Preprint typeset in JHEP style - HYPER VERSION

# Quantum Field Theory in de Sitter Space

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Abstract: In these notes I review the computation of correlation functions for quantum fluctuations in de Sitter space. My focus is on the conceptual rather than the computational.

## Contents

## 1. Motivation

These notes discuss the primordial origin of the temperature variations in the cosmic microwave background (CMB). The main goal will be to show how quantum fluctuations in quasi-de Sitter space produce a spectrum of fluctuations that accurately matches the observations.

Let me begin by reminding you of the metric for the de Sitter spacetime

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a^2(t)\mathrm{d}\mathbf{x}^2 \ , \quad \text{with} \quad a(t) = e^{Ht} \ , \tag{1.1}$$

or, in conformal time $\mathrm{d}\tau = \mathrm{d}t/a(t)$,

$$\mathrm{d}s^2 = a^2(\tau)\left[-\mathrm{d}\tau^2 + \mathrm{d}\mathbf{x}^2\right] \ , \quad \text{with} \quad a(\tau) = -\frac{1}{H\tau} \ , \tag{1.2}$$

where $H = \partial_t \ln a$ is the Hubble parameter. Recall that perfect de Sitter space is defined by constant $H$, while inflation (or quasi-de Sitter space) is characterized by a small time-evolution of $H$,

$$\varepsilon = -\frac{\dot{H}}{H^2} \ll 1 \ . \tag{1.3}$$

For a perfect fluid with energy density $\rho$ and pressure $p$, the Hubble expansion is determined by the Einstein equations

$$H^2 = \frac{\rho}{3M_{\rm pl}^2} \qquad \text{and} \qquad \dot{H} + H^2 = -\frac{1}{6M_{\rm pl}^2}(\rho + 3p) \ , \tag{1.4}$$

where $M_{\rm pl}^{-2} = 8\pi G$. This implies

$$\varepsilon = \frac{3}{2}(1+w) \ , \tag{1.5}$$

where $w = p/\rho$ is the equation of state of the fluid. The de Sitter limit is $w = -1$, while slow-roll inflation corresponds to $w \approx -1$. As I have discussed elsewhere[1], the simplest way to realize such a negative pressure component in the stress tensor of the early universe is to exploit the slow-roll dynamics of a scalar field $\phi$ on a sufficiently flat potential $V(\phi)$:

$$\varepsilon \approx \frac{M_{\rm pl}^2}{2}\left(\frac{V'}{V}\right)^2 \equiv \epsilon_{\rm v} \ \ll \ 1 \ . \tag{1.6}$$

In general, the evolution of a scalar field in the FRW background (1.1) is governed by the Klein-Gordon equation

$$\ddot{\phi} + 3H\dot{\phi} + V' = 0 \ , \tag{1.7}$$

[1] D. Baumann, *Basics of Inflation.*
D. Baumann, *TASI Lectures on Inflation.*

where

$$H^2 = \frac{1}{3M_{\rm pl}^2}\left(\frac{1}{2}\dot{\phi}^2 + V(\phi)\right) \, . \tag{1.8}$$

The slow-roll limit is a systematic approximation scheme to solve Eqns. (1.7) and (1.8). For the purpose of the present discussion it is only important that this gives a classical background $a(t)$ and $\phi(t)$. In these notes we will be interested in small fluctuations around the inflationary background.

## 2. Classical Perturbations

Why is it so interesting to study fluctuations during inflation? As we have just seen, the inflaton evolution $\phi(t)$ governs the energy density of the early universe $\rho(t)$ and hence the end of inflation. Essentially, $\bar{\phi}(t) + \delta\phi(t, \mathbf{x})$ plays the role of a local clock reading off the amount of inflationary expansion remaining. The space-dependent fluctuations $\delta\phi$ imply that different regions of space inflate by different amounts. Intuitively, microscopic clocks are quantum mechanical objects with necessarily some variance (by the uncertainty principle). In quantum theory, local fluctuations in $\rho$ and hence ultimately in the CMB temperature $T(t, \mathbf{x})$ are therefore unavoidable.

The main purpose of these notes is to compute this effect. For concreteness we will consider single-field slow-roll models of inflation

$$S = \int \mathrm{d}^4x\sqrt{-g}\left[\frac{M_{\rm pl}^2}{2}R_{(4)} - \frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - V(\phi)\right] \, . \tag{2.1}$$

However, in the end we will explain that the quadratic action for small fluctuations is in fact (almost) universal and can be derived using much more general considerations[2] without assuming a specific action sourcing the inflationary background $H(t)$.

We will study both scalar and tensor fluctuations. For the scalar modes we have to be careful to identify the true physical degrees of freedom. A priori, we have 5 scalar modes: 4 metric perturbations–$\delta g_{00}, \delta g_{ii}, \delta g_{0i} \sim \partial_i B$ and $\delta g_{ij} \sim \partial_i\partial_j H$–and 1 scalar field perturbation $\delta\phi$. Gauge invariances associated with the invariance of (2.1) under scalar coordinate transformations–$t \to t + \epsilon_0$ and $x_i \to x_i + \partial_i\epsilon$–remove two modes. The Einstein constraint equations remove two more modes. so that we are left with 1 physical scalar mode. Deriving the quadratic action for this mode is the aim of this section.

[2]Cheung et al., *The Effective Theory of Inflation.*

### 2.1 Comoving Gauge

I will work in a fixed gauge throughout. For a number of reason I like *comoving gauge*[3]:

$$\delta\phi = 0 \tag{2.2}$$

$$\delta g_{ij} = a^2(1-2\mathcal{R})\delta_{ij} + a^2 h_{ij} \ . \tag{2.3}$$

Here, $h_{ij}$ is a transverse ($\nabla_i h^{ij} = 0$), traceless ($h^i_i = 0$) tensor and $\mathcal{R}$ is a scalar. One can show that the comoving spatial slices $\phi = const.$ have 3-curvature $R_{(3)} = \frac{4}{a^2}\nabla^2\mathcal{R}$. Hence, we refer to $\mathcal{R}$ as the *curvature perturbation*.

