



Master's Thesis
Theoretical Physics

Decoherence in Inflation

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‘What’re quantum mechanics?’

‘I don’t know. People who repair quantum, I suppose.’

—Terry Pratchett, *Eric*

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<p>In this thesis, we study the decoherence of cosmological scalar perturbations during inflation. We first discuss the FRW model and cosmic inflation. Inflation is a period of accelerated expansion in the early universe, in typical models caused by a scalar field called inflaton. We review cosmological perturbation theory, where perturbations of the inflaton field and scalar degrees of freedom of the metric tensor are combined into the gauge-invariant Sasaki-Mukhanov variable ν. We quantize this variable using canonical quantization. Then, we discuss how interactions between the perturbations and their environment can lead to decoherence.</p> <p>In decoherence, the reduced density operator of the perturbations becomes diagonal with respect to a particular pointer basis. We argue that the pointer basis for the cosmological scalar perturbations consists of approximate eigenstates of the field value operator. Finally, we discuss how decoherence can help understand the transition from quantum theory to classical perturbation theory, and justify the standard treatment of perturbations and their initial conditions in cosmology. We conclude that since decoherence should not spoil the observationally successful predictions of this standard treatment, it is unlikely that the actual amount of decoherence could be observed in, say, the CMB radiation.</p>			
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1. Introduction

According to cosmology, our universe is about 13.8 billion years old [1], and was born from a hot, dense state called the Big Bang. In the early universe, physics was ruled by high energy phenomena, and all particles moved at relativistic speeds. After the Big Bang, space expanded and temperature dropped. Eventually, atomic matter was formed, and the universe became transparent; the radiation that we today observe as the cosmic microwave background (CMB) was released. Long after this, matter cooled down enough to form gravitationally bound structures: galaxies, stars, and, eventually, planets.

However, this basic model has several problems, related to the homogeneity, isotropy and flatness of the universe. To solve these problems, physicists introduced cosmic inflation, a period of rapid, accelerated expansion of space at early times, before other events of the traditional Big Bang model. According to typical inflationary models, this expansion was driven by a field called inflaton.

While inflation solved the above mentioned problems, it answered another question as well: What is the origin of structure in the universe? Why are there inhomogeneities, like galaxies and stars, instead of a maximally symmetric space with constant energy density? The answer comes from quantum mechanics. When perturbations of the inflaton and space-time itself are treated as quantum fields, even their vacuum state is not empty in the classical sense, but undergoes constant fluctuation. Their small-scale quantum fluctuations are stretched out by the rapid

expansion during inflation, and they act as seeds of the classical structure and the CMB anisotropy we see around us today.

The spectrum of these quantum fluctuations can be calculated theoretically. Predictions of the best-fitting models match incredibly well the measurements made of the CMB radiation. This is the first time that space-time, or at least its small perturbations, have been quantized to observational success, providing a glimpse of quantum gravity. However, in standard cosmology perturbations are treated classically, with no reference to quantum mechanics. A question arises: how is this transition from quantum mechanical initial conditions to classical treatment justified?

Such questions are not unique to cosmology. How exactly classical mechanics arises from the fundamental quantum theory is an open question in physics till this day. This question is partially answered by decoherence. In decoherence, the system becomes entangled with its environment, which brings the original quantum state into an ensemble of classical looking ones. This explains how, for example, a particle traversing through material becomes to look classical with relatively well-defined position and momentum. The same idea can be applied to cosmological perturbations. In this thesis, we first introduce the necessary ingredients of inflation, cosmological perturbation theory and quantum field theory, and then study how decoherence can be used to understand the transition from quantum mechanics to classical physics in the case of cosmological scalar perturbations during inflation.

In chapter 2, we show how a homogeneous and isotropic universe can be modelled using the theory of general relativity, and how this model with realistic matter content predicts the Big Bang. We discuss some of the problems of the original Big Bang model, and show how inflation can solve them. We also show how inflation can be induced by a slowly rolling scalar field.

In chapter 3, we study small perturbations around the mean values of the

inflaton field and the space-time using cosmological perturbation theory. We derive the classical equations of motion for the scalar perturbations to first order.

Chapter 4 adds quantum mechanics to the mix. We learn how to quantize the scalar perturbations, what their vacuum state looks like, and how this state evolves in time. We find that the vacuum state indeed has fluctuations around the mean value, and as time goes on, these fluctuations become highly squeezed: the quantum mechanical uncertainties of the perturbations and their canonical momenta increase, while a certain linear combination of them gets a well-defined value. We argue that such a state is very much quantum mechanical, and can't be treated classically without further justification.

In chapter 5, we tackle the problem of classicalisation of the quantum perturbations. We show how decoherence can bring the vacuum quantum state into an ensemble of classical looking states with well-defined perturbation field values. We discuss the implications and limitations of this approach with respect to observations of the cosmic microwave background radiation and the quantum mechanical measurement problem.

1.1 Conventions

We use the metric convention $(-, +, +, +)$, that is, the metric tensor of Minkowski space reads

$$\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1).$$

We use the usual index conventions, where upper indices represent contravariant components and lower indices represent covariant components of vectors and tensors. Index 0 corresponds to time, and indices 1–3 correspond to spatial directions. Repeated indices are summed over according to the Einstein summation convention.

Other notations include:

\dot{a}	Derivative of a with respect to cosmic time t
a'	Derivative of a with respect to conformal time η
v^μ, v^i	Components of vector v : Greek indices run from 0 to 3, Latin indices run from 1 to 3
\mathbf{v}	Three-vector with components v^i
∂_μ	Partial derivative with respect to x^μ , where x is the coordinate vector
$b_{,\mu}$	Another notation for partial derivative of b with respect to x^μ
c^*	Complex conjugate of complex number c
$\text{Re } c, \text{Im } c$	Real and complex parts of complex number $c = \text{Re } c + i \text{Im } c$
\hat{A}	Operator that corresponds to the observable A
\hat{A}^\dagger	Hermitean conjugate of operator \hat{A}
tr	Trace of a matrix or an operator
δ_{ij}	Kronecker delta: one if $i = j$, zero otherwise
\equiv	Equal by definition
\propto	Proportional to
\sim	Of the same order of magnitude as

We use natural units, where the speed of light and the reduced Planck constant are set to one:

$$c = \hbar = 1.$$

2. Background

In cosmology, the universe is approximated as spatially isotropic and homogeneous, which means that each location and each direction looks the same. Such a universe is described in the framework of general relativity by the Friedmann–Robertson–Walker (FRW) metric and the accompanying Friedmann equations. These equations, together with observations, show that the universe is expanding and that it started some 13.8 billion years ago [1] with an era of high temperature and enormous energy density—the Big Bang.

However, if the universe is assumed to only contain ordinary matter and radiation, this model has several problems. One of them is related to the cosmic microwave background radiation. When the universe was 380 000 years old, free electrons combined with nuclei to produce electrically neutral atoms. After this, electromagnetic radiation could travel through space freely, without scattering. The released black-body radiation is highly isotropic, with fluctuations of only order 10^{-4} around the mean temperature [2]. The problem is that, due to the finite speed of light, far-away regions appearing identical to us shouldn't have had time to interact with each other at the time of last scattering, so the CMB has no reason to appear isotropic.

To solve this and other problems of the Big Bang model, cosmic inflation was introduced [3–7]. Inflation is a period of accelerated expansion at the beginning of the universe. If inflation happened, the regions from which we receive the CMB ra-

diation could have been in causal contact at early times, and only spread out during the rapid inflationary expansion. In general relativity, such expansion requires negative pressure. The pressure of ordinary matter and radiation is positive, but a scalar field can have negative pressure and cause inflation under the right circumstances.

In this chapter, we take a look at the FRW solution and inflation. We introduce the concept of a scalar field and derive the corresponding field equation and the Friedmann equations. We also show how a scalar field can cause inflation in the slow-roll approximation. Unmodified theory of general relativity is used throughout the thesis; for a reference, see [8] and appendix A.

2.1 FRW model

2.1.1 FRW metric

At the background level, we assume that space is homogeneous and isotropic. The universe is then described by the FRW model, see e.g. [8, p. 329]. The metric is given in spherical coordinates by the line element

$$ds^2 = -dt^2 + a^2(t) \left(\frac{dr^2}{1 - Kr^2} + r^2 d\Omega^2 \right), \quad (2.1)$$

where t is the cosmic time, r is the radial coordinate and $d\Omega^2$ is the differential solid angle. We assume from now on that there is no spatial curvature, which means that $K = 0$. This assumption agrees with observations [1] and it makes things mathematically easier; in particular, it enables us to use Fourier transforms of fields. Then (2.1) can be written in Cartesian coordinates as

$$ds^2 = -dt^2 + a^2(t) (dx^2 + dy^2 + dz^2). \quad (2.2)$$

The metric (2.2) has one remaining degree of freedom, the scale factor $a(t)$, which describes the expansion of the universe. We define the Hubble parameter character-

using the expansion rate as

$$H \equiv \frac{\dot{a}}{a}, \quad (2.3)$$

where dot indicates derivative with respect to the cosmic time t .

Next, we define conformal time η by

$$dt = a d\eta \quad \Rightarrow \quad \eta = \int_{t_0}^t \frac{dt'}{a(t')}, \quad (2.4)$$

where t_0 sets the zero point of η . We denote derivatives with respect to η by a prime and define

$$\mathcal{H} \equiv \frac{a'}{a} = \dot{a}. \quad (2.5)$$

In terms of the conformal time, the line element (2.2) takes the simple form

$$ds^2 = a^2(\eta) (-d\eta^2 + dx^2 + dy^2 + dz^2). \quad (2.6)$$

In this chapter, we mostly use the cosmic time t with the accompanying metric (2.2), but from chapter 3 onward we change to the more convenient conformal time.

2.1.2 Time Evolution

Time dependence of the scale factor a is determined by the Einstein equation:

$$G_{\mu\nu} = \frac{1}{M_{\text{Pl}}^2} T_{\mu\nu}. \quad (2.7)$$

Here $G_{\mu\nu}$ is the Einstein tensor determined by the metric (see appendix A), $M_{\text{Pl}} = 1/\sqrt{8\pi G}$ is the reduced Planck mass with G being the gravitational constant, and $T_{\mu\nu}$ is the stress-energy tensor which depends on the matter content of the universe.

To satisfy the symmetry of the FRW model, matter is described by an ideal fluid, and the stress-energy tensor takes the form

$$T^\mu{}_\nu = \text{diag}(-\rho, p, p, p), \quad (2.8)$$

where ρ is the fluid's energy density, assumed to be positive, and p is its pressure. Then the Einstein equation (2.7) with (2.2) and (2.8) gives the Friedmann equations

$$H^2 = \frac{\rho}{3M_{\text{Pl}}^2}, \quad (2.9)$$

$$\frac{\ddot{a}}{a} = -\frac{1}{6M_{\text{Pl}}^2}(\rho + 3p). \quad (2.10)$$

If pressure depends on energy density in the simple way

$$p = w\rho, \quad (2.11)$$

where w is a constant and $w > -1$, then equations (2.9)–(2.10) can be solved to give

$$a \propto t^{\frac{2}{3(1+w)}}, \quad (2.12)$$

$$\ddot{a} \propto -(1 + 3w)t^{-\frac{4+6w}{3(1+w)}}. \quad (2.13)$$

There is a singularity at $t = 0$: there the scale factor goes to zero and energy density diverges. This is the Big Bang.

As long as $w > -1/3$, expansion is decelerating according to (2.13). This is true for ordinary matter and radiation, which have

$$w_{\text{m}} = 0, \quad w_{\text{r}} = 1/3. \quad (2.14)$$

For accelerated expansion, something different is needed; according to (2.10), we need a matter component with sufficiently negative pressure:

$$p < -\rho/3. \quad (2.15)$$

This can be achieved with a simple scalar field, as we will see below.

2.2 Scalar Field Matter

We next introduce another source of energy and pressure, apart from ordinary matter and radiation. It is given by a scalar field $\varphi(x)$, which takes a real value for each

space-time point x . Our starting point is an action integral chosen so that minimising it with respect to the metric $g_{\mu\nu}$ and the scalar field φ gives the Einstein equation and a field equation for φ . Such an approach will be useful for quantization in chapter 4. The action reads [8, p. 159]

$$S = \underbrace{\frac{M_{\text{Pl}}^2}{2} \int d^4x \sqrt{-g} R}_{S_{\text{grav}}} + \underbrace{\int d^4x \sqrt{-g} \left(-\frac{1}{2} g^{\alpha\beta} \partial_\alpha \varphi \partial_\beta \varphi - V(\varphi) \right)}_{S_\varphi = \int d^4x \sqrt{-g} \mathcal{L}_\varphi}. \quad (2.16)$$

Here g is the determinant of the metric tensor $g_{\mu\nu}$, R is the curvature scalar, and the first term is the usual Hilbert action. The second term is the scalar field action, formed from the Lagrangian density \mathcal{L}_φ which contains a kinetic term and a potential term. The potential $V(\varphi)$ is an analytical function of the scalar field. The metric only enters \mathcal{L}_φ by contracting indices in the kinetic term; this is called minimal coupling.

Minimizing S with respect to φ , we get the field equation¹

$$\frac{1}{\sqrt{-g}} \partial_\mu (\sqrt{-g} g^{\mu\nu} \partial_\nu \varphi) - V'(\varphi) = 0. \quad (2.17)$$

Minimizing S with respect to $g_{\mu\nu}$ gives the Einstein equation (2.7), with the stress-energy tensor

$$T_{\mu\nu} = \left(-\frac{1}{2} g^{\alpha\beta} \partial_\alpha \varphi \partial_\beta \varphi - V(\varphi) \right) g_{\mu\nu} + \partial_\mu \varphi \partial_\nu \varphi. \quad (2.18)$$

In the case of the FRW universe, symmetry dictates that $\partial_i \varphi = 0$. With the metric (2.2), the stress-energy tensor has the components

$$T^\mu{}_\nu = \left(\frac{1}{2} \dot{\varphi}^2 - V(\varphi) \right) \delta^\mu{}_\nu - \delta^\mu{}_0 \delta^0{}_\nu \dot{\varphi}^2 \quad (2.19)$$

$$\Rightarrow \rho = \frac{1}{2} \dot{\varphi}^2 + V(\varphi), \quad p = \frac{1}{2} \dot{\varphi}^2 - V(\varphi). \quad (2.20)$$

¹Prime here denotes taking a derivative with respect to the scalar field φ . This should not be confused with derivative with respect to the conformal time η ; potential V is a function of φ only.

Notably, the pressure p can be negative even for a positive potential V . The first Friedmann equation (2.9) and the scalar field equation (2.17) now determine the evolution of the system:

$$H^2 = \frac{1}{3M_{\text{Pl}}^2} \left(\frac{1}{2} \dot{\varphi}^2 + V(\varphi) \right), \quad (2.21)$$

$$\ddot{\varphi} + 3H\dot{\varphi} + V'(\varphi) = 0. \quad (2.22)$$

In conformal time, we get

$$\mathcal{H}^2 = \frac{1}{3M_{\text{Pl}}^2} \left(\frac{1}{2} \varphi'^2 + a^2 V(\varphi) \right), \quad (2.23)$$

$$\varphi'' + 2\mathcal{H}\varphi' + a^2 V'(\varphi) = 0. \quad (2.24)$$

The second Friedmann equation is not independent but can be derived from these two. We will return to a solution of these equations in section 2.3.4, after introducing inflation and some general concepts related to it.

2.3 Inflation

2.3.1 Horizon Problem

In this section, we motivate inflation by showing how it can solve the horizon problem mentioned at the beginning of the chapter.

At early times, the scale factor a gets arbitrarily small and any two points in space get close to each other. However, this doesn't mean that all points are in causal contact. To see this, let's consider a light pulse sent at the time of the Big Bang, $t = 0$. Due to homogeneity and isotropy of space, we can choose the light pulse to travel radially away from the origin in the coordinate system of the metric (2.1). Light follows a null geodesic:

$$ds^2 = 0 \Rightarrow dr = \frac{dt}{a(t)}. \quad (2.25)$$

At time t , the light pulse has travelled the coordinate distance

$$d_{\text{hor}}^c(t) = r(t) = \int_0^t \frac{dt'}{a(t')}. \quad (2.26)$$

This is the comoving particle horizon, the maximum coordinate distance between two points that have been in causal contact at some point up until time t . It is also equal to the conformal time (2.4), up to an additive constant.

Let's now turn to the question of isotropy of the CMB mentioned at the beginning of the chapter. Call the time of birth of the CMB t_1 , and the time now t_2 . The coordinate distance traversed by light during this interval is

$$\Delta r_{12} = \int_{t_1}^{t_2} \frac{dt'}{a(t')} = d_{\text{hor}}^c(t_2) - d_{\text{hor}}^c(t_1). \quad (2.27)$$

For the CMB to appear isotropic, points at this coordinate distance should have been in causal contact earlier, that is,

$$\Delta r_{12} < d_{\text{hor}}^c(t_1). \quad (2.28)$$

For a matter- or radiation-dominated universe, (2.12) gives

$$d_{\text{hor}}^c(t) \propto \frac{1}{a(t)H(t)} \propto t^{\frac{1+3w}{3(1+w)}}, \quad (2.29)$$

and the causality condition (2.28) becomes

$$\frac{t_2}{t_1} < 2^{\frac{3(1+w)}{1+3w}} \lesssim 10. \quad (2.30)$$

We used the radiation and matter values w_r and w_m (2.14) in the last approximation. However, realistic estimates give $t_1 \approx 380\,000$ years and $t_2 \approx 13.8 \cdot 10^9$ years [1, 9], and thus the inequality is violated.

One way to fix this is to introduce a phase of accelerated expansion at the early universe. This period is called cosmic inflation [3, 4] (other historically important papers include [5–7]), and during it we have

$$\ddot{a} > 0. \quad (2.31)$$

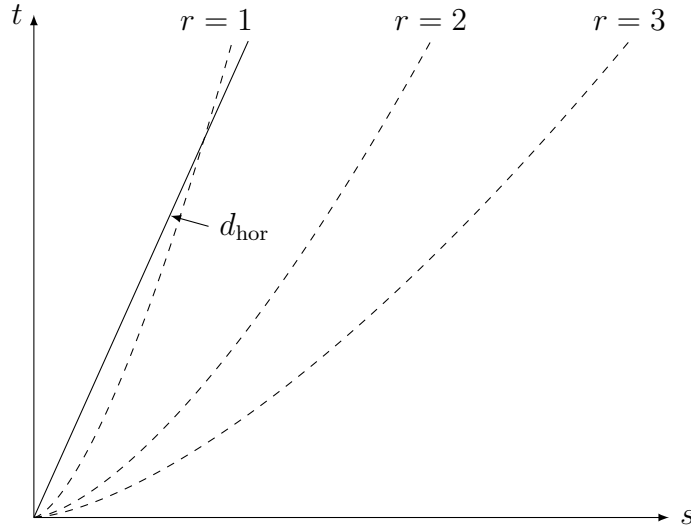


Figure 2.1: Matter-dominated universe. On vertical axis is the cosmic time t , and on horizontal axis is the spatial distance s measured along a constant-time hypersurface. Dashed lines correspond to constant coordinate distances r and the solid line is the horizon distance $d_{\text{hor}}(t) = a(t)d_{\text{hor}}^c(t)$, the distance reached by a light pulse sent at $t = 0, s = 0$.

Inflation does not affect the evolution of the scale factor after t_1 , so Δr_{12} remains unchanged. However, the horizon distance $d_{\text{hor}}^c(t_1)$ increases: due to accelerated expansion, the scale factor spends more time at small values at the beginning, and only later catches up with the post-inflation values (compare figures 2.1 and 2.2). Thus the integral (2.26) gives a bigger value, and the causality condition (2.28) for the CMB can be satisfied.

The problem with the above analysis is that we used the FRW metric from the start and thus implicitly assumed homogeneity and isotropy. However, even if the universe starts in some chaotic state, it can be argued that inhomogeneity and anisotropy tend to damp out locally; see [4] and references therein. A locally homogeneous and isotropic region would follow the FRW metric, and could expand during inflation to become our observed universe.

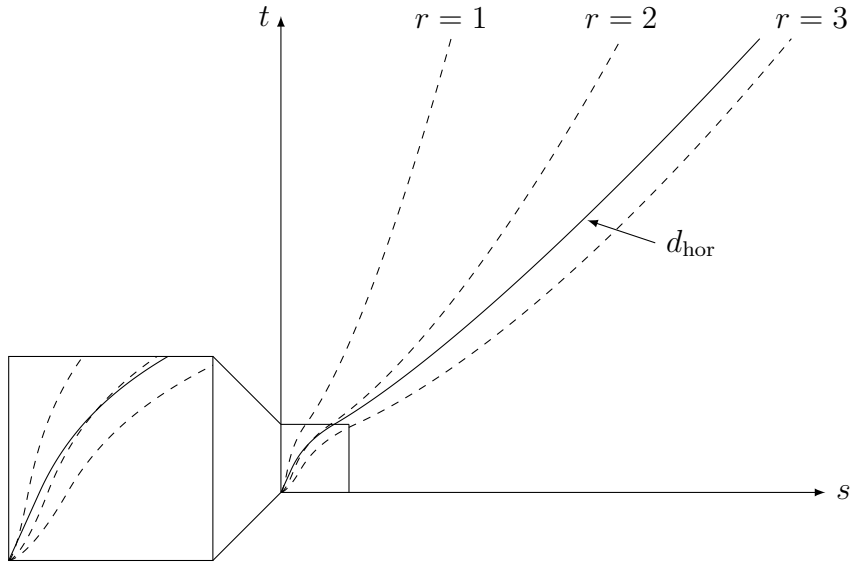


Figure 2.2: Universe with an inflationary period. Same as figure 2.1, but with a short period of exponential expansion between two matter-dominated epochs. Scales don't correspond to a realistic model, but we see that even a short period of inflation can result in a large increase in the particle horizon.

