Assigning Quantum-Mechanical Initial Conditions to Cosmological Perturbations

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Abstract

Quantum-mechanical initial conditions for the fluctuations of the geometry can be assigned in excess of a given physical wavelength. The two-point functions of the scalar and tensor modes of the geometry will then inherit corrections depending on which Hamiltonian is minimized at the initial stage of the evolution. The energy density of the background geometry is compared with the energy-momentum pseudo-tensor of the fluctuations averaged over the initial states, minimizing each different Hamiltonian. The minimization of adiabatic Hamiltonians leads to initial states whose back-reaction on the geometry is negligible. The minimization of non-adiabatic Hamiltonians, ultimately responsible for large corrections in the two-point functions, is associated with initial states whose energetic content is of the same order as the energy density of the background.

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I. INTRODUCTION

In cosmology, classical and quantum fluctuations share some features, which can hide radical differences. For instance, in the linearized approximation, classical and quantum fluctuations obey the same evolution equations, but while classical fluctuations are given once forever (on a given space-like hypersurface) quantum fluctuations keep on reappearing all the time during the inflationary phase.

Inflation has to last approximately 60-efolds. One reason to demand such a minimal duration is that, today, the total curvature of the Universe receives a leading contribution from the extrinsic curvature and a subleading contribution from the intrinsic (spatial) curvature. The ratio between the intrinsic and extrinsic curvature goes as $1/\dot{a}^2$ (where $a(t)$ is the scale factor of the Friedmann–Robertson–Walker Universe and the dot denotes derivation with respect to the cosmic time coordinate). During an epoch of decelerated expansion (i.e. $\ddot{a} < 0$, $\dot{a} > 0$) such as the ordinary radiation and matter-dominated phases, $1/\dot{a}^2$ can become very large. The role of inflation is, in this context, to make $1/\dot{a}^2$ very minute at the end of inflation, so that it can easily be of order 1 today. The minimal duration of inflation required in order to achieve this goal is about 60-efolds.

If the duration of inflation is minimal (or close to minimal) classical fluctuations, which were super-horizon sized at the onset of inflation will be affected neither by the inflationary phase nor by the subsequent post-inflationary epoch and can have computable large scale effects [1,2]. If the fluctuations are classical, there are, virtually no ambiguities in normalizing them: it is sufficient to assign the values of the various inhomogeneities over a typical scale and at a given time. For instance, one can imagine that at the onset of inflation the tensor modes of the geometry had some classical initial conditions; this observation leads to predictable consequences provided the duration of inflation is minimal [3].

When the duration of inflation is much longer than 60-efolds, the large scale fluctuations are probably all of quantum-mechanical nature, at least in the case of inflationary models driven by a single inflaton field. Quantum-mechanical fluctuations result from the zero-point
energy of the metric inhomogeneities present during the inflationary epoch. The predictions of inflationary cosmology are partially imprinted in the correlation functions of the scalar and tensor modes of the geometry. For a reliable calculation of these correlators, it is mandatory to correctly normalize the inhomogeneity of the geometry to their quantum-mechanical value.

The main theme of the present investigation will be to present various ways of assigning quantum-mechanical initial conditions in the treatment of cosmological perturbations. The leading term of the scalar and tensor power spectra will not be affected by the different prescriptions. However, there will be computable corrections, which change according to the choice of normalization assignment. The second step of the present paper will be to select one of the different prescriptions, according to the requirement that the initial state of the evolution of the fluctuations will not carry too much energy density if compared with the background geometry.

A naive (but correct) answer to the problem of normalizing quantum fluctuations is to demand that the initial state for the evolution of the various modes of the geometry minimizes the corresponding (quantum) Hamiltonian at the onset of the time evolution. In spite of the correctness of the previous statement, ambiguities are hidden in so far as the Hamiltonian is time-dependent.

One way of assigning quantum-mechanical initial conditions consists in normalizing the mode functions to their “vacuum” value for $\eta \to -\infty$. The Hamiltonians of the scalar and tensor modes of the geometry will then be minimized for $\eta \to -\infty$, which is a physical limit, not a mathematical one. In fact, inflation cannot last indefinitely in the past. Thus, metric fluctuations are normalized to their quantum mechanical amplitude at a time very close to the onset of inflation.

The standard way of normalizing the fluctuations of the geometry was recently scrutinized

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†In this paper $\eta$ denotes the conformal time coordinate, simply related to the cosmic time coordinate by the standard differential relation $a(\eta)d\eta = dt$. 

