = a_{\max}$ [27], as we will outline below.

Since we consider here a flat FLRW universe, we have to solve the Friedmann equation for flat spatial sections with a GCG matter content. The resulting equations can be integrated analytically and yield the solution

$$\mathbf{B}\left[\frac{1}{2(1+\beta)}, \frac{2\beta+1}{2(1+\beta)} \right] - \mathbf{B}\left[\left(\frac{a}{a_{\max}} \right)^{3(1+\beta)}, \frac{1}{2(1+\beta)}, \frac{2\beta+1}{2(1+\beta)} \right] \tag{8.22}$$
$$= \sqrt{3}\kappa\, |A|^{\frac{1}{2(1+\beta)}} (1+\beta)\, t\,,$$

where $\mathbf{B}[\gamma, \delta]$ and $\mathbf{B}[x, \gamma, \delta]$ stand for the beta function and the incomplete beta function, respectively (see section 6.2. in [1]). The time t stands for the time that elapses from a given finite value of the scale factor to its maximum value $a_{\max}$. As long as $-1/2 < \beta \leq 0$ holds, t is finite. However, in the limiting case $\beta \to -1/2$, it becomes infinite. Using equation 15.1.20 in [1], one can rewrite (8.22) as

$$2(1+\beta)\Bigg\{ \mathbf{F}\left[\frac{1}{1+\beta}, \frac{1}{1+\beta}; 1 + \frac{1}{1+\beta}; 1 \right] \tag{8.23}$$
$$- \left(\frac{a}{a_{\max}} \right)^{\frac{3}{2}} \mathbf{F}\left[\frac{1}{1+\beta}, \frac{1}{1+\beta}; 1 + \frac{1}{1+\beta}; \left(\frac{a}{a_{\max}} \right)^{3(1+\beta)} \right] \Bigg\}$$
$$= \sqrt{3}\kappa\, |A|^{\frac{1}{2(1+\beta)}} (1+\beta)\, t\,.$$

Here, $\mathbf{F}[\gamma, \delta; \epsilon; x]$ denotes a hypergeometric function (see chapter 15 in [1]). This expression directly shows that t stays finite for $-1/2 < \beta \leq 0$, but becomes infinite for $\beta \to -1/2$.

At the maximum scale factor, $a = a_{\max}$, the n-th derivative of the Hubble parameter H diverges in the case $\beta \neq 1/(2p) - 1/2$, $p \in \mathbb{N}$. One can express n as

$$n = 1 + E\Big((1 + 2\beta)^{-1}\Big) \tag{8.24}$$

using the integer value function E [27]. This implies that the $(n-1)$-th derivative of the scalar curvature diverges as well at $a = a_{\max}$ and, hence, we have a type IV singularity at $a = a_{\max}$.

We can describe a universe filled with this kind of GCG as dust-dominated at small scale factors, which means that $P/\rho \ll 1$, and there is a Big Bang singularity at $a = 0$. In the cases $\beta \neq 1/(2p) - 1/2$, $p \in \mathbb{N}$, the universe expands up to $a_{\max}$, where it assumes its maximum size and faces a type IV singularity. In the limiting case $\beta = -1/2$, it takes the universe an infinite time to reach its maximum size, therefore the Hubble parameter and all its cosmic time derivatives remain finite and there is no type IV singularity.

As we have described before, we now have to implement this type of generalized Chaplygin gas dynamically by a minimally coupled scalar field, for which the energy density and pressure are given by

$$\rho_\phi = \frac{1}{2}\,\dot{\phi}^2 + V(\phi), \qquad P_\phi = \frac{1}{2}\,\dot{\phi}^2 - V(\phi). \tag{8.25}$$

Here, we have used a dot to denote derivatives with respect to cosmic time t. We can consequently express the kinetic energy $\dot{\phi}^2$ and the potential $V(\phi)$ of the scalar field in terms of the scale factor as follows

$$\dot{\phi}^2 = |A|^{\frac{1}{1+\beta}} \frac{\left(\frac{a_{\max}}{a}\right)^{3(1+\beta)}}{\left[\left(\frac{a_{\max}}{a}\right)^{3(1+\beta)} - 1\right]^{\frac{\beta}{1+\beta}}}, \qquad V(\phi) = \frac{1}{2}\,|A|^{\frac{1}{1+\beta}} \frac{\left(\frac{a_{\max}}{a}\right)^{3(1+\beta)} - 2}{\left[\left(\frac{a_{\max}}{a}\right)^{3(1+\beta)} - 1\right]^{\frac{\beta}{1+\beta}}}. \tag{8.26}$$

The relation between the scalar field and the scale factor is therefore given by

$$|\phi - \phi_{\max}|(a) = \frac{2\sqrt{3}}{3\kappa|1+\beta|} \ln\left[\left(\frac{a_{\max}}{a}\right)^{\frac{3}{2}(1+\beta)} + \sqrt{\left(\frac{a_{\max}}{a}\right)^{3(1+\beta)} - 1}\,\right], \tag{8.27}$$

where $\phi_{\max}$ denotes the value ϕ acquires at the maximum scale factor $a = a_{\max}$, where the type IV singularity is located. We set $\phi_{\max} = 0$ for simplicity.

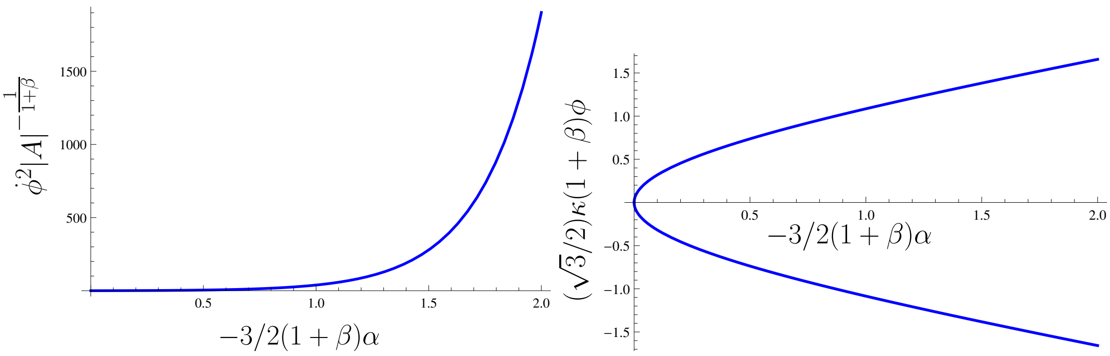

Figure 8.1: Plot of the dependence of the kinetic energy $\dot{\phi}^2$ on the logarithmic scale factor $\alpha = \ln(a/a_{\text{max}})$ (left) and of the scalar field ϕ on α (right). In the left figure, the value $\beta = -\sqrt{2}/3$ is chosen. The type IV singularity is located at $\phi = 0$, where $a = a_{\text{max}}$. From [30].

Figure 8.1 shows the dependence of the kinetic energy $\dot{\phi}^2$ on the logarithmic scale factor α as well as the dependence of the field ϕ on α, which is the classical trajectory in configuration space.

Finally, we can write down the potential of the scalar field

$$V(\phi) = V_1 \left[\sinh^{\frac{2}{1+\beta}} \left(\frac{\sqrt{3}}{2} \kappa |1+\beta||\phi| \right) - \sinh^{-\frac{2\beta}{1+\beta}} \left(\frac{\sqrt{3}}{2} \kappa |1+\beta||\phi| \right) \right], \quad (8.28)$$

where we have defined, analogously to [31],

$$V_1 := \frac{|A|^{\frac{1}{1+\beta}}}{2}. \quad (8.29)$$

In figure 8.2, we present a plot of this potential for a typical value of β.

Note that near the singularity, $a = a_{\text{max}}$, $\phi = 0$, the potential is negative and finite, which reflects the fact that at a type IV singularity both the energy density and the pressure remain finite.

The potential (8.28) has the form of a double-well potential and is regular everywhere, in contrast to the cases discussed in [41, 61, 31]. The reason is the mild nature of the type IV singularity, which will be reflected in the quantized model later on.

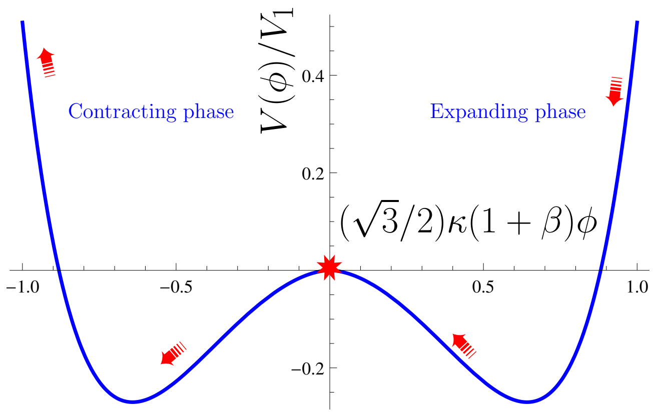

Figure 8.2: Plot of the potential defined in equation (8.28) as a function of the scalar field ϕ using the value $\beta = -\sqrt{2}/3$, which has been chosen to make sure that β cannot be written as $1/(2p) - 1/2$, $p \in \mathbb{N}$. The potential has the form of a double-well potential widely used in quantum mechanics. From [30].

Like it was done in [31], we can approximate the potential close to the type IV singularity, $a = a_{\text{max}}$, $\phi = 0$, as

$$V(\phi) \simeq -V_1 \left(\frac{\sqrt{3}}{2} \kappa \, |1 + \beta| |\phi| \right)^{-\frac{2\beta}{1+\beta}} . \tag{8.30}$$

For the limiting case $\beta = -1/2$, we thus have an inverted harmonic oscillator in this approximation.