2.3.2 The Flatness and Relic Problems

The horizon problem is not the only shortcoming of the traditional Big Bang model. We next briefly review the two other historically important problems solved by inflation, the flatness and relic problems [4], [10, p. 307].

The flatness problem arises if we drop the assumption that the curvature parameter K is exactly zero in (2.1). For non-zero K , the first Friedmann equation (2.9) takes the form

$$H^2 = \frac{\rho}{3M_{\text{Pl}}^2} - \frac{K}{a^2} \quad (2.32)$$

$$\Leftrightarrow 1 = \frac{\rho}{3M_{\text{Pl}}^2 H^2} - \frac{K}{a^2 H^2}, \quad (2.33)$$

while the second equation stays intact. The problem is that the spatial curvature term behaves in a matter- or radiation dominated universe as

$$\frac{K}{a^2 H^2} = K \dot{a}^{-2} \propto t^{\frac{2+6w}{3(1+w)}} \xrightarrow{t \rightarrow \infty} \infty, \quad (2.34)$$

so it quickly becomes dominant over the energy density term. In practice, this leads to the collapse of the universe for $K > 0$, or rapid expansion and decrease in the energy density for $K < 0$. This is also called the oldness problem: the universe couldn't have reached the age of 13.8 billion years and been in the state we observe it in, unless K was fine-tuned to be close to zero.

However, during inflation, since $\ddot{a} > 0$, the term (2.34) decreases. Inflation then naturally adjusts this term to be very small at the beginning of the radiation dominated era, solving the flatness problem.

A third problem solved by inflation is related to grand unified theories (GUTs), which try to describe physics at high energy scales, beyond the standard model of particle physics. Such theories predict the existence of exotic particles called relics, which nevertheless have not been observed in nature. Inflation can solve the relic problem: if the relics were born before inflation, then the rapid expansion would typically have diluted the relic density so much that there wouldn't be any relics around to observe today.

2.3.3 Evolution of Scales

Expansion rate of the universe gives an important time- and length-scale, the Hubble length:

$$\ell_H \equiv \frac{1}{H}. \quad (2.35)$$

Dividing this by the scale factor, we get the comoving Hubble length, which can be compared with coordinate distances:

$$\ell_H^c \equiv \frac{1}{aH} = \dot{a}^{-1}. \quad (2.36)$$

This quantity often pops up in equations, dividing coordinate scales into two categories: those shorter than ℓ_H^c , called subhorizon modes, and those longer than ℓ_H^c , called superhorizon modes. From the definition (2.36) it follows that during infla-

tion, ℓ_H^c decreases, and during matter- or radiation-domination ℓ_H^c decreases. During inflation scales are then ‘leaving the horizon’, that is, moving from subhorizon to superhorizon, and after inflation they start to re-enter the horizon again. The word ‘horizon’ does not here refer to the particle horizon, but to the comoving Hubble length; we use such terminology for the rest of this thesis.

2.3.4 Slow-Roll Inflation

As seen earlier, cold matter and radiation can’t cause inflation. A scalar field, on the other hand, can; in the context of inflation, such a scalar field is called the inflaton. To see how inflation emerges, let’s plug the inflaton energy density and pressure (2.20) into the inflation condition (2.15):

$$p < -\frac{\rho}{3} \Leftrightarrow \dot{\varphi}^2 < V. \quad (2.37)$$

Inflation occurs if the potential term V dominates over the kinetic term $\dot{\varphi}^2$.

We consider slow-roll inflation, see e.g. [11, p. 42], which is well compatible with observations. We demand

$$\dot{\varphi}^2 \ll V, \quad (2.38)$$

$$|\ddot{\varphi}| \ll 3H|\dot{\varphi}|. \quad (2.39)$$

These are the slow-roll conditions: the field value changes slowly as it ‘rolls down’ towards a minimum of the potential V . With them, the time evolution equations (2.21), (2.22) take the simple form

$$H^2 \approx \frac{V}{3M_{\text{Pl}}^2}, \quad (2.40)$$

$$3H\dot{\varphi} \approx -V'. \quad (2.41)$$

Slow-roll is characterised by the slow-roll parameters:

$$\epsilon_V \equiv \frac{1}{2} M_{\text{Pl}}^2 \left(\frac{V'}{V} \right)^2 \ll 1, \quad (2.42)$$

$$\eta_V \equiv M_{\text{Pl}}^2 \frac{V''}{V} \ll 1, \quad (2.43)$$

$$\xi_V \equiv M_{\text{Pl}}^4 \frac{V''' V'}{V^2} \ll 1. \quad (2.44)$$

The third parameter is considered to be second-order small compared to the first two. Smallness of the slow-roll parameters follows from (2.38)–(2.41) and is a necessary condition for slow-roll inflation, but not a sufficient one: the parameters define a region for the field φ compatible with slow-roll, depending on the potential V , but in addition we need $\dot{\varphi}$ to be small. Fortunately, slow-roll solution is an attractor: systems with wildly different initial conditions tend towards it as the field value changes.

Equations (2.40)–(2.41) hold to zeroth order in the slow-roll parameters. Using them and the definitions (2.42)–(2.44), we can derive the following higher order results:

$$-\frac{\dot{H}}{H^2} = \epsilon_V + \mathcal{O}(\epsilon_V^2), \quad (2.45)$$

$$\dot{\epsilon}_V = H(4\epsilon_V^2 - 4\eta_V \epsilon_V) + \mathcal{O}(\epsilon_V^3), \quad (2.46)$$

$$\dot{\eta}_V = H(2\epsilon_V \eta_V - \xi) + \mathcal{O}(\epsilon_V^3), \quad (2.47)$$

$$\frac{\dot{\varphi}}{H} = -\sqrt{2\epsilon_V} M + \mathcal{O}(\epsilon_V). \quad (2.48)$$

Although only ϵ_V is written explicitly, the higher order corrections can contain any of the slow-roll parameters. Parameters ϵ_V and η_V are constant to first order in the slow-roll parameters, as implied by (2.46) and (2.47)². We can then integrate (2.45)

²To be precise, we should show that higher time derivatives are small as well. When calculating these, we encounter higher derivatives of the potential V and need to introduce new slow-roll parameters which must be higher order small, see [12].

to obtain

$$H = H_0(1 - H_0\epsilon_V t) + \mathcal{O}(\epsilon_V^2), \quad (2.49)$$

$$a(t) \propto e^{H_0 t} \left(1 - H_0 \frac{\epsilon_V t^2}{2} \right) + \mathcal{O}(\epsilon_V^2). \quad (2.50)$$

This quasi-exponential expansion continues until the field rolls out of the slow-roll region and inflation ends. In conformal time, (2.49)–(2.50) become:

$$\mathcal{H} = -\frac{1 + \epsilon}{\eta} + \mathcal{O}(\epsilon_V^2), \quad (2.51)$$

$$a(\eta) \propto -\frac{1}{\eta} [1 - \epsilon_V \ln(-\eta)] + \mathcal{O}(\epsilon_V^2), \quad (2.52)$$

where we chose the integration constant of (2.4) so that always $\eta < 0$ and $\eta \rightarrow 0$ as $t \rightarrow \infty$. To the lowest slow-roll order, we then have

$$H_0^{-1} = \frac{a}{\dot{a}} = \frac{a}{\mathcal{H}} = -a\eta \quad (2.53)$$

and

$$\ell_H^c = -\eta. \quad (2.54)$$

Slow-roll is a general inflationary scenario. It doesn't specify the shape of the potential V , and the differences only come in as corrections to the zeroth-order result through the small slow-roll parameters. Its merits are its simplicity and the attractor behaviour which renders it insensitive to initial conditions. It also provides a good match with observations. The slow-roll solution obtained above will be used as a background solution for the space-time and the inflaton field for the rest of this thesis; on top of it, we'll add small deviations from homogeneity and isotropy, starting in the next chapter.

3. Perturbations

In the previous chapter, we argued that during inflation, the observed universe can become extremely homogeneous and isotropic. However, small inhomogeneities always exist due to quantum fluctuations. These fluctuations are amplified during inflation, and eventually they lead to the anisotropies of the CMB and the present structure on all scales from stars to galaxy clusters and beyond. Predicting details of this structure correctly is the true strength of the inflation hypothesis.

To study the primordial fluctuations, small perturbations are added to the inflaton field φ and the metric tensor $g_{\mu\nu}$. In the theory of first order (or linear) perturbations, the background solution obtained in chapter 2 remains unchanged, but on top of it fluctuations evolve according to the Einstein and scalar field equations.

Perturbations in the metric introduce extra freedom: not all perturbations correspond to different physical situations, since some are related to each other by coordinate transformations. These coordinate transformations can be thought of as gauge transformations, resulting in gauge freedom.

In this chapter, we introduce a gauge-invariant combination of the perturbations in the metric tensor $g_{\mu\nu}$ and the inflaton field φ , the Sasaki-Mukhanov variable ν [13], which fully describes linear scalar perturbations. We use linear perturbation theory to obtain classical equations of motion for this variable. This will be the starting point for quantizing the perturbations in chapter 4.

3.1 Perturbations Introduced

For this chapter, our starting point is the conformal background metric (2.6), denoted from now on by $\bar{g}_{\mu\nu}$. Our notation follows mostly that of [11]; for a classic review on the subject, see [14]. To study small deviations from (2.6), we write the metric tensor in the general form

$$g_{\mu\nu} = \bar{g}_{\mu\nu} + \delta g_{\mu\nu} = a^2 \begin{pmatrix} -(1 + 2A) & -B_i \\ -B_i & (1 - 2D)\delta_{ij} + 2E_{ij} \end{pmatrix}. \quad (3.1)$$

Here A and D are scalars, B_i is a 3-vector, and E_{ij} is a symmetric, traceless three-dimensional rank two tensor. They are functions of both time and space coordinates, and thus introduce deviations from the homogeneity of the FRW model. The positions of the indices are fixed: we don't raise or lower them with any sort of metric tensor. Repeated indices are summed over regardless of their position.

Similarly, we split the inflaton field into a homogeneous background part and a perturbation as

$$\varphi(\eta, x_i) = \bar{\varphi}(\eta) + \delta\varphi(\eta, x_i). \quad (3.2)$$

The background metric $\bar{g}_{\mu\nu}$ and the inflaton field $\bar{\varphi}$ follow the slow-roll solution of section 2.3.4. For the deviations from the background, we use first order perturbation theory: only terms up to first order in perturbations are kept, while second-order and higher contributions are neglected as smaller corrections. All equations are then linear in perturbations. This is a good approximation during inflation, even though it breaks down later.

3.1.1 Scalar, Vector and Tensor Perturbations

In the case of flat space, we can categorise the metric perturbations further. Every three-vector, including B_i , can in flat space be written as

$$B_i = B_i^V + B_i^S, \quad (3.3)$$

$$B_{i,i}^V = 0, \quad (3.4)$$

$$B_i^S = -B_{,i}, \quad (3.5)$$

where B_i^V is a vector part with zero divergence, and B_i^S is a scalar part with zero curl given by the gradient of a new scalar field B . The minus sign in (3.5) is a matter of convention.

Similarly, any three-dimensional symmetric traceless rank two tensor E_{ij} can be decomposed into tensor, vector and scalar parts as

$$E_{ij} = E_{ij}^T + E_{ij}^V + E_{ij}^S, \quad (3.6)$$

$$E_{ij,j}^T = 0, \quad E_{ii}^T = 0, \quad (3.7)$$

$$E_{ij}^V = -\frac{1}{2}(E_{i,j} + E_{j,i}), \quad E_{ii}^V = 0, \quad (3.8)$$

$$E_{ij}^S = E_{,ij} - \frac{1}{3}\delta_{ij}E_{,kk}. \quad (3.9)$$

Here E_{ij}^T is a pure tensor contribution: it cannot be written in terms of vector or scalar fields, and we cannot form vector or scalar fields out of it at linear order because it is traceless and divergenceless. Similarly B_i^V and E_i (a building block of E_{ij}^V) are pure vector contributions, whereas A , B , D and E (a building block of E_{ij}^S) are scalars, and they transform accordingly in spatial rotations.

The decomposition (3.1), (3.3)–(3.9) can be uniquely done to any symmetric four-dimensional rank two tensor [15, 16]. In particular, the Einstein tensor $G_{\mu\nu}$ is composed only of the metric tensor and its derivatives, and in the linear approximation the scalar sector of the perturbation $\delta G_{\mu\nu}$ can only contain the $\delta g_{\mu\nu}$ scalar quantities, the vector sector of $\delta G_{\mu\nu}$ can only contain $\delta g_{\mu\nu}$ vectors, and $\delta G_{\mu\nu}$ tensors

consist of $\delta g_{\mu\nu}$ tensors. The stress-energy perturbation $\delta T_{\mu\nu}$ during inflation is built from the scalar perturbation $\delta\varphi$; there are no vector or tensor perturbations. Due to uniqueness of the decomposition, tensor equations like the Einstein equation (2.7) must be satisfied sector by sector for the perturbations. Thus the scalar, vector and tensor sectors evolve independently of each other, with no linear order couplings between them.

Vector perturbations are not expected to be generated during inflation [11, p. 339], and tensor perturbations correspond to primordial gravitational waves, which have not been detected [1]. To study the evolution of matter perturbations, it is enough to consider the scalar sector, since the inflaton field resides there. We can then use a metric with only scalar perturbations:

$$ds^2 = a^2 \left\{ -(1 + 2A)d\eta^2 + 2B_{,i}dx^i d\eta + [(1 - 2\psi)\delta_{ij} + 2E_{,ij}]dx^i dx^j \right\}, \quad (3.10)$$

where

$$\psi \equiv D + \frac{1}{3}E_{,ii}. \quad (3.11)$$

After some general considerations in the next section, we will use this metric for the rest of this thesis.

3.2 Gauge Freedom

3.2.1 Gauge Transformations

In general relativity, the same space-time can be described using different coordinate systems. Especially, in perturbation theory, there are many coordinate systems where the metric (3.1) remains close to the background metric (2.6), and we are free to choose any of them. This choice fixes the values of the perturbations in (3.1) and (3.2). The freedom to choose the functional form of the perturbations by choice of coordinate system is called gauge freedom, and transformations between

such nearby coordinate systems are called gauge transformations.

We adopt the passive approach to gauge transformations [17, 18]. Two manifolds are considered, see figure 3.1. One of them is the perturbed universe \mathcal{N} , with different coordinate systems corresponding to different gauges on it, while the other, \mathcal{M} , is the unperturbed, homogeneous and isotropic universe with the coordinate system given by (2.6). We can build a map from the unperturbed manifold onto the perturbed manifold so that a point on \mathcal{M} is mapped into a point with the same coordinate values on \mathcal{N} . Different gauges then correspond to different maps.

If two points on the manifold \mathcal{N} , \tilde{P} and \hat{P} , correspond to the same point P on manifold \mathcal{M} but in different gauges, then the difference between \tilde{P} and \hat{P} on \mathcal{N} is small. At first order accuracy, in a fixed gauge, perturbations take the same values at both points. We say that perturbations live on the unperturbed manifold, and evaluate them at point P instead of \tilde{P} or \hat{P} .

Next, we will find out how perturbations in different gauges are related to each other. Let x^μ be the coordinates on the unperturbed manifold, and let \tilde{x}^μ and \hat{x}^μ be two sets of coordinates in the perturbed universe, corresponding to different gauges. For the aforementioned points, we have

$$x^\mu(P) = \tilde{x}^\mu(\tilde{P}) = \hat{x}^\mu(\hat{P}). \quad (3.12)$$

The gauge transformation between \tilde{x}^μ and \hat{x}^μ is defined by a vector field $\xi^\mu(P)$, with first order small components, so that

$$\tilde{x}^\mu(\tilde{P}) = \hat{x}^\mu(\tilde{P}) + \xi^\mu(P), \quad (3.13)$$

$$\hat{x}^\mu(\hat{P}) = \tilde{x}^\mu(\hat{P}) - \xi^\mu(P). \quad (3.14)$$

Using (3.12), these become

$$\tilde{x}^\mu(\hat{P}) = \tilde{x}^\mu(\tilde{P}) + \xi^\mu(P), \quad (3.15)$$

$$\hat{x}^\mu(\tilde{P}) = \hat{x}^\mu(\hat{P}) - \xi^\mu(P). \quad (3.16)$$

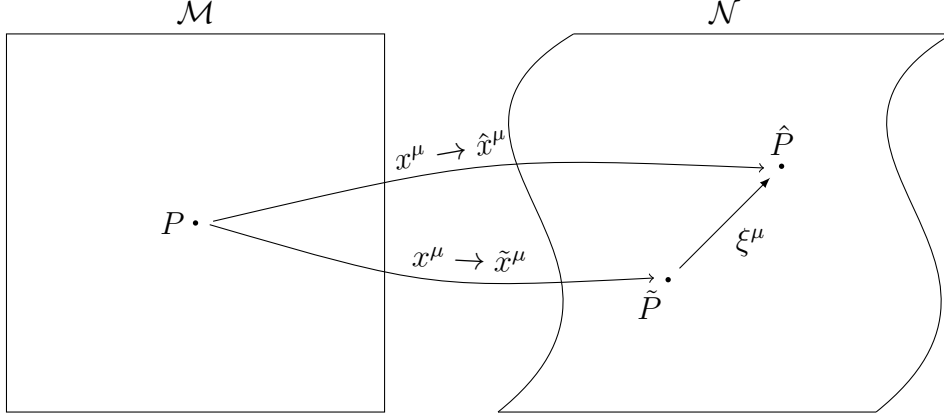


Figure 3.1: Gauge freedom. Point P on the background manifold \mathcal{M} is mapped into point \tilde{P} or \hat{P} on the perturbed manifold \mathcal{N} , depending on where on \mathcal{N} we set the coordinates $x^\mu(P)$. This is called the passive approach to gauge transformations.

Metric tensors in the coordinate systems of the perturbed manifold are $\tilde{g}_{\alpha\beta}$ and $\hat{g}_{\alpha\beta}$, and their perturbations $\delta\tilde{g}_{\alpha\beta}$, $\delta\hat{g}_{\alpha\beta}$ are defined to satisfy

$$\tilde{g}_{\alpha\beta}(\tilde{P}) = \bar{g}_{\alpha\beta}(P) + \delta\tilde{g}_{\alpha\beta}(P), \quad (3.17)$$

$$\hat{g}_{\alpha\beta}(\hat{P}) = \bar{g}_{\alpha\beta}(P) + \delta\hat{g}_{\alpha\beta}(P), \quad (3.18)$$

in accordance with (3.1). Here we used the short hand notation

$$\hat{g}_{\mu\nu}(A) \equiv \hat{g}_{\mu\nu}(\hat{x}^\gamma(A)), \quad (3.19)$$

$$\tilde{g}_{\mu\nu}(A) \equiv \tilde{g}_{\mu\nu}(\tilde{x}^\gamma(A)), \quad (3.20)$$

for any point A on \mathcal{N} . Now a coordinate transformation of the metric tensor gives

$$\begin{aligned} \tilde{g}_{\alpha\beta}(\tilde{P}) &= \frac{\partial \hat{x}^\mu(\tilde{P})}{\partial \tilde{x}^\alpha(\tilde{P})} \frac{\partial \hat{x}^\nu(\tilde{P})}{\partial \tilde{x}^\beta(\tilde{P})} \hat{g}_{\mu\nu}(\tilde{P}) \\ &= (\delta_\alpha^\mu - \xi^\mu_{,\alpha}(P)) (\delta_\beta^\nu - \xi^\nu_{,\beta}(P)) \left(\hat{g}_{\mu\nu}(\hat{P}) - \left[\frac{\partial}{\partial \hat{x}^\gamma} \hat{g}_{\mu\nu}(\hat{P}) \right] \xi^\gamma(P) \right) \\ &= \hat{g}_{\alpha\beta}(\hat{P}) - \xi^\mu_{,\alpha}(P) \bar{g}_{\mu\beta}(P) - \xi^\nu_{,\beta}(P) \bar{g}_{\alpha\nu}(P) - \xi^\gamma(P) \bar{g}_{\alpha\beta,\gamma}(P), \end{aligned} \quad (3.21)$$

where we used (3.13) and (3.16) with (3.18), and dropped terms of second or higher order. Substituting (3.17) and (3.18) into (3.21) gives the gauge transformation of

the metric perturbations:

$$\delta\tilde{g}_{\alpha\beta} = \delta\hat{g}_{\alpha\beta} - \xi^\mu{}_{,\alpha}\bar{g}_{\mu\beta} - \xi^\nu{}_{,\beta}\bar{g}_{\alpha\nu} - \xi^\gamma\bar{g}_{\alpha\beta,\gamma}, \quad (3.22)$$

where all quantities are evaluated on the background manifold at point P .