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in different contexts (see [4] and [5] for recent reviews covering also this subject). The approach of these investigations is from different perspectives. In [6–8] (see also [9–11]), the robustness of inflationary predictions is discussed from a conservative point of view. In [12–15] modifications of the dispersion relations (arising from different contexts) are invoked as a possible source of deviation from the standard lore.

In order to explain in simple terms why the standard prescription might be questioned, let us consider the situation where inflation lasts more than the (minimal) 60-e-folds. Consider also, for concreteness, the case of the tensor modes of the geometry in de Sitter space described by a scale factor \( a(\eta) = (-\eta_1/\eta) \), for \( \eta \leq -\eta_1 \). In this case the evolution equation for each tensor polarization is particularly simple and it is given by:

\[
h_k'' - \frac{2}{\eta} h_k' + k^2 h_k = 0.
\] (1.1)

This equation of motion can be obtained from different Hamiltonians. For instance, following [8] and defining \( \mu = a h \) we will have

\[
H(\eta) = \frac{1}{2} \int d^3x \left[ \pi^2 - \frac{2}{\eta} \mu \pi + (\partial_i \mu)^2 \right], \quad \pi = \mu' + \frac{1}{\eta} \mu, \quad (1.2)
\]

\[
\tilde{H}(\eta) = \frac{1}{2} \int d^3x \left[ \tilde{\pi}^2 - \frac{2}{\eta^2} \mu^2 + (\partial_i \mu)^2 \right], \quad \tilde{\pi} = \mu'. \quad (1.3)
\]

Using the explicit expression for the canonical momenta, the Hamilton equations derived from either (1.2) or (1.3) will always lead, when combined, to (1.1). It is expected that the two Hamiltonians will lead to exactly the same dynamical evolution, since (1.2) and (1.3) are related by a canonical transformation. Furthermore, in the limit \( \eta \to -\infty \), Eqs. (1.2) and (1.3) coincide, since \( \tilde{\pi} \sim \pi \). Consequently, if, as in the standard treatment, quantum-mechanical initial conditions are assigned for \( \eta \to -\infty \), the state minimizing \( H \) will also minimize \( \tilde{H} \). On the contrary, when initial conditions are imposed at a finite (but large) conformal time \( \eta_0 \), the states minimizing \( H \) and \( \tilde{H} \) will differ. This is, ultimately, the reason why [8] the various authors in [6,7] get different corrections in the (late-time) two-point function of \( h(\vec{x}, \eta) \). Different Hamiltonians (not necessarily coinciding with (1.2) or (1.3)) are minimized at the initial time of the evolution: while the dynamical evolution is the
same for both Hamiltonians, the quantum-mechanical states minimizing one or the other are different.

Concerning the initial time of the evolution of the fluctuations there are two possibilities: it could be independent of the comoving scale or it could be different depending on the comoving scale. In order to illustrate the first possibility, recall that, in the conformal time parametrization the scale factor $a(\eta) \to 0$ for $\eta \to -\infty$. Thus, the physical wavelength

$$\lambda_{\text{ph}}(\eta) = \lambda_0 a(\eta)$$

(1.4)

of the fluctuations will go to zero for $\eta \to -\infty$. The typical amplitude of the tensor fluctuations is given by the power spectrum, i.e. the Fourier transform of the two-point function which is, up to numerical factors $\delta_h \sim k^{3/2}|h_k|$. The fluctuations described by Eq. (1.1) should be normalized to quantum-mechanical fluctuations before they leave the horizon, i.e. in the regime $k\eta \gg 1$. In this regime, $h_k \sim 1/a$ and the fluctuation is said to be adiabatically suppressed. It is clear that for a quantum-mechanical fluctuation, i.e. $|h_k| \sim \ell_P/\sqrt{2\pi}$ we will have $\delta_h \sim \omega(\eta)/M_P$, where $\omega(\eta) = \lambda(\eta)^{-1} = k/a(\eta)$ is the physical frequency. It is also clear that when $\omega(\eta) \sim M_P$, $\delta_h \sim \mathcal{O}(1)$.

There might be nothing wrong with the fact that $\lambda_{\text{ph}}$ goes to zero; however one can also imagine that the physical description contains a fundamental length scale $\Lambda^{-1}$. In this case the time at which the normalization is assigned changes depends on the physical scale. Suppose then that a quantum-mechanical normalization is assigned to the fluctuations, at a given conformal time $\eta_0$ in such a way that the physical wavelength $^\dagger$ is defined as

$$\lambda_{\text{ph}}(\eta_0) = \Lambda^{-1},$$

(1.5)

where $\Lambda^{-1}$ is a typical length scale which is of the order of the Planck scale $[^6,^7,^4]$. The condition (1.5) defines a New Physics Hypersurface (NPH) $[^8]$, in the sense that, unlike in

$^\dagger$We will denote with $\lambda_{\text{ph}}(\eta)$ the physical wavelength and with $\omega(\eta) = k/a(\eta)$ the physical frequency
the standard case, different physical frequencies become of order $\Lambda$ at different conformal times.