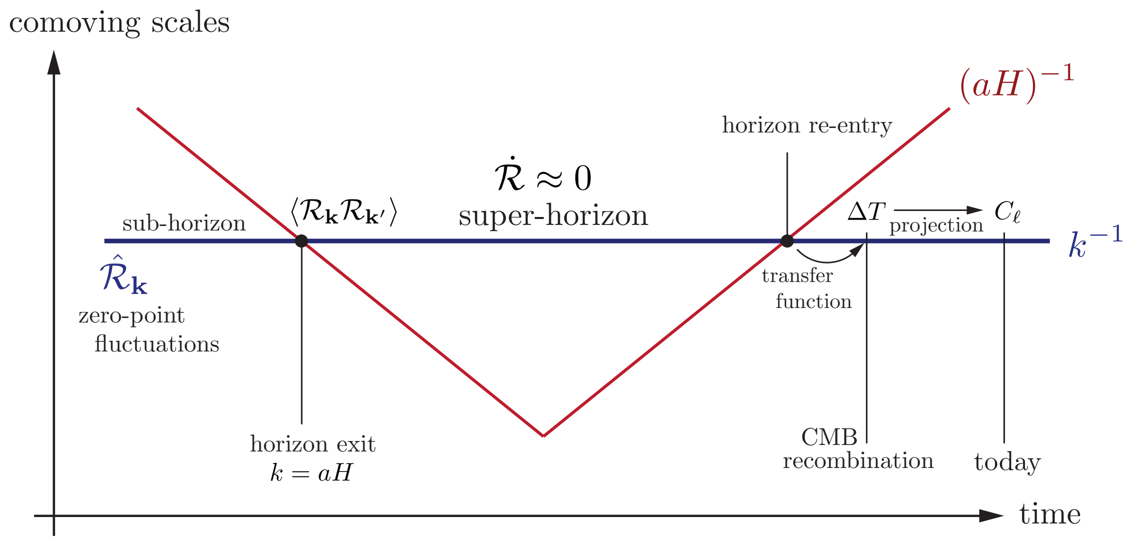


**Figure 1:** *Curvature perturbations in de Sitter: The comoving horizon $(aH)^{-1}$ shrinks during inflation and grows in the subsequent FRW evolution. This implies that comoving scales $k^{-1}$ exit the horizon at early times and re-enter the horizon at late times. While the curvature perturbations $\mathcal{R}$ are outside of the horizon they don't evolve, so our computation for the correlation function $\langle \mathcal{R}_{\mathbf{k}}\mathcal{R}_{\mathbf{k}'}\rangle$ at horizon exit during the early de Sitter phase can be related directly to CMB observables at late times.*

The perturbation $\mathcal{R}$ has several nice properties:

1) it is time-independent on superhorizon scales:

$$\lim_{k \ll aH} \dot{\mathcal{R}}_{\mathbf{k}} = 0 \tag{2.4}$$

[3]In Appendix B we use the Einstein equations to replace the additional (non-dynamical) metric perturbations $\delta g_{00}$ and $\delta g_{0i}$ in terms of $\mathcal{R}$. This results in an action purely for $\mathcal{R}$ which is why we can afford to be a bit implicit about the remaining metric perturbations.

2) it can straightforwardly be related to cosmological observables: e.g.

$$a_{\ell m} = 4\pi(-i)^\ell \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}} \mathcal{R}_\mathbf{k}\, \Delta_{T\ell}(k) Y_{\ell m}(\hat{\mathbf{k}}) \tag{2.5}$$

$$C_\ell = \frac{2}{\pi} \int k^2 dk\, P_\mathcal{R}(k)\, \Delta_{T\ell}(k)^2 \ , \tag{2.6}$$

where $\Delta_{T\ell}(k)$ is a well-known transfer function supplied by CMBFast.

The constancy of $\mathcal{R}$ on superhorizon scales allows us to relate CMB observations directly to the inflationary dynamics (at the time when a given fluctuation crosses the horizon) while allowing us to be completely ignorant about the high-energy physics during the intervening history of the universe.

### 2.2 Constraint Equations

Solving the Einstein equations for the non-dynamical metric perturbations $\delta g_{00}$ and $\delta g_{0i}$ in terms of $\mathcal{R}$ is a bit tedious and would interrupt the flow of these notes. I show the full calculation in Appendix B, but for now ask you to trust me that it can be done. We can then proceed to the result for the quadratic action for the perturbation $\mathcal{R}$.

### 2.3 Quadratic Action

Substituting $\delta g_{00}(\mathcal{R})$ and $\delta g_{0i}(\mathcal{R})$ from Appendix B into (2.1) and expanding in powers of $\mathcal{R}$ we find

$$S = \int \mathrm{d}t\, \mathrm{d}^3\mathbf{x}\, \frac{a^3 \dot{\phi}^2}{2H^2} \left[ \dot{\mathcal{R}}^2 - \frac{1}{a^2} (\nabla \mathcal{R})^2 \right] + \cdots \tag{2.7}$$

where we defined $M_{\rm pl} \equiv 1$. The ellipses in (2.7) refer to terms that are higher order in $\mathcal{R}$. Being interested only in the quadratic action of $\mathcal{R}$ we will now drop these terms. We will come back to these terms when we discuss higher-order correlations and non-Gaussianity.[4] We define the canonically-normalized Mukhanov variable

$$v \equiv z \mathcal{R} \ , \tag{2.8}$$

where

$$z^2 \equiv a^2 \frac{\dot{\phi}^2}{H^2} = 2a^2 \varepsilon \ . \tag{2.9}$$

Switching to conformal time, results in

$$S = \frac{1}{2} \int \mathrm{d}\tau\, \mathrm{d}^3\mathbf{x} \left[ (v')^2 - (\nabla v)^2 + \frac{z''}{z} v^2 \right] \ . \tag{2.10}$$

[4] D. Baumann, *Non-Gaussianity*.

We recognize this as the action of an *harmonic oscillator with time-dependent mass*

$$S = \int \mathrm{d}\tau\, \mathrm{d}^3\mathbf{x} \left[ -\frac{1}{2}\eta^{\mu\nu}\partial_\mu v \partial_\nu v - \frac{1}{2} m_{\text{eff}}^2(\tau) v^2 \right] \ , \tag{2.11}$$

where

$$m_{\text{eff}}^2(\tau) \equiv -\frac{z''}{z} = -\frac{H}{a\dot{\phi}} \frac{\partial^2}{\partial \tau^2} \left( \frac{a\dot{\phi}}{H} \right) \ . \tag{2.12}$$

Given a solution for the homogeneous background $a(t)$ and $\phi(t)$ one obtains $m_{\text{eff}}(\tau)$, i.e. all of de Sitter is encoded in $m_{\text{eff}}(\tau)$. The time-dependence of the effective mass accounts for the interaction of the scalar field $\mathcal{R}$ with the gravitational background.

### 2.4 Mukhanov-Sasaki Equation

Varying the action $S$ and expanding $v$ in Fourier modes,

$$v(\tau, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}}\, v_{\mathbf{k}}(\tau) e^{i\mathbf{k}\cdot\mathbf{x}} \ , \tag{2.13}$$

we arrive at the classical equation of motion (the *Mukhanov-Sasaki equation*)[5]

$$v_{\mathbf{k}}'' + \omega_k^2(\tau) v_{\mathbf{k}} = 0 \ , \qquad \text{where} \qquad \omega_k^2(\tau) \equiv k^2 - \frac{z''}{z} \ . \tag{2.14}$$

In de Sitter the effective frequency reduces to

$$\omega_k^2(\tau) \equiv k^2 - \frac{2}{\tau^2} \qquad \text{(de Sitter)}. \tag{2.15}$$

It is interesting to study special limits of (2.14): For modes with wavelengths much smaller than the horizon we get

$$v_{\mathbf{k}}'' + k^2 v_{\mathbf{k}} = 0 \qquad \text{(subhorizon)}. \tag{2.16}$$

This leads to oscillating solutions: $v_{\mathbf{k}} \propto e^{\pm ik\tau}$. For modes with wavelengths much larger than the horizon we find instead

$$\frac{v_{\mathbf{k}}''}{v_{\mathbf{k}}} = \frac{z''}{z} \approx \frac{2}{\tau^2} \qquad \text{(superhorizon)}. \tag{2.17}$$

This has the growing solution $v_{\mathbf{k}} \propto z \propto \tau^{-1}$ (and the decaying solution $v_{\mathbf{k}} \propto \tau^2$). This implies that $\mathcal{R}$ indeed freezes on superhorizon scales: $\mathcal{R}_{\mathbf{k}} = z^{-1} v_{\mathbf{k}} \propto const.$

[5] The Mukhanov-Sasaki equation is hard to solve in full generality since the function $z(\tau)$ depends on the background dynamics. For a given inflationary background, $\phi(\tau)$ and $a(\tau)$, one may of course solve (2.14) numerically. However, to gain a more intuitive understanding of the solutions, we will discuss approximate analytical solutions in the pure de Sitter limit (Section 4) as well as in the slow-roll expansion of quasi-de Sitter space (Appendix A).