After some algebra, (3.22) reads in the notation of (3.1):

$$\tilde{A} = \hat{A} - \xi^{0'} - \mathcal{H}\xi^0, \quad (3.23)$$

$$\tilde{B}_i = \hat{B}_i + \xi^{i'} - \xi^0{}_{,i}, \quad (3.24)$$

$$\tilde{D} = \hat{D} + \frac{1}{3}\xi^k{}_{,k} + \mathcal{H}\xi^0, \quad (3.25)$$

$$\tilde{E}_{ij} = \hat{E}_{ij} - \frac{1}{2}(\xi^i{}_{,j} + \xi^j{}_{,i}) + \frac{1}{3}\delta_{ij}\xi^k{}_{,k}. \quad (3.26)$$

These hold component by component; to match the positions of the indices, one can write $\xi^i = \delta_{ij}\xi^j$.

According to the discussion in section 3.1.1, the vector field ξ^i can be decomposed into scalar and vector parts:

$$\xi^i = \xi^{iV} + \xi^{iS}, \quad (3.27)$$

$$\xi^{kV}{}_{,k} = 0, \quad (3.28)$$

$$\xi^{iS} = -\xi_{,i}, \quad (3.29)$$

where the scalar ξ generates transformations of the scalar quantities B and E . Substituting ξ^{iS} for ξ^i in (3.24) and (3.26), and using the definition of ψ (3.11), we get

$$\tilde{B} = \hat{B} + \xi' + \xi^0, \quad (3.30)$$

$$\tilde{E} = \hat{E} + \xi, \quad (3.31)$$

$$\tilde{\psi} = \hat{\psi} + \mathcal{H}\xi^0. \quad (3.32)$$

Inflaton field perturbations also change in gauge transformations. From definition

(3.2),

$$\tilde{\varphi}(\tilde{P}) = \bar{\varphi}(P) + \delta\tilde{\varphi}(P), \quad (3.33)$$

$$\hat{\varphi}(\hat{P}) = \bar{\varphi}(P) + \delta\hat{\varphi}(P), \quad (3.34)$$

and for scalars we have

$$\tilde{\varphi}(\tilde{P}) = \hat{\varphi}(\tilde{P}) = \hat{\varphi}(\hat{P}) - \xi^\mu(P)\partial_\mu\bar{\varphi}(P), \quad (3.35)$$

so that

$$\delta\tilde{\varphi} = \delta\hat{\varphi} - \xi^0\bar{\varphi}' \quad (3.36)$$

due to the homogeneity of $\bar{\varphi}$.

3.2.2 Invariant Quantities

The purpose of the previous section was to obtain the transformation equations (3.23)–(3.26), (3.30)–(3.32), (3.36) for the perturbations so that we can build gauge invariant quantities out of them. Gauge invariance means that the expression of the quantity, presented in terms of the components A , B , etc., does not change in gauge transformations.

Two examples of gauge invariant quantities are the Bardeen potentials [14, 15]

$$\Phi \equiv A + \mathcal{H}(B - E') + (B - E')', \quad (3.37)$$

$$\Psi \equiv \psi - \mathcal{H}(B - E'). \quad (3.38)$$

Their invariance can be seen by substituting (3.23), (3.30)–(3.32) into (3.37) and (3.38). The inflaton field perturbation $\delta\varphi$ can also be made gauge invariant by adding an appropriate counter term:

$$\delta\varphi_{\text{inv}} \equiv \delta\varphi + \bar{\varphi}'(B - E'). \quad (3.39)$$

Combining (3.38) and (3.39), we can define the gauge-invariant Sasaki-Mukhanov variable [13]:

$$\nu \equiv a \left(\delta\varphi_{\text{inv}} + \frac{\bar{\varphi}'}{\mathcal{H}}\Psi \right) = a \left(\delta\varphi + \frac{\bar{\varphi}'}{\mathcal{H}}\psi \right). \quad (3.40)$$

In the next section, we will see that ν is enough to describe the time evolution of the whole scalar sector. It is this variable that we will work with in the following chapters. The advantage of using a gauge invariant variable is that we can omit the question of a gauge choice. There are also formal arguments why ν is the right choice for a canonical variable for quantization [19].

3.3 Time Evolution

3.3.1 Equation of Motion

We want to eventually quantize the scalar perturbations, and for this, a suitable action integral is useful. Substituting the perturbed metric (3.10) and the inflaton expansion (3.2) into the action (2.16), we get an expression of the form

$$S = S_0 + S_1 + S_2 + S'. \quad (3.41)$$

Here S_0 contains the terms that do not depend on the perturbations, S_1 contains the terms that are first order in perturbations, S_2 contains the second-order terms, and S' contains the higher order corrections. Varying S_1 with respect to the perturbations gives the background equations, whereas variation of S_2 gives first-order time evolution equations and constraint equations for the perturbations. As discussed in [13], using these equations and simple but lengthy algebra, and dropping boundary terms, S_2 can be written in terms of a single variable, the Sasaki-Mukhanov variable from the previous section:

$$S_2 = \frac{1}{2} \int d^4x \left(\nu'^2 - \nu_{,i} \nu_{,i} + \frac{z''}{z} \nu^2 \right), \quad (3.42)$$

where

$$z \equiv a \frac{\bar{\varphi}'}{\mathcal{H}}. \quad (3.43)$$

This looks like an action for a free field with a time-dependent mass in Minkowski space, fit for quantization. Using (2.46)–(2.48), (2.52), we get the time evolution of

the mass term to first order in the slow-roll parameters:

$$\frac{z''}{z} = \frac{2 + 9\epsilon_V - 3\eta_V}{\eta^2}. \quad (3.44)$$

Varying (3.42) with respect to ν gives its equation of motion:

$$\nu'' - \nu_{,ii} - \frac{z''}{z}\nu = 0. \quad (3.45)$$

Once the time evolution of ν is solved from (3.45), other perturbations can be calculated from it using the constraint equations.

3.3.2 Solutions in Fourier Space

To solve (3.45), we write ν in terms of its spatial Fourier transform:

$$\mu_{\mathbf{k}}(\eta) \equiv \frac{1}{(2\pi)^{3/2}} \int d^3\mathbf{x} \nu(\eta, \mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}}, \quad (3.46)$$

$$\nu(\eta, \mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int d^3\mathbf{k} \mu_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (3.47)$$

Then (3.44), (3.45) give for the Fourier components

$$\mu_{\mathbf{k}}'' + \omega_{\mathbf{k}}^2 \mu_{\mathbf{k}} = 0, \quad (3.48)$$

where the time-dependent angular frequency is

$$\omega_{\mathbf{k}}^2(\eta) \equiv k^2 - \frac{z''}{z} = k^2 - \frac{2 + 9\epsilon_V - 3\eta_V}{\eta^2}, \quad (3.49)$$

and $k \equiv |\mathbf{k}|$. We work to first order in the slow-roll parameters, so ϵ_V and η_V are constant according to (2.46) and (2.47). Substituting $\mu_{\mathbf{k}} = \sqrt{-\eta} s$ and $k\eta = -x$ we get the Bessel equation

$$x^2 \frac{d^2}{dx^2} s(x) + x \frac{d}{dx} s(x) + (x^2 - \gamma^2) s(x) = 0 \quad (3.50)$$

with

$$\gamma \equiv \sqrt{\frac{9}{4} + 9\epsilon_V - 3\eta_V} \approx \frac{3}{2} + 3\epsilon_V - \eta_V, \quad (3.51)$$

so the general solution of (3.48) is

$$\mu_{\mathbf{k}}(\eta) = \sqrt{-\eta k} [A_{\mathbf{k}} J_{\gamma}(-k\eta) + B_{\mathbf{k}} J_{-\gamma}(-k\eta)], \quad (3.52)$$

where J_{γ} is the Bessel function of the first kind [20, p. 643] and $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are time-independent constants.

In general, the Fourier transform (3.47) is complex. Perturbations are described by real numbers; to get a real solution, we add together (3.47) and its complex conjugate and write

$$\nu(\eta, \mathbf{x})_{\text{real}} = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} [c_{\mathbf{k}} \mu_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} + c_{\mathbf{k}}^* \mu_{\mathbf{k}}^*(\eta) e^{-i\mathbf{k}\cdot\mathbf{x}}], \quad (3.53)$$

where the constants $c_{\mathbf{k}}$ were added for future convenience. This is our final result. It's just another way to write the general real solution of (3.45), since for real ν , it reverts back to (3.47), up to the constants.

3.3.3 Hamiltonian Formalism

As a prelude for the next chapter, let us take a look at the system in Hamiltonian formalism (see e.g. [21]). The Lagrangian density corresponding to the action (3.42) is

$$\mathcal{L} = \frac{1}{2} \nu'^2 - \frac{1}{2} \nu_{,i} \nu_{,i} + \frac{z''}{2z} \nu^2, \quad (3.54)$$

the canonical momentum and the Hamiltonian density read

$$p = \frac{\partial \mathcal{L}}{\partial \nu'} = \nu', \quad (3.55)$$

$$\mathcal{H} = p\nu' - \mathcal{L}_{\nu} = \frac{1}{2} p^2 + \frac{1}{2} \nu_{,i} \nu_{,i} - \frac{z''}{2z} \nu^2, \quad (3.56)$$

and the full Hamiltonian is

$$H = \int d^3\mathbf{x} \mathcal{H}. \quad (3.57)$$

For reference, their dimensions in natural units are

$$[\nu] = E, \quad [p] = E^2, \quad (3.58)$$

$$[\mathcal{L}] = E^4, \quad [\mathcal{H}] = E^4, \quad [H] = E, \quad (3.59)$$

where E is a unit of energy, for example the electron volt.

Let A and B be two functionals of ν and p . Their Poisson bracket is defined as

$$\{A, B\}(\eta) \equiv \int d^3\mathbf{x} \left[\frac{\delta A}{\delta \nu(\eta, \mathbf{x})} \frac{\delta B}{\delta p(\eta, \mathbf{x})} - \frac{\delta A}{\delta p(\eta, \mathbf{x})} \frac{\delta B}{\delta \nu(\eta, \mathbf{x})} \right]. \quad (3.60)$$

In particular,

$$\{\nu(\eta, \mathbf{x}), p(\eta, \mathbf{y})\} = \delta^3(\mathbf{x} - \mathbf{y}), \quad (3.61)$$

$$\{\nu(\eta, \mathbf{x}), \nu(\eta, \mathbf{y})\} = \{p(\eta, \mathbf{x}), p(\eta, \mathbf{y})\} = 0, \quad (3.62)$$

where $\delta^3(\mathbf{x})$ is the three-dimensional Dirac delta function, with dimension

$$[\delta^3(\mathbf{x})] = [x]^{-3} = E^3. \quad (3.63)$$

Time evolution of ν and p is given by

$$\nu' = \frac{\delta H}{\delta p} = \{\nu, H\} = p, \quad (3.64)$$

$$p' = -\frac{\delta H}{\delta \nu} = \{p, H\} = \nu_{,ii} + \frac{z''}{z}\nu, \quad (3.65)$$

and for a general functional,

$$A' = \frac{\delta A}{\delta \nu} \nu' + \frac{\delta A}{\delta p} p' = \{A, H\}. \quad (3.66)$$

As we will see in the next chapter, equations (3.61)–(3.62), (3.64)–(3.66) have direct counterparts in quantum theory.

4. Quantum Description

In the previous chapter, we derived the equations of motion for the cosmological scalar perturbations. To fully solve these equations, the constants in the general solution (3.52) must be fixed by some initial conditions. Quantum field theory provides such initial conditions. It also explains the origin of fluctuations: vacuum is not an eigenstate of the field operator, so the field has no definite value there.

A possible complication of quantization is that we don't have a general theory of quantum gravity. However, in the limit of first order perturbations, well-established field theory methods can be used to quantize the gauge-invariant Sasaki-Mukhanov variable from Chapter 3. In this chapter we do exactly this and study the resulting quantum operators, states and their evolution using both the Heisenberg picture and wave function formalism. We find that the time evolution results in a 'squeezed' quantum state, where a linear combination of the field values and momenta has a vanishingly small uncertainty.

4.1 Formalism of Quantum Mechanics

4.1.1 Hilbert Space

In this section, the basic formalism of quantum mechanics is summarised. For a comprehensive treatment, see [22].

In quantum mechanics and quantum field theory, the state of a physical system

is described by a vector in a complex Hilbert space. We use the bra-ket notation, where ket-vectors

$$|\psi\rangle \tag{4.1}$$

belong to the Hilbert space, and bra-vectors

$$\langle\phi| \tag{4.2}$$

belong to its dual space. There is a one-to-one correspondence between ket- and bra-vectors, and we define an inner product between two states:

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \in \mathbb{C}. \tag{4.3}$$

Physical states are normalised:

$$\langle\psi|\psi\rangle = 1. \tag{4.4}$$

The usual physical interpretation of the inner product is that if the system is prepared to state $|\psi\rangle$, then

$$P = |\langle\phi|\psi\rangle|^2 \tag{4.5}$$

is the probability to find it in state $|\phi\rangle$ in a measurement. We will discuss the role of measurements in quantum mechanics in section 5.3.2.

4.1.2 Observables

In quantization, an observable quantity A is replaced by a linear Hermitian operator acting in the Hilbert space:

$$A \rightarrow \hat{A}, \quad \hat{A}^\dagger = \hat{A}, \tag{4.6}$$

where hat marks an operator and dagger marks a Hermitian conjugate. In the following, we assume that \hat{A} has a complete set of eigenstates $|a_i\rangle$ that satisfy

$$\hat{A}|a_i\rangle = a_i|a_i\rangle, \quad a_i \in \mathbb{R}, \quad (4.7)$$

$$\langle a_i|a_j\rangle = \delta_{ij}, \quad (4.8)$$

$$\sum_i |a_i\rangle\langle a_i| = \mathbb{1}, \quad (4.9)$$

where $\mathbb{1}$ is the unit operator. This is always true for Hermitean operators in a finite dimensional space. For a continuous set of eigenvalues, the sum is replaced by an integral and the Kronecker delta is replaced by a Dirac delta function. For simplicity, we assume that there is no degeneracy, that is, for each eigenvalue there is exactly one linearly independent eigenvector.

It is usually postulated that when the value of the observable A is measured, one of the eigenvalues is obtained, and the system moves to the corresponding eigenstate. The result of the measurement is random; the probability to obtain eigenvalue a_j from state $|\psi\rangle$ is

$$P(a_j) = |\langle a_j|\psi\rangle|^2. \quad (4.10)$$

Expectation value of A is given by, using (4.9) and (4.10),

$$\langle A \rangle \equiv \sum_i a_i P(a_i) = \sum_i \langle \psi|\hat{A}|a_i\rangle\langle a_i|\psi\rangle = \langle \psi|A|\psi\rangle. \quad (4.11)$$

Uncertainty of A is defined as

$$\Delta A \equiv \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}. \quad (4.12)$$

4.1.3 Pictures of Time Evolution

One way to introduce time evolution to the system is to have the operators corresponding to the observables evolve in time. This is called the Heisenberg picture. Relations between operators are obtained from those between the classical observ-

ables by replacing the Poisson brackets in section 3.3.3 by commutators:

$$\{A, B\} \rightarrow -i[\hat{A}, \hat{B}] \equiv -i(\hat{A}\hat{B} - \hat{B}\hat{A}). \quad (4.13)$$

Time evolution of an operator $\hat{A}_H(\eta)$, where H stands for Heisenberg, follows from (3.66):

$$\hat{A}'_H(\eta) = -i[\hat{A}_H(\eta), \hat{H}_H(\eta)]. \quad (4.14)$$

The Hermitian Hamilton operator $\hat{H}_H(\eta)$ is formed from the classical Hamiltonian by replacing the observables by Heisenberg picture operators. Because of the similar algebraic properties of the Poisson bracket and the commutator, the equations of motion for the Heisenberg operators resemble their classical counterparts.

Formally equation (4.14) is solved by

$$\hat{A}_H(\eta) = \hat{U}^\dagger(\eta)\hat{A}_H(\eta_{\text{ini}})\hat{U}(\eta), \quad (4.15)$$

where $\hat{U}(\eta)$ is a unitary time evolution operator evolving the system from the initial time η_{ini} to time η , with

$$\hat{U}(\eta_{\text{ini}}) = \mathbb{1}, \quad (4.16)$$

$$\hat{U}(\eta)^\dagger\hat{U}(\eta) = \hat{U}(\eta)\hat{U}(\eta)^\dagger = \mathbb{1}. \quad (4.17)$$

Equation (4.14) is satisfied when \hat{U} evolves in time as

$$\hat{U}'(\eta) = -i\hat{U}(\eta)\hat{H}_H(\eta). \quad (4.18)$$

In the Heisenberg picture, the state vector $|\psi\rangle_H$ does not change in time. Alternatively, we can use the Schrödinger picture, where operators corresponding to observables are constant and the state vector evolves:

$$\hat{A}_S \equiv \hat{U}(\eta)\hat{A}_H(\eta)\hat{U}^\dagger(\eta) = \hat{A}_H(\eta_{\text{ini}}), \quad (4.19)$$

$$|\psi(\eta)\rangle_S \equiv \hat{U}(\eta)|\psi\rangle_H, \quad (4.20)$$

where S stands for Schrödinger. We also introduce the Schrödinger picture Hamilton operator:

$$\hat{H}_S(\eta) \equiv \hat{U}(\eta) \hat{H}_H(\eta) \hat{U}^\dagger(\eta). \quad (4.21)$$

This is of the form (4.19), but \hat{H}_S may still contain intrinsic time dependence, which we assumed to be absent from \hat{A}_S . In practice, \hat{H}_S is obtained from \hat{H}_H by replacing the Heisenberg picture operators of observables in it with the Schrödinger picture equivalents. Equation (4.18) can then be written as¹

$$\hat{U}'(\eta) = -i \hat{H}_S(\eta) \hat{U}(\eta), \quad (4.22)$$

and the state vector $|\psi\rangle_S$ satisfies the Schrödinger equation

$$|\psi(\eta)\rangle'_S = -i \hat{H}_S(\eta) |\psi(\eta)\rangle_S. \quad (4.23)$$

Heisenberg and Schrödinger pictures are both equally valid representations of the physics. Especially, expectation values have the same time dependence in both pictures:

$$\langle A \rangle(\eta) = \langle \psi |_H \hat{A}_H(\eta) | \psi \rangle_H = \langle \psi(\eta) |_S \hat{A}_S | \psi(\eta) \rangle_S, \quad (4.24)$$

as can be seen from (4.19)–(4.20).

4.2 Quantizing Scalar Perturbations

4.2.1 Operators

We now follow the procedure outlined in the previous sections to quantize the cosmological scalar perturbations. The Sasaki-Mukhanov variable, the corresponding

¹Solution of (4.22) can be formally written by means of the time ordered exponential:

$$\hat{U}(\eta) = \mathcal{T} \exp\left(-i \int_{\eta_0}^{\eta} \hat{H}_S(\eta') d\eta'\right).$$

canonical momentum, and the Hamiltonian (3.57) become Hermitian operators:

$$\nu \rightarrow \hat{\nu}, \quad p \rightarrow \hat{p}, \quad (4.25)$$

$$H \rightarrow \hat{H} = \frac{1}{2} \int d^3\mathbf{x} \left(\hat{p}^2 + \hat{\nu}_{,i} \hat{\nu}_{,i} - \frac{z''}{z} \hat{\nu}^2 \right), \quad (4.26)$$

$$\hat{\nu}^\dagger = \hat{\nu}, \quad \hat{p}^\dagger = \hat{p}, \quad \hat{H} = \hat{H}^\dagger. \quad (4.27)$$

In this section, we work in the Heisenberg picture, but the index H is omitted for brevity.

Replacing the canonical Poisson brackets (3.61)–(3.62) with commutators using the rule (4.13), we get the canonical commutation relations:

$$[\hat{\nu}(\eta, \mathbf{x}), \hat{p}(\eta, \mathbf{y})] = i\delta^3(\mathbf{x} - \mathbf{y}), \quad (4.28)$$

$$[\hat{\nu}(\eta, \mathbf{x}), \hat{\nu}(\eta, \mathbf{y})] = [\hat{p}(\eta, \mathbf{x}), \hat{p}(\eta, \mathbf{y})] = 0. \quad (4.29)$$

Time evolution follows from (4.14), (4.26) and (4.28)–(4.29):

$$\hat{\nu}' = -i[\hat{\nu}, \hat{H}] = \hat{p}, \quad (4.30)$$

$$\hat{p}' = -i[\hat{p}, \hat{H}] = \hat{\nu}_{,ii} + \frac{z''}{z} \hat{\nu} \quad (4.31)$$

$$\Rightarrow \hat{\nu}'' - \hat{\nu}_{,ii} - \frac{z''}{z} \hat{\nu} = 0. \quad (4.32)$$

We next build representations of $\hat{\nu}$ and \hat{p} that satisfy the properties (4.27), (4.28), and (4.30)–(4.32).