In the first part of this investigation the corrections to the power spectrum of scalar and tensor fluctuations of the geometry will be computed. It will be shown that the minimization of different Hamiltonians, characterized by a different degree of adiabaticity, lead to different corrections to the power spectrum of curvature fluctuations. The same ambiguities arising in the case of the tensor modes of the geometry [8] are also present in the case of the curvature and metric fluctuations.

In general one cannot assign a localized energy density to the gravitational field, and this is one of the problems in the analysis of the back-reaction of gravitational fluctuations. One possible approach is the one of [17] (see, for a different perspective, also [18]). The energy density of tensor fluctuations of the geometry will be estimated for different initial states (minimizing different Hamiltonians) and it will be shown that this analysis pins down a specific class of Hamiltonians.

The present paper is organized as follows. In Section II the main equations for the scalar modes of the geometry will be briefly reviewed. In Section III it will be shown that minimizing different Hamiltonians will lead to different corrections in the scalar power spectra. Then, in Section IV the issue of the selection of the Hamiltonian will be addressed. The energy density of the tensor modes off the geometry (derived from the pseudo-tensor of gravitational waves) will be averaged over the quantum states, minimizing different Hamiltonians. It will be shown that different initial states can be distinguished by requiring that their energetic content is always sub-leading with respect to the energy density of the background geometry. Finally in Section V some concluding remarks will be proposed.

**II. CURVATURE AND METRIC FLUCTUATIONS**

Consider an accelerated phase of expansion driven by a single inflaton field $\varphi$ in a spatially flat Friedmann–Robertson–Walker metric whose line element can be written, in the
conformal time parametrization, as

\[ ds^2 = a^2(\eta)[d\eta^2 - d\vec{x}^2]. \tag{2.1} \]

The evolution equations for the background will then be §

\[ \mathcal{H}^2 M_P^2 = \frac{1}{3} \left( \frac{\varphi'^2}{2} + V a^2 \right), \tag{2.2} \]
\[ 2(\mathcal{H}^2 - \mathcal{H}' M_P^2 = \varphi'^2, \tag{2.3} \]
\[ \varphi'' + 2\mathcal{H} \varphi' + \frac{\partial V}{\partial \varphi} a^2 = 0, \tag{2.4} \]

where the prime denotes a derivation with respect to the conformal time coordinate and \( \mathcal{H} = a'/a \).

The two Bardeen [19] potentials (\( \Psi \) and \( \Phi \)) and the gauge-invariant scalar field fluctuation \( \chi \) define the coupled system of scalar fluctuations of the geometry (see, for instance, [20]):

\[ \nabla^2 \Psi - 3\mathcal{H}(\mathcal{H}\Phi + \Psi') = \frac{a^2}{2M_P^2} \delta \rho_\varphi, \tag{2.5} \]
\[ \mathcal{H}\Phi + \Psi' = \frac{1}{2M_P^2} \varphi' \chi, \tag{2.6} \]
\[ \Psi'' + \mathcal{H}(\Phi' + 2\Psi') + (\mathcal{H}^2 + 2\mathcal{H}')\Phi = \frac{a^2}{2M_P^2} \delta p_\varphi \tag{2.7} \]

where Eqs. (2.5)–(2.7) are, respectively, the perturbed (00), (0i) and (ij) components of Einstein equations and

\[ \delta \rho_\varphi = \frac{1}{a^2} \left[ -\varphi'^2 \Phi + \varphi' \chi' + \frac{\partial V}{\partial \varphi} \chi \right], \]
\[ \delta p_\varphi = \frac{1}{a^2} \left[ -\varphi'^2 \Phi + \varphi' \chi' - \frac{\partial V}{\partial \varphi} \chi \right], \tag{2.8} \]

are the gauge-invariant energy and pressure density fluctuations. In the absence of any shear in the perturbed energy-momentum tensor) the \( (i \neq j) \) component of the perturbed Einstein equations leads to \( \Phi = \Psi \).