### 2.5 Mode Expansion

Since the frequency $\omega_k(\tau)$ in (2.14) depends only on $k \equiv |\mathbf{k}|$, the most general solution of (2.14) can be written as[6]

$$v_{\mathbf{k}} = a^-_{\mathbf{k}} v_k(\tau) + a^+_{-\mathbf{k}} v^*_k(\tau) \ . \tag{2.18}$$

Here, $v_k(\tau)$ and its complex conjugate $v^*_k(\tau)$ are two linearly independent solutions of (2.14). As indicated by dropping the vector notation $\mathbf{k}$ on the subscript the mode functions, $v_k(\tau)$ and $v^*_k(\tau)$, are the same for all Fourier modes with $k \equiv |\mathbf{k}|$. The Wronskian of the mode functions is

$$W[v_k, v^*_k] \equiv v'_k v^*_k - v_k v^{*\prime}_k = 2i \,\mathrm{Im}(v'_k v^*_k) \ . \tag{2.19}$$

From the equation of motion (2.14) it follows that $W[v_k, v^*_k]$ is time-independent. Furthermore, by rescaling the mode functions as $v_k \to \lambda v_k$ (giving $W[v_k, v^*_k] \to |\lambda|^2 W[v_k, v^*_k]$) we can always normalize $v_k$ such that $W[v_k, v^*_k] \equiv -i$. The reason for this particular choice of normalization will become clear momentarily.

The two time-independent integration constants $a^\pm_{\mathbf{k}}$ in (2.18) are

$$a^-_{\mathbf{k}} = \frac{v^{*\prime}_k v_{\mathbf{k}} - v^*_k v'_{\mathbf{k}}}{v^{*\prime}_k v_k - v^*_k v'_k} = \frac{W[v^*_k, v_{\mathbf{k}}]}{W[v^*_k, v_k]} \qquad \text{and} \qquad a^+_{\mathbf{k}} = (a^-_{\mathbf{k}})^* \ , \tag{2.20}$$

where the relation between $a^+_{\mathbf{k}}$ and $a^-_{\mathbf{k}}$ follows from the reality of $v$. Note that the constants $a^\pm_{\mathbf{k}}$ may depend on the direction of the wave vector $\mathbf{k}$.

Finally, substituting (2.18) into (2.13) gives

$$v(\tau, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}} \left[ a^-_{\mathbf{k}} v_k(\tau) + a^+_{-\mathbf{k}} v^*_k(\tau) \right] e^{i\mathbf{k}\cdot\mathbf{x}} \tag{2.21}$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}} \left[ a^-_{\mathbf{k}} v_k(\tau) e^{i\mathbf{k}\cdot\mathbf{x}} + a^+_{\mathbf{k}} v^*_k(\tau) e^{-i\mathbf{k}\cdot\mathbf{x}} \right] \ , \tag{2.22}$$

where the second line is manifestly real, since $a^+_{\mathbf{k}} = (a^-_{\mathbf{k}})^*$.

[6] The $-\mathbf{k}$ on $a^+_{-\mathbf{k}}$ was chosen for later convenience.

# 3. Quantum Origin of Cosmological Perturbations

Our task now is to quantize the field $v$. This is not much more complicated than quantizing the simple harmonic oscillator in quantum mechanics, except for a small subtlety in the vacuum choice arising from the time-dependence of the oscillator frequencies $\omega_k(\tau)$.[7]

## 3.1 Quantization

The canonical quantization procedure proceeds in the standard way: the field $v$ and its canonically conjugate momentum $\pi \equiv v'$ are promoted to quantum operators $\hat{v}$ and $\hat{\pi}$, which satisfy the standard equal-time commutation relations[8]

$$[\hat{v}(\tau, \mathbf{x}), \hat{\pi}(\tau, \mathbf{y})] = i\delta(\mathbf{x} - \mathbf{y}) \tag{3.1}$$

and

$$[\hat{v}(\tau, \mathbf{x}), \hat{v}(\tau, \mathbf{y})] = [\hat{\pi}(\tau, \mathbf{x}), \hat{\pi}(\tau, \mathbf{y})] = 0 \ . \tag{3.2}$$

It follows from (2.14) that the commutation relation (3.1) holds at all times if it holds at any one time. The Hamiltonian is

$$\hat{H}(\tau) = \frac{1}{2}\int \mathrm{d}^3\mathbf{x} \left[\hat{\pi}^2 + (\nabla \hat{v})^2 + m_{\rm eff}^2(\tau)\hat{v}^2\right] \ . \tag{3.3}$$

The constants of integration $a_{\mathbf{k}}^{\pm}$ in the mode expansion of $v$ become operators $\hat{a}_{\mathbf{k}}^{\pm}$, so that the field operator $\hat{v}$ is expanded as

$$\hat{v}(\tau, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}} \left[\hat{a}_{\mathbf{k}}^{-} v_k(\tau) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{a}_{\mathbf{k}}^{+} v_k^*(\tau) e^{-i\mathbf{k}\cdot\mathbf{x}}\right] \ . \tag{3.4}$$

Substituting (3.4) into (3.1) and (3.2) implies

$$[\hat{a}_{\mathbf{k}}^{-}, \hat{a}_{\mathbf{k}'}^{+}] = \delta(\mathbf{k} - \mathbf{k}') \qquad \text{and} \qquad [\hat{a}_{\mathbf{k}}^{-}, \hat{a}_{\mathbf{k}'}^{-}] = [\hat{a}_{\mathbf{k}}^{+}, \hat{a}_{\mathbf{k}'}^{+}] = 0 \ . \tag{3.5}$$

We realize that our normalization for the mode functions

$$W[v_k, v_k^*] = v_k' v_k^* - v_k v_k^{*\prime} \equiv -i \tag{3.6}$$

was wisely chosen to make (3.5) simple. The operators $\hat{a}_{\mathbf{k}}^{+}$ and $\hat{a}_{\mathbf{k}}^{-}$ may then be interpreted as creation and annihilation operators, respectively.

[7] For a nice treatment of quantum field theory in curved backgrounds I strongly recommend: V. Mukhanov and S. Winitzki, *Introduction to Quantum Effects in Gravity*.

[8] Here, we defined $\hbar \equiv 1$.