Hermiticity and the equation of motion (4.32) suggest that we can expand $\hat{\nu}$ like the classical real solution (3.53):

$$\hat{\nu}(\eta, \mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \hat{\nu}_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \left[\hat{c}_{\mathbf{k}} \mu_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{c}_{\mathbf{k}}^\dagger \mu_{\mathbf{k}}^*(\eta) e^{-i\mathbf{k}\cdot\mathbf{x}} \right], \quad (4.33)$$

$$\hat{p}(\eta, \mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \hat{p}_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \left[\hat{c}_{\mathbf{k}} \mu'_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{c}_{\mathbf{k}}^\dagger \mu'^*_{\mathbf{k}}(\eta) e^{-i\mathbf{k}\cdot\mathbf{x}} \right]. \quad (4.34)$$

Here $\hat{c}_{\mathbf{k}}$ are constant operators. Time dependence resides in the mode functions $\mu_{\mathbf{k}}$, and we only consider functions that are independent of the direction of \mathbf{k} (this follows

from direction-independent time evolution (3.48)–(3.49) and initial conditions; see section 4.2.3). The Fourier components read

$$\hat{v}_{\mathbf{k}}(\eta) = \int \frac{d^3\mathbf{x}}{(2\pi)^{3/2}} \hat{v}(\eta, \mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} = \mu_k(\eta) \hat{c}_{\mathbf{k}} + \mu_k^*(\eta) \hat{c}_{-\mathbf{k}}^\dagger, \quad (4.35)$$

$$\hat{p}_{\mathbf{k}}(\eta) = \int \frac{d^3\mathbf{x}}{(2\pi)^{3/2}} \hat{p}(\eta, \mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} = \mu'_k(\eta) \hat{c}_{\mathbf{k}} + \mu'_k{}^*(\eta) \hat{c}_{-\mathbf{k}}^\dagger. \quad (4.36)$$

They are not Hermitian and not all independent, but satisfy

$$\hat{v}_{\mathbf{k}} = \hat{v}_{-\mathbf{k}}^\dagger, \quad \hat{p}_{\mathbf{k}} = \hat{p}_{-\mathbf{k}}^\dagger. \quad (4.37)$$

Inverting (4.35)–(4.36), we get

$$\hat{c}_{\mathbf{k}} = (\mu_k'^* \hat{v}_{\mathbf{k}} - \mu_k^* \hat{p}_{\mathbf{k}}) (\mu_k' \mu_k - \mu_k^* \mu_k'^*)^{-1}, \quad (4.38)$$

$$\hat{c}_{\mathbf{k}}^\dagger = (\mu_k \hat{p}_{\mathbf{k}}^\dagger - \mu_k' \hat{v}_{\mathbf{k}}^\dagger) (\mu_k' \mu_k - \mu_k^* \mu_k'^*)^{-1}. \quad (4.39)$$

From commutation relations (4.28)–(4.29) it follows for the Fourier components

$$[\hat{v}_{\mathbf{k}}(\eta), \hat{p}_{\mathbf{k}'}^\dagger(\eta)] = i\delta^3(\mathbf{k} - \mathbf{k}'), \quad (4.40)$$

$$[\hat{v}_{\mathbf{k}}(\eta), \hat{v}_{\mathbf{k}'}(\eta)] = [\hat{p}_{\mathbf{k}}(\eta), \hat{p}_{\mathbf{k}'}(\eta)] = 0, \quad (4.41)$$

and for the the operators $\hat{c}_{\mathbf{k}}$ and $\hat{c}_{\mathbf{k}}^\dagger$

$$[\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}] = [\hat{c}_{\mathbf{k}}^\dagger, \hat{c}_{\mathbf{k}'}^\dagger] = 0, \quad (4.42)$$

$$[\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}^\dagger] = i(\mu_k'^* \mu_k - \mu_k^* \mu_k')^{-1} \delta^3(\mathbf{k} - \mathbf{k}'). \quad (4.43)$$

Using the time evolution of the mode functions (3.48), we see that

$$\frac{d}{d\eta} (\mu_k'^* \mu_k - \mu_k^* \mu_k') = \mu_k''^* \mu_k - \mu_k^* \mu_k'' = \mu_k \mu_k^* \omega_k^2 - \mu_k^* \mu_k \omega_k^2 = 0, \quad (4.44)$$

so the prefactor in (4.43) is a constant. Its choice determines the normalisation of the mode functions μ_k , but does not change the total field operator (4.33). We choose

$$\mu_k'^* \mu_k - \mu_k^* \mu_k' = i, \quad (4.45)$$

so that

$$[\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}^\dagger] = \delta^3(\mathbf{k} - \mathbf{k}'), \quad (4.46)$$

that is, $\hat{c}_{\mathbf{k}}$ and $\hat{c}_{\mathbf{k}}^\dagger$ satisfy the usual algebra for ladder operators.

4.2.2 States

According to the commutation relations (4.42), (4.46), \hat{c}^\dagger and \hat{c} are the usual ladder operators [23, p. 21], creating and annihilating excitations, or particles, of the field ν . In particular, we define the vacuum state $|0\rangle$ with no particles by

$$\hat{c}_{\mathbf{k}} |0\rangle = 0 \quad \forall \mathbf{k} \in \mathbb{R}^3. \quad (4.47)$$

It is normalised:

$$\langle 0|0\rangle = 1. \quad (4.48)$$

States containing particles with definite momenta are formed from the vacuum state by acting on it with the creation operators. For example, a one particle state with a single particle with momentum \mathbf{k} is

$$|\mathbf{k}\rangle \equiv \hat{c}^\dagger |\mathbf{k}\rangle, \quad (4.49)$$

and the normalisation of such states follows from the commutation relations (4.46):

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \delta^3(\mathbf{k} - \mathbf{k}'). \quad (4.50)$$

We assume that the universe is in the vacuum state of ν during inflation. Using the field operator (4.33) with (4.47), we see that the field expectation value is zero:

$$\langle 0|\hat{\nu}(\eta, \mathbf{x})|0\rangle = 0. \quad (4.51)$$

However, the variance is non-zero:

$$\langle 0|\hat{\nu}^2(\eta, \mathbf{x})|0\rangle = \int \frac{dk}{2\pi^2} k^2 |\mu_k|^2. \quad (4.52)$$

Vacuum is not an eigenstate of the field operator, and the field fluctuates around the expectation value.

4.2.3 Adiabatic Vacuum

We are now ready to tackle the question of proper initial conditions for the mode functions μ_k , that is, the coefficients A_k and B_k in (3.52). Effectively, we are choosing the vacuum state, since the mode functions determine the properties of the vacuum. Features of the CMB and details of structure formation arise from this choice.

We choose the adiabatic vacuum state [24, 25], where μ_k is near some initial time η_{ini} given by the WKB-like, positive frequency solution

$$f_{\mathbf{k}} = \frac{1}{\sqrt{2\omega_k(\eta)}} \exp\left(-i \int_{\eta_{\text{ini}}}^{\eta} \omega_k(\eta') d\eta'\right). \quad (4.53)$$

This is possible at early times. Let $\eta, \eta_{\text{ini}} \rightarrow -\infty$ so that their difference stays finite. Then we get for the angular frequency (3.49)

$$\omega_k \rightarrow k, \quad (4.54)$$

and thus

$$f_k \rightarrow \frac{1}{\sqrt{2k}} \exp(-ik(\eta - \eta_{\text{ini}})). \quad (4.55)$$

This satisfies the equation of motion (3.48), which takes the form

$$f_k'' + k^2 f_k = 0. \quad (4.56)$$

At this limit, the mode functions f_k resemble those of a massless scalar field in a stationary Minkowski space-time. Using time evolution of z (3.44) with (2.54), we see that the mode in question is deep inside the horizon:

$$k \gg \left(\frac{z''}{z}\right)^{1/2} \sim -\frac{1}{\eta} = (\ell_H^c)^{-1}. \quad (4.57)$$

These modes don't feel the curvature of the space-time, and it is possible to define a sensible vacuum state.

The initial conditions for μ_k are then that they should approach the asymptotic form (4.55) as $\eta \rightarrow -\infty$. At this limit, the solution (3.52) becomes [20, p. 693]

$$\mu_k(\eta) \rightarrow \sqrt{\frac{2}{\pi}} \left\{ A_k \cos \left[-k\eta - \left(\frac{1}{2} + \gamma\right) \frac{\pi}{2} \right] + B_k \cos \left[-k\eta - \left(\frac{1}{2} - \gamma\right) \frac{\pi}{2} \right] \right\}. \quad (4.58)$$

This is equal to (4.55) when we take

$$A_k = \sqrt{\frac{\pi}{k}} \frac{\exp(ik\eta_{\text{ini}} + i3\pi/4 - i\gamma\pi/2)}{2 \sin(\pi\gamma)}, \quad (4.59)$$

$$B_k = -A_k \exp(i\gamma\pi). \quad (4.60)$$

To zeroth order in the slow-roll parameters, (3.51) gives $\gamma = 3/2$, and the solution (3.52) with the constants (4.59)–(4.60) is

$$\mu_k(\eta) = \frac{1}{\sqrt{2k}} \left(1 - \frac{i}{k\eta} \right) e^{-ik(\eta - \eta_{\text{ini}})}. \quad (4.61)$$

This gives us the time evolution and the full form of the operator $\hat{\nu}$, completing quantization.

4.3 Functional Approach

4.3.1 Field Value Basis

Quantization is usually done in the Heisenberg picture description of section 4.2, and the vacuum state is most easily defined there. However, our ultimate goal is to examine the rise of classical behaviour from our quantum system, and for this we want to know how the Fourier components of the field ν behave. This can be readily seen in the functional approach. There the vacuum state is described by a wave function giving probability amplitudes for different field configurations in Fourier space. In this section, we build such a wave function, and find out how it evolves in time. We work in the Schrödinger picture (omitting again the index S): the state vector evolves in time, while operators stay constant.

We follow the approach of [25], and start by writing the Hamilton operator (4.26) in Fourier space. Inserting the Fourier expansions (4.33) and (4.34), we get:

$$\hat{H} = \frac{1}{2} \int d^3\mathbf{k} [\hat{p}_{\mathbf{k}} \hat{p}_{\mathbf{k}}^\dagger + \omega_k^2 \hat{\nu}_{\mathbf{k}} \hat{\nu}_{\mathbf{k}}^\dagger]. \quad (4.62)$$

The problem with expression (4.62) is that, according to (4.37), all Fourier modes are not independent. To get rid of the extra freedom, we divide the integration space \mathbb{R}^3 into two halves by the sign of the first component of \mathbf{k} ; call the half with $k^1 > 0$ by the name \mathbb{R}_+^3 . It can be seen from the properties of the Fourier space operators (4.37), (4.41) that both halves give the same contribution to \hat{H} , so we can write

$$\hat{H} = \int_{\mathbb{R}_+^3} d^3\mathbf{k} [\hat{p}_{\mathbf{k}}\hat{p}_{\mathbf{k}}^\dagger + \omega_k^2\hat{\nu}_{\mathbf{k}}\hat{\nu}_{\mathbf{k}}^\dagger]. \quad (4.63)$$

From now on, we only consider the independent wave vectors in \mathbb{R}_+^3 . Since the field values are real, fixing one Fourier component with wave vector $\mathbf{k} \in \mathbb{R}_+^3$ also fixes the Fourier component with $-\mathbf{k} \in \mathbb{R}^3 \setminus \mathbb{R}_+^3$.

Another problem with the Fourier space operators is their non-Hermiticity. However, we can use them to build the Hermitian operators

$$\hat{\nu}_{\mathbf{k}}^R \equiv \frac{1}{\sqrt{2}}(\hat{\nu}_{\mathbf{k}} + \hat{\nu}_{\mathbf{k}}^\dagger), \quad \hat{\nu}_{\mathbf{k}}^I \equiv -\frac{i}{\sqrt{2}}(\hat{\nu}_{\mathbf{k}} - \hat{\nu}_{\mathbf{k}}^\dagger), \quad (4.64)$$

$$\hat{p}_{\mathbf{k}}^R \equiv \frac{1}{\sqrt{2}}(\hat{p}_{\mathbf{k}} + \hat{p}_{\mathbf{k}}^\dagger), \quad \hat{p}_{\mathbf{k}}^I \equiv -\frac{i}{\sqrt{2}}(\hat{p}_{\mathbf{k}} - \hat{p}_{\mathbf{k}}^\dagger), \quad (4.65)$$

or equivalently,

$$\hat{\nu}_{\mathbf{k}} = \frac{1}{\sqrt{2}}(\hat{\nu}_{\mathbf{k}}^R + i\hat{\nu}_{\mathbf{k}}^I), \quad \hat{\nu}_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{2}}(\hat{\nu}_{\mathbf{k}}^R - i\hat{\nu}_{\mathbf{k}}^I), \quad (4.66)$$

$$\hat{p}_{\mathbf{k}} = \frac{1}{\sqrt{2}}(\hat{p}_{\mathbf{k}}^R + i\hat{p}_{\mathbf{k}}^I), \quad \hat{p}_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{2}}(\hat{p}_{\mathbf{k}}^R - i\hat{p}_{\mathbf{k}}^I). \quad (4.67)$$

Using the commutation relations (4.40)–(4.41) with (4.64)–(4.65), and considering only wave vectors in \mathbb{R}_+^3 so that $\delta^3(\mathbf{k} + \mathbf{k}') = 0$, we get

$$[\hat{\nu}_{\mathbf{k}}^R, \hat{p}_{\mathbf{k}'}^R] = [\hat{\nu}_{\mathbf{k}}^I, \hat{p}_{\mathbf{k}'}^I] = i\delta^3(\mathbf{k} - \mathbf{k}'), \quad (4.68)$$

while other commutators between the operators (4.64)–(4.65) are zero. Thus $\nu_{\mathbf{k}}^A$ and $p_{\mathbf{k}}^A$, where A is either R or I and \mathbf{k} takes all values in \mathbb{R}_+^3 , are suitable real, independent canonical variables that describe the field ν . The Hamilton operator becomes

$$\hat{H} = \int_{\mathbb{R}_+^3} d^3\mathbf{k} \sum_{A=R,I} \left[\frac{1}{2}\hat{p}_{\mathbf{k}}^{A2} + \frac{\omega_k^2(\eta)}{2}\hat{\nu}_{\mathbf{k}}^{A2} \right]. \quad (4.69)$$

For mathematical convenience, we next restrict ourselves to a finite volume of space, a cube with edges of coordinate length L . Imposing periodic boundary conditions, the wave vectors can take only the discrete values

$$\mathbf{k} = \frac{2\pi}{L} \mathbf{n}, \quad n^i \in \mathbb{Z}, \quad (4.70)$$

where the components of \mathbf{n} are integers. Sums over \mathbf{n} then become integrals in the continuum limit $L \rightarrow \infty$. Using this we get the discrete expressions from the continuum ones by making the replacements

$$\int d^3\mathbf{k} \rightarrow \frac{(2\pi)^3}{V} \sum_{\mathbf{k}}, \quad (4.71)$$

$$\delta^3(\mathbf{k} - \mathbf{k}') \rightarrow \frac{V}{(2\pi)^3} \delta_{\mathbf{k}\mathbf{k}'}, \quad (4.72)$$

where $V \equiv L^3$. We rescale the field and momentum operators:

$$\hat{\nu}_{\mathbf{k}}^A \rightarrow \frac{\sqrt{V}}{(2\pi)^{3/2}} \hat{\nu}_{\mathbf{k}}^A, \quad (4.73)$$

$$\hat{p}_{\mathbf{k}}^A \rightarrow \frac{\sqrt{V}}{(2\pi)^{3/2}} \hat{p}_{\mathbf{k}}^A, \quad (4.74)$$

so that the Fourier expansions read

$$\hat{\nu}(\eta, \mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{\sqrt{2}} \left(\hat{\nu}_{\mathbf{k}}^R + i \hat{\nu}_{\mathbf{k}}^I \right) e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (4.75)$$

$$\hat{p}(\eta, \mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{\sqrt{2}} \left(\hat{p}_{\mathbf{k}}^R + i \hat{p}_{\mathbf{k}}^I \right) e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (4.76)$$

The Fourier components now have dimensions

$$[\nu_{\mathbf{k}}^A] = E^{-1/2}, \quad [p_{\mathbf{k}}^A] = E^{1/2}, \quad (4.77)$$

and follow the canonical commutation relations

$$[\hat{\nu}_{\mathbf{k}}^R, \hat{p}_{\mathbf{k}'}^R] = [\hat{\nu}_{\mathbf{k}}^I, \hat{p}_{\mathbf{k}'}^I] = i \delta_{\mathbf{k}\mathbf{k}'}. \quad (4.78)$$

The Hamilton operator (4.69) becomes

$$\hat{H} = \sum_{\mathbf{k} \in \mathbb{R}_+^3} \left[\hat{H}_{\mathbf{k},R}(\eta) + \hat{H}_{\mathbf{k},I}(\eta) \right], \quad (4.79)$$

where

$$\hat{H}_{\mathbf{k},A}(\eta) \equiv \frac{1}{2}\hat{p}_{\mathbf{k}}^{A2} + \frac{\omega_{\mathbf{k}}^2(\eta)}{2}\hat{v}_{\mathbf{k}}^{A2}. \quad (4.80)$$

Now the operator (4.79) is a sum of Hamilton operators of independent oscillators, two for each wave vector \mathbf{k} in \mathbb{R}_+^3 . The values of the independent, compatible observables $\nu_{\mathbf{k}}^R, \nu_{\mathbf{k}}^I$ determine the whole field configuration $\nu(\mathbf{x})$. The Hilbert space is then a direct product of Hilbert spaces for the different Fourier components, and an eigenstate of the field operator can be written as

$$|\nu\rangle = |\nu_{\mathbf{k}_1}^R\rangle \otimes |\nu_{\mathbf{k}_1}^I\rangle \otimes |\nu_{\mathbf{k}_2}^R\rangle \otimes |\nu_{\mathbf{k}_2}^I\rangle \otimes \dots \quad (4.81)$$

where the wave vectors \mathbf{k}_i take all the allowed values in \mathbb{R}_+^3 . Each component of the Hamiltonian acts in one of the spaces in the product.

If a state can be initially decomposed as

$$|\Psi(\eta)\rangle = |\psi_{\mathbf{k}_1,R}(\eta)\rangle \otimes |\psi_{\mathbf{k}_1,I}(\eta)\rangle \otimes |\psi_{\mathbf{k}_2,R}(\eta)\rangle \otimes \dots, \quad (4.82)$$

that is, if there is no entanglement between the Fourier modes, then it stays like this for all times, since the Hamiltonian contains no mixing between modes. The probability amplitude of measuring the field configuration ν in state $|\Psi\rangle$ is then the wave function

$$\Psi(\nu, \eta) \equiv \langle \nu | \Psi(\eta) \rangle = \prod_{\mathbf{k} \in \mathbb{R}_+^3} \psi_{\mathbf{k}}^R(\nu_{\mathbf{k}}^R, \eta) \psi_{\mathbf{k}}^I(\nu_{\mathbf{k}}^I, \eta), \quad (4.83)$$

where the component wave functions are defined as

$$\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A, \eta) \equiv \langle \nu_{\mathbf{k}}^A | \psi_{\mathbf{k},A}(\eta) \rangle. \quad (4.84)$$

They are the probability amplitudes for measuring the corresponding Fourier component values in the state $|\Psi\rangle$, and they evolve according to the Schrödinger equation (4.23),

$$\psi_{\mathbf{k}}^{\prime A}(\nu_{\mathbf{k}}^A, \eta) = -i \langle \nu_{\mathbf{k}}^A | \hat{H}_{\mathbf{k},A}(\eta) | \psi_{\mathbf{k},A}(\eta) \rangle. \quad (4.85)$$

Here

$$\hat{\nu}_{\mathbf{k}}^A |\nu_{\mathbf{k}}^A\rangle = \nu_{\mathbf{k}}^A |\nu_{\mathbf{k}}^A\rangle, \quad (4.86)$$

and we choose the following representation for $\hat{p}_{\mathbf{k}}^A$:

$$\langle \nu_{\mathbf{k}}^A | \hat{p}_{\mathbf{k}}^A | \nu_{\mathbf{k}}^A \rangle = -i \frac{\partial}{\partial \nu_{\mathbf{k}}^A} \delta(\nu_{\mathbf{k}}^A - \nu_{\mathbf{k}}^A) \quad (4.87)$$

$$\Rightarrow \langle \nu_{\mathbf{k}}^A | \hat{p}_{\mathbf{k}}^A | \psi_{\mathbf{k}}^A \rangle = -i \frac{\partial}{\partial \nu_{\mathbf{k}}^A} \psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A, \eta). \quad (4.88)$$

This satisfies the commutation relations (4.78). Then (4.85) becomes

$$\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A, \eta) = -i \left(-\frac{1}{2} \frac{\partial^2}{\partial (\nu_{\mathbf{k}}^A)^2} + \frac{\omega_{\mathbf{k}}^2(\eta)}{2} \nu_{\mathbf{k}}^A \right) \psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A, \eta), \quad (4.89)$$

a wave mechanical version of the Schrödinger equation.