On the other hand, for small scale factors, corresponding to large values of the scalar field ϕ, an approximation of the potential leads to the following exponential form

$$V(\phi) \simeq 2^{-\frac{2}{1+\beta}} V_1 \exp\left(\sqrt{3}\kappa|\phi|\right) . \tag{8.31}$$

An exponential potential like this also occurs for a Big Rip with a phantom field [41] and for the Big Bang in the model containing an anti-Chaplygin gas as presented in [61], which also contains a Big Brake singularity. As we have discussed before, in this model the big-bang singularity is avoided simultaneously with the big-brake singularity for the normalizable solutions of the Wheeler–DeWitt equation. Also in the model discussed in [31], where a big-freeze singularity is induced by a standard generalized Chaplygin gas, but where the universe behaves dust-like ($P/\rho \sim 0$) for large rather than for small scale factors, one finds a similar expression to (8.31).

8.3.2 Phantom generalized Chaplygin gas

Apart from the standard generalized Chaplygin gas, we also want to analyze a universe that contains a *phantom* generalized Chaplygin gas that, as we have mentioned before, violates the null energy condition. According to [27], such a type of matter can induce a type IV singularity in the *past* in the following cases

$$A > 0\,, \quad B < 0\,, \quad \text{and} \quad -\frac{1}{2} < \beta < 0\,, \quad \text{where} \quad \beta \neq \frac{1}{2p} - \frac{1}{2}\,, \tag{8.32}$$

and p is again a positive integer. We can write the energy density (8.18) and the pressure of the phantom GCG as

$$\rho = |A|^{\frac{1}{1+\beta}} \left[1 - \left(\frac{a_{\min}}{a}\right)^{3(1+\beta)}\right]^{\frac{1}{1+\beta}}\,, \quad P = -|A|^{\frac{1}{1+\beta}} \left[1 - \left(\frac{a_{\min}}{a}\right)^{3(1+\beta)}\right]^{\frac{-\beta}{1+\beta}}\,. \tag{8.33}$$

In this model, the scale factor a has a minimum value $a_{\min}$ instead of a maximum value as for the standard GCG (8.21). This minimum value, where the type IV singularity is located, is given by

$$a_{\min} := \left|\frac{B}{A}\right|^{\frac{1}{3(1+\beta)}}\,. \tag{8.34}$$

The cosmic time derivatives of the Hubble rate are of a similar form as the ones of the previous subsection. We can thus see that there is a type IV singularity at $a = a_{\min}$.

We can integrate the Friedmann equations analytically, which leads to (see section 6.2. in [1])

$$\mathbf{B}\left[\left(\frac{a}{a_{\min}}\right)^{3(1+\beta)}, 0, \frac{2\beta+1}{2(1+\beta)}\right] = \sqrt{3}\,\kappa A^{\frac{1}{2(1+\beta)}}\,(1+\beta)\,t\,. \tag{8.35}$$

Here, t denotes the time that has elapsed from the beginning of the expansion of the universe at the minimum scale factor, $a = a_{\min}$, where the type IV singularity is situated, until the universe has reached a given finite size a. For very large values of the scale factor a, the universe asymptotically takes the form of a de Sitter universe. The incomplete beta function used in (8.35) is well-defined even though it has the value zero in its second argument.

Now we want to realize the phantom GCG by a minimally coupled scalar field. Because of the phantom nature of this field, the kinetic terms in the expressions for energy density and pressure change their sign compared to (8.25) and read

$$\rho_\phi = -\frac{1}{2}\,\dot{\phi}^2 + V(\phi)\,, \qquad P_\phi = -\frac{1}{2}\,\dot{\phi}^2 - V(\phi)\,. \tag{8.36}$$

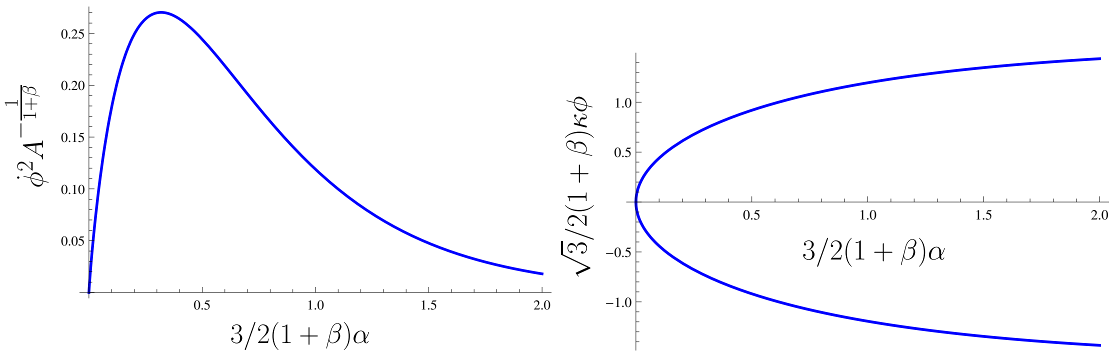

Figure 8.3: Plot of the dependence of the kinetic energy $\dot{\phi}^2$ on the logarithmic scale factor $\alpha = \ln(a/a_{\text{min}})$ (left) and of the scalar field ϕ on α (right). In the left figure, the value $\beta = -\sqrt{2}/3$ is chosen. The type IV singularity is located at $\phi = 0$, where $a = a_{\text{min}}$. From [30].

We can then write out the kinetic energy $\dot{\phi}^2$ and the potential $V(\phi)$ of the scalar field in terms of the scale factor a and get

$$\dot{\phi}^2 = A^{\frac{1}{1+\beta}} \frac{\left(\frac{a_{\text{min}}}{a}\right)^{3(1+\beta)}}{\left[1-\left(\frac{a_{\text{min}}}{a}\right)^{3(1+\beta)}\right]^{\frac{\beta}{1+\beta}}}, \qquad V(\phi) = \frac{1}{2} A^{\frac{1}{1+\beta}} \frac{2-\left(\frac{a_{\text{min}}}{a}\right)^{3(1+\beta)}}{\left[1-\left(\frac{a_{\text{min}}}{a}\right)^{3(1+\beta)}\right]^{\frac{\beta}{1+\beta}}}. \quad (8.37)$$

For the dependence of the scalar field ϕ on the scale factor a, we therefore obtain

$$|\phi - \phi_{\text{min}}|(a) = \frac{2}{\kappa\sqrt{3}} \frac{1}{1+\beta} \arccos\left[\left(\frac{a_{\text{min}}}{a}\right)^{\frac{3(1+\beta)}{2}}\right]. \quad (8.38)$$

Here, we denote the minimum value of the scalar field at $a = a_{\text{min}}$, where the singularity is located, by ϕ_{min}. In the following we set $\phi_{\text{min}} = 0$ for simplicity. Figure 8.3 shows the absolute value of the kinetic energy of the scalar field $\dot{\phi}^2$ as well as the dependence of the field ϕ on the logarithmic scale factor α.

We can express the potential of the scalar field $V(\phi)$ as

$$V(\phi) = V_{-1}\left[\sin^{-\frac{2\beta}{1+\beta}}\left(\frac{\sqrt{3}}{2}\kappa\,|1+\beta||\phi|\right) + \sin^{\frac{2}{1+\beta}}\left(\frac{\sqrt{3}}{2}\kappa\,|1+\beta||\phi|\right)\right], \quad (8.39)$$

where we have defined

$$V_{-1} := \frac{A^{\frac{1}{1+\beta}}}{2} \quad (8.40)$$

and we have to restrict the values the scalar field ϕ can take to (cf. equation (21) in [31])

$$0 < \frac{\sqrt{3}}{2}\kappa\,|1+\beta|\,|\phi| \leq \frac{\pi}{2}. \quad (8.41)$$

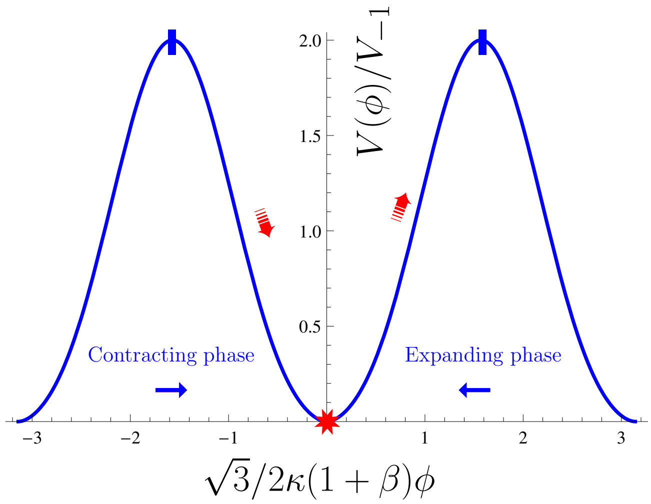

Figure 8.4: Plot of the potential defined in equation (8.39) as a function of the scalar field ϕ using the value $\beta = -\sqrt{2}/3$, which has been chosen to make sure that β cannot be written as $1/(2p) - 1/2$, $p \in \mathbb{N}$. While the potential is periodic, the model we consider here corresponds to the range of values of ϕ between two consecutive maxima indicated by blue vertical lines. From [30].

We see that near the location of the singularity, $a = a_{\text{min}}$, $\phi = 0$, the potential is positive and finite, which is again contrary to the situation presented in [31]. As before, this can be attributed to the fact that at a type IV singularity both the energy density and the pressure remain finite.

However, the potential (8.39) is periodic in ϕ, which is a significant difference compared to the standard field. Figure 8.4 displays the shape of the potential in terms of the scalar field ϕ. The branch we consider here is the expanding branch, where the evolution of the universe starts from the type IV singularity $\phi = 0$. The scalar field then rolls up the potential and for $a \to \infty$ asymptotically reaches the top of the potential, which is situated at

$$\phi = \frac{\pi}{\sqrt{3}(\beta+1)\kappa}. \tag{8.42}$$

The other parts of the potential displayed in figure 8.4, which are located outside the maxima of the potential marked with vertical lines, correspond to different classical solutions, which may have consequences for the quantized model.

We add that one can approximate the potential $V(\phi)$ close to the singularity by

$$V(\phi) \simeq V_{-1}\left(\frac{\sqrt{3}}{2}\kappa|1+\beta||\phi|\right)^{-\frac{2\beta}{1+\beta}}. \tag{8.43}$$

Now we will discuss the quantization of these classical models.