Quantum states in the Hilbert space are then constructed by defining the vacuum state $|0\rangle$ via

$$\hat{a}_{\mathbf{k}}^{-}|0\rangle = 0 \ , \tag{3.7}$$

and by producing excited states by repeated application of creation operators

$$|m_{\mathbf{k}_1}, n_{\mathbf{k}_2}, \cdots\rangle = \frac{1}{\sqrt{m!n!\cdots}}\left[(a_{\mathbf{k}_1}^{+})^m (a_{\mathbf{k}_2}^{+})^n \cdots\right]|0\rangle \ . \tag{3.8}$$

### 3.2 Non-Uniqueness

An unambiguous physical interpretation of the states in (3.7) and (3.8) arises only after the mode functions $v_k(\tau)$ are selected.[9] However, the normalization (3.6) is not sufficient to completely fix the solutions $\chi_k(\tau)$ to the second-order ODE (2.14). An unambiguous definition of the vacuum still requires additional physical input.

To illustrate this ambiguity explicitly, consider the following functions

$$u_k(\tau) = \alpha_k v_k(\tau) + \beta_k v_k^*(\tau) \ , \tag{3.9}$$

where $\alpha_k$ and $\beta_k$ are complex constants. The functions $u_k(\tau)$ of course also satisfy the equation of motion (2.14). Moreover, they satisfy the normalization (3.6), i.e. $W[u_k, u_k^*] = -i$, if the coefficients $\alpha_k$ and $\beta_k$ obey

$$|\alpha_k|^2 - |\beta_k|^2 = 1 \ . \tag{3.10}$$

At this point there is therefore nothing that permits us to favor $v_k(\tau)$ over $u_k(\tau)$ in our choice of mode functions. In terms of $u_k(\tau)$ the expansion of $\hat{v}$ takes the form

$$\hat{v}(\tau, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}}\left[\hat{b}_{\mathbf{k}}^{-} u_k(\tau) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{b}_{\mathbf{k}}^{+} u_k^*(\tau) e^{-i\mathbf{k}\cdot\mathbf{x}}\right] \ , \tag{3.11}$$

where $\hat{b}_{\mathbf{k}}^{\pm}$ are alternative creation and annihilation operators satisfying (3.5). Comparing (3.11) to (3.4) leads to the *Bogolyubov transformation* between $\hat{b}_{\mathbf{k}}^{\pm}$ operators and $\hat{a}_{\mathbf{k}}^{\pm}$ operators:

$$\hat{a}_{\mathbf{k}}^{-} = \alpha_k^* \hat{b}_{\mathbf{k}}^{-} + \beta_k \hat{b}_{-\mathbf{k}}^{+} \qquad \text{and} \qquad \hat{a}_{\mathbf{k}}^{+} = \alpha_k \hat{b}_{\mathbf{k}}^{+} + \beta_k^* \hat{b}_{-\mathbf{k}}^{-} \ . \tag{3.12}$$

Both sets of operators can be used to construct a basis of states in the Hilbert space:

$$\hat{a}_{\mathbf{k}}^{-}|0\rangle_a = 0 \qquad \hat{b}_{\mathbf{k}}^{-}|0\rangle_b = 0 \tag{3.13}$$

[9] Changing $v_k(\tau)$ while keeping $\hat{v}$ fixed, changes $\hat{a}_{\mathbf{k}}^{\pm}$ [cf. (2.20)] and hence changes the vacuum $|0\rangle$ and the excited states $|m, n, \cdots\rangle$.

and

$$|m_{\mathbf{k}_1}, n_{\mathbf{k}_2}, \cdots\rangle_a = \frac{1}{\sqrt{m!n!\cdots}}\left[(a^+_{\mathbf{k}_1})^m (a^+_{\mathbf{k}_2})^n \cdots\right]|0\rangle_a \tag{3.14}$$

$$|m_{\mathbf{k}_1}, n_{\mathbf{k}_2}, \cdots\rangle_b = \frac{1}{\sqrt{m!n!\cdots}}\left[(b^+_{\mathbf{k}_1})^m (b^+_{\mathbf{k}_2})^n \cdots\right]|0\rangle_b \tag{3.15}$$

It should be clear that the $b$-states are in general *different* form the $a$-states. In particular, the $b$-vacuum contains $a$-particles:

$$\begin{aligned} {}_b\langle 0|\hat{N}^{(a)}_{\mathbf{k}}|0\rangle_b &= {}_b\langle 0|\hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}}|0\rangle_b & (3.16)\\ &= {}_b\langle 0|(\alpha_k \hat{b}^+_{\mathbf{k}} + \beta^*_k \hat{b}^-_{-\mathbf{k}})(\alpha^*_k \hat{b}^-_{\mathbf{k}} + \beta_k \hat{b}^+_{-\mathbf{k}})|0\rangle_b & (3.17)\\ &= |\beta_k|^2 \delta(0)\ . & (3.18) \end{aligned}$$

The divergent factor $\delta(0)$ arises because we are considering an infinite spatial volume, but the mean density of $a$-particles in the $b$-vacuum is finite (and typically not zero):

$$n \equiv \int \mathrm{d}^3\mathbf{k}\ n_{\mathbf{k}} = \int \mathrm{d}^3\mathbf{k}\ |\beta_k|^2\ . \tag{3.19}$$

### 3.3 Choice of the Physical Vacuum

Clearly, we are still missing some essential physical input to define the unique vacuum state.

#### 3.3.1 Vacuum in Minkowski Space

How do we usually do this? In a *time-independent* spacetime a preferable set of mode functions and thus an unambiguous physical vacuum can be defined by requiring that the expectation value of the Hamiltonian in the vacuum state is minimized. To illustrate this let us consider the Mukhanov-Sasaki equation in Minkowski space (i.e. the $a \equiv 0$ limit of (2.14)):

$$v''_k + k^2 v_k = 0\ . \tag{3.20}$$

We aim to find the mode functions $v_k$ that minimize the expectation value of the Hamiltonian in the vacuum. We will therefore compute ${}_v\langle 0|\hat{H}|0\rangle_v$ for an arbitrary mode function $v$ and then find the preferred function $v$ that minimize the result. In terms of our mode expansion, the Hamiltonian (3.3) becomes

$$\hat{H} = \frac{1}{2}\int \mathrm{d}^3\mathbf{k}\left[\hat{a}^-_{\mathbf{k}}\hat{a}^-_{-\mathbf{k}}F^*_k + \hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}}F_k + \left(2\hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}} + \delta(0)\right)E_k\right]\ , \tag{3.21}$$

where

$$E_k \equiv |v'_k|^2 + k^2|v_k|^2\ , \tag{3.22}$$

$$F_k \equiv v'^2_k + k^2 v^2_k\ . \tag{3.23}$$

Since $\hat{a}^-_{\mathbf{k}}|0\rangle_v = 0$, we have

$$ {}_v\langle 0|\hat{H}|0\rangle_v = \frac{\delta(0)}{4}\int \mathrm{d}^3\mathbf{k}\, E_k \ . \tag{3.24} $$