4.3.2 Vacuum Wave Function

Now that we have introduced the formalism, it's time to find the wave function of the adiabatic vacuum state. We write the ladder operators in the definition of the Heisenberg picture vacuum (4.47) in terms of the Fourier space operators using (4.38), (4.45):

$$-i(\mu_k^{I*} \hat{\nu}_{\mathbf{k}H} - \mu_k^* \hat{p}_{\mathbf{k}H}) |0\rangle_H = 0. \quad (4.90)$$

Multiplying from left by the time evolution operator \hat{U} and the bra-vector $\langle \nu_{\mathbf{k}}^A |$, this becomes

$$\langle \nu_{\mathbf{k}}^A | \underbrace{\hat{U}(\eta) (-i(\mu_k^{I*} \hat{\nu}_{\mathbf{k}H} - \mu_k^* \hat{p}_{\mathbf{k}H}) \hat{U}^\dagger(\eta))}_{-i(\mu_k^{I*} \hat{\nu}_{\mathbf{k}S} - \mu_k^* \hat{p}_{\mathbf{k}S})} \underbrace{\hat{U}(\eta) |0\rangle_H}_{|0\rangle_S} = 0. \quad (4.91)$$

Equations for different Fourier modes are independent, so clearly the vacuum state is of the form (4.82). Using the operator representations (4.86) and (4.87), we get for the component wave functions:

$$\left(-i\mu_k^{I*} \nu_{\mathbf{k}}^A + \mu_k^* \frac{\partial}{\partial \nu_{\mathbf{k}}^A} \right) \psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A, \eta) = 0. \quad (4.92)$$

The solution is

$$\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A, \eta) = C(\eta) e^{-\Omega_{\mathbf{k}}(\eta) \nu_{\mathbf{k}}^A{}^2}, \quad (4.93)$$

where C is an arbitrary function of time (it may also depend on \mathbf{k} and A), and

$$\Omega_k(\eta) \equiv -\frac{i \mu_k'^*}{2 \mu_k^*}. \quad (4.94)$$

We will need the real and imaginary parts of $\Omega_k = \text{Re } \Omega_k + i \text{Im } \Omega_k$. Using the mode function (4.61) obtained earlier, we get

$$\text{Re } \Omega_k(\eta) = \frac{k^3 \eta^2}{2(k^2 \eta^2 + 1)}, \quad (4.95)$$

$$\text{Im } \Omega_k(\eta) = \frac{1}{2\eta(k^2 \eta^2 + 1)}, \quad (4.96)$$

to zeroth order in slow-roll parameters; we will use this approximation in what follows.

For C , we write

$$C(\eta) \equiv N(\eta) e^{i\theta(\eta)}, \quad \theta \in \mathbb{R}, \quad N > 0. \quad (4.97)$$

The magnitude is fixed by normalisation:

$$\int d\nu_k^A \psi_{\mathbf{k}}^A(\nu_k^A, \eta) \psi_{\mathbf{k}}^{A*}(\nu_k^A, \eta) = 1 \quad (4.98)$$

$$\Rightarrow N(\eta) = \left(\frac{2 \text{Re } \Omega_k(\eta)}{\pi} \right)^{\frac{1}{4}}. \quad (4.99)$$

Substituting the wave function (4.93) into the Schrödinger equation (4.89), we see that the vacuum solution evolves in time properly when the phase is

$$\theta(\eta) = - \int_{\eta_{\text{ini}}}^{\eta} d\eta' \text{Re } \Omega_k(\eta'). \quad (4.100)$$

Thus, the vacuum wave functions are Gaussian wave packets with expectation value zero and non-trivial, time dependent width and phase. If interactions with other fields are neglected, the phase (4.100) is unimportant. Uncertainties of $\nu_{\mathbf{k}}^A$ and $p_{\mathbf{k}}^A$ are

$$\Delta \nu_{\mathbf{k}}^A = \frac{1}{2\sqrt{\text{Re } \Omega_k}} \xrightarrow{\eta \rightarrow 0} \infty, \quad (4.101)$$

$$\Delta p_{\mathbf{k}}^A = \frac{|\Omega_k|}{\sqrt{\text{Re } \Omega_k}} \xrightarrow{\eta \rightarrow 0} \infty, \quad (4.102)$$

and

$$\Delta\nu_{\mathbf{k}}^A \Delta p_{\mathbf{k}}^A = \frac{1}{2} \sqrt{1 + \frac{1}{\eta^6 k^6}}. \quad (4.103)$$

Comparing this with the Heisenberg uncertainty relation derived from the commutation relation (4.78),

$$\Delta\nu_{\mathbf{k}}^A \Delta p_{\mathbf{k}}^A \geq \frac{1}{2}, \quad (4.104)$$

we see that initially, at $\eta \rightarrow -\infty$, the wave packet has minimum uncertainty, but as time goes on, the packet spreads. However, a certain linear combination of $\nu_{\mathbf{k}}^A$ and $p_{\mathbf{k}}^A$ gets a well-defined value with small uncertainty, and the resulting state is called squeezed. This is the topic of the next section.

4.4 Squeezed State

4.4.1 Wigner Function

Properties of quantum states can be visualised with a Wigner function [26] [27, p. 81]. Consider a general one-dimensional quantum mechanical system with canonical variables x and p , satisfying the commutation relation

$$[\hat{x}, \hat{p}] = i, \quad (4.105)$$

and a state $|\psi\rangle$ described by the wave function $\psi(x) \equiv \langle x|\psi\rangle$. Then the Wigner function corresponding to this state is

$$W_{\psi}(x, p) \equiv \frac{1}{\pi} \int dy \psi^*(x+y) \psi(x-y) e^{2ipy}. \quad (4.106)$$

Some important properties include

$$\int dx dp W_{\psi}(x, p) = 1, \quad (4.107)$$

$$\int dp W_{\psi}(x, p) = |\psi(x)|^2, \quad (4.108)$$

$$\int dx W_{\psi}(x, p) = |\psi(p)|^2, \quad (4.109)$$

$$2\pi \int dx dp W_{\psi}(x, p) W_{\phi}(x, p) = |\langle \psi | \phi \rangle|^2, \quad (4.110)$$

where $\psi(p) \equiv \langle p|\psi\rangle$ is the wave function in momentum representation, which is the Fourier transform of $\psi(x)$.

Properties (4.107)–(4.109) suggest that W_ψ behaves like a probability distribution in (x, p) phase space: expectation values of functions of x can be obtained as

$$\langle f(x) \rangle_\psi = \int dx dp f(x) W_\psi(x, p), \quad (4.111)$$

and the same is true for functions of p . However, W_ψ can take negative values, so it is not a true probability distribution. Moreover, points in the (x, p) space do not represent actual states of the system: according to the Heisenberg uncertainty principle, the values of x and p can't be determined exactly at the same time.

In any case, the Wigner function can be used to visualise correlations between different x and p values. For example, we can ask what is the probability to find the system in a Gaussian state centered around (x_0, p_0) . The wave function of such a minimum uncertainty state is

$$\phi(x) = \left(\frac{1}{\pi D}\right)^{\frac{1}{4}} e^{-(x-x_0)^2/(2D)+ip_0x}, \quad (4.112)$$

with a positive constant D , and its Wigner function reads

$$W_\phi(x, p) = \frac{1}{\pi} e^{-(x-x_0)^2/D-D(p-p_0)^2}. \quad (4.113)$$

This is positive and peaked around (x_0, p_0) in the phase space. Then the integral in (4.110), which gives the probability $|\langle\psi|\phi\rangle|^2$, is strongly affected by the average value of W_ψ at the vicinity of this point. Thus, the bigger the system's Wigner function is at (x_0, p_0) , the greater is the probability to find the system nearby.

4.4.2 Squeezed Vacuum

Let us now return to cosmological scalar perturbations, which in linear perturbation theory are a collection of independent one-dimensional systems. The canonical

variables for one degree of freedom are $\nu_{\mathbf{k}}^A$ and $p_{\mathbf{k}}^A$, and the Wigner function corresponding to the wave function (4.93) reads

$$W_0(\nu_{\mathbf{k}}^A, p_{\mathbf{k}}^A) = \frac{|\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A)|^2}{\sqrt{2\pi \operatorname{Re} \Omega_k}} \exp\left[-\frac{1}{2 \operatorname{Re} \Omega_k} (p_{\mathbf{k}}^A + 2\nu_{\mathbf{k}}^A \operatorname{Im} \Omega_k)^2\right]. \quad (4.114)$$

From (4.95)–(4.96) we see that as time goes on,

$$\operatorname{Re} \Omega \xrightarrow{\eta \rightarrow 0} 0, \quad (4.115)$$

$$\operatorname{Im} \Omega \xrightarrow{\eta \rightarrow 0} -\infty. \quad (4.116)$$

Using [20, p. 76]

$$\frac{1}{\sqrt{\pi\epsilon}} e^{-x^2/\epsilon} \xrightarrow{\epsilon \rightarrow 0} \delta(x), \quad (4.117)$$

the first limit (4.115) implies that

$$W_0(\nu_{\mathbf{k}}^A, p_{\mathbf{k}}^A) \xrightarrow{\eta \rightarrow 0} |\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A)|^2 \delta(p_{\mathbf{k}}^A + 2\nu_{\mathbf{k}}^A \operatorname{Im} \Omega_k). \quad (4.118)$$

At the same time, the wave function widens. The state is ‘squeezed’ into a thin, long line with

$$p_{\mathbf{k}}^A + 2\nu_{\mathbf{k}}^A \operatorname{Im} \Omega_k = 0. \quad (4.119)$$

In other words, measuring the quantity $p_{\mathbf{k}}^A + 2\nu_{\mathbf{k}}^A \operatorname{Im} \Omega_k$ gives zero with high accuracy:

$$\Delta(p_{\mathbf{k}}^A + 2\nu_{\mathbf{k}}^A \operatorname{Im} \Omega_k) = \operatorname{Re} \Omega_k \xrightarrow{\eta \rightarrow 0} 0, \quad (4.120)$$

and using the example from section 4.4.1, for a fixed $p_{\mathbf{k}}^A$ or $\nu_{\mathbf{k}}^A$ value, the probability to find the system in a narrow Gaussian state reaches its maximum along the line (4.119) at late times. The values of $p_{\mathbf{k}}^A$ and $\nu_{\mathbf{k}}^A$ become correlated. Probability densities of field values, or the corresponding momenta, are given by $|\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A)|^2$.

The second limit (4.116) means that as the Wigner function narrows, it also rotates from the $\nu_{\mathbf{k}}^A$ direction towards the $p_{\mathbf{k}}^A$ axis. This is visualised in figure 4.1.

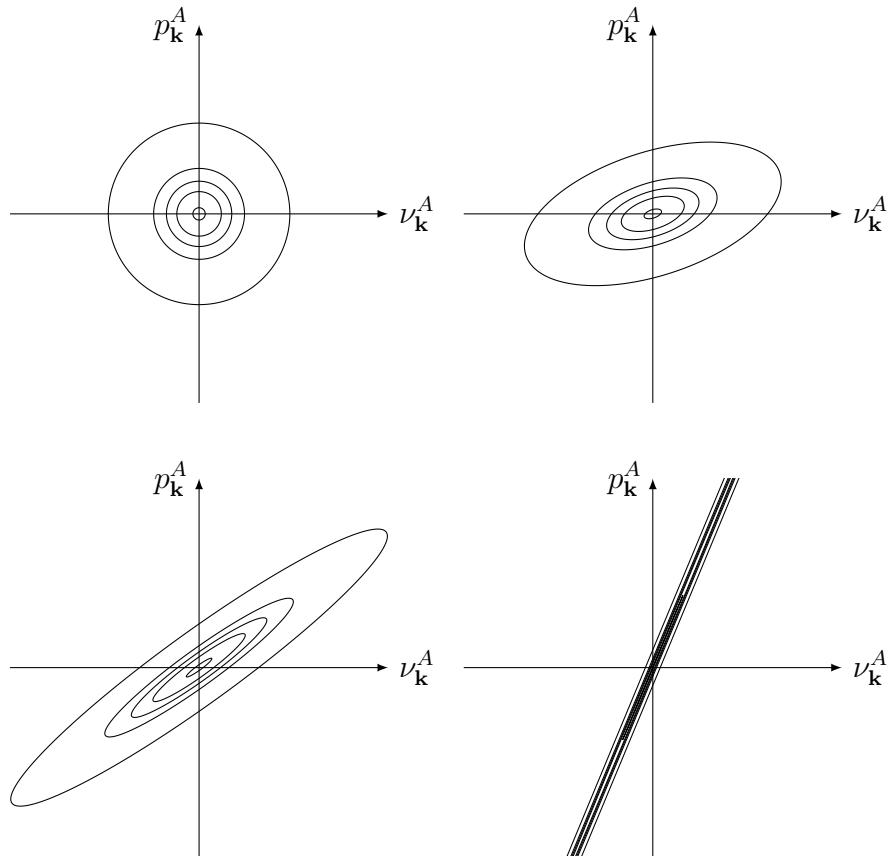


Figure 4.1: Squeezed state. The Wigner function (4.114) evolves from its initial state (top left) to late times (bottom right). The function is at its maximum at the origin and decreases when moving outwards; the closed lines correspond to constant values. As time goes on, the Wigner function elongates and rotates counterclockwise.

4.4.3 Classical or Not?

We now turn to the question of the transition from quantum mechanics to classical theory. According to inflation the cosmological perturbations have quantum mechanical origins, but when examining the evolution of the universe they are typically treated as classical stochastic variables, with great observational success. In the rest of this thesis, we will discuss how this classical behaviour arises.

By classicality, we mean that some classical observables have well-defined values, and evolve according to the classical equations of motion. This is true if the wave function of the system is localised so that the uncertainties of these variables are small at all times.

The natural guess for classical variables in the case of cosmological scalar perturbations would be the field strengths $\nu_{\mathbf{k}}^A$ and the canonical momenta $p_{\mathbf{k}}^A$. Their classical time evolution follows from the method of quantization: commutators like (4.14) produce expressions that resemble those of classical mechanics, with canonical variables replaced by operators. Taking expectation values on each side, we get

$$\frac{d}{d\eta} \langle x \rangle_{\psi} = \langle \psi | -i[x, H] | \psi \rangle = \langle \psi | \{x, H\} |_{x \rightarrow \hat{x}, p \rightarrow \hat{p}} | \psi \rangle, \quad (4.121)$$

$$\frac{d}{d\eta} \langle p \rangle_{\psi} = \langle \psi | -i[p, H] | \psi \rangle = \langle \psi | \{p, H\} |_{x \rightarrow \hat{x}, p \rightarrow \hat{p}} | \psi \rangle, \quad (4.122)$$

leading to the Ehrenfest theorem [22, p. 87] for a Hamiltonian quadratic in the momentum: the time derivative of $\langle x \rangle_{\psi}$ is proportional to $\langle p \rangle_{\psi}$, and the time derivative of $\langle p \rangle_{\psi}$ is given by the expectation value of the x -derivative of the potential function. When the state vector is an approximate eigenstate of the canonical variables, the state is accurately described by these expectation values, and the Ehrenfest theorem leads to classical equations of motion for $\langle x \rangle_{\psi}$ and $\langle p \rangle_{\psi}$.

In the case of cosmological scalar perturbations, the vacuum state is not localised in phase space at late times, as discussed above. However, the state can be thought of as a sum of local wave packets along the squeezing direction. It is then

tempting to interpret the system as an ensemble of such classical states, so that when the observables are measured, the system collapses into one of these states and evolves classically onwards. Canonical variables $\nu_{\mathbf{k}}^A, p_{\mathbf{k}}^A$ become stochastic random variables, with the corresponding probability densities given by the Wigner function (4.114). However, this approach is not sufficient to explain the transition to classicality, for several reasons.

Firstly, the whole concept of measurements and collapsing state vectors is difficult. It is not clear what qualifies as a measurement, especially in the early universe with no human influence. Also, as we have seen in this chapter, even quantum states with minimal uncertainty tend to spread in position and momentum space, so that a state ‘classicalised’ by a collapse may not remain classical forever without subsequent collapses. When does the state vector collapse, and why?

Secondly, there is no obvious reason why the field values or the canonical momenta become the classical variables. Why do we see a universe with well-defined, classical perturbation field values, and not, for example, superpositions of multiple field values?

Lastly, the question of classicality is hardly relevant if the system is isolated, as we have assumed so far. For cosmological perturbations to affect the evolution of the universe, they must interact with their environment. Considering these interactions can solve the above-mentioned problems, at least to a certain degree. This will be discussed in the next chapter.

5. Decoherence

We have thus far seen how cosmological scalar perturbations can be treated quantum mechanically, and how this treatment gives rise to a highly squeezed vacuum state. This state is still very much quantum mechanical. We would like to justify the classical treatment of the perturbations, common in standard cosmology.

In this chapter, we shall see how classical behaviour arises from environment-induced decoherence. There the quantum mechanical system becomes entangled with its environment, resulting in an ensemble of classical looking states. We first introduce the formalism of density operators, and use it to discuss decoherence in a laboratory setting as in the Schrödinger's cat thought experiment, where the quantum mechanical system becomes entangled with the classical environment of the laboratory. We then move on to the decoherence of cosmological scalar perturbations. We review some realistic models for the environment in the cosmological case, and discuss how interactions between the perturbations and their environment can give rise to decoherence. In the end, we return to the question of classicalisation of the perturbations. We take a look at the measurement problem of quantum mechanics and its relation to decoherence, and consider the possibility of detecting the effects of decoherence in the CMB.

5.1 Density Operator

5.1.1 Definition and Properties

As mentioned in section 4.4.3, we would like to interpret the cosmological scalar perturbations as a collection of classical states with some probabilities. Such ensembles of states are described by density operators, see [22, p. 176]. These are Hilbert space operators of the form

$$\hat{\rho} = \sum_i w_i |\psi_i\rangle\langle\psi_i|. \quad (5.1)$$

Here $|\psi_i\rangle$ are the states in the ensemble. They can be any normalised vectors in the Hilbert space, and in particular, they don't have to be orthogonal. The weights w_i are their corresponding statistical probabilities, positive real numbers whose sum is one:

$$w_i \geq 0, \quad (5.2)$$

$$\sum_i w_i = 1. \quad (5.3)$$

The point of such a representation is that it simplifies the calculation of expectation values of observables. For an observable A with the complete set of orthonormal eigenvectors $|a_j\rangle$ as in (4.7)–(4.9), we get

$$\begin{aligned} \langle A \rangle &= \sum_i w_i \sum_j a_j P_{\psi_i}(a_j) = \sum_i \sum_j w_i |\langle\psi_i|a_j\rangle|^2 a_j \\ &= \sum_j \langle a_j | \sum_i w_i |\psi_i\rangle\langle\psi_i| \hat{A} |a_j\rangle = \text{tr}(\hat{\rho}\hat{A}). \end{aligned} \quad (5.4)$$

Here tr stands for the trace of an operator. It is defined as

$$\text{tr} \hat{X} \equiv \sum_i \langle b_i | \hat{X} | b_i \rangle, \quad (5.5)$$

where $|b_i\rangle$ is some complete set of orthonormal basis vectors. In (5.4), we used the eigenstates of \hat{A} , but the trace is independent of the choice of basis.

Important properties of the density operator include hermiticity,

$$\hat{\rho} = \hat{\rho}^\dagger, \quad (5.6)$$

which is evident from (5.1), and the fact that the trace of $\hat{\rho}$ is one:

$$\text{tr } \hat{\rho} = \sum_i w_i \underbrace{\text{tr } |\psi_i\rangle\langle\psi_i|}_{=1} = 1. \quad (5.7)$$

Density operators are also non-negative, that is,

$$\langle\phi|\hat{\rho}|\phi\rangle = \sum_i w_i |\langle\psi_i|\phi\rangle|^2 \geq 0 \quad (5.8)$$

for any state $|\phi\rangle$.

Working in the Schrödinger picture, the states $|\psi_i\rangle$ evolve in time according to the Schrödinger equation (4.23), giving the von Neumann equation

$$\hat{\rho}(\eta)' = -i \sum_i w_i \left\{ \hat{H}(\eta) |\psi_i(\eta)\rangle\langle\psi_i(\eta)| - |\psi_i(\eta)\rangle\langle\psi_i(\eta)| \hat{H}(\eta) \right\} = -i [\hat{H}(\eta), \hat{\rho}(\eta)]. \quad (5.9)$$

This leads to

$$\hat{\rho}(\eta) = \hat{U}(\eta) \hat{\rho}(\eta_0) \hat{U}^\dagger(\eta), \quad (5.10)$$

where $\hat{U}(\eta)$ is the time evolution operator from section 4.1.3.

The density operator description introduced here is an expansion of the quantum mechanics discussed in chapter 4. If the quantum state of the system is known with certainty to be $|\psi\rangle$, the density operator becomes

$$\hat{\rho}_{\text{pure}} = |\psi\rangle\langle\psi|. \quad (5.11)$$

We say that $\hat{\rho}_{\text{pure}}$ describes a pure state. Clearly,

$$\text{tr } \hat{\rho}_{\text{pure}}^2 = \text{tr } \hat{\rho}_{\text{pure}} = 1, \quad (5.12)$$

and this is both a necessary and a sufficient condition for the purity of a density operator [22, p. 179]. For pure states, relations like (5.4), (5.9) are reduced to their counterparts (4.11), (4.23) from chapter 4.

Non-pure states are called mixed. In this chapter, we show how the pure vacuum state of cosmological scalar perturbations can look to an observer like a

mixed ensemble of classically behaving states. This may sound surprising: even if a pure state can be written as a superposition of classical states,

$$|\psi\rangle = \sum_i b_i |\psi_i\rangle, \quad (5.13)$$

the corresponding density operator is

$$\hat{\rho}_\psi = \sum_i |b_i|^2 |\psi_i\rangle\langle\psi_i| + \sum_{i \neq j} b_i b_j^* |\psi_i\rangle\langle\psi_j|, \quad (5.14)$$

including cross terms absent from the form (5.1). Moreover, using the purity condition (5.12), we see that since unitary time evolution preserves the trace, it keeps pure states pure and mixed states mixed. However, we will see that the transition from a pure state to an ensemble can be achieved if we take into account interactions between the perturbations and their environment.