8.4 Analysis of the quantized models

In order to find out whether the type IV singularities are resolved after a canonical quantization of the models discussed in the previous section, we have to find a solution to the Wheeler–DeWitt equations describing these models in some approximation. While the quantum cosmology of a generalized Chaplygin gas was first discussed in [32], we will use here the methods presented in [41, 61, 31].

After the preparation done in chapter 3 and using the Laplace–Beltrami factor ordering, we obtain the following Wheeler–DeWitt equation for the wave function $\Psi\left(\alpha,\phi\right)$ with $\alpha := \ln(a/a_0)$

$$\frac{\hbar^2}{2}\left(\frac{\kappa^2}{6}\frac{\partial^2}{\partial\alpha^2} - \ell\frac{\partial^2}{\partial\phi^2}\right)\Psi\left(\alpha,\phi\right) + a_0^6\,\mathrm{e}^{6\alpha}\,V(\phi)\,\Psi\left(\alpha,\phi\right) = 0\,. \tag{8.44}$$

Since we want to treat the cases of a standard and a phantom generalized Chaplygin gas, that is standard and phantom scalar field, at once, we have introduced a parameter ℓ, which takes the value $\ell = 1$ for the standard case and $\ell = -1$ for the phantom case.

We set the reference scale factor a_0 to the location of the type IV singularity, i.e. $a_0 = a_{\max}$ for the model with the standard field and $a_0 = a_{\min}$ for the model with the phantom field. The potential $V(\phi)$ has to be taken from (8.28) for the standard case and from (8.39) for the phantom case.

In order to find a solution to equation (8.44), we use the Born–Oppenheimer type of ansatz that was first used in [66] and separate the wave function $\Psi\left(\alpha,\phi\right)$ in the following way

$$\Psi(\alpha,\phi) = \varphi_k(\alpha,\phi)\,C_k(\alpha)\,, \tag{8.45}$$

where we have introduced k as a general complex parameter. Furthermore, we require that in the Born–Oppenheimer limit, the matter part φ_k of the wave function Ψ satisfy the subsequent differential equation with an energy function $E_k(\alpha)$

$$-\ell\,\frac{\hbar^2}{2}\frac{\partial^2\varphi_k}{\partial\phi^2} + a_0^6\,\mathrm{e}^{6\alpha}\,V(\phi)\,\varphi_k = E_k(\alpha)\,\varphi_k\,. \tag{8.46}$$

8.4.1 Standard field

We start with the analysis of the case of a standard field, that means we have $\ell = 1$. Furthermore, we set $\hbar = 1$ from now on for simplicity.

Since it is difficult to solve equation (8.46) analytically for a general value of β, we have to choose a particular value for β. Our choice is

$$\beta = -\frac{1}{2}\,, \tag{8.47}$$

which is strictly speaking a value where a type IV singularity does *not* occur, as it lies outside the range $-1/2 < \beta < 0$, which was imposed in the previous section. Nevertheless, since the form of the potential 8.2 remains the same for $\beta = -1/2$ and $\beta = -1/2 + \epsilon$, $0 < \epsilon \ll 1$ one can expect that the qualitative features of the limiting case $\beta = -1/2$ are carried over to the more general case, where a type IV singularity occurs.

Using $\beta = -1/2$, the differential equation of the matter part (8.46) reads

$$-\frac{1}{2}\frac{\partial^2\varphi_k}{\partial\phi^2} + a_0^6\,V_1\,\mathrm{e}^{6\alpha}\left[\sinh^4\left(\frac{\sqrt{3}}{4}\kappa\,\phi\right) - \sinh^2\left(\frac{\sqrt{3}}{4}\kappa\,\phi\right)\right]\varphi_k = E_k(\alpha)\,\varphi_k\,. \tag{8.48}$$

In order to simplify this equation, we introduce a new variable x as follows

$$x := \sinh\left(\frac{\sqrt{3}}{4}\kappa\,\phi\right). \tag{8.49}$$

In figure 8.1 (right) the range $x > 0$ corresponds to the upper branch of the trajectory, while the range $x < 0$ corresponds to the lower branch. From now on, we will skip the index k in order to simplify the notation. Using the new variable x, equation (8.48) reads

$$\left(1 + x^2\right)\frac{\partial^2\varphi}{\partial x^2} + x\,\frac{\partial\varphi}{\partial x} - \xi\,x^2\,(x^2 - 1)\,\varphi = -\,\epsilon\,\varphi\,, \tag{8.50}$$

where we have introduced the parameters ξ and ϵ, whose dependence on α we do not explicitly state and which are defined as

$$\xi := \frac{32\,V_1\,a_0^6\,\mathrm{e}^{6\alpha}}{3\,\kappa^2} > 0\,, \qquad \epsilon := \frac{32\,E_k(\alpha)}{3\,\kappa^2}\,. \tag{8.51}$$

The resulting equation (8.50) is symmetric under $x \mapsto -x$, such that we can treat both branches on an equal footing.

We now use the separation ansatz

$$\varphi = \exp\left(-\frac{\sqrt{\xi}}{2}\,x^2\right)\mathrm{H}(x) \tag{8.52}$$

and consequently find that the newly introduced function $\mathrm{H}(x)$ obeys the subsequent differential equation

$$\left(1+x^2\right)\frac{\mathrm{d}^2\mathrm{H}}{\mathrm{d}x^2}+\left(x-2x\left(1+x^2\right)\sqrt{\xi}\right)\frac{\mathrm{d}\mathrm{H}}{\mathrm{d}x}-\left(\left(1+2x^2\right)\sqrt{\xi}-2x^2\xi\right)\mathrm{H}=-\epsilon\,\mathrm{H}. \tag{8.53}$$

Note that we write an ordinary differential here, because we specify only the dependence on the variable x. Using the transformation

$$z := -x^2\,, \tag{8.54}$$

equation (8.53) takes the form

$$\frac{\mathrm{d}^2\mathrm{H}}{\mathrm{d}z^2}+\frac{\sqrt{\xi}z^2-\left(\sqrt{\xi}-1\right)z-\frac{1}{2}}{z\,(z-1)}\frac{\mathrm{d}\mathrm{H}}{\mathrm{d}z}-\frac{\left(2\xi-2\sqrt{\xi}\right)z+\sqrt{\xi}-\epsilon}{4z\,(z-1)}\mathrm{H}=0\,. \tag{8.55}$$

This is one of the standard forms for the confluent Heun differential equation, which is discussed in detail in [95]. The solutions to this differential equation are called *confluent Heun functions* and are denoted using five parameters as $\mathcal{H}_\mathrm{c}(u,v,w,\delta,\eta;z)$. Using these parameters, the canonical form of the confluent Heun differential equation reads, see e.g. p. 59, eq. (13) in [42],

$$\begin{aligned}\frac{\mathrm{d}^2\mathcal{H}_\mathrm{c}}{\mathrm{d}z^2}&+\frac{u\,z^2-(u-v-w-2)\,z-v-1}{z\,(z-1)}\frac{\mathrm{d}\mathcal{H}_\mathrm{c}}{\mathrm{d}z}\\&+\frac{\left(\delta+\frac{1}{2}u\,(v+w+2)\right)z+\frac{1}{2}(w-u)(v+1)+\frac{v}{2}+\eta}{z\,(z-1)}\mathcal{H}_\mathrm{c}=0\,.\end{aligned} \tag{8.56}$$

A comparison of this general form with our equation (8.55) yields that we can write the solution of (8.55) in the following form

$$\mathrm{H}(z)=\mathcal{H}_\mathrm{c}\left(\sqrt{\xi},-\frac{1}{2},-\frac{1}{2},-\frac{\xi}{2},\frac{3}{8}+\frac{\epsilon}{4};z\right) \tag{8.57}$$

and we immediately see that (8.53) is solved by

$$\mathrm{H}(x)=\mathcal{H}_\mathrm{c}\left(\sqrt{\xi},-\frac{1}{2},-\frac{1}{2},-\frac{\xi}{2},\frac{3}{8}+\frac{\epsilon}{4};-x^2\right). \tag{8.58}$$

According to p. 61, proposition 2-1, in [42], we can write a linearly independent solution of (8.53) as follows

$$\mathrm{H}(x)=x\,\mathcal{H}_\mathrm{c}\left(\sqrt{\xi},\frac{1}{2},-\frac{1}{2},-\frac{\xi}{2},\frac{3}{8}+\frac{\epsilon}{4};-x^2\right). \tag{8.59}$$

Note the sign change of the second parameter. Hence, we can write our solution for φ as the subsequent linear combination with constants c_1 and c_2

$$\varphi(x) = c_1\,\mathrm{e}^{-\frac{\sqrt{\xi}}{2}x^2}\,\mathcal{H}_{\mathrm{c}}\left(\sqrt{\xi}, -\frac{1}{2}, -\frac{1}{2}, -\frac{\xi}{2}, \frac{3}{8}+\frac{\epsilon}{4}; -x^2\right) + c_2\,x\,\mathrm{e}^{-\frac{\sqrt{\xi}}{2}x^2}\,\mathcal{H}_{\mathrm{c}}\left(\sqrt{\xi}, \frac{1}{2}, -\frac{1}{2}, -\frac{\xi}{2}, \frac{3}{8}+\frac{\epsilon}{4}; -x^2\right). \tag{8.60}$$

Even though it is not known up to now what kind of Hilbert space one has to choose in quantum gravity [69], we proceed here as for the normalizability condition in quantum mechanics and require that the physically allowed wave functions $\varphi(x)$ go to zero for large x.

The Heun function $\mathcal{H}_{\mathrm{c}}$ that appears in our solution (8.60) has the property that it is regular at the origin $x = 0$, see [95], p. 98,

$$\mathcal{H}_{\mathrm{c}}(\cdot,\cdot,\cdot,\cdot,\cdot;0) = 1\,, \tag{8.61}$$

and that it increases as a power for large x, see [95], p. 101. However, the decrease due to the Gaussian factor appearing in (8.60) dominates over the increase as a power due to $\mathcal{H}_{\mathrm{c}}$, such that the wave function $\varphi(x)$ in (8.60) goes to zero at infinity and thus satisfies our requirement.