Dividing out the uninteresting divergence, $\delta(0)$, we infer that the energy density in the vacuum state is

$$ \varepsilon = \frac{1}{4}\int \mathrm{d}^3\mathbf{k}\, E_k \ . \tag{3.25} $$

It is clear that this is minimized if each $\mathbf{k}$ mode $E_k$ is minimized separately. We therefore now determine the $v_k$ and $v_k'$ that minimize the expression

$$ E_k = |v_k'|^2 + k^2|v_k|^2 \ . \tag{3.26} $$

We mustn't forget that the mode functions $\chi_k$ satisfy the normalization (3.6),

$$ v_k' v_k^* - v_k v_k^{*\prime} = -i \ . \tag{3.27} $$

Using the parameterization $v_k = r_k e^{i\alpha_k}$, for real $r_k$ and $\alpha_k$, (3.27) becomes

$$ r_k^2 \alpha_k' = -\frac{1}{2} \tag{3.28} $$

and (3.26) gives

$$ E_k = r_k'^2 + r_k^2\alpha_k'^2 + k^2 r_k^2 \tag{3.29} $$

$$ = r_k'^2 + \frac{1}{4r_k^2} + k^2 r_k^2 \ . \tag{3.30} $$

It easily seen that (3.30) is minimized if $r_k' = 0$ and $r_k = \frac{1}{\sqrt{2k}}$. Integrating (3.28) gives $\alpha_k = -k\tau$ (up to an irrelevant constant that doesn't affect any observables; e.g. this constant phase factor drops out in the computation of the power spectrum) and hence

$$ v_k(\tau) = \frac{1}{\sqrt{2k}} e^{-ik\tau} \ . \tag{3.31} $$

This defines the preferred mode functions for fluctuations in Minkowski space. Note that for these mode functions we find $E_k = k \equiv \omega_k$ and $F_k = 0$, so the Hamiltonian is

$$ \hat{H} = \int \mathrm{d}^3\mathbf{k}\ \omega_k \left[\hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}} + \frac{1}{2}\delta(0)\right] \ . \tag{3.32} $$

Hence, the Hamiltonian is diagonal in the eigenbasis of the occupation number operator $\hat{N}_{\mathbf{k}} \equiv \hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}}$.

### 3.3.2 Vacuum in Time-Dependent Spacetimes

The vacuum prescription which we just applied to Minkowski space does *not* generalize straightforwardly to *time-dependent* spacetimes.

In this case the mode equation (2.14) involves time-dependent frequencies $\omega_k(\tau)$ and the 'minimum-energy vacuum' depends on the time $\tau_0$ at which it is defined. Repeating the above argument, one can nevertheless determine the vacuum which *instantaneously* minimizes the expectation value of the Hamiltonian at some time $\tau_0$. One finds that the initial conditions

$$v_k(\tau_0) = \frac{1}{\sqrt{2\omega_k(\tau_0)}} e^{-i\omega_k(\tau_0)\tau_0} \ , \qquad v_k'(\tau_0) = -i\omega_k(\tau_0)\chi_k(\tau_0) \tag{3.33}$$

select the preferred mode functions which determine the vacuum $|0\rangle_{\tau_0}$. However, since $\omega_k(\tau)$ changes with time, the mode functions satisfying (3.33) at $\tau = \tau_0$ will typically be different from the mode functions that satisfy the same conditions at a different time $\tau_1 \neq \tau_0$. This implies that $|0\rangle_{\tau_1} \neq |0\rangle_{\tau_0}$ and the state $|0\rangle_{\tau_0}$ is not the lowest-energy state at a later time $\tau_1$.

### 3.3.3 Bunch-Davies Vacuum

How do we resolve this ambiguity for the inflationary quasi-de Sitter spacetime?

From Fig. 1 we note that a sufficiently early times (large negative conformal time $\tau$) all modes of cosmological interest were deep inside the horizon:

$$\frac{k}{aH} \sim |k\tau| \gg 1 \qquad\qquad \text{(subhorizon)} \tag{3.34}$$

This means that in the remote past all observable modes had time-independent frequencies; e.g. in perfect de Sitter space:

$$\omega_k^2 = k^2 - \frac{2}{\tau^2} \to k^2 \ . \tag{3.35}$$

The corresponding modes are therefore not affected by gravity and behave like in Minkowski space:

$$v_k'' + k^2 v_k = 0 \ . \tag{3.36}$$

The two independent solutions of (3.36) are $v_k \propto e^{\pm ik\tau}$. As we have seen above only the positive frequency mode $v_k \propto e^{-ik\tau}$ is the 'minimal excitation state', cf. Eqn. (3.31).

Given that at sufficiently early times all modes have time-independent frequencies, we can now avoid the ambiguity in defining the initial conditions for the mode functions that afflicts the treatment in more general time-dependent spacetimes. In practice, this means solving the Mukhanov-Sasaki equation with the (Minkowski) initial condition

$$\lim_{\tau \to -\infty} v_k(\tau) = \frac{1}{\sqrt{2k}} e^{-ik\tau} . \tag{3.37}$$

This defines a preferable set of mode functions and a unique physical vacuum, the *Bunch-Davies vacuum*.

# 4. Results for de Sitter Space

We are now ready to derive the correlation functions for quantum fluctuations in de Sitter space.

## 4.1 de Sitter Mode Functions

In de Sitter space the Mukhanov-Sasaki equation is:

$$v_k'' + \left(k^2 - \frac{2}{\tau^2}\right) v_k = 0 . \tag{4.1}$$

The exact solution of (4.1) is

$$v_k(\tau) = \alpha \frac{e^{-ik\tau}}{\sqrt{2k}} \left(1 - \frac{i}{k\tau}\right) + \beta \frac{e^{ik\tau}}{\sqrt{2k}} \left(1 + \frac{i}{k\tau}\right) . \tag{4.2}$$

The initial condition (3.37) fixes $\beta = 0$, $\alpha = 1$. Hence, the unique mode function is

$$v_k(\tau) = \frac{e^{-ik\tau}}{\sqrt{2k}} \left(1 - \frac{i}{k\tau}\right) . \tag{4.3}$$

This determines the future evolution of the mode including its superhorizon dynamics:

$$\lim_{k\tau \to 0} v_k(\tau) = \frac{1}{i\sqrt{2}} \cdot \frac{1}{k^{3/2}\, \tau} . \tag{4.4}$$

Since $z \propto a \propto \tau^{-1}$ in de Sitter, this implies

$$\lim_{k\tau \to 0} \mathcal{R}_k(\tau) = \frac{1}{z} \lim_{k\tau \to 0} v_k(\tau) = const. , \tag{4.5}$$

i.e. as advertized, $\mathcal{R}$ freezes on superhorizon scales.

### 4.2 Zero-Point Fluctuations

Knowledge of the mode functions for canonically-normalized fields in de Sitter space allows us to compute the effect of quantum zero-point fluctuations:

$$\begin{aligned}
\langle \hat{v}_{\mathbf{k}} \hat{v}_{\mathbf{k}'} \rangle &= \langle 0 | \hat{v}_{\mathbf{k}} \hat{v}_{\mathbf{k}'} | 0 \rangle & (4.6)\\
&= \langle 0 | \left( a^-_{\mathbf{k}} v_k + a^+_{-\mathbf{k}} v_k^* \right) \left( a^-_{\mathbf{k}'} v_{k'} + a^+_{-\mathbf{k}'} v_{k'}^* \right) | 0 \rangle & (4.7)\\
&= v_k v^*_{k'} \langle 0 | a^-_{\mathbf{k}} a^+_{-\mathbf{k}'} | 0 \rangle & (4.8)\\
&= v_k v^*_{k'} \langle 0 | \left[ a^-_{\mathbf{k}} \, , \, a^+_{-\mathbf{k}'} \right] | 0 \rangle & (4.9)\\
&= |v_k|^2 \, \delta(\mathbf{k} + \mathbf{k}') & (4.10)\\
&\equiv P_v(k) \, \delta(\mathbf{k} + \mathbf{k}') \, . & (4.11)
\end{aligned}$$

On superhorizon scales this approaches [cf. Eqn. (4.4)]

$$P_v = \frac{1}{2k^3} \frac{1}{\tau^2} = \frac{1}{2k^3} (aH)^2 \, . \tag{4.12}$$

All power spectra for fields in de Sitter space are simple rescalings of this power spectrum for the canonically-normalized field.