5.1.2 Reduced Density Operator

To be able to handle the environment of the perturbations, we need to introduce one more piece of formalism. Consider a direct product Hilbert space:

$$H = H_1 \otimes H_2. \quad (5.15)$$

Here H_1 and H_2 are Hilbert spaces with the orthonormal bases

$$|b_i\rangle \in H_1, \quad \langle b_i | b_j \rangle = \delta_{ij}, \quad \sum_i |b_i\rangle\langle b_i| = \mathbb{1}, \quad (5.16)$$

$$|c_i\rangle \in H_2, \quad \langle c_i | c_j \rangle = \delta_{ij}, \quad \sum_i |c_i\rangle\langle c_i| = \mathbb{1}. \quad (5.17)$$

An observable A residing in only H_1 has the operator form

$$\hat{A}_{\text{tot}} = \hat{A} \otimes \mathbb{1}. \quad (5.18)$$

We introduce the reduced density operator

$$\hat{\rho}_1 \equiv \text{tr}_2 \hat{\rho} \equiv \sum_{j,k,m} |b_m\rangle\langle b_m c_j| \hat{\rho} |b_k c_j\rangle\langle b_k|, \quad (5.19)$$

where tr_2 means tracing over the Hilbert space H_2 , and we have abbreviated $|b_k c_j\rangle \equiv |b_k\rangle \otimes |c_j\rangle$. The resulting operator operates in H_1 and follows the usual properties of density operators, (5.6)–(5.8). Moreover, expectation values of H_1 -observables can be written as

$$\begin{aligned}
\langle A \rangle &= \text{tr} \left\{ \hat{\rho} (\hat{A} \otimes \mathbb{1}) \right\} = \sum_{i,j} \langle b_i c_j | \hat{\rho} (\hat{A} \otimes \mathbb{1}) | b_i c_j \rangle \\
&= \sum_{i,j,k,l} \langle b_i c_j | \hat{\rho} | b_k c_l \rangle \langle b_k c_l | \hat{A} \otimes \mathbb{1} | b_i c_j \rangle \\
&= \sum_{i,j,k,l,m} \underbrace{\delta_{im}}_{\langle b_i | b_m \rangle} \langle b_m c_j | \hat{\rho} | b_k c_l \rangle \langle b_k | \hat{A} | b_i \rangle \underbrace{\delta_{lj}}_{\langle c_l | c_j \rangle} \\
&= \sum_i \langle b_i | \left(\sum_{j,k,m} |b_m\rangle \langle b_m c_j| \hat{\rho} | b_k c_j\rangle \langle b_k| \right) \hat{A} | b_i \rangle \\
&\equiv \text{tr}_1 (\hat{\rho}_1 \hat{A}),
\end{aligned} \tag{5.20}$$

where tr_1 is the usual trace over space H_1 . Any effects of H_2 are hidden inside the reduced density operator.

When working only with degrees of freedom from the Hilbert space H_1 , we can thus ignore the space H_2 by using the reduced density operator instead of the full one. However, if there are interactions between the two spaces, then H_2 still affects the form of $\hat{\rho}_1$ and in particular its time evolution. In this case, the Hamilton operator of the system can be split into three parts:

$$\hat{H} = \hat{H}_1 \otimes \mathbb{1} + \mathbb{1} \otimes \hat{H}_2 + \hat{H}_{\text{int}}. \tag{5.21}$$

The third term includes the interactions between H_1 and H_2 . Due to the interactions, $\hat{\rho}_1$ does not follow the unitary evolution (5.10), unlike the full $\hat{\rho}$. Instead, its time dependence is described by a more complicated master equation. In particular, the H_1 -subsystem may end up in a mixed state, where $\hat{\rho}_1$ does not satisfy the purity condition (5.12), even if it starts out in a pure state with no mixing between the two Hilbert spaces. In this case, the H_1 -part of the system starts in a well-defined state, but after the mixing this is no longer true, and we need the density operator

$\hat{\rho}_1$ to describe the H_1 -subsystem, which is then a true statistical ensemble a la (5.1).

We will return to the the specifics of time evolution in section 5.2.2.

5.2 Decoherence

5.2.1 Laboratory Setting

We now apply the approach of the previous section to see how classical behaviour can arise from quantum mechanics, following the treatment in [27, p. 40]. Consider a quantum mechanical system interacting with its environment in a laboratory, for example the Schrödinger’s cat thought experiment, where the quantum state of radioactive substance (dacyed or not decayed) determines whether poison is released in a box, which would kill a cat inside. We can ask, what is the quantum state of the cat during the experiment: is it in a superposition state of ‘dead’ and ‘alive’, corresponding to the superposition state of ‘decayed’ and ‘not decayed’ of the radioactive material?

We want to model the process of observing the system by writing the Hilbert space as a direct product of two parts: the system itself, and the environment, including the degrees of freedom that aren’t being observed. We assume these parts to be initially uncorrelated, so that the quantum state of the system is the direct product

$$|\Psi\rangle = |\psi\rangle \otimes |E\rangle, \quad (5.22)$$

where $|\psi\rangle$ is the initial state of the system, and $|E\rangle$ is the initial state of the classical environment.

As time goes on, the state evolves according to the Hamiltonian

$$\hat{H} = \hat{H}_S \otimes \mathbb{1} + \mathbb{1} \otimes \hat{H}_E + \hat{H}_{\text{int}}, \quad (5.23)$$

of the form (5.21), so that H_S evolves the system state, H_E evolves the environmental

state, and H_{int} mixes them together. We take the interaction part to be of the von Neumann form

$$\hat{H}_{\text{int}} = \sum_i |\psi_i\rangle\langle\psi_i| \otimes \hat{A}_i, \quad (5.24)$$

where the states $|\psi_i\rangle$ form a complete orthonormal basis, so we can write the initial state as

$$|\Psi\rangle = \left[\sum_i c_i |\psi_i\rangle \right] \otimes |E\rangle \quad (5.25)$$

with some complex constants c_i . Considering only the interaction part of the Hamiltonian for the moment, time evolution keeps the system states constant and changes the environmental states according to the operators \hat{A}_i . In laboratory, we work with the usual time t instead of the conformal time η , and get

$$|\Psi(t)\rangle = \sum_i c_i |\psi_i\rangle \otimes \exp(-i\hat{A}_i t) |E\rangle \equiv \sum_i c_i |\psi_i\rangle \otimes |E_i(t)\rangle. \quad (5.26)$$

In other words, the interaction correlates the environment with the system. As discussed earlier, the vectors $|E_i(t)\rangle$ correspond to classical environmental states. As classically distinguishable, they are orthogonal:

$$\langle E_i(t) | E_j(t) \rangle = \delta_{ij}. \quad (5.27)$$

Since we are not interested in the environment, we trace over it, getting a reduced density operator for the system:

$$\begin{aligned} \hat{\rho}_{\text{red}} &= \sum_{i,j,k} c_i c_j^* |\psi_i\rangle\langle\psi_j| \otimes \underbrace{\langle E_k | E_i \rangle}_{\delta_{ki}} \underbrace{\langle E_j | E_k \rangle}_{\delta_{jk}} \\ &= \sum_i |c_i|^2 |\psi_i\rangle\langle\psi_i|. \end{aligned} \quad (5.28)$$

Normalisation of the state $|\Psi\rangle$ dictates that the factors $|c_i|^2$ sum up to one. This is then an ensemble of states like (5.1), a collection of system states linked to classical environments, observed with probabilities $|c_i|^2$.

The process described above is called environment-induced decoherence. A comprehensive review is given in [27]. The word ‘coherent’ describes situations

where phases between different parts of the system are well defined, such as in coherent light. In decoherence, such phase information is lost. After tracing over the environment, only the magnitudes of the factors c_i remain visible in the reduced density operator, while information about their phases—that is, the relative phases of the states $|\psi_i\rangle$ in the superposition (5.25)—is lost. This is related to the loss of interference terms of the form $|\psi_i\rangle\langle\psi_j|$ in the reduced density operator (5.28).

Decoherence now explains how the observation of classical reality arises from quantum theory. The reduced density operator (5.28) contains all the information available for observers, when the environment is disregarded. Instead of a quantum mechanical superposition, we have an ensemble of states, each observed with a certain probability. These states, singled out by the interaction (5.24), are called pointer states, since in our laboratory example they are linked to definite positions of a pointer in a classical measuring device. In decoherence, the reduced density operator of the system gets diagonalised in the pointer state basis.

In the case of Schrödinger’s cat, the pointer states correspond to the combinations ‘no decay and a living cat’ and ‘decay and a dead cat’. The different environmental states correspond to slightly different movements in the air in the laboratory, or perhaps different positions of scientists around the box, or other indistinguishable or unimportant details not under observation. After decoherence, instead of a cat in a superposition, we have a statistical ensemble of two classical realities, one with a living cat and the other with a dead one. We will discuss such an interpretation and its limitations in more detail in section 5.3.

In the next sections, we apply this logic to cosmological scalar perturbations: via interactions the perturbations become entangled with their environment, and trace over the environment gives a statistical ensemble of universes with different, observable realisations of the perturbations. However, in the cosmological context, there is no classical laboratory to play the role of an environment. By environment

we mean the degrees of freedom that are invisible to us today, and thus can be traced over when examining observations of the perturbations. To see if, and how, this works in practice, we need to answer the following questions: What is the ‘environment’ in the case of cosmological perturbations? What kind of interactions are there between this environment and the perturbations? What kind of pointer basis is singled out? Is decoherence fast enough to make the perturbations classical during inflation, and are the results in line with our expectations and observations? We start by studying a simple model for the interactions (section 5.2.2) and the corresponding pointer states (section 5.2.3). After demonstrating that decoherence can work, we consider some realistic models for the environment and the interactions found in the literature in section 5.2.5.

5.2.2 A Simple Model

To study decoherence and the details of the process (5.26), we need to find the time evolution of the reduced density operator. As mentioned in section 5.1.2, the evolution of the reduced density operator does not follow the von Neumann equation (5.9). In principle, we could first solve the evolution of the full system and then trace out the environment, but for this we would need full knowledge of the environment and its interactions with the system. Instead, we use here a phenomenological master equation which gives a plausible time evolution directly for the reduced density operator. A fairly general form of such an equation is given by Lindblad [28]:

$$\dot{\hat{\rho}}_{\text{red}} = -i[\hat{H}_S, \hat{\rho}_{\text{red}}] - \frac{1}{2} \sum_k \left(\hat{L}_k^\dagger \hat{L}_k \hat{\rho} + \hat{\rho} \hat{L}_k^\dagger \hat{L}_k - 2\hat{L}_k \hat{\rho} \hat{L}_k^\dagger \right). \quad (5.29)$$

Here \hat{H}_S is the free system Hamiltonian from (5.23). The last terms introduce a deviation from the von Neumann time evolution, and the operators \hat{L}_k model the effects of the environment. For this kind of an equation to hold for all times, certain

conditions must be met. Most notably, the environment should be large in the sense that it is only perturbed a little by changes in the system, and the correlation time scale of said perturbations should be shorter than the time scale of interactions, so that the process is Markovian (for more details, see [29], [27, p. 229]).

In the case of cosmological scalar perturbations, and a specific Fourier mode $\nu_{\mathbf{k}}^A$, any interaction operator should be built out of the operators $\hat{\nu}_{\mathbf{k}}^A$ and $\hat{p}_{\mathbf{k}}^A$. In quantum field theory, interactions between different fields typically couple the field strengths instead of the canonical momenta. We thus choose a model where the only \hat{L} -operator is

$$\hat{L} = \Lambda \hat{\nu}_{\mathbf{k}}^A, \quad (5.30)$$

where Λ is a positive constant.

To solve (5.29), we define the density matrix:

$$\rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}) \equiv \langle \nu_{\mathbf{k}}^A | \hat{\rho}_{\text{red}} | \nu_{\mathbf{k}}^{\prime A} \rangle. \quad (5.31)$$

Using this, we can write the reduced density operator in the form

$$\hat{\rho}_{\text{red}} = \int d\nu_{\mathbf{k}}^A d\nu_{\mathbf{k}}^{\prime A} | \nu_{\mathbf{k}}^A \rangle \rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}) \langle \nu_{\mathbf{k}}^{\prime A} |. \quad (5.32)$$

With the Hamiltonian of cosmological scalar perturbations (4.80), the Lindblad equation (5.29) now becomes a differential equation for the density matrix elements:

$$\begin{aligned} \rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}, \eta)' = & \left[\frac{i}{2} \left(\frac{\partial^2}{\partial (\nu_{\mathbf{k}}^A)^2} - \frac{\partial^2}{\partial (\nu_{\mathbf{k}}^{\prime A})^2} \right) - i \frac{\omega_{\mathbf{k}}^2}{2} (\nu_{\mathbf{k}}^{A2} - \nu_{\mathbf{k}}^{\prime A2}) \right. \\ & \left. - \frac{\Lambda}{2} (\nu_{\mathbf{k}}^A - \nu_{\mathbf{k}}^{\prime A})^2 \right] \rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}, \eta). \end{aligned} \quad (5.33)$$

For diagonal matrix elements with $\nu_{\mathbf{k}}^{\prime A} = \nu_{\mathbf{k}}^A$, the last term vanishes. The diagonal elements evolve with just the free system Hamiltonian, unaffected by the environment.

On the other hand, the non-diagonal elements with $\nu_{\mathbf{k}}^{\prime A} \neq \nu_{\mathbf{k}}^A$ are affected by the interaction term. For them, (5.33) could be solved using an exponential

trial function, as detailed in [27, p. 288]. However, the full solution is messy, and for the purposes of decoherence it is more instructive to concentrate just on the interaction term, which captures the essential effect of decoherence. Forgetting the von Neumann part of (5.33), we have

$$\rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}, \eta)' = -\frac{\Lambda}{2}(\nu_{\mathbf{k}}^A - \nu_{\mathbf{k}}^{\prime A})^2 \rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}, \eta) \quad (5.34)$$

$$\Rightarrow \rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}, \eta) = \rho_{\text{red}}(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}, \eta_{\text{ini}}) \exp\left\{-\frac{\Lambda}{2}(\nu_{\mathbf{k}}^A - \nu_{\mathbf{k}}^{\prime A})^2(\eta - \eta_{\text{ini}})\right\} \xrightarrow{\eta - \eta_{\text{ini}} \rightarrow \infty} 0. \quad (5.35)$$

The non-diagonal terms are suppressed, and vanish exponentially as time goes on. The reduced density operator thus approaches the form

$$\hat{\rho}_{\text{red}} \xrightarrow{\eta \rightarrow 0} \frac{1}{\delta(0)} \int d\nu_{\mathbf{k}}^A |\nu_{\mathbf{k}}^A\rangle \rho(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^A) \langle \nu_{\mathbf{k}}^A| = \frac{1}{\delta(0)} \int d\nu_{\mathbf{k}}^A |\nu_{\mathbf{k}}^A\rangle |\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A)|^2 \langle \nu_{\mathbf{k}}^A|, \quad (5.36)$$

where $\delta(0)$ is the formally infinite Dirac delta function at zero, needed for normalisation, and $\psi_{\mathbf{k}}^A(\nu_{\mathbf{k}}^A)$ is the vacuum wave function from (4.93).

This suggests that our pointer states, the states that we can observe, are those of definite field values $\nu_{\mathbf{k}}^A$. This is good, since in cosmology perturbations are assumed to take well-defined values after their formation and evolve classically from then on. This is exactly what happens here. Notably, the interaction operator \hat{L} just induces decoherence, but does not otherwise affect the evolution of the perturbations: the diagonal matrix elements are unaffected by the interactions, and after decoherence they capture the full classical stochastic evolution of the perturbations.

5.2.3 Pointer States

In the last section, we found out that states with definite field values are good candidates for pointer states. In this section, we explain the general properties of good pointer states [30], and show that the field value eigenstates obey them.

First of all, good pointer states should be eigenstates of the system part of the

interaction Hamiltonian, as in (5.24). This guarantees that the pointer states are stable with respect to the interaction, so that decoherence happens in the pointer basis. Let's formulate this mathematically. Let $|\psi_i\rangle$ be some orthonormal would-be pointer states, eigenstates of a non-degenerate pointer observable B :

$$\hat{B} \equiv \sum_i |\psi_i\rangle b_i \langle\psi_i| \otimes \mathbb{1}, \quad b_i \in \mathbb{R}. \quad (5.37)$$

For $|\psi_i\rangle$ to be eigenstates of \hat{H}_{int} , the operator \hat{B} must commute with \hat{H}_{int} :

$$[\hat{B}, \hat{H}_{\text{int}}] = 0. \quad (5.38)$$

This is a necessary condition for $|\psi_i\rangle$ to be good pointer states.

We also want that the pointer states stay pointer states as time goes on. In the Schrödinger picture this means that a pointer state should not spread into a superposition of multiple such states, and a density operator diagonal in the pointer states should stay diagonal. The classical property linked to the pointer state $|\psi_i\rangle$ then has a well-defined value which may change in time, but whose uncertainty stays small at all times. In the Heisenberg picture, where the operators corresponding to observables evolve in time instead of states and density operators, this means that an eigenstate of \hat{B} at time η_1 should still be an eigenstate of \hat{B} at a later time η_2 , albeit possibly with a different eigenvalue. In other words, we demand

$$[\hat{B}(\eta_1), \hat{B}(\eta_2)] = 0 \quad (5.39)$$

as another necessary condition for $|\psi_i\rangle$ to be good pointer states.

For cosmological perturbations, we assumed that \hat{H}_{int} contains the field value operators $\hat{\nu}_{\mathbf{k}}^A$ and not the canonical momenta $\hat{p}_{\mathbf{k}}^A$. Then, choosing $\hat{B} = \hat{\nu}_{\mathbf{k}}^A$, the condition (5.38) is satisfied. To study the second condition (5.39), we can use the expressions of the canonical operators (4.35)–(4.36) in terms of ladder operators

(4.38)–(4.39) with the transformation (4.64)–(4.65) to solve

$$\hat{\nu}_{\mathbf{k}}^A(\eta_2) = 2 \operatorname{Im}[\mu_{\mathbf{k}}(\eta_1)\mu_{\mathbf{k}}^*(\eta_2)]\hat{p}_{\mathbf{k}}^A(\eta_1) + 2 \operatorname{Im}[\mu_{\mathbf{k}}^*(\eta_1)\mu_{\mathbf{k}}(\eta_2)]\hat{\nu}_{\mathbf{k}}^A(\eta_1), \quad (5.40)$$

$$\hat{p}_{\mathbf{k}}^A(\eta_2) = 2 \operatorname{Im}[\mu_{\mathbf{k}}(\eta_1)\mu_{\mathbf{k}}^*(\eta_2)]\hat{p}_{\mathbf{k}}^A(\eta_1) + 2 \operatorname{Im}[\mu_{\mathbf{k}}^*(\eta_1)\mu_{\mathbf{k}}'(\eta_2)]\hat{\nu}_{\mathbf{k}}^A(\eta_1). \quad (5.41)$$

In the late time limit $k\eta_2 \rightarrow 0$, with $\eta_1 \equiv \eta_{\text{ini}} \rightarrow -\infty$, our solution (4.61) for the mode function $\mu_{\mathbf{k}}$ gives

$$\hat{\nu}_{\mathbf{k}}^A(\eta) \approx \frac{1}{k^2\eta}\hat{p}_{\mathbf{k}0}^A - \frac{1}{3}k^2\eta^2\hat{\nu}_{\mathbf{k}0}^A, \quad (5.42)$$

$$\hat{p}_{\mathbf{k}}^A(\eta) \approx -\frac{1}{k^2\eta^2}\hat{p}_{\mathbf{k}0}^A - \frac{2}{3}k^2\eta\hat{\nu}_{\mathbf{k}0}^A, \quad (5.43)$$

where $\hat{\nu}_{\mathbf{k}0}^A, \hat{p}_{\mathbf{k}0}^A$ are the initial canonical operators at early times. Only the terms of lowest order in $k\eta$ are written out (see e.g. [31] for a similar calculation). At late times and in the superhorizon limit $k\eta \rightarrow 0$, the first terms dominate, so that

$$\hat{\nu}_{\mathbf{k}}^A(\eta) = \frac{1}{k^2\eta}\hat{p}_{\mathbf{k}0}^A, \quad (5.44)$$

$$\hat{p}_{\mathbf{k}}^A(\eta) = -\frac{1}{k^2\eta^2}\hat{p}_{\mathbf{k}0}^A. \quad (5.45)$$

We thus get

$$\hat{p}_{\mathbf{k}}^A(\eta) = -\frac{1}{\eta}\hat{\nu}_{\mathbf{k}}^A(\eta), \quad (5.46)$$

that is, the commutator of the field and its momentum becomes vanishingly small in comparison to the field strength. The field operators at different times are also proportional to each other:

$$\hat{\nu}_{\mathbf{k}}^A(\eta_1) = \frac{\eta_2}{\eta_1}\hat{\nu}_{\mathbf{k}}^A(\eta_2). \quad (5.47)$$

Thus $\hat{\nu}_{\mathbf{k}}^A(\eta)$ satisfies (5.39), confirming that the states $|\nu_{\mathbf{k}}^A\rangle$ are indeed an excellent choice for pointer states.