One can also see that in the first term of (8.60) the variable x appears only quadratically, which makes this part of the wave function symmetric, whereas the additional factor of x in the second term of (8.60) makes this part antisymmetric, such that it assumes the value zero at the origin. Given that $x = 0$ corresponds to the location of the type IV singularity at $\phi = 0$, we can conclude that this second antisymmetric part fulfills the condition of singularity avoidance, while the first symmetric part does not.

Since in the general case, where a type IV singularity is present, i.e. for $-1/2 < \beta < 0$, $\beta \neq 1/(2p) - 1/2$, $p \in \mathbb{N}$, the equations take a much more complicated form and are generally not analytically solvable, we restrict ourselves to draw general conclusions from our solution for $\beta = -1/2$ without making explicit calculations, using the following arguments.

As we have mentioned, a sufficient criterium for singularity avoidance is that the wave function vanishes at the point where the classical singularity is located, which in our case is at $\phi = 0$. The question we thus have to answer is whether we can implement $\varphi(\alpha, 0) = 0$. In ordinary quantum mechanics, double-well potentials that take a similar form as the one displayed in figure 8.2 lead to a spectrum of infinitely many discrete bound states, where the ground state φ_0 has a symmetric form, while the symmetry of the excited states φ_n, which have n nodes, alternates between antisymmetric and symmetric. If we consider two consecutive nodes of φ_n, we find that there is always a node of φ_{n-1} located between them. Hence, we can conclude that the antisymmetric solutions vanish at $\phi = 0$, whereas the symmetric ones do not.

Therefore, there is a crucial difference for the case discussed here when compared to how singularities were resolved in the earlier articles [61] and [31]. In some of the cases considered in these former papers, the requirement that the wave function is normalizable with respect to the $\mathcal{L}^2$ inner product already enforces that the wave function vanishes at the point of the classical singularity. This is not the case for type IV singularities, were singularity-avoiding solutions are allowed, but not enforced. We can therefore construct singularity-avoiding solutions using superpositions of states of the form (8.45), where φ_k is chosen to be an antisymmetric eigenstate of (8.50), but solutions that do not vanish at the classical singularity are equally allowed.

This argument is valid for general β fulfulling $-1/2 < \beta < 0$, $\beta \neq 1/(2p) - 1/2$, $p \in \mathbb{N}$. The solutions for $\beta = -1/2$ presented above in terms of Heun functions correspond to a special case where explicit solutions can be given.

Apart from the solutions for the matter part φ_k, one also has to solve the gravitational part of the wave function (8.45). Plugging the ansatz (8.45) into the Wheeler–DeWitt equation (8.44) leads to the following equation for $C_k(\alpha)$,

$$\frac{\kappa^2}{6}\left(2\,\dot{C}_k\,\dot{\varphi}_k + C_k\,\ddot{\varphi}_k\right) + \left(\frac{\kappa^2}{6}\,\ddot{C}_k + 2\,E_k(\alpha)\,C_k\right)\varphi_k = 0\,, \tag{8.62}$$

where we now use a dot to denote a derivative with respect to α. We now assume as it is usually done in the Born–Oppenheimer approximation that C_k varies much more rapidly with α than with φ_k and that one can neglect the backreaction of the matter part φ_k on the gravitational part C_k. This allows us to neglect the terms where α-derivatives of φ_k appear, i.e. $\dot{C}_k\dot{\varphi}_k$ and $C_k\ddot{\varphi}_k$ [66]. Consequently, the matter part influences the gravitational part only by contributing its energy via the term $E_k(\alpha)$. Hence, using this approximation, we end up with

$$\left(\frac{\kappa^2}{6}\,\ddot{C}_k + 2\,E_k(\alpha)\,C_k\right)\varphi_k = 0\,. \tag{8.63}$$

Since the parameter ℓ does not appear in this equation, it can be used for both the standard case and the phantom case.

Since we cannot write out the exact expression for $E_k(\alpha)$ due to the fact that these are the eigenvalues of (8.46) and cannot be given in explicit form, we have to solve (8.63) using a WKB approximation. This leads to the following approximate solution

$$C_k(\alpha) \sim \left(\frac{12\,E_k(\alpha)}{\kappa^2}\right)^{-\frac{1}{4}} \left(b_1 \exp\left[\mathrm{i}\int \sqrt{\frac{12\,E_k(\alpha)}{\kappa^2}}\,\mathrm{d}\alpha\right] + b_2 \exp\left[-\mathrm{i}\int \sqrt{\frac{12\,E_k(\alpha)}{\kappa^2}}\,\mathrm{d}\alpha\right]\right), \tag{8.64}$$

where b_1 and b_2 are constants. The function $E_k(\alpha)$ is real because it is an eigenvalue of the Hermitian operator appearing in (8.48). The $E_k(\alpha)$ are positive in the classically allowed region, that is for $a \leq a_{\max}$, and negative in the classically forbidden region, i.e. for $a > a_{\max}$.

We have to make sure that the wave functions $C_k(\alpha)$ decrease exponentially for $\alpha \to \infty$, that is in the classically forbidden region, such that we respect the correspondence to the classical limit [76]. This important consistency condition then leads to a relation between the parameters b_1 and b_2 in (8.64) using standard WKB connection formulae. Given the fact that all these solutions are regular, they do not influence the conclusions we made on singularity avoidance.

In principle, one could get a solution to the Wheeler–DeWitt equation (8.44) that vanishes at the type IV singularity by demanding that the functions C_k vanish at this point, which would lead to a certain condition between the parameters b_1 and b_2. However, this would mean that the resulting functions C_k would not decrease in the classically forbidden region, which is why we do not consider this option.

8.4.2 Phantom field

In order to analyze the case of a phantom generalized Chaplygin gas, we can proceed largely analogously to the standard case discussed above, which is why we only describe the main steps. If we choose $\ell = -1$, $\beta = -1/2$ and insert the potential for the phantom scalar field (8.39), we obtain the following differential equation for the matter part φ_k

$$-\frac{1}{2}\frac{\partial^2\varphi_k}{\partial\phi^2} - V_{-1}\,\mathrm{e}^{6\alpha}\left[\sin^4\left(\frac{\sqrt{3}}{4}\kappa\,\phi\right) + \sin^2\left(\frac{\sqrt{3}}{4}\kappa\,\phi\right)\right]\varphi_k = -\,E_k(\alpha)\,\varphi_k\,. \tag{8.65}$$

In this case, we introduce the variable y defined as

$$y := \sin\left(\frac{\sqrt{3}}{4}\kappa\,\phi\right), \tag{8.66}$$

such that we obtain the following equation for φ_k, where we omit again the index k from now on

$$(1-y^2)\,\frac{\partial \varphi}{\partial y^2} - y\,\frac{\partial \varphi}{\partial y} + \xi\, y^2\,(1+y^2)\,\varphi = \epsilon\,\varphi\,. \tag{8.67}$$

Here, we have defined

$$\xi := \frac{32\,V_{-1}\,a_0^6\,\mathrm{e}^{6\alpha}}{3\,\kappa^2}\,, \qquad \epsilon := \frac{32\,E_k(\alpha)}{3\,\kappa^2}\,. \tag{8.68}$$

As before, we use the separation ansatz

$$\varphi = \exp\left(-\frac{\sqrt{\xi}}{2}\,y^2\right)\mathrm{H}(y) \tag{8.69}$$

and we can infer that $\mathrm{H}(y)$ obeys the following differential equation

$$\left(1-y^2\right)\frac{\mathrm{d}^2\mathrm{H}}{\mathrm{d}y^2} - \left(y + 2y\left(1-y^2\right)\sqrt{\xi}\right)\frac{\mathrm{d}\mathrm{H}}{\mathrm{d}y} + \left(\left(2y^2-1\right)\sqrt{\xi} + 2y^2\xi\right)\mathrm{H} = \epsilon\,\mathrm{H}\,, \tag{8.70}$$

which can be transformed into a standard form for the confluent Heun differential equation using the transformation $z := y^2$. Consequently, equation (8.70) is converted into the following form

$$\frac{\mathrm{d}^2\mathrm{H}}{\mathrm{d}z^2} - \frac{\sqrt{\xi}z^2 - \left(\sqrt{\xi}+1\right)z + \frac{1}{2}}{z\,(z-1)}\,\frac{\mathrm{d}\mathrm{H}}{\mathrm{d}z} - \frac{\left(2\xi + 2\sqrt{\xi}\right)z - \sqrt{\xi} - \epsilon}{4z\,(z-1)}\,\mathrm{H} = 0\,. \tag{8.71}$$

A comparison with the canonical form of the confluent Heun differential equation given in (8.56) yields that equation (8.71) is solved by

$$\mathrm{H}(z) = \mathcal{H}_{\mathrm{c}}\left(-\sqrt{\xi}, -\frac{1}{2}, -\frac{1}{2}, -\frac{\xi}{2}, \frac{3}{8} + \frac{\epsilon}{4}; z\right), \tag{8.72}$$

from which we immediately see that the solution to (8.70) is given by

$$\mathrm{H}(y) = \mathcal{H}_{\mathrm{c}}\left(-\sqrt{\xi}, -\frac{1}{2}, -\frac{1}{2}, -\frac{\xi}{2}, \frac{3}{8} + \frac{\epsilon}{4}; -y^2\right). \tag{8.73}$$

We see that the main difference to the case with a standard generalized Chaplygin gas is the sign of the first argument of the Heun functions. Furthermore, y is a periodic variable, which is why normalizability of the wave function is not required, even though we still have to demand that the wave functions do not increase exponentially for large values of y. Apart from this sign change, the solution for $\varphi(y)$ is identical to the earlier solution $\varphi(x)$ in (8.60).