### 4.3 Curvature Fluctuations in Quasi-de Sitter

Strictly speaking, the curvature fluctuations $\mathcal{R} = z^{-1} v$ are ill-defined in perfect de Sitter since $z^2 = a^2 \frac{\dot{\phi}^2}{H^2} = 2a^2 \varepsilon$ vanishes in that limit. We therefore consider quasi-de Sitter space where $\varepsilon$ is small but finite.[10] In this case, the power spectrum of $\mathcal{R}$ is simply given by rescaling the power spectrum of $v$:

$$P_{\mathcal{R}} = \frac{1}{z^2} P_v = \frac{1}{4k^3} \frac{H^2}{\varepsilon} = \frac{1}{2k^3} \frac{H^4}{\dot{\phi}^2} \, . \tag{4.13}$$

Evaluating the r.h.s at horizon crossing $k = aH$ this becomes a function purely of $k$:

$$P_{\mathcal{R}}(k) = \frac{1}{4k^3} \frac{H^2}{\varepsilon} \bigg|_{k=aH} \, . \tag{4.14}$$

Defining the dimensionless power spectrum $\Delta_s^2(k) \equiv \frac{k^3}{2\pi^2} P_{\mathcal{R}}(k)$ we get

$$\Delta_s^2(k) = \frac{1}{8\pi^2} \frac{H^2}{\varepsilon} \bigg|_{k=aH} \, . \tag{4.15}$$

[10] For a more systematic treatment of the slow-roll approximation please refer to Appendix A.

Since $H$ and possibly $\varepsilon$ are now functions of time, the power spectrum will deviate slightly from the scale-invariant form $\Delta_s^2 \sim k^0$. The common way to quantify the deviation from scale-invariance is via the scalar spectral index $n_s$:

$$n_s - 1 \equiv \frac{d \ln \Delta_\mathrm{s}^2}{d \ln k} \, . \tag{4.16}$$

We split the r.h.s. into two factors

$$\frac{d \ln \Delta_\mathrm{s}^2}{d \ln k} = \frac{d \ln \Delta_\mathrm{s}^2}{dN} \times \frac{dN}{d \ln k} \, . \tag{4.17}$$

The derivative with respect to $e$-folds is

$$\frac{d \ln \Delta_\mathrm{s}^2}{dN} = 2 \frac{d \ln H}{dN} - \frac{d \ln \varepsilon}{dN} \, . \tag{4.18}$$

The first term is just $-2\varepsilon$ and the second term is $-\eta$.[11] The second factor in Eqn. (4.17) is evaluated by recalling the horizon crossing condition $k = aH$, or

$$\ln k = N + \ln H \, . \tag{4.19}$$

Hence

$$\frac{dN}{d \ln k} = \left[ \frac{d \ln k}{dN} \right]^{-1} = \left[ 1 + \frac{d \ln H}{dN} \right]^{-1} \approx 1 + \varepsilon \, . \tag{4.20}$$

To first order in the Hubble slow-roll parameters we therefore find

$$n_\mathrm{s} - 1 = -2\varepsilon - \eta \, . \tag{4.21}$$

The parameter $n_s$ is an interesting probe of the inflationary dynamics.

### 4.4 Gravitational Waves in de Sitter

The formalism we just introduced can also be applied to compute the quantum generation of tensor perturbations to the spatial metric $h_{ij}$, cf. Eqn. (2.3). In this case, our job is considerably simplified by the fact that first-order tensor perturbation are gauge-invariant and don't backreact on the inflationary background.

Expansion of the Einstein-Hilbert action gives the second-order action for tensor fluctuations

$$S = \frac{M_\mathrm{pl}^2}{8} \int \mathrm{d}\tau \, \mathrm{d}^3\mathbf{x} \; a^2 \left[ (h_{ij}')^2 - (\nabla h_{ij})^2 \right] \, . \tag{4.22}$$

[11] D. Baumann, *Classical Dynamics of Inflation.*

Here, we have reintroduced the explicit factor of $M_{\rm pl}^2$ to make $h_{ij}$ manifestly dimensionless. Up to the normalization factor of $\frac{M_{\rm pl}}{2}$ this is the same as the action for a massless scalar field in an FRW universe.

We define the standard Fourier representation for transverse, traceless tensors

$$h_{ij}(\tau, \mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^{3/2}} \sum_{\gamma=+,\times} \epsilon_{ij}^\gamma(k) h_{\mathbf{k}}^\gamma(\tau) e^{i\mathbf{k}\cdot\mathbf{x}} \, , \tag{4.23}$$

where $\epsilon_{ii}^\gamma = k^i \epsilon_{ij}^\gamma = 0$ and $\epsilon_{ij}^\gamma \epsilon_{ij}^{\gamma'} = 2\delta_{\gamma\gamma'}$. The fields $h_{\mathbf{k}}^\gamma$ describe the two polarization modes of the gravitational waves ($+$ and $\times$). Eqn. (4.22) then becomes

$$S = \sum_\gamma \int \mathrm{d}\tau \, \mathrm{d}^3\mathbf{k} \, \frac{a^2}{4} M_{\rm pl}^2 \left[ h_{\mathbf{k}}^{\gamma\prime} h_{\mathbf{k}}^{\gamma\prime} - k^2 h_{\mathbf{k}}^\gamma h_{\mathbf{k}}^\gamma \right] \, . \tag{4.24}$$

For the canonically-normalized fields

$$v_{\mathbf{k}}^\gamma \equiv \frac{a}{2} M_{\rm pl} h_{\mathbf{k}}^\gamma \tag{4.25}$$

this reads

$$S = \sum_\gamma \frac{1}{2} \int \mathrm{d}\tau \, \mathrm{d}^3\mathbf{k} \left[ (v_{\mathbf{k}}^{\gamma\prime})^2 - \left(k^2 - \frac{a''}{a}\right) (v_{\mathbf{k}}^\gamma)^2 \right] \, , \tag{4.26}$$

where for a de Sitter background

$$\frac{a''}{a} = \frac{2}{\tau^2} \, . \tag{4.27}$$

Eqn. (4.26) should be recognized as essentially two copies of the action (2.10). Hence, we can jump straight to Eqn. (4.12):

$$P_v = \frac{1}{2k^3} (aH)^2 \, . \tag{4.28}$$

Defining the tensor power spectrum $P_t$ as the sum of the power spectra for each polarization mode of $h_{ij}$, we find

$$P_t = 2 \cdot P_h = 2 \cdot \left(\frac{2}{aM_{\rm pl}}\right)^2 \cdot P_v = \frac{4}{k^3} \frac{H^2}{M_{\rm pl}^2} \, , \tag{4.29}$$

or

$$\Delta_t^2(k) = \frac{2}{\pi^2} \frac{H^2}{M_{\rm pl}^2} \bigg|_{k=aH} \, . \tag{4.30}$$

This completes our treatment of the quantum generation of scalar and tensor fluctuations in the inflationary quasi-de Sitter space.