Above we dropped operators in the expansions because the factors multiplying them were small. However, smallness of Hilbert space operators is not a straightforward concept. Ignoring the $\hat{\nu}_{\mathbf{k}0}^A$ -terms in (5.42)–(5.43) is justified only for expectation

values in states where the typical scales of the initial field values are not much bigger than those of the initial momenta:

$$\langle p_{\mathbf{k}0}^{A2} \rangle \gtrsim k^2 \langle \nu_{\mathbf{k}0}^{A2} \rangle. \quad (5.48)$$

This is true for all states that are of interest to us: the relevant pointer states are those which form the vacuum state of chapter 4 as their superposition, and at early times, this vacuum state was a Gaussian with minimum uncertainty and $\langle p_{\mathbf{k}0}^{A2} \rangle = k^2 \langle \nu_{\mathbf{k}0}^{A2} \rangle$ (see section 4.3.2). From (5.44)–(5.47), we then get for the pointer states at late times:

$$\langle \nu_{\mathbf{k}}^A(\eta_2) \rangle = \frac{\eta_1}{\eta_2} \langle \nu_{\mathbf{k}}^A(\eta_1) \rangle, \quad (5.49)$$

$$\langle p_{\mathbf{k}}^A(\eta) \rangle = -\frac{1}{\eta} \langle \nu_{\mathbf{k}}^A(\eta) \rangle, \quad (5.50)$$

$$\Delta p_{\mathbf{k}}^A(\eta) = \frac{1}{\eta} \Delta \nu_{\mathbf{k}}^A(\eta). \quad (5.51)$$

We see that the uncertainty of $p_{\mathbf{k}}^A$ increases faster than that of $\nu_{\mathbf{k}}^A$, a result already encountered for the squeezed vacuum state in section 4.4.2. In addition, looking at an exact eigenstate of $\nu_{\mathbf{k}}^A$ at time η_1 , we see that at a later time η_2 ,

$$\begin{aligned} \Delta \nu_{\mathbf{k}}^A(\eta_2) &= \left[\langle \nu_{\mathbf{k}}^A(\eta_1) | \hat{\nu}_{\mathbf{k}}^{A2}(\eta_1) \left(\frac{\eta_1}{\eta_2} \right)^2 + \mathcal{O} \left(\frac{\eta_1}{\eta_2} \right) | \nu_{\mathbf{k}}^A(\eta_1) \rangle \right. \\ &\quad \left. - \langle \nu_{\mathbf{k}}^A(\eta_1) | \hat{\nu}_{\mathbf{k}}^A(\eta_1) \left(\frac{\eta_1}{\eta_2} \right) + \mathcal{O}(1) | \nu_{\mathbf{k}}^A(\eta_1) \rangle^2 \right]^{\frac{1}{2}} \\ &= \left[\nu_{\mathbf{k}}^{A2}(\eta_1) \left(\frac{\eta_1}{\eta_2} \right)^2 - \nu_{\mathbf{k}}^{A2}(\eta_1) \left(\frac{\eta_1}{\eta_2} \right)^2 + \mathcal{O} \left(\frac{\eta_1}{\eta_2} \right) \right]^{\frac{1}{2}} \\ &= \mathcal{O} \left(\sqrt{\frac{\eta_1}{\eta_2}} \right). \end{aligned} \quad (5.52)$$

The uncertainty of $\nu_{\mathbf{k}}^A$ in such a state increases slower than the expectation value (5.49). Effectively, an approximate field eigenstate spreads in the momentum direction, stays at almost constant width in the field direction, and moves according to the classical evolution. This corresponds approximately to a classical universe that has a well-defined field value $\nu_{\mathbf{k}}^A$.

5.2.4 Rate of Decoherence

An interesting question to ask is, whether there is enough time during inflation for decoherence to happen. There are many ways to study how fast decoherence is. We could, say, look at the rate of change of entropy, since pure states have lower entropy than mixed ones. Another way to quantify the speed of decoherence is given by the rate of de-separation [32] [27, p. 45]:

$$\mathcal{A} = \sum_{i \neq 0, j \neq 0} \left| \langle \nu_i \phi_j | \hat{H} | \nu_0 \phi_0 \rangle \right|^2. \quad (5.53)$$

Here ϕ is some environmental field, and the states $|\nu_i\rangle, |\phi_j\rangle$ form orthonormal bases for the cosmological perturbations and the environment. The free parts of the Hamiltonian (5.23) do not contribute to \mathcal{A} , since either the perturbation part or the environmental part of the product vanishes due to orthogonality of the states in the sum (5.53). We can thus replace \hat{H} by \hat{H}_{int} in (5.53).

The value of \mathcal{A} quantifies the rate at which an initial product state $|\nu_0 \phi_0\rangle \equiv |\nu_0\rangle \otimes |\phi_0\rangle$ becomes entangled. The conformal time scale of decoherence is then

$$\Delta\eta_D \sim \frac{1}{\sqrt{\mathcal{A}}}. \quad (5.54)$$

Using $dt = a d\eta$, the corresponding cosmic time scale is

$$\Delta t_D \sim \frac{a}{\sqrt{\mathcal{A}}}. \quad (5.55)$$

As a demonstration, we next calculate \mathcal{A} and the decoherence time scale for a simplified model. Our calculation follows the one presented in [33]; for the end result, see also [34].

Consider each Fourier mode of the cosmological perturbations separately, and assume that the interaction Hamiltonian couples each mode $\nu_{\mathbf{k}}$ to a corresponding environmental mode $\phi_{\mathbf{k}}$ as presented in [33]:

$$\begin{aligned} H_{\text{int } \mathbf{k}} &= gk^2 (\hat{\nu}_{\mathbf{k}} \otimes \hat{\phi}_{\mathbf{k}}^\dagger + \hat{\nu}_{\mathbf{k}}^\dagger \otimes \hat{\phi}_{\mathbf{k}}) \\ &= gk^2 (\hat{\nu}_{\mathbf{k}}^R \otimes \hat{\phi}_{\mathbf{k}}^R + \hat{\nu}_{\mathbf{k}}^I \otimes \hat{\phi}_{\mathbf{k}}^I). \end{aligned} \quad (5.56)$$

Here we used (4.66) to move to the real and imaginary modes, giving for each independent mode:

$$\hat{H}_{\text{int } \mathbf{k}}^A = gk^2 \hat{\nu}_{\mathbf{k}}^A \otimes \hat{\phi}_{\mathbf{k}}^A. \quad (5.57)$$

The rate of de-separation now becomes

$$\begin{aligned} \mathcal{A} &= \sum_{j \neq 0, i \neq 0} \left| \left\langle \nu_{\mathbf{k}i}^A \phi_{\mathbf{k}j}^A \middle| \hat{H}_{\text{int } \mathbf{k}}^A \middle| \nu_{\mathbf{k}0}^A \phi_{\mathbf{k}0}^A \right\rangle \right|^2 \\ &= \left\langle \nu_{\mathbf{k}0}^A \phi_{\mathbf{k}0}^A \middle| \hat{H}_{\text{int } \mathbf{k}}^A \sum_{i \neq 0, j \neq 0} \left| \nu_{\mathbf{k}i}^A \phi_{\mathbf{k}j}^A \right\rangle \left\langle \nu_{\mathbf{k}i}^A \phi_{\mathbf{k}j}^A \middle| \hat{H}_{\text{int } \mathbf{k}}^A \middle| \nu_{\mathbf{k}0}^A \phi_{\mathbf{k}0}^A \right\rangle \right. \\ &= g^2 k^4 \left\langle \nu_{\mathbf{k}0}^A \middle| \hat{\nu}_{\mathbf{k}0}^A \left(\mathbb{1} - \left| \nu_{\mathbf{k}0}^A \right\rangle \left\langle \nu_{\mathbf{k}0}^A \right| \right) \hat{\nu}_{\mathbf{k}0}^A \middle| \nu_{\mathbf{k}0}^A \right\rangle \\ &\quad \cdot \left\langle \phi_{\mathbf{k}0}^A \middle| \hat{\phi}_{\mathbf{k}0}^A \left(\mathbb{1} - \left| \phi_{\mathbf{k}0}^A \right\rangle \left\langle \phi_{\mathbf{k}0}^A \right| \right) \hat{\phi}_{\mathbf{k}0}^A \middle| \phi_{\mathbf{k}0}^A \right\rangle \\ &= g^2 k^4 \left(\Delta \nu_{\mathbf{k}}^A \right)^2 \left(\Delta \phi_{\mathbf{k}}^A \right)^2. \end{aligned} \quad (5.58)$$

Let the perturbations be in the squeezed vacuum state. Then (4.101) gives

$$\left(\Delta \nu_{\mathbf{k}}^A \right)^2 = \frac{1}{4 \text{Re } \Omega_k} = \frac{k^2 \eta^2 + 1}{2k^3 \eta^2}. \quad (5.59)$$

Assume further that the environmental field ϕ is in a minimum uncertainty Gaussian state, like the cosmological perturbations at $\eta \rightarrow -\infty$. Now (4.101) gives

$$\left(\Delta \phi_{\mathbf{k}}^A \right)^2 = \frac{1}{2k}. \quad (5.60)$$

The rate of de-separation in the superhorizon limit in this model is thus

$$\mathcal{A} = \frac{g^2}{4} \left(k^2 + \frac{1}{\eta^2} \right) \xrightarrow{k\eta \rightarrow 0} \frac{g^2}{4\eta^2}, \quad (5.61)$$

and with (2.53), the cosmic time scale of decoherence (5.55) becomes

$$\Delta t_D \sim g^{-1}(-a\eta) = g^{-1} H_0^{-1}. \quad (5.62)$$

In high energy scale inflationary models, inflation continues typically for at least 50–60 e-folds (that is, 50–60 Hubble times H_0^{-1}) after the scales of cosmic importance today left the horizon [11, p. 46]. This simple model thus suggests that it is possible that a significant amount of decoherence occurred during inflation. Since the

interaction Hamiltonian (5.57) is diagonal in the field basis, it becomes the pointer basis, and its evolution is not affected by H_{int} , as discussed in section 5.2.3. The interaction acts as an ‘ideal measurement’ [34], entangling the perturbations with their environment without disturbing the time evolution of the observable $\nu_{\mathbf{k}}^A$. However, the interaction presented here is just a toy model; for accurate predictions we need realistic models for the environment and interactions. This is the subject of the next section.

5.2.5 Models for the Environment

Modelling the environment of the inflaton field during inflation is no easy task. Two main types of environment are considered in the literature: the short wavelength perturbation modes can act as an environment for the observable, long wavelength modes, or the environment can consist of additional fields. In this section, we briefly review both possibilities.

The first approach is to split the perturbations into short and long wavelength modes, with the cut-off placed at the Hubble scale H_0^{-1} . The long wavelength modes are the ones we can observe in the large scale structure of the universe and the anisotropy of the CMB, while the short wavelength modes play the role of the environment. This corresponds to coarse-graining the perturbations. This is the approach taken in stochastic inflation [35], [36], where the inflaton field is treated classically, but the short wavelength modes have random values and act as a source of randomness for the long wavelength modes. Quantum mechanics can be used to justify such a model from first principles [37]. Furthermore, if we go beyond the linear perturbation theory, we get interaction terms between different modes, and possible decoherence. Recent studies of such models include [29, 38, 39].

For example, in [38], the authors split the Sasaki-Mukhanov variable into short and long wavelength modes, and extract the leading interaction term between them.

Then the authors move to density operator formalism and trace over the short wavelength modes to obtain a master equation similar to (5.29). It is approximated that the resulting decoherence in the field basis takes 20 e-folds after the particular mode leaves the horizon.

Authors of [29, 37] analyse the perturbations using a Lindblad-like master equation, paying more attention to the details that we did above. They estimate that decoherence is likely to happen before the long wavelength modes enter the horizon again after inflation has ended, and that decoherence is not very sensitive to the details of the coupling between the long and short wavelength sectors. On the other hand, it is unclear whether a considerable amount of decoherence can happen during inflation. In particular, the validity of the master equation approach during inflation used in [38] is questioned by [29], where it is argued that it might not be enough to consider the leading interaction term only. Such an approach is sufficient only when the correlation time between the system and the environment is short enough; otherwise, higher order corrections must be taken into account when considering time evolution over long time scales.

An alternate approach is to consider interactions between the inflaton and some additional fields. One simple model of this type is examined in [39], where an inflaton-like field is coupled to an environmental scalar field. While decoherence is not studied directly, the authors trace over the environment and conclude that the interactions modify slightly the perturbation power spectrum. However, decoherence can be achieved even if such observable effects are negligible, since it only requires entanglement between inflaton and the environment.

5.3 Quantum to Classical Transition

In the previous sections, we have seen how during decoherence the reduced density operator for cosmological scalar perturbations gets diagonalised, and becomes

an ensemble of pointer states with well defined field values. These are the natural choice for classically observable states. Indeed, taking a step back and comparing our analysis of the perturbations to that of the laboratory setting in section 5.2.1, we can argue that the pointer states and their respective environmental states correspond to different classical universes, evolving onwards along classical trajectories. Eventually, they get linked to us as classical observers. This explains the transition from a quantum mechanical vacuum state to classical perturbation theory: tracing over the unobservable degrees of freedom, we get an ensemble of different classical universes, with different classical realisations of the perturbations. We don't have to interpret this as a literal collection of different universes, but mathematically, for the purposes of observables and expectation values, it looks like one.

Let us now return to the questions regarding the quantum to classical transition posed at the end of chapter 4. We have seen how the perturbation field values naturally become the well-defined variables of the classical theory, when we take into account the effects of the environment. We have also seen that the field values stay well-defined, that is, due to decoherence, their uncertainties do not increase uncontrollably in time. We are left with the question of measurements and the collapse of the state vector. This will be discussed in section 5.3.2. Before that, we make a brief comment on the subject of 'decoherence without decoherence' found in the literature in section 5.3.1. In the end, in section 5.3.3, we discuss how decoherence affects the observations of the CMB anisotropy.

5.3.1 Decoherence without Decoherence?

As seen in section 5.2.3, it follows from squeezing that the typical values of the Sasaki-Mukhanov variable and its momentum are much larger than their commutator. For the purpose of expectation values, the commutator vanishes and the perturbations look like classical stochastic variables, even without considering the

effects of the environment. Another way to look at this is to divide the field and momentum operators into growing and decaying modes; the growing modes commute with each other, and become dominant as time goes on [33, 40, 41]. This is sometimes called ‘decoherence without decoherence’ [40].

It should be noted that squeezing alone does not lead to decoherence in the sense we defined it above, that is, the vanishing of the non-diagonal elements of the density matrix. Using the vacuum wave function (4.93), we can write the density matrix elements of the pure state as [42]

$$\begin{aligned} \rho(\nu_{\mathbf{k}}^A, \nu_{\mathbf{k}}^{\prime A}) &= \langle \nu_{\mathbf{k}}^A | \psi_{\mathbf{k},A} \rangle \langle \psi_{\mathbf{k},A} | \nu_{\mathbf{k}}^{\prime A} \rangle \\ &= |C|^2 \exp\left\{-\operatorname{Re} \Omega_k (\nu_{\mathbf{k}}^{A2} + \nu_{\mathbf{k}}^{\prime A2}) - i \operatorname{Im} \Omega_k (\nu_{\mathbf{k}}^{A2} - \nu_{\mathbf{k}}^{\prime A2})\right\}. \end{aligned} \quad (5.63)$$

In the limits $\operatorname{Re} \Omega_k \xrightarrow{\eta \rightarrow 0} 0$ and $\operatorname{Im} \Omega_k \xrightarrow{\eta \rightarrow 0} -\infty$ from (4.95)–(4.96), the off-diagonal elements $\nu_{\mathbf{k}}^A \neq \nu_{\mathbf{k}}^{\prime A}$ are of the same order of magnitude as the diagonal elements $\nu_{\mathbf{k}}^A = \nu_{\mathbf{k}}^{\prime A}$ at late times. The only difference is that the off-diagonal elements start to oscillate rapidly due to the $\operatorname{Im} \Omega_k$ -term. Interactions with the environment are needed to achieve decoherence as we defined it. Also, we see from (4.93) and (4.94) that the growing and decaying modes of the perturbations reside in the exponent of the wave function; the state $|\nu_{\mathbf{k}}^A\rangle$ is not a superposition of growing and decaying components whose cross-terms could die away so that the state would decohere.

The merit of ‘decoherence without decoherence’ is that the non-diagonal elements of the density matrix are not needed when calculating the expectation values of physically relevant quantities. Using (5.46), we see that the field eigenstates $|\nu_{\mathbf{k}}^A\rangle$ are approximate eigenstates of both $\hat{\nu}_{\mathbf{k}}^A$ and $\hat{p}_{\mathbf{k}}^A$, and we have

$$\begin{aligned} \langle F(\nu_{\mathbf{k}}^A, p_{\mathbf{k}}^A) \rangle &= \operatorname{tr} [\hat{\rho} F(\hat{\nu}_{\mathbf{k}}^A, \hat{p}_{\mathbf{k}}^A)] \\ &= \int d\nu_{\mathbf{k}}^A \langle \nu_{\mathbf{k}}^A | \hat{\rho} F\left(\hat{\nu}_{\mathbf{k}}^A, -\frac{1}{\eta} \hat{\nu}_{\mathbf{k}}^A\right) | \nu_{\mathbf{k}}^A \rangle \\ &= \int d\nu_{\mathbf{k}}^A \langle \nu_{\mathbf{k}}^A | \hat{\rho} | \nu_{\mathbf{k}}^A \rangle F\left(\nu_{\mathbf{k}}^A, -\frac{1}{\eta} \nu_{\mathbf{k}}^A\right) \end{aligned} \quad (5.64)$$

for a general function F of the fields and canonical momenta. A more appropriate

term for this situation might be ‘classicalisation without decoherence’: expectation values can be calculated just as for classical stochastic variables with a phase space probability distribution given by $\langle \nu_{\mathbf{k}}^A | \hat{\rho} | \nu_{\mathbf{k}}^A \rangle \delta(p_{\mathbf{k}}^A + \frac{1}{\eta} \nu_{\mathbf{k}}^A)$. At least a level of semi-classicality is achieved, even though we argued in section 4.4.3 that this is not enough to fully explain the transition from quantum mechanics to classical physics: it does not explain what the classical observables are, and how they obtain their observed, well-defined values.

5.3.2 The Measurement Problem

Up until this point, we have concentrated on the unitary time evolution of states and density operators, generated by the Hamilton operator. This can result into a state which does not correspond directly to any classical situation, like in the Schrödinger’s cat thought experiment in section 5.2.1. We can then ask, what is the relationship between the quantum formalism and our observations when we measure some property of a quantum mechanical system? This is the measurement problem.

The usual answer offered by the Copenhagen interpretation of quantum mechanics states that when a measurement is made, the state vector of the system ‘collapses’ to a state corresponding to the measurement result, and the probabilities of different results are given by (4.5). This raises several questions: What counts as a measurement, and who qualifies as a measurer? In particular, what is the role of measurements in the time evolution of cosmological perturbations, when there are no human observers present in the early universe?

Using decoherence, we can try to evade these questions, and breach the gap between quantum mechanics and observations with unitary time evolution alone, without invoking collapses. Decoherence brings the reduced density operator of the system naturally to an ensemble of classically observable universes, as discussed in the beginning of section 5.3. One of the universes gets selected as the observed one.

Decoherence does not solve the measurement problem: it does not explain how a certain universe is singled out to be observed. However, some progress can be made compared to the pure Copenhagen interpretation. There is no need to consider collapses of the state vector before the current moment: information of all possibilities and their probabilities—whether they are purely quantum mechanical or resemble classical physics—is correctly encoded in the density operator, and when considering the system together with its environment, time evolution is unitary and deterministic. Decoherence also naturally selects the pointer states as the classical, observable ones. All that is left is to invoke the collapse at the time of measurement to select the observed state from the pointer states.

Decoherence and its role in the measurement problem in the case of cosmological perturbations have been discussed, and criticised, in [43]. Besides pointing out that decoherence does not solve the measurement problem (for example, it does not explain how the observed inhomogeneities emerge from the homogeneous and isotropic vacuum state), it is argued in [43] that decoherence in the case of cosmological perturbations might not be as straightforward as presented previously in this chapter. For example, if inflation drives all additional fields towards their vacuum states, can they act as an effective environment for inflaton for the purposes of decoherence? It is also questioned what constitutes a good environment in the cosmological case: it seems strange to give special significance to some degrees of freedom just because we can't observe them with our current technology.

An alternative approach to the problem of quantum-to-classical transition is provided by models where the wave function collapses dynamically, by some yet unknown physics; two such model are presented in [44] and [45]. Recent arguments for and against such models and decoherence can be found in [46], [47].

5.3.3 Decoherence and Observations

We can ask whether the amount of decoherence of the cosmological perturbations could be detected in, say, the CMB radiation. Is there an observable difference in the CMB between a universe where no decoherence has happened, and a universe where the reduced density matrix has decohered to the form (5.36)? Based on the considerations above, the answer seems to be ‘no’ for decoherence with respect to the field basis. For the Gaussian case, the CMB anisotropy depends on the power spectrum of the perturbations, that is, the expectation value of the square of the Sasaki-Mukhanov variable (see appendix B). As shown in (5.64), such a quantity only depends on the diagonal elements of the density matrix, and is thus not affected by decoherence. The same prediction for the power spectrum, which coincides very well with the CMB measurements, is obtained with or without decoherence. The same is true for higher correlators of the field operators, which measure non-Gaussianity.