Hence, the arguments we presented for the standard case are still valid and we conclude as before that type IV singularities in the phantom case are only avoided for a subset of the solutions. We have already remarked that the solution for the gravitational part does not depend on the parameter ℓ and is therefore given also here by (8.64).

8.5 Comparison with other approaches

Universes with a type IV singularity have also been studied in loop quantum cosmology [101, 102]. Using a numerical investigation, it was found that type IV singularities occurring in the past are only avoided for certain choices of parameters in a closed universe. For type IV singularities occurring at late times, there is a singularity resolution only if one considers a “baby universe”. In the context of loop quantum gravity related theories, one can also avoid singularities due to a maximum acceleration that appears in spinfoam theory [98]. This has, however, not yet been applied to type IV singularities.

In a certain class of $f(R, T)$ gravity models, it was shown that type IV singularities are not resolved by invoking quantum effects due to the conformal anomaly present in these models [57].

If one applies a different formalism or a different interpretation like the one used in [62], where the method of *time-depending gauge fixing* and *reduction to physical degrees of freedom* instead of the Wheeler–DeWitt equation was used, one finds that at the quantum level weak singularities like the Big Brake are not avoided, which was claimed to hold for all kinds of weak singularities, hence, also for the ones of type IV.

9

Conclusions and outlook

In the first part of this dissertation, we have derived quantum-gravitational corrections to the power spectra of cosmological perturbations during the inflationary phase of the universe. We considered first scalar-field perturbations in a de Sitter model and then moved to gauge-invariant scalar and tensor perturbations, which were investigated both for a pure de Sitter universe as well as for a quasi-de Sitter model in the context of slow-roll inflation. In all cases, we performed a canonical quantization of the respective model and obtained a Wheeler–DeWitt equation. From a semiclassical Born–Oppenheimer type of approximation of this equation, we derived a Schrödinger equation for the individual perturbation modes, which we could use to calculate the power spectrum of the perturbations. At the next order of the approximation, the Schrödinger equation was modified by a quantum-gravitational correction term. Using a modified Gaussian ansatz, we were able to give analytic solutions for the corrected Schrödinger equation in de Sitter case and, after a suitable approximation, also for the slow-roll model.

We demanded that the quantum-gravitational corrections vanish for late times in order to set our boundary condition. However, there remained an ambiguity in the solution and in order to single out one solution, we had to use an additional criterion like continuity of the imaginary part of the solution or minimal oscillatory behavior.

After calculating the corrected power spectrum, we found that for the non-gauge-invariant scalar-field perturbations there was an enhancement of the power on the largest scales, while for both the gauge-invariant scalar and tensor perturbations there is a suppression of the same order of magnitude. The slow-roll parameters give a subdominant contribution that does not change this behavior if one constrains these parameters from observation. Furthermore, we found a correction to the tensor-to-scalar ratio, which is, however, of the second order in the slow-roll parameters.

The significant qualitative change of the correction when going from non-gauge-invariant scalar field perturbations to gauge-invariant perturbations can be attributed to the fact that one multiplies the perturbation variables with the scale factor a at the classical level. This rescaling causes that in the quantity $\Omega_k^{(0)}$ used to calculate the power spectrum, an additional imaginary term appears. This term does not have an influence on the uncorrected power spectrum, because in order to calculate it one has to take the real part of $\Omega_k^{(0)}$. However, in order to calculate the quantum-gravitational correction of this quantity, one has to insert the full solution of $\Omega_k^{(0)}$, which is then cubed and hence changes the differential equation one has to solve. The qualitative change of the result might be unexpected, but one has to consider that we multiply the perturbation variable with a background variable, which is quantized as well. Thus we are dealing with a different quantum (gravity) theory in the gauge-invariant case compared to the scalar-field case and can in principle not expect that the results are identical. Deciding from within the theory, which approach is the correct one, that is, which perturbation variables to choose, might not be possible and would have to be decided by actual observation.

However, as we have seen, the corrections calculated here are several orders of magnitude too small to be measurable in CMB anisotropies, especially because of Cosmic Variance, and – in the case of CMB anisotropies – unavoidable statistical uncertainty. For the large-scale structure of the universe, which can be investigated by looking at the distribution of galaxies, Cosmic Variance is not present. Thus it cannot be excluded that such a quantum-gravitational effect could be easier measurable in this case. But this would have to be checked explicitly by relating the corrected power spectrum of scalar fluctuations to the respective quantities used to describe the large-scale structure, which we leave for further research.

The actual form of the quantum-gravitational corrections derived here is given by

$$1 + \frac{C}{k^3}\frac{H^2}{m_{\rm P}^2} + \mathcal{O}\left(\frac{H^4}{m_{\rm P}^4}\right),$$

where C is a numerical factor that depends on the nature of the perturbations and can also include the slow-roll parameters. Such a k^{-3}-dependence was also found in [59] and [64] using a different semiclassical approximation method to the Wheeler–DeWitt equation. One should investigate further, whether this dependence is a generic prediction of Wheeler–DeWitt quantum cosmology.

With regard to extensions of the models used here, it seems unlikely that one can go further using only analytic solutions of the equations. Our slow-roll model covers every inflationary model where the slow-roll approximation can be applied. In order to investigate any model beyond the slow-roll approximation, one would have to express the quantity z''/z in terms of canonical momenta and convert these to derivatives after quantization, which would complicate the resulting differential equation enormously and one would probably have to use numerics to analyze it, which is beyond the scope of this work.

An interesting further model, which one could possibly investigate analytically with regard to quantum-gravitational corrections is the so-called R^2 inflation, which is also known as the Starobinsky model of inflation [104]. Here one could also study whether those quantum-gravitational corrections lead to new constraints on the parameters of R^2 inflation. But since this model predicts a very low tensor-to-scalar ratio, it is only realistic if the polarization measurements of the Planck satellite that have only been partly released at the writing of this dissertation [2] dispute the claim by the BICEP2 measurements that r is of about 0.2 [3].

In the second part of the thesis, we have investigated whether type IV singularities are avoided in quantum cosmology. We modeled a universe containing such a singularity using a generalized Chaplygin gas both as a standard scalar field as well as a phantom scalar field. We could give an analytic solution to the matter part of the Wheeler–DeWitt equation of this model after using a Born–Oppenheimer approximation and found both for the standard and phantom field that only a subclass of the allowed wave functions vanish at the point where the type IV singularity is located, which we used as a criterion for singularity avoidance. This is in contrast with the results found earlier for our types of singularities, where imposing normalizability of the wave function already selected wave functions that vanish at the classical singularities.

In loop quantum cosmology, it was also found that type IV singularities can only be avoided in very specific models. One could therefore investigate whether this is a general feature of mild singularities like the type IV singularity in canonical quantum gravity.

Another further study that can be done with these models is to investigate whether the type IV singularity can be avoided by tunneling, which in the case of the standard scalar field is motivated by the double-well form of the potential. In the phantom case, the potential is periodic and a branch between two maxima entirely describes a classical solution, while the other branches describe different, but equivalent, entirely independent classical solutions. Hence, in this case tunneling between different branches would allude to concepts like the multiverse.

Appendix

Further analysis of the solution for the quantum-gravitational corrections in the scalar-field case

We follow [22] and consider equation (5.114). When introducing the new variable z defined as

$$z = 1 + \mathrm{i}\xi, \tag{0.1}$$

one can write (5.114) as

$$\frac{\mathrm{d}\Omega_k^{(1)}}{\mathrm{d}z} = 2\left(1 - \frac{1}{z}\right)\Omega_k^{(1)} + \frac{3}{2}\left(7 - 2z - \frac{9}{z} + \frac{5}{z^2} - \frac{1}{z^3}\right), \tag{0.2}$$

whose solution is given by

$$\Omega_k^{(1)}(z) = P_1\,\frac{\mathrm{e}^{2z}}{z^2} + \frac{3}{8z^2}\left[4z^3 - 8z^2 + 10z - 5 + 4\,\mathrm{e}^{2z}\,\mathrm{Ei}(1, 2z)\right]. \tag{0.3}$$

The constant P_1 is chosen such that $\Omega_k^{(1)}(1) = 0$.

In order to study it grafically, we introduce the complex polar representation for

$$z = \rho\,\mathrm{e}^{\mathrm{i}\theta} \tag{0.4}$$

and insert it into the definition of $\Omega_k^{(1)}(z)$. We use the definitions

$$f_\rho(\theta) := \mathfrak{Re}\left[\Omega_k^{(1)}(\rho\mathrm{e}^{\mathrm{i}\theta})\right], \quad g_\rho(\theta) := \mathfrak{Im}\left[\Omega_k^{(1)}(\rho\mathrm{e}^{\mathrm{i}\theta})\right], \tag{0.5}$$

and show the behavior of these functions in figures 0.1 and 0.2.

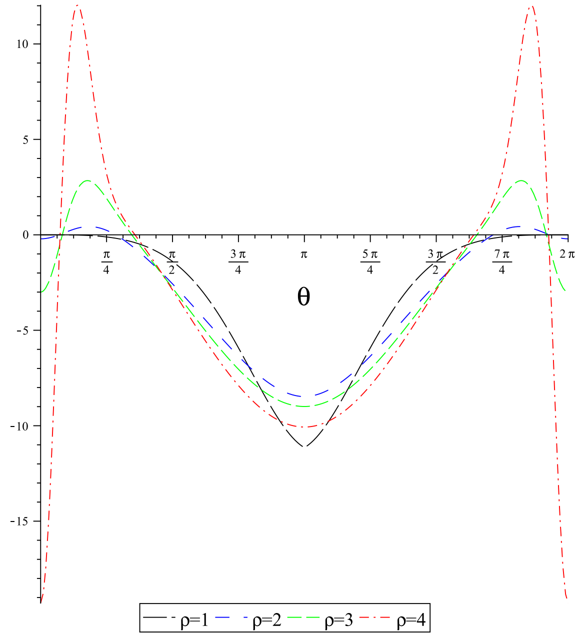

Figure 0.1: Plots of $f_\rho(\theta)$, $\rho = 1,2,3,4$. As ρ increases, the curves show two enhanced peaks at around $\theta = 0$ and $\theta = 2\pi$, from [22].