## 5. Conclusions

We conclude by summarizing the predictions of inflation for primordial scalar and tensor perturbations. We then briefly discuss present constraints and future test of the inflationary paradigm.

### 5.1 Theory

The power spectra of scalar and tensor fluctuations are

$$\Delta_s^2(k) = \frac{1}{8\pi^2}\frac{H^2}{\varepsilon}\bigg|_{k=aH} \qquad \text{and} \qquad \Delta_t^2(k) = \frac{2}{\pi^2}\frac{H^2}{M_{\rm pl}^2}\bigg|_{k=aH} . \tag{5.1}$$

This implies that the tensor-to-scalar ratio is determined by the inflationary equation of state:

$$r \equiv \frac{\Delta_t^2}{\Delta_s^2} = 16\varepsilon \ , \tag{5.2}$$

The scale-dependence of the spectra is

$$n_s - 1 \equiv \frac{d\ln\Delta_s^2}{d\ln k} = -2\varepsilon - \eta \tag{5.3}$$

and

$$n_t \equiv \frac{d\ln\Delta_t^2}{d\ln k} = -2\varepsilon \ . \tag{5.4}$$

Here, we have defined a second slow-roll parameter $\eta \equiv \frac{\dot{\varepsilon}}{H\varepsilon}$ (see Appendix A). Note that while the scalar spectrum can be red ($n_s < 1$) or blue ($n_s > 1$) (depending on the sign of $\eta$), the tensor spectrum is always red ($n_t < 0$). Finally, in single-field slow-roll models we find a consistency relation between tensor observables

$$r = -8n_t \ . \tag{5.5}$$

### 5.2 Observations

Scalar (density) fluctuations have been measured from the imprints they leave in the CMB temperature anisotropies. The inferred amplitude of fluctuations is

$$\Delta_s \sim 10^{-5} \ . \tag{5.6}$$

Its scale-dependence is

$$n_s \sim 0.96 \ . \tag{5.7}$$

No non-Gaussian and/or non-adiabatic contributions have been found.

Primordial tensor modes have not yet been detected, but will be hunted in the B-mode polarization of the CMB. So far we just have upper limits on the tensor-to scalar ratio

$$r \lesssim 0.2 \; . \tag{5.8}$$

The future will be tremendously exciting, with a number of CMB experiments going after the elusive gravitational waves predicted by inflation.

# A. Results for Slow-Roll Inflation

In this appendix we compute the power spectrum of curvature fluctuation in a systematic expansion in slow-roll parameters:

$$\epsilon \equiv -\frac{\dot{H}}{H^2}\ , \qquad \eta \equiv \frac{\dot{\varepsilon}}{H\varepsilon}\ , \qquad \kappa \equiv \frac{\dot{\eta}}{H\eta}\ . \tag{A.1}$$

This will involve a slow-roll expansion of the Mukhanov-Sasaki equation (2.14):

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

Given $z^2 = 2a^2\varepsilon$ we find

$$\frac{z'}{z} = (aH)\left[1 + \frac{1}{2}\eta\right] \qquad \text{(exact)} \tag{A.3}$$

$$\frac{z''}{z} = (aH)^2\left[2 - \varepsilon + \frac{3}{2}\eta - \frac{1}{2}\varepsilon\eta + \frac{1}{4}\eta^2 + \eta\kappa\right] \qquad \text{(exact)} \tag{A.4}$$

Despite the appearance of the slow-roll parameters, both expressions above are exact. From the definition of $\varepsilon$ we furthermore get

$$\frac{d}{d\tau}\left(\frac{1}{aH}\right) = \varepsilon - 1 \qquad \text{(exact)} \tag{A.5}$$

Expanding the expressions to first order in the slow-roll parameters, $\{\varepsilon, |\eta|, |\delta|\} \ll 1$, gives

$$aH = -\frac{1}{\tau}(1+\varepsilon) \qquad \text{(first order in SR)} \tag{A.6}$$

and

$$\frac{z''}{z} = \frac{1}{\tau^2}\left[2 + 3\left(\varepsilon + \frac{1}{2}\eta\right)\right] \equiv \frac{\nu^2 - \frac{1}{4}}{\tau^2} \qquad \text{(first order in SR)} \tag{A.7}$$

where

$$\nu \equiv \frac{3}{2} + \varepsilon + \frac{1}{2}\eta\ . \tag{A.8}$$

For constant $\nu$, the Mukhanov-Sasaki equation

$$v_k'' + \left(k^2 - \frac{\nu^2 - \frac{1}{4}}{\tau^2}\right) v_k = 0 \tag{A.9}$$

has an exact solution in terms of Hankel function of the first and second kind:

$$v_k(\tau) = \sqrt{-\tau}\left[\alpha H_\nu^{(1)}(-k\tau) + \beta H_\nu^{(2)}(-k\tau)\right] \tag{A.10}$$

To impose the Bunch-Davies boundary condition at early times, we consider the limit

$$\lim_{k\tau\to-\infty} v_k(\tau) = \sqrt{\frac{2}{\pi}}\left[\alpha\frac{1}{\sqrt{k}}e^{-ik\tau} + \beta\frac{1}{\sqrt{k}}e^{ik\tau}\right] \,, \tag{A.11}$$

where we used

$$\lim_{k\tau\to-\infty} H_\nu^{(1,2)}(-k\tau) = \sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{-k\tau}}e^{\pm ik\tau}e^{\pm i\frac{\pi}{2}(\nu+\frac{1}{2})} \tag{A.12}$$

and dropped the unimportant phase factors $e^{\pm i\frac{\pi}{2}(\nu+\frac{1}{2})}$. Comparing (A.11) to (3.37) we find

$$\beta = 0 \qquad \text{and} \qquad \alpha = \sqrt{\frac{\pi}{2}} \,. \tag{A.13}$$

Hence, the Bunch-Davies mode functions to first order in slow-roll are:

$$v_k(\tau) = \sqrt{\frac{\pi}{2}}(-\tau)^{1/2}H_\nu^{(1)}(-k\tau) \qquad\qquad \nu \equiv \frac{3}{2} + \varepsilon + \frac{1}{2}\eta \,. \tag{A.14}$$

To compute the power spectrum of curvature fluctuations, $P_{\mathcal{R}} = z^{-2}P_v$, we use $z \sim \tau^{\frac{1}{2}-\nu}$ (first order in SR)

$$P_{\mathcal{R}} \sim \frac{\pi}{2}(-\tau)^{2\nu}|H_\nu^{(1)}(-k\tau)|^2 \,. \tag{A.15}$$

In the superhorizon limit, $-k\tau \ll 1$, this reduces to

$$\Delta_s^2 \equiv \frac{k^3}{2\pi^2}P_{\mathcal{R}} \sim k^{3-2\nu} \,, \tag{A.16}$$

where we used

$$\lim_{k\tau\to 0} H_\nu^{(1)}(-k\tau) = \frac{i}{\pi}\Gamma(\nu)\left(\frac{-k\tau}{2}\right)^{-\nu} \,. \tag{A.17}$$

Finally, the scale-dependence of the scalar spectrum is

$$n_s - 1 \equiv \frac{d\ln\Delta_s^2}{d\ln k} = 3 - 2\nu \tag{A.18}$$

$$= -2\varepsilon - \eta \,. \tag{A.19}$$

This shows that the spectrum is perfectly scale-invariant in de Sitter space, while slow-roll corrections to de Sitter led to percent level deviations from $n_s = 1$.