On the other hand, if decoherence happened in some other basis, say the particle number basis, this might affect the power spectrum and the Gaussianity and ruin the observational success of the theory (see [30]). As a demonstration, let’s calculate the expectation value needed to predict the power spectrum in some general basis:

$$\begin{aligned}
 \text{tr}_{\text{system}} \left[\hat{\rho}_{\text{red}} \hat{\nu}_{\mathbf{k}}^{A2} \right] &= \text{tr}_{\text{system}} \left[\sum_{i,j} |i\rangle \rho_{\text{red } ij} \langle j| \hat{\nu}_{\mathbf{k}}^{A2} \right] \\
 &= \int d\nu_{\mathbf{k}}^A \langle \hat{\nu}_{\mathbf{k}}^A | \sum_{i,j} |i\rangle \rho_{\text{red } ij} \langle j| \hat{\nu}_{\mathbf{k}}^{A2} | \hat{\nu}_{\mathbf{k}}^A \rangle \\
 &= \int d\nu_{\mathbf{k}}^A \nu_{\mathbf{k}}^{A2} \sum_{i,j} \rho_{\text{red } ij} \langle j | \nu_{\mathbf{k}}^A \rangle \langle \nu_{\mathbf{k}}^A | i \rangle.
 \end{aligned} \tag{5.65}$$

In general, the non-diagonal elements with $i \neq j$ do affect the result, so that we get a different power spectrum whether these elements are zero (decoherence) or non-zero (no decoherence). Then decoherence could lead to a discrepancy between theory and observations. Only if the basis vectors $|i\rangle$, $|j\rangle$ are eigenstates of $\hat{\nu}_{\mathbf{k}}^A$ are the non-diagonal elements unimportant, since then $\langle \hat{\nu}_{\mathbf{k}}^A | \hat{\nu}_{\mathbf{k}}^A \rangle = \delta(\hat{\nu}_{\mathbf{k}}^A - \hat{\nu}_{\mathbf{k}}^A)$ (and

the sums are replaced by integrals).

Besides the power spectrum of the primordial perturbations, the CMB is affected by acoustic oscillations of the baryon-photon fluid at the time of decoupling, causing oscillations in the CMB angular power spectrum (see figure 5.1 and [11, p. 125]). The initial conditions of said oscillations come from the primordial scalar perturbations and their time derivatives. Classically, the time derivatives take some well-defined values, and this leads to the peak structure of the power spectrum. Quantum mechanically, the time derivatives correspond to the canonical momenta, and they get the classically right values if the correlation between them and the perturbation field values, (5.46), is satisfied. Decoherence should not destroy this correlation, or the peak structure in the angular power spectrum would be lost [48]. This once again excludes decoherence with respect to many pointer bases, such as the particle number basis.

Another way to formulate this is to consider the entropy of the perturbations [30, 48–50], defined as

$$S \equiv \text{tr}(\hat{\rho}_{\text{red}} \ln \hat{\rho}_{\text{red}}). \quad (5.66)$$

Entropy is related to the shape of the Wigner function of the system (see section 4.4.1), and thus the correlation between $\nu_{\mathbf{k}}$ and $p_{\mathbf{k}}$. As entropy increases, this correlation gets weaker and the peaks in the power spectrum are smeared out. Observations thus set an upper limit on the entropy. Since entropy changes in decoherence in a way that depends on the pointer basis, this restricts the possible pointer bases for the perturbations. When decoherence happens with respect to the field value basis, entropy is significantly lower than its maximum value, preserving the peak structure [30].

Ultimately, the problem in directly observing the effects of decoherence is that we have already made successful predictions for the CMB spectrum without invoking decoherence, and decoherence shouldn't spoil these predictions. Observations set

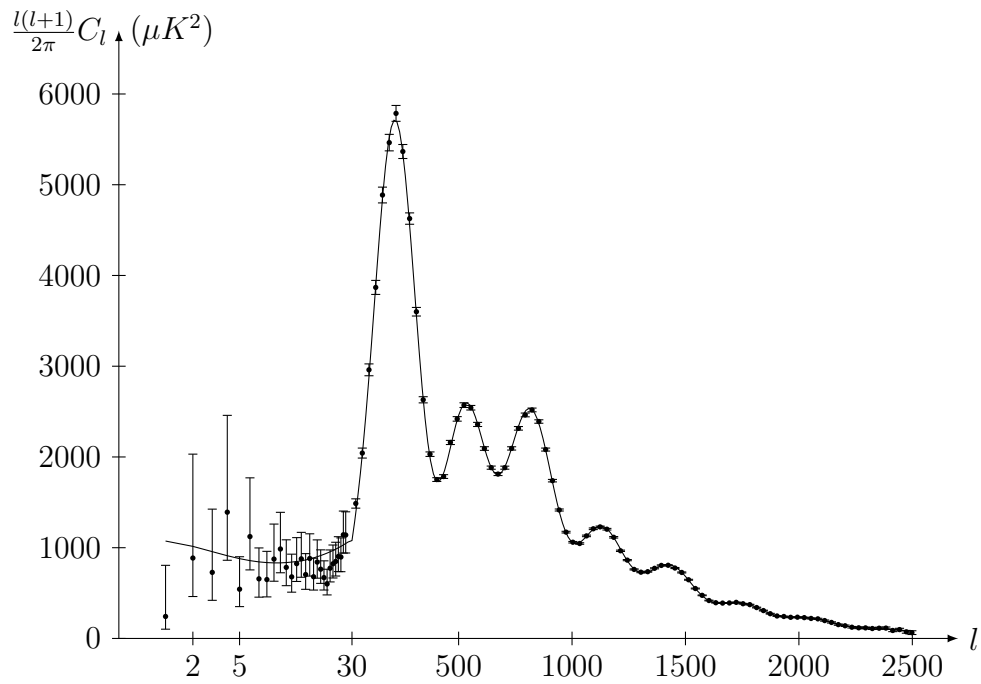


Figure 5.1: The CMB angular power spectrum. The energy density of the baryon-photon fluid was oscillating when the CMB was released, and these oscillations got imprinted as peaks in the CMB power spectrum. The points with error bars are the measurements and their uncertainties, and the line is the prediction from the best fitting Λ CDM model. Source: Planck Legacy Archive, <http://pla.esac.esa.int/pla/>.

limits on the decoherence process, rather than the other way around, at least for the data currently available to us. The role of decoherence is then mostly a conceptual one, explaining the transition from quantum description to classical physics, and justifying the predictions made by combining these theories.

6. Conclusions

In this thesis, we have discussed the formalism of cosmological perturbation theory and quantum field theory needed to describe the quantum fluctuations of scalar perturbations during inflation. We have studied environmental decoherence, a process where the perturbations get entangled with their environment. This results in the vanishing of the non-classical interference terms in the reduced density operator of the perturbations.

The role of decoherence is to justify the usage of classical perturbation theory at late times, even though the origin of the perturbations lies in quantum mechanics. As we have discussed, decoherence does not solve the measurement problem of quantum mechanics, but nonetheless offers valuable insights into the quantum-to-classical transition.

Decoherence as such is an inevitable physical process, but its details in the case of inflation and cosmological perturbations are hard to grasp based on theoretical considerations alone. On the other hand, we have seen that it is difficult to observe the amount of decoherence from the cosmic microwave background, since the observables there only depend on the diagonal elements of the density matrix in the field eigenstate basis, presumably untouched by decoherence. For now, decoherence has played only a conceptual role: it explains why the theory works, without altering its predictions. The natural next step would be to devise some means to detect the effects of decoherence directly, maybe through observational data from some other

source. From the CMB, we can only measure correlators involving the perturbation fields; if we could also measure the canonical momenta, the results could be different for the cases with or without decoherence, even though these differences would be suppressed by squeezing.

An alternative route forward would be to calculate the effects of decoherence with respect to a basis other than the field eigenvalue basis. As discussed above, this could lead to deviations from the predictions of the traditional models, including non-Gaussianity in the CMB. It would be instructive to study what kind of bounds the CMB observations set on the pointer basis.

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A. Notes on General Relativity

In this appendix, we go through the basic formalism of general relativity, and show how the Friedmann equations (2.9) and (2.10) arise from the metric (2.2) and the stress-energy tensor of an ideal fluid (2.8). Good references on the subject include [8, 51].

General relativity is a theory of the structure of space-time and its interactions with matter. To describe this structure, we first choose a system of coordinates x^μ , accompanied by a metric tensor $g_{\mu\nu}$. The metric determines the geometry of the space-time by giving the inner product between two vectors:

$$a \cdot b \equiv g_{\mu\nu} a^\mu b^\nu \equiv a_\nu b^\nu. \quad (\text{A.1})$$

In practice, we use the metric to raise and lower the indices of tensors, and sum over repeated indices (see section 1.1).

The geometry of space-time determines how matter moves through it. Objects in free fall follow geodesics $x^\mu(\lambda)$, given by the equation

$$\frac{d^2 x^\mu}{d\lambda^2} + \Gamma_{\rho\sigma}^\mu \frac{dx^\rho}{d\lambda} \frac{dx^\sigma}{d\lambda} = 0. \quad (\text{A.2})$$

These are the equivalent of straight lines in a curved space-time. The symbols $\Gamma_{\rho\sigma}^\mu$ are the connection coefficients that describe how the basis vectors of our coordinate system change from point to point; they can be calculated from the metric as

$$\Gamma_{\mu\nu}^\lambda = \frac{1}{2} g^{\lambda\sigma} (\partial_\mu g_{\nu\sigma} + \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu}). \quad (\text{A.3})$$

Starting from the connection coefficients, we can define other objects related to different aspects of the geometry. An important one is the Riemann tensor:

$$R^\rho{}_{\sigma\mu\nu} \equiv \partial_\mu \Gamma^\rho_{\nu\sigma} - \partial_\nu \Gamma^\rho_{\mu\sigma} + \Gamma^\rho_{\mu\lambda} \Gamma^\lambda_{\nu\sigma} - \Gamma^\rho_{\nu\lambda} \Gamma^\lambda_{\mu\sigma}, \quad (\text{A.4})$$

together with the Ricci tensor and curvature scalar obtained by contracting the indices of $R^\rho{}_{\sigma\mu\nu}$:

$$R_{\mu\nu} \equiv R^\lambda{}_{\mu\lambda\nu}, \quad (\text{A.5})$$

$$R \equiv g^{\mu\nu} R_{\mu\nu}. \quad (\text{A.6})$$

With these, we define the Einstein tensor:

$$G_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}. \quad (\text{A.7})$$

This is the geometric quantity which appears on the left-hand side of the Einstein equation.

While the geodesic equation (A.2) tells us how matter moves through space, the Einstein equation tells how space is curved by matter. It relates the structure of space-time, described by the Einstein tensor, to its matter content given by the stress-energy tensor $T_{\mu\nu}$:

$$G_{\mu\nu} = \frac{1}{M_{\text{Pl}}^2} T_{\mu\nu}, \quad (\text{A.8})$$

where M_{Pl} is the reduced Planck mass.

As a demonstration of this formalism, we can take the FRW-metric (2.2) in Cartesian coordinates and calculate from it the connection coefficients and eventually the Ricci tensor. Its non-zero components turn out to be

$$R_{00} = -3\frac{\ddot{a}}{a}, \quad (\text{A.9})$$

$$R_{ii} = a\ddot{a} + a\dot{a}^2, \quad (\text{A.10})$$

with no sum implied in the second expression. The curvature scalar is then

$$R = 6 \left[\frac{\ddot{a}}{a} + \left(\frac{\dot{a}}{a} \right)^2 \right], \quad (\text{A.11})$$

and the Einstein tensor reads

$$G_{\mu\nu} = \begin{pmatrix} 3H^2 & 0_{1\times 3} \\ 0_{3\times 1} & (-2a\ddot{a} - \dot{a}^2) \cdot \mathbb{1}_{3\times 3} \end{pmatrix}. \quad (\text{A.12})$$

For the stress-energy tensor of an ideal fluid, (2.8), the right-hand side of the Einstein equation (A.8) becomes

$$\frac{1}{M_{\text{Pl}}^2} T_{\mu\nu} = \frac{1}{M_{\text{Pl}}^2} \begin{pmatrix} \rho & 0_{1\times 3} \\ 0_{3\times 1} & a^2 p \cdot \mathbb{1}_{3\times 3} \end{pmatrix}. \quad (\text{A.13})$$

With straightforward manipulations, the Einstein equation then gives the Friedmann equations (2.9) and (2.10),

$$H^2 = \frac{\rho}{3M_{\text{Pl}}^2}, \quad (\text{A.14})$$

$$\frac{\ddot{a}}{a} = -\frac{1}{6M_{\text{Pl}}^2}(\rho + 3p), \quad (\text{A.15})$$

which serve as the starting point of our analysis in section 2.1.2.

B. From Primordial Scalar Perturbations to the CMB

In this appendix, we go briefly through some steps needed to get from the primordial scalar perturbations to the CMB angular power spectrum. For more details, see [10, 11].

The CMB radiation is black body radiation whose spectrum depends on only one parameter, the temperature T . The temperature is slightly different in different directions. To quantify this anisotropy, we expand the temperature fluctuations in terms of the spherical harmonic functions Y_{lm} (see [20, p. 756]):

$$\frac{\delta T}{T}(\theta, \phi) = \sum_{l=-\infty}^{\infty} \sum_{m=-l}^l a_{lm} Y_{lm}(\theta, \phi), \quad (\text{B.1})$$

where θ and ϕ are the polar angles and a_{lm} , $m = -l \dots l$ are the independent expansion coefficients. The angular power spectrum C_l is defined as an average of $|a_{lm}|^2$ over m :

$$C_l \equiv \frac{1}{2l+1} \sum_{m=-l}^l |a_{lm}|^2. \quad (\text{B.2})$$

These values can be predicted from theory by calculating the expectation values of $|a_{lm}|^2$, or measured from the observed coefficients a_{lm} (see figure 5.1). Since the coefficients are random stochastic variables, and we can only observe one realisation of them on the sky, we expect the observations to sometimes deviate from the theoretical averages. We can calculate the expected magnitude of these deviations.

It is given by the cosmic variance [10, p. 155]:

$$\Delta C_l \equiv \sqrt{\langle (C_{l\text{theor}} - C_{l\text{obs}})^2 \rangle} = \sqrt{\frac{2}{2l+1}} C_{l\text{theor}}. \quad (\text{B.3})$$

For big l , where $C_{l\text{obs}}$ is calculated from many observed a_{lm} -coefficients, this variance becomes small. Indeed, the Planck satellite has measured C_l for l -values over 2000 [52]; for this high multipoles, the predictions and observations should agree with high accuracy, giving a powerful test of any theory that tries to predict the form and origin of the temperature fluctuations.

In practice, C_l can be calculated from the Fourier components of the temperature fluctuation at the time of last scattering. In this section, we use the Fourier convention

$$\frac{\delta T}{T}(\mathbf{x}) = \sum_{\mathbf{k}} \left(\frac{\delta T}{T} \right)_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (\text{B.4})$$

We also define the power spectrum of these fluctuations:

$$\mathcal{P}_T(k) \equiv \frac{L^3}{2\pi^2} k^3 \left\langle \left| \left(\frac{\delta T}{T} \right)_{\mathbf{k}} \right|^2 \right\rangle. \quad (\text{B.5})$$

We work here in a finite box of comoving size L , where the wave vector \mathbf{k} gets discrete values, like in section 4.3.1. Due to isotropy, \mathcal{P}_T only depends on the magnitude $|\mathbf{k}| = k$. Using properties of the spherical harmonics, (B.2) can be manipulated into the form

$$C_l = 4\pi \int_0^\infty \frac{dk}{k} j_l^2(k\eta_0) \mathcal{P}_T(k), \quad (\text{B.6})$$

where we have moved to the continuum limit again, j_l is a spherical Bessel function, and η_0 is the conformal time of the last scattering. Due to the Bessel function, C_l gets the biggest contribution from the Fourier modes with $k = l/\eta_0$.

To get the dependence on the primordial scalar perturbations, we want to write \mathcal{P}_T in terms of the power spectrum of the Sasaki-Mukhanov variable,

$$\begin{aligned} \mathcal{P}_\nu(k) &\equiv \frac{L^3}{2\pi^2} k^3 \left\langle \left| L^{-3/2} \nu_{\mathbf{k}} \right|^2 \right\rangle \\ &= \frac{k^3}{2\pi^2} \left\langle \nu_{\mathbf{k}}^{A2} \right\rangle. \end{aligned} \quad (\text{B.7})$$

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Note the correction made to $\nu_{\mathbf{k}}$ due to the different Fourier conventions in (B.4) and (4.75).

As is conventional, we first define an intermediate variable, the covariant curvature perturbation \mathcal{R} . For this, we go to the covariant gauge, where the time-space parts of the metric and stress-energy tensor vanish [17, p. 39], leading to the gauge conditions for scalars

$$\delta\varphi^C = 0, \quad (\text{B.8})$$

$$B^C = 0. \quad (\text{B.9})$$

\mathcal{R} is then defined as the perturbation ψ (see (3.11)) in this gauge:

$$\mathcal{R} \equiv \psi^C. \quad (\text{B.10})$$

A gauge transformation from a general gauge to the covariant gauge gives, using (3.32) and (3.36),

$$\psi^C = \psi + \mathcal{H}\xi^0, \quad (\text{B.11})$$

$$0 = \delta\varphi^C = \delta\varphi - \xi^0\bar{\varphi}', \quad (\text{B.12})$$

and from these and the definition of ν (3.40), we can solve

$$\xi^0 = \frac{\delta\varphi}{\bar{\varphi}'} \quad (\text{B.13})$$

$$\Rightarrow \mathcal{R} = \psi^C = \psi + \mathcal{H}\frac{\delta\varphi}{\bar{\varphi}'} = \frac{\mathcal{H}}{\bar{\varphi}'}\left(\delta\varphi + \frac{\bar{\varphi}'}{\mathcal{H}}\psi\right) = \frac{H}{a\dot{\bar{\varphi}}}\nu. \quad (\text{B.14})$$

Thus \mathcal{R} and ν have an intimate connection. Since during slow-roll inflation H and $\dot{\bar{\varphi}}$ are approximately constants, we can see from (2.52) and (5.47) that the Fourier-components $\mathcal{R}_{\mathbf{k}}$ freeze to constant values at superhorizon scales. The advantage of using $\mathcal{R}_{\mathbf{k}}$ instead of $\nu_{\mathbf{k}}$ is that $\mathcal{R}_{\mathbf{k}}$ is defined in terms of purely metric quantities, and stays constant at superhorizon even when inflation ends and the inflaton φ decays into particles of other fields. When the corresponding mode then re-enters

the horizon after inflation, we can calculate the ensuing time evolution of $\mathcal{R}_{\mathbf{k}}$ using cosmological perturbation theory for a radiation- or matter-dominated universe.

We define the power spectrum of \mathcal{R} to be calculated at the time when the mode in question has just left the horizon during inflation, that is, when $aH = k$. It can then be written as

$$\mathcal{P}_{\mathcal{R}}(k) \equiv \frac{L^3}{2\pi^2} k^3 \langle |\mathcal{R}_{\mathbf{k}}|^2 \rangle \Big|_{aH=k} = \left(\frac{H}{a\dot{\varphi}} \right)^2 \mathcal{P}_{\nu}(k) \Big|_{aH=k}. \quad (\text{B.15})$$

Since the scalar perturbations are described by just one variable in the adiabatic case, and since we work in linear perturbation theory, we can write in general

$$\mathcal{P}_T(k) = \mathcal{T}^2(k) \mathcal{P}_{\mathcal{R}}(k). \quad (\text{B.16})$$

Here $\mathcal{T}(k)$ is the transfer function that relates $(\delta T/T)_{\mathbf{k}}$ at the time of last scattering to the superhorizon value of $\mathcal{R}_{\mathbf{k}}$, and it depends only on k . Its exact form is a complicated matter, but in general we can use it to write the result (B.6) as

$$\begin{aligned} C_l &= 4\pi \int_0^\infty \frac{dk}{k} j_l^2(k\eta_0) \mathcal{T}^2(k) \mathcal{P}_{\mathcal{R}}(k) \\ &= 4\pi \int_0^\infty \frac{dk}{k} j_l^2(k\eta_0) \mathcal{T}^2(k) \left(\frac{H}{a\dot{\varphi}} \right)^2 \mathcal{P}_{\nu}(k) \Big|_{aH=k} \\ &= 4\pi \int_0^\infty \frac{dk}{k} j_l^2(k\eta_0) \mathcal{T}^2(k) \left(\frac{H}{a\dot{\varphi}} \right)^2 \frac{k^3}{2\pi^2} \langle \nu_{\mathbf{k}}^{A2} \rangle \Big|_{aH=k}. \end{aligned} \quad (\text{B.17})$$

So C_l depends directly on the expectation value of $\nu_{\mathbf{k}}^{A2}$, taken at a time when the scale has crossed the horizon and freezed out in the sense of (5.47). How decoherence affects this expectation value and the observed CMB spectrum is discussed in section 5.3.3.

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