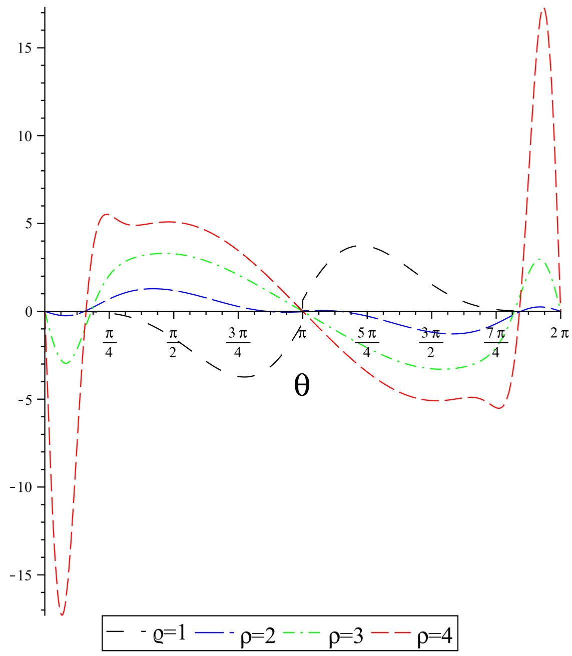

Figure 0.2: Plots of $g_\rho(\theta)$, $\rho = 1,2,3,4$. As ρ increases the curves show two enhanced peaks at around $\theta = 0$ and $\theta = 2\pi$, from [22].

In order to study the deep quantum-gravity regime, one can consider the inverse of ξ as new variable

$$\widetilde{\xi} \equiv \frac{1}{\xi}. \tag{0.6}$$

With this redefinition, we can write (0.2) as

$$\frac{\mathrm{d}}{\mathrm{d}\widetilde{\xi}}\Omega_k^{(1)} = \frac{2\mathrm{i}}{\widetilde{\xi}^2\left(\mathrm{i}\widetilde{\xi}-1\right)}\Omega_k^{(1)} + \frac{3}{2}\frac{\left(\mathrm{i}\widetilde{\xi}-2\right)}{\widetilde{\xi}^3\left(1-\mathrm{i}\widetilde{\xi}\right)^3}. \tag{0.7}$$

Defining again the complex variable

$$z := 1 + \frac{\mathrm{i}}{\xi}, \tag{0.8}$$

we want to plot $\Omega_k^{(1)}$ as a function of z and in order to do so, we introduce the complex polar representation as above and plot in figures 0.3 and 0.4 the real and imaginary part of the solution of (0.7). In order to compare this with figures 0.1 and 0.2, we plot the function when the amplitude ρ takes the same values considered in figures 0.1 and 0.2.

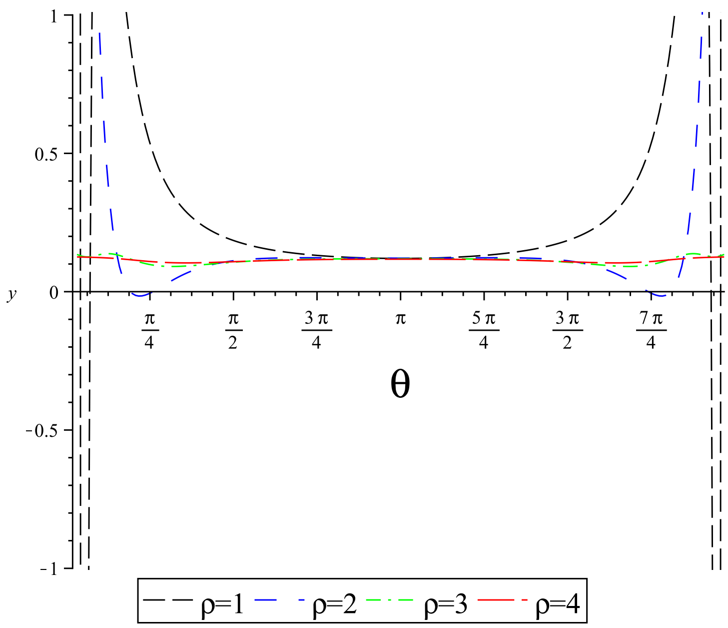

Figure 0.3: Plot of the real part of the solution of (0.7) when the amplitude ρ of the complex variable $z = 1 + \frac{i}{\xi}$ takes the values $1, 2, 3, 4$, from [22].

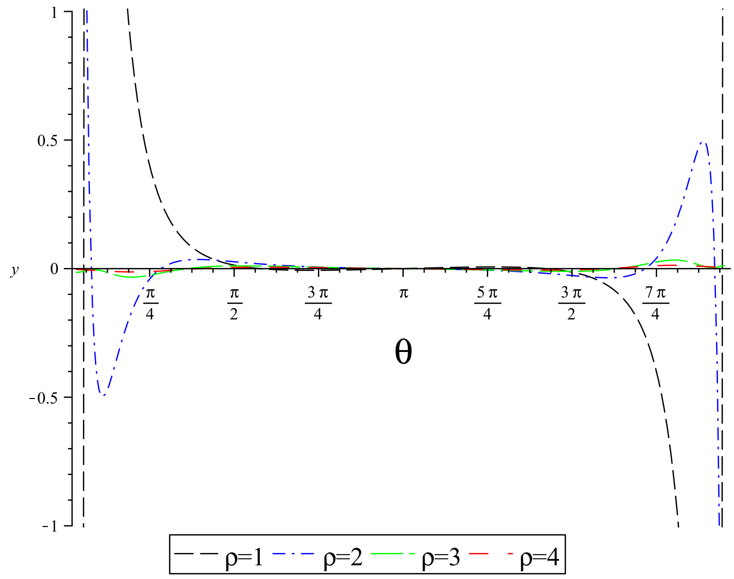

Figure 0.4: Plot of the imaginary part of the solution of (0.7) when the amplitude ρ of the complex variable $z = 1 + \frac{i}{\xi}$ takes the values $1, 2, 3, 4$, from [22].

Bibliography

[1] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, U.S. Government Printing Office, 1964.

[2] R. Adam et al., *Planck intermediate results. XXX. The angular power spectrum of polarized dust emission at intermediate and high Galactic latitudes*, arXiv: 1409.5738 (2014).

[3] P. A. R. Ade et al., *Detection of B-Mode Polarization at Degree Angular Scales by BICEP2*, Phys. Rev. Lett. **112** (2014), 241101.

[4] P. A. R. Ade et al., *Planck 2013 results. XVI. Cosmological parameters*, Astron. Astrophys. **571** (2014), A16.

[5] I. Agulló, A. Ashtekar, and W. Nelson, *Quantum Gravity Extension of the Inflationary Scenario*, Phys. Rev. Lett. **109** (2012), 251301.

[6] I. Agulló, A. Ashtekar, and W. Nelson, *Extension of the quantum theory of cosmological perturbations to the Planck era*, Phys. Rev. D **87** (2013), 043507.

[7] I. Agulló, A. Ashtekar, and W. Nelson, *The pre-inflationary dynamics of loop quantum cosmology: Confronting quantum gravity with observations*, Class. Quant. Grav. **30** (2013), 085014.

[8] J. Ambjørn, A. Gorlich, J. Jurkiewicz, and R. Loll, *CDT - an Entropic Theory of Quantum Gravity*, (2010).

[9] R. Arnowitt, S. Deser, and C. W. Misner, *The dynamics of general relativity,* in: Gravitation: An Introduction to Current Research (edited by Louis Witten), ch. 7, pp. 227–265, Wiley, 1962.

[10] A. Ashtekar, *New Variables for Classical and Quantum Gravity*, Phys. Rev. Lett. **57** (1986), 2244–2247.

[11] A. Ashtekar, *New Hamiltonian formulation of general relativity*, Phys. Rev. D **36** (1987), 1587–1602.

[12] K. Bamba, S. Nojiri, and S. D. Odintsov, *The Universe future in modified gravity theories: Approaching the finite-time future singularity*, JCAP **0810** (2008), 045.

[13] E. M. J. Barbaoza and N. A. Lemos, *Does the Big Rip survive quantization?*, Gen. Rel. Grav. **38** (2006), 1609–1622.

[14] J. D. Barrow, G. J. Galloway, and F. J. Tipler, *The closed-universe recollapse conjecture*, Mon. Not. R. Astro. Soc. **223** (1986), 835–844.

[15] J. D. Barrow, *Sudden future singularities*, Class. Quant. Grav. **21** (2004), L79–L82.

[16] N. Bartolo, E. Komatsu, S. Matarrese, and A. Riotto, *Non-Gaussianity from inflation: Theory and observations*, Phys. Rept. **402** (2004), 103–266.

[17] D. Baumann, *TASI Lectures on Inflation*, arXiv: 0907.5424 (2009).

[18] D. Baumann et al., *CMBPol Mission Concept Study: Probing Inflation with CMB Polarization*, AIP Conf. Proc. **1141** (2009), 10–120.

[19] M. C. Bento, O. Bertolami, and A. A. Sen, *Generalized Chaplygin gas, accelerated expansion and dark energy matter unification*, Phys. Rev. D **66** (2002), 043507.

[20] C. Bertoni, F. Finelli, and G. Venturi, *The Born-Oppenheimer approach to the matter - gravity system and unitarity*, Class. Quant. Grav. **13** (1996), 2375–2384.

[21] N. Bilić, G. B. Tupper, and R. D. Viollier, *Unification of dark matter and dark energy: The Inhomogeneous Chaplygin gas*, Phys. Lett. B **535** (2002), 17–21.

[22] D. Bini, G. Esposito, C. Kiefer, M. Krämer, and F. Pessina, *On the modification of the cosmic microwave background anisotropy spectrum from canonical quantum gravity*, Phys. Rev. D **87** (2013), 104008.