## B. Free Field Action for $\mathcal{R}$

In this appendix we compute the second-order action for the comoving curvature perturbation $\mathcal{R}$, cf. Eqn. (2.7). This is a basic element for the quantization of cosmological scalar perturbations.

### Slow-Roll Background

We consider slow-roll models of inflation which are described by a canonical scalar field $\phi$ minimally coupled to gravity

$$S = \frac{1}{2} \int \mathrm{d}^4 x \sqrt{-g} \left[ R - (\nabla \phi)^2 - 2V(\phi) \right] , \tag{B.1}$$

in units where $M_{\mathrm{pl}}^{-2} \equiv 8\pi G = 1$. We will study perturbations of this action due to fluctuations in the scalar field $\delta\phi(t, x^i) \equiv \phi(t, x^i) - \bar{\phi}(t)$ and the metric. We will treat metric fluctuations in the ADM formalism (Arnowitt-Deser-Misner).

We consider a flat background metric

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a^2(t) \delta_{ij} \mathrm{d}x^i \mathrm{d}x^j = a^2(\tau)(-\mathrm{d}\tau^2 + \delta_{ij}\mathrm{d}x^i \mathrm{d}x^j) , \tag{B.2}$$

with scale factor $a(t)$ and Hubble parameter $H(t) \equiv \partial_t \ln a$ satisfying the Friedmann equations

$$3H^2 = \frac{1}{2}\dot{\phi}^2 + V(\phi) \qquad \text{and} \qquad \dot{H} = -\frac{1}{2}\dot{\phi}^2 . \tag{B.3}$$

The scalar field satisfies the Klein-Gordon equation

$$\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} = 0 . \tag{B.4}$$

The standard slow-roll parameters are

$$\epsilon_{\mathrm{v}} = \frac{1}{2}\left(\frac{V_{,\phi}}{V}\right)^2 \approx \frac{1}{2}\frac{\dot{\phi}^2}{H^2} , \qquad \eta_{\mathrm{v}} = \frac{V_{,\phi\phi}}{V} \approx -\frac{\ddot{\phi}}{H\dot{\phi}} + \frac{1}{2}\frac{\dot{\phi}^2}{H^2} . \tag{B.5}$$

### ADM Formalism

We treat fluctuations in the ADM formalism where spacetime is sliced into three-dimensional hypersurfaces

$$\mathrm{d}s^2 = -N^2 \mathrm{d}t^2 + g_{ij}(\mathrm{d}x^i + N^i \mathrm{d}t)(\mathrm{d}x^j + N^j \mathrm{d}t) . \tag{B.6}$$

Here, $g_{ij}$ is the three-dimensional metric on slices of constant $t$. The lapse function $N(\mathbf{x})$ and the shift function $N_i(\mathbf{x})$ appear as non-dynamical Lagrange multipliers in the action, i.e. their equations of motion are purely algebraic. For our purposes this is the main advantage of the ADM formalism. The action (B.1) becomes

$$S = \frac{1}{2}\int \mathrm{d}^4x\sqrt{-g}\Big[NR^{(3)} - 2NV + N^{-1}(E_{ij}E^{ij} - E^2) + N^{-1}(\dot{\phi} - N^i\partial_i\phi)^2 - Ng^{ij}\partial_i\phi\partial_j\phi - 2V\Big]\,, \tag{B.7}$$

where

$$E_{ij} \equiv \frac{1}{2}(\dot{g}_{ij} - \nabla_i N_j - \nabla_j N_i)\,, \qquad E = E^i_i\,. \tag{B.8}$$

$E_{ij}$ is related to the extrinsic curvature of the three-dimensional spatial slices $K_{ij} = N^{-1}E_{ij}$.

To fix time and spatial reparameterizations we choose the following gauge for the dynamical fields $g_{ij}$ and $\phi$

$$\delta\phi = 0\,, \qquad g_{ij} = a^2[(1-2\mathcal{R})\delta_{ij} + h_{ij}]\,, \qquad \partial_i h_{ij} = h^i_i = 0\,. \tag{B.9}$$

In this gauge the inflaton field is unperturbed and all scalar degrees of freedom are parameterized by the metric fluctuation $\mathcal{R}(t, \mathbf{x})$.

### Solving the Constraint Equations

The ADM action (B.7) implies the following constraint equations for the Lagrange multipliers $N$ and $N^i$

$$\nabla_i[N^{-1}(E^i_j - \delta^i_j E)] = 0\,, \tag{B.10}$$

$$R^{(3)} - 2V - N^{-2}(E_{ij}E^{ij} - E^2) - N^{-2}\dot{\phi}^2 = 0\,. \tag{B.11}$$

To solve the constraints, we split the shift vector $N_i$ into irrotational (scalar) and incompressible (vector) parts

$$N_i \equiv \psi_{,i} + \tilde{N}_i\,, \qquad \text{where} \qquad \partial_i\tilde{N}_i = 0\,, \tag{B.12}$$

and define the lapse perturbation as

$$N \equiv 1 + \alpha\,. \tag{B.13}$$

The quantities $\alpha$, $\psi$ and $\tilde{N}_i$ then admit expansions in powers of $\mathcal{R}$,

$$\begin{aligned} \alpha &= \alpha_1 + \alpha_2 + \dots\,, \\ \psi &= \psi_1 + \psi_2 + \dots\,, \\ \tilde{N}_i &= \tilde{N}^{(1)}_i + \tilde{N}^{(2)}_i + \dots\,, \end{aligned} \tag{B.14}$$

where, e.g. $\alpha_n = \mathcal{O}(\mathcal{R}^n)$. The constraint equations may then be set to zero order-by-order:

At first order Eqn. (B.11) implies

$$\alpha_1 = \frac{\dot{\mathcal{R}}}{H}\,, \qquad \partial^2 \tilde{N}_i^{(1)} = 0\,, \tag{B.15}$$

where $\tilde{N}_i^{(1)} \equiv 0$ with an appropriate choice of boundary conditions. Furthermore, at first order Eqn. (B.10) implies

$$\psi_1 = -\frac{\mathcal{R}}{H} + \frac{a^2}{H}\epsilon_{\rm v}\,\partial^{-2}\dot{\mathcal{R}}\,, \tag{B.16}$$

where $\partial^{-2}$ is defined via $\partial^{-2}(\partial^2\phi) = \phi$.

### The Free Field Action

Substituting the first-order solutions for $N$ and $N_i$ back into the action, one finds the following second-order action[12]

$$S_{(2)} = \frac{1}{2}\int \mathrm{d}^4x\, a^3 \frac{\dot{\phi}^2}{H^2}\left[\dot{\mathcal{R}}^2 - a^{-2}(\partial_i\mathcal{R})^2\right]\,. \tag{B.17}$$

[12]To arrive at Eqn. (B.17) requires integration by parts and use of the background equations of motion.

## C. Quantum-to-Classical Transtion

[to be included.]