[23] M. Bojowald, G. Calcagni, and S. Tsujikawa, *Observational constraints on loop quantum cosmology*, Phys. Rev. Lett. **107** (2011), 211302.

[24] M. Bojowald, G. Calcagni, and S. Tsujikawa, *Observational test of inflation in loop quantum cosmology*, JCAP **1111** (2011), 046.

[25] M. Bouhmadi-López, P. Chen, Y.-C. Huang, and Y.-H. Lin, *Slow-roll inflation preceded by a topological defect phase à la Chaplygin gas*, Phys. Rev. D **87** (2013), 103513.

[26] M. Bouhmadi-López, P. Chen, and Y.-W. Liu, *Cosmological Imprints of a Generalized Chaplygin Gas Model for the Early Universe*, Phys. Rev. D **84** (2011), 023505.

[27] M. Bouhmadi-López, P. F. González-Díaz, and P. Martín-Moruno, *On the generalised Chaplygin gas: Worse than a big rip or quieter than a sudden singularity?*, Int. J. Mod. Phys. D **17** (2008), 2269–2290.

[28] M. Bouhmadi-López, P. F. González-Díaz, and P. Martín-Moruno, *Worse than a big rip?*, Phys. Lett. B **659** (2008), 1–5.

[29] M. Bouhmadi-López and J. A. Jiménez Madrid, *Escaping the big rip?*, JCAP **0505** (2005), 005.

[30] M. Bouhmadi-López, C. Kiefer, and M. Krämer, *Resolution of type IV singularities in quantum cosmology*, Phys. Rev. D **89** (2014), 064016.

[31] M. Bouhmadi-López, C. Kiefer, B. Sandhöfer, and P. V. Moniz, *On the quantum fate of singularities in a dark-energy dominated universe*, Phys. Rev. D **79** (2009), 124035.

[32] M. Bouhmadi-López and P. Vargas Moniz, *FRW quantum cosmology with a generalized Chaplygin gas*, Phys. Rev. D **71** (2005), 063521.

[33] T. S. Bunch and P. C. W. Davies, *Quantum Field Theory in de Sitter Space: Renormalization by Point Splitting*, Proc. Roy. Soc. Lond. A **360** (1978), 117–134.

[34] G. Calcagni, *Classical and quantum cosmology*, Lecture notes, AEI Potsdam (2011).

[35] G. Calcagni, *Observational effects from quantum cosmology*, Annalen Phys. **525** (2013), no. 5, 323–338.

[36] R. R. Caldwell, *A Phantom menace?*, Phys. Lett. B **545** (2002), 23–29.

[37] R. R. Caldwell, M. Kamionkowski, and N. N. Weinberg, *Phantom energy and cosmic doomsday*, Phys. Rev. Lett. **91** (2003), 071301.

[38] C. Cattoen and M. Visser, *Necessary and sufficient conditions for big bangs, bounces, crunches, rips, sudden singularities, and extremality events*, Class. Quant. Grav. **22** (2005), 4913–4930.

[39] M. P. Dąbrowski and T. Denkiewicz, *Barotropic index w-singularities in cosmology*, Phys. Rev. D **79** (2009), 063521.

[40] M. P. Dąbrowski and T. Denkiewicz, *Exotic-singularity-driven dark energy*, AIP Conf. Proc. **1241** (2010), 561–570.

[41] M. P. Dąbrowski, C. Kiefer, and B. Sandhöfer, *Quantum phantom cosmology*, Phys. Rev. D **74** (2006), 044022.

[42] A. Decarreau, M.-C. Dumont-Lepage, P. Maroni, A. Robert, and A. Ronveaux, *Formes canoniques des équations confluentes de l'équation de Heun*, Annales de la Société Scientifique de Bruxelles **92** (1978), I–II 53–78.

[43] B. S. DeWitt, *Quantum Theory of Gravity. 1. The Canonical Theory*, Phys. Rev. **160** (1967), 1113–1148.

[44] P. A. M. Dirac, *Lectures on Quantum Mechanics*, Belfer Graduate School of Science Monograph Series, vol. 2, Yeshiva University, 1964.

[45] S. Dodelson, *Modern Cosmology*, Academic Press, 2003.

[46] L. Fernandez-Jambrina and R. Lazkoz, *Classification of cosmological milestones*, Phys. Rev. D **74** (2006), 064030.

[47] L. Fernandez-Jambrina and R. Lazkoz, *Geodesic behaviour of sudden future singularities*, Phys. Rev. D. **70** (2004), 121503.

[48] W. Frank, D. Land, and R. Spector, *Singular potentials*, Rev. Mod. Phys. **43** (1971), 36–98.

[49] G. Gamow, *Expanding universe and the origin of elements*, Phys. Rev. **70** (1946), 572–573.

[50] U. H. Gerlach, *Derivation of the Ten Einstein Equations from the Semiclassical Approximation to Quantum Geometrodynamics*, Phys. Rev. **177** (1969), 1929–1941.

[51] V. Gorini, A. Y. Kamenshchik, U. Moschella, and V. Pasquier, *Tachyons, scalar fields and cosmology*, Phys. Rev. D **69** (2004), 123512.

[52] A. Guth, *The Inflationary Universe: A Possible Solution to the Horizon and Flatness Problems*, Phys. Rev. D **23** (1981), 347–356.

[53] J. Guven, B. Lieberman, and C. T. Hill, *Schrödinger Picture Field Theory in Robertson-Walker Flat Space-times*, Phys. Rev. D **39** (1989), 438.

[54] J. J. Halliwell, *Introductory Lectures on Quantum Cosmology (1990)*, arXiv: 0909.2566 (2009).

[55] J. J. Halliwell and S. W. Hawking, *The Origin of Structure in the Universe*, Phys. Rev. D **31** (1985), 1777–1791.

[56] G. Hinshaw et al., *Nine-Year Wilkinson Microwave Anisotropy Probe (WMAP) Observations: Cosmological Parameter Results*, Astrophys. J. Suppl. **208** (2013), 19.

[57] M. J. S. Houndjo, C. E. M. Batista, J. P. Campos, and O. F. Piattella, *Finite-time singularities in f(R,T) gravity and the effect of conformal anomaly*, Can. J. Phys. **91** (2013), 548–553.

[58] W. Hu and S. Dodelson, *Cosmic Microwave Background Anisotropies*, Ann. Rev. Astron. Astrophys. **40** (2002), 171–216.

[59] A. Y. Kamenshchik, A. Tronconi, and G. Venturi, *Inflation and Quantum Gravity in a Born-Oppenheimer Context*, Phys. Lett. B **726** (2013), 518–522.

[60] A. Y. Kamenshchik, *Quantum cosmology and late-time singularities*, Class. Quant. Grav. **30** (2013), 173001.

[61] A. Y. Kamenshchik, C. Kiefer, and B. Sandhöfer, *Quantum cosmology with big-brake singularity*, Phys. Rev. D **76** (2007), 064032.

[62] A. Y. Kamenshchik and S. Manti, *Classical and quantum Big Brake cosmology for scalar field and tachyonic models*, Phys. Rev. D **85** (2012), 123518.

[63] A. Y. Kamenshchik, U. Moschella, and V. Pasquier, *An Alternative to quintessence*, Phys. Lett. B **511** (2001), 265–268.

[64] A. Y. Kamenshchik, A. Tronconi, and G. Venturi, *Signatures of quantum gravity in a Born–Oppenheimer context*, Phys. Lett. B **734** (2014), 72–78.

[65] C. Kiefer, *Continuous Measurement of Minisuperspace Variables by Higher Multipoles*, Class. Quant. Grav. **4** (1987), 1369.

[66] C. Kiefer, *Wave Packets in Minisuperspace*, Phys. Rev. D **38** (1988), 1761–1772.

[67] C. Kiefer, *Can singularities be avoided in quantum cosmology?*, Annalen Phys. **19** (2010), 211–218.

[68] C. Kiefer, *On the Avoidance of Classical Singularities in Quantum Cosmology*, J. Phys. Conf. Ser. **222** (2010), 012049.

[69] C. Kiefer, *Quantum Gravity*, 3rd ed., Oxford University Press, 2012.

[70] C. Kiefer and M. Krämer, *Can effects of quantum gravity be observed in the cosmic microwave background?*, Int. J. Mod. Phys. D **21** (2012), 1241001.

[71] C. Kiefer and M. Krämer, *Quantum gravitational contributions to the cosmic microwave background anisotropy spectrum*, Phys. Rev. Lett. **108** (2012), 021301.

[72] C. Kiefer, I. Lohmar, D. Polarski, and A. A. Starobinsky, *Pointer states for primordial fluctuations in inflationary cosmology*, Class. Quant. Grav. **24** (2007), 1699–1718.

[73] C. Kiefer and D. Polarski, *Why do cosmological perturbations look classical to us?*, Adv. Sci. Lett. **2** (2009), 164–173.

[74] C. Kiefer, D. Polarski, and A. A. Starobinsky, *Quantum-to-classical transition for fluctuations in the early universe*, Int. J. Mod. Phys. D **7** (1998), 455–462.

[75] C. Kiefer and T. P. Singh, *Quantum gravitational corrections to the functional Schrödinger equation*, Phys. Rev. D **44** (1991), 1067–1076.

[76] C. Kiefer and H.-D. Zeh, *Arrow of time in a recollapsing quantum universe*, Phys. Rev. D **51** (1995), 4145–4153.

[77] E. W. Kolb and M. S. Turner, *The Early Universe*, Westview Press, 1990.

[78] M. Krämer, *Quantum Gravitational Corrections to the Primordial Power Spectrum of Density Fluctuations Within the Framework of Quantum Geometrodynamics*, Diplomarbeit, Rheinische Friedrich-Wilhelms-Universität Bonn, 2010.

[79] F. Kühnel and D. J. Schwarz, *Large-Scale Suppression from Stochastic Inflation*, Phys. Rev. Lett. **105** (2010), 211302.

[80] C. Lämmerzahl, *A Hamilton operator for quantum optics in gravitational fields*, Phys. Lett. A **203** (1995), 12–17.

[81] D. Langlois, *Hamiltonian formalism and gauge invariance for linear perturbations in inflation*, Class. Quant. Grav. **11** (1994), 389–407.

[82] A. R. Liddle, *An introduction to cosmological inflation*, arXiv: astro-ph/9901124v1 (1999).

[83] A. R. Liddle and D. H. Lyth, *Cosmological Inflation and Large-Scale Structure*, Cambridge University Press, 2000.

[84] A. D. Linde, *A New Inflationary Universe Scenario: A Possible Solution of the Horizon, Flatness, Homogeneity, Isotropy and Primordial Monopole Problems*, Phys. Lett. B **108** (1982), 389–393.

[85] A. D. Linde, *Chaotic Inflation*, Phys. Lett. B **129** (1983), 177–181.

[86] J. Martin, V. Vennin, and P. Peter, *Cosmological inflation and the quantum measurement problem*, Phys. Rev. D **86** (2012), 103524.

[87] V. F. Mukhanov, H. A. Feldman, and R. H. Brandenberger, *Theory of cosmological perturbations*, Phys. Rep. **215** (1992), 203–333.

[88] S. Nojiri, S. D. Odintsov, and S. Tsujikawa, *Properties of singularities in (phantom) dark energy universe*, Phys. Rev. D. **71** (2005), 063004.

[89] T. Padmanabhan, *Structure formation in the universe*, Cambridge University Press, 1993.

[90] L. Parker and D. Toms, *Quantum Field Theory in Curved Spacetime: Quantized Fields and Gravity*, Cambridge University Press, September 2009.

[91] A. A. Penzias and R. W. Wilson, *A measurement of excess antenna temperature at 4080 Mc/s*, Astrophys. J. **142** (1965), 419–421.

[92] P. Peter and J.-P. Uzan, *Primordial cosmology*, Oxford University Press, 2009.

[93] E. Ramirez and D. J. Schwarz, *Predictions of just-enough inflation*, Phys. Rev. D **85** (2012), 103516.

[94] M. Reuter and F. Saueressig, *Quantum Einstein Gravity*, New J. Phys. **14** (2012), 055022.

[95] A. Ronveaux (ed.), *Heun's Differential Equations*, Oxford University Press, 1995.

[96] J. L. Rosales, *Quantum state correction of relic gravitons from quantum gravity*, Phys. Rev. D **55** (1997), 4791–4794.

[97] C. Rovelli and L. Smolin, *Loop Space Representation of Quantum General Relativity*, Nucl. Phys. B **331** (1990), 80–152.

[98] C. Rovelli and F. Vidotto, *Evidence for Maximal Acceleration and Singularity Resolution in Covariant Loop Quantum Gravity*, Phys. Rev. Lett. **111** (2013), 091303.

[99] P. Schneider, *Extragalactic Astronomy and Cosmology: An Introduction*, Springer, 2006.

[100] D. Schuch, *Riccati and Ermakov equations in time-dependent and time-independent quantum systems*, SIGMA **4** (2008), 043.

[101] P. Singh, *Are loop quantum cosmos never singular?*, Class. Quant. Grav. **26** (2009), 125005.

[102] P. Singh and F. Vidotto, *Exotic singularities and spatially curved Loop Quantum Cosmology*, Phys. Rev. D **83** (2011), 064027.

[103] A. A. Starobinsky, *Spectrum of relict gravitational radiation and the early state of the universe*, JETP Lett. **30** (1979), 682–685.

[104] A. A. Starobinsky, *A New Type of Isotropic Cosmological Models Without Singularity*, Phys. Lett. B **91** (1980), 99–102.

[105] A. A. Starobinsky, *Spectrum of initial perturbations in open and closed inflationary models*, (1996).

[106] A. A. Starobinsky, *Future and origin of our universe: Modern view*, Grav. Cosmol. **6** (2000), 157–163.

[107] C. F. Steinwachs, *Non-minimal Higgs inflation and frame dependence in cosmology*, Springer, 2014.

[108] S. Tsujikawa, R. Maartens, and R. Brandenberger, *Noncommutative inflation and the CMB*, Phys. Lett. B **574** (2003), 141–148.

[109] S. Tsujikawa, P. Singh, and R. Maartens, *Loop quantum gravity effects on inflation and the CMB*, Class. Quant. Grav. **21** (2004), 5767–5775.

[110] J. A. Wheeler, *Superspace and the nature of quantum geometrodynamics*, in: Battelle rencontres (1968), 242–307.

Acknowledgements

Zunächst gilt mein Dank meinem Betreuer Herrn Prof. Dr. Claus Kiefer für die zahlreichen Diskussionen und hilfreichen Kommentare, dafür dass er mich seinen langjährigen Kollaborateuren vorstellte, was zu interessanten Projekten geführt hat, und dass er mich ermutigte, meine Resultate auf wissenschaftlichen Konferenzen zu präsentieren, und hierzu großzügig finanzielle Mittel bereitstellte.

Ebenso bedanken möchte ich mich bei Herrn Prof. Dr. Domenico Giulini, der als Zweitgutachter für diese Dissertation zur Verfügung steht, sowie bei Herrn Prof. Dr. Andreas Eckart und Herrn Privatdozent Dr. Rochus Klesse für die Übernahme des Vor- bzw. Beisitzes der Prüfungskommission.

Inoltre, ringrazio ai miei collaboratori Dr. Giampiero Esposito, Francesco Pessina e Dr. Donato Bini, tal como agradezco a mis colaboradores Dr. Mariam Bouhmadi-López y Dr. David Brizuela. En particular, doy las gracias a David por sus comentarios en cuanto a varias partes de esta tesis.

Furthermore, I would like to thank my office mates and other colleagues from the institute – Jens Boos, Arezu Dehghanfar, Pranjal Dhole, Dr. Alberto Favaro, Thaisa Guio, Prof. Dr. Friedrich W. Hehl, Branislav Nikolić, Christian Schell, Hannes Schenck, Sebastian Schuster, Dr. Christian Steinwachs, Nassim Tanha and Patrick J. Wong – for creating a nice work environment and for numerous discussions. Insbesondere danke ich Jens für seine Unterstützung bei der Tippfehlersuche.

Dalej chciałbym podziękować członkom Szczecińskiej Grupy Kosmologicznej a zwłaszcza profesorowi dr hab. Mariuszowi Dąbrowskiemu za wsparcie w ostatnich tygodniach pisania tej dysertacji.

I would also like to thank the Bonn–Cologne Graduate School of Physics and Astronomy for financial support.

Nicht zuletzt danke ich meinen Eltern für ihre moralische Unterstützung.

Erklärung

Ich versichere, dass ich die von mir vorgelegte Dissertation selbständig angefertigt, die benutzten Quellen und Hilfsmittel vollständig angegeben und die Stellen der Arbeit – einschließlich Tabellen, Karten und Abbildungen –, die anderen Werken im Wortlaut oder dem Sinn nach entnommen sind, in jedem Einzelfall als Entlehnung kenntlich gemacht habe; dass diese Dissertation noch keiner anderen Fakultät oder Universität zur Prüfung vorgelegen hat; dass sie – abgesehen von unten angegebenen Teilpublikationen – noch nicht veröffentlicht worden ist, sowie, dass ich eine solche Veröffentlichung vor Abschluss des Promotionsverfahrens nicht vornehmen werde. Die Bestimmungen der Promotionsordnung sind mir bekannt. Die von mir vorgelegte Dissertation ist von Herrn Prof. Dr. Claus Kiefer betreut worden.

Köln, den ________________ ______________________________

Manuel Krämer

Teilpublikationen

Veröffentlichungen in Fachzeitschriften mit Peer-Review-Verfahren

Claus Kiefer und Manuel Krämer,
Quantum Gravitational Contributions to the Cosmic Microwave Background Anisotropy Spectrum,
Physical Review Letters **108**, 021301 (2012), `arXiv:1103.4967v3`.

Anm.: Die erste im März 2011 auf den Preprint-Server `arXiv` gestellte Version `1103.4967v1` basierte auf meiner Diplomarbeit [78]. Die bei *Physical Review Letters* veröffentlichte Version `1103.4967v3` vom Oktober 2011 wurde allerdings an wesentlichen Stellen überarbeitet.

Donato Bini, Giampiero Esposito, Claus Kiefer, Manuel Krämer und Francesco Pessina,
On the modification of the cosmic microwave background anisotropy spectrum from canonical quantum gravity,
Physical Review D **87**, 104008 (2013), `arXiv:1303.0531v2`.

Mariam Bouhmadi-López, Claus Kiefer und Manuel Krämer,
Resolution of type IV singularities in quantum cosmology,
Physical Review D **89**, 064016 (2014), `arXiv:1312.5976v2`.

Beitrag zum Aufsatzwettbewerb der *Gravity Research Foundation*

Claus Kiefer und Manuel Krämer,
Can effects of quantum gravity be observed in the cosmic microwave background?,
International Journal of Modern Physics D **21**, 1241001 (2012),
arXiv:1205.5161.

Beiträge zu Konferenz-Proceedings

Manuel Krämer,
Can one observe effects of quantum gravity in the cosmic microwave background?,
in: Proceedings of the Barcelona Postgrad Encounters on Fundamental Physics,
hrsg. von D. Fernández, M. B. Fröb, I. Latella und A. Dector;
Universitat de Barcelona, 2013, S. 25–30.

Claus Kiefer und Manuel Krämer,
On the Observability of Quantum-Gravitational Effects in the Cosmic Microwave Background,
in: Relativity and Gravitation – 100 years after Einstein in Prague,
hrsg. von J. Bičák und T. Ledvinka;
Springer Proceedings in Physics **157**, 531–538 (2014).

Manuel Krämer,
Can one observe quantum-gravitational effects in the cosmic microwave background?,
in: The Thirteenth Marcel Grossmann Meeting,
hrsg. von K. Rosquist, R. T. Jantzen und R. Ruffini;
World Scientific, 2015, S. 1622–1624; arXiv:1303.1544.