§If not stated otherwise, units \( M_P = 1/\sqrt{8\pi G} \) will be used.
Following [19] and [21], it is convenient to introduce the fluctuations of the spatial curvature on comoving spatial hypersurfaces

\[ \mathcal{R} = -\Psi - \mathcal{H} \frac{X}{\varphi'} = -\Psi - \frac{\mathcal{H}(\mathcal{H}\Phi + \Psi')}{\mathcal{H}^2 - \mathcal{H}'} , \]  

where the equality follows from the use of Eq. (2.6) and of the background equations. The definition of (2.9) and a linear combination of Eqs. (2.5) and (2.7) leads to the following simple equation

\[ \mathcal{R}' = -\frac{4\mathcal{H}}{\varphi'^2}\nabla^2\Psi , \]  

which implies the constancy of \( \mathcal{R} \) for modes \( k\eta \ll 1 \) [19,21]. The power spectrum of the scalar modes amplified during the inflationary phase is customarily expressed in terms of \( \mathcal{R} \), which is conserved on super-horizon scales. Taking the time derivative of Eq. (2.10) and using, repeatedly, Eq. (2.9) and Eqs. (2.5)–(2.7), the following second-order equation can be obtained:

\[ \mathcal{R}'' + 2z\frac{z'}{z}\mathcal{R}' - \nabla^2\mathcal{R} = 0 , \]  

where

\[ z = \frac{a\varphi'}{\mathcal{H}} . \]  

Going to Fourier space, Eq. (2.11) has a simple solution for modes outside the horizon, i.e.

\[ \mathcal{R}_k = A_k + B_k \int^{\eta'} \frac{d\eta'}{z^2(\eta')} , \]  

namely, for the case of single field inflationary backgrounds with polynomial or exponential potential, a constant and a decaying solution.

The curvature perturbations on comoving spatial hypersurfaces can also be simply related to the curvature perturbations on the constant density hypersurfaces, denoted by \( \zeta \)

\[ \zeta = -\Psi - \mathcal{H} \frac{\delta \rho_\phi}{\rho_\phi} \equiv -\Psi + \frac{a^2\delta \rho_\phi}{3\varphi'^2} . \]
It is clear that, taking the difference in the definitions (2.9) and (2.14), and using Eq. (2.5):

\[
\zeta - \mathcal{R} \equiv \frac{\mathcal{H}}{\varphi} + \frac{a^2 \delta \rho_\varphi}{3 \varphi'^2} = \frac{2M_\text{Pl}^2}{3} \frac{\nabla^2 \Psi}{\varphi'^2} ,
\]  

(2.15)

\( \mathcal{R} \) and \( \zeta \) differ by Laplacians of the Bardeen potential.

For the purposes of the present investigation, it is desirable to treat the evolution of the scalar fluctuations of the geometry in terms of a suitable variational principle. On this basis consistent Hamiltonians for the evolution of the fluctuations can be defined.

Instead of perturbing the Einstein equations to first order, the Einstein-Hilbert and scalar field actions should be perturbed to second order. The result of this procedure is usefully expressed in terms of the gauge-invariant curvature fluctuation:

\[
S^{(1)} = \frac{1}{2} \int d^4x \ z^2 \left[ \mathcal{R}'^2 - (\partial_i \mathcal{R})^2 \right] .
\]  

(2.16)

Defining now the canonical momentum \( \pi_\mathcal{R} = z^2 \mathcal{R}' \) the Hamiltonian related to the action (2.16) becomes

\[
H^{(1)}(\eta) = \frac{1}{2} \int d^3x \ \left[ \frac{\pi_\mathcal{R}^2}{z^2} + z^2 (\partial_i \mathcal{R})^2 \right] ,
\]  

(2.17)

and the Hamilton equations

\[
\pi_\mathcal{R}' = z^2 \nabla^2 \mathcal{R} ,
\]  

(2.18)

\[
\mathcal{R}' = \frac{\pi_\mathcal{R}}{z^2} .
\]  

(2.19)

Combining these equations in a single second-order equation Eq. (2.11) is again obtained.

The physical interpretation of \( \mathcal{R} \) has been already introduced in terms of the curvature fluctuations on comoving spatial hypersurfaces. The canonically conjugate momentum, \( \pi_\mathcal{R} \) is related to the density contrast on comoving hypersurfaces, namely, in the case of a single scalar field source [19],

\[
\epsilon_m = \frac{\delta \rho_\varphi + 3 \mathcal{H}(\rho_\varphi + p_\varphi) V}{\rho_\varphi} = \frac{a^2 \delta \rho_\varphi + 3 \mathcal{H} \varphi' \chi}{a^2 \rho_\varphi} ,
\]  

(2.20)

where the second equality can be obtained using that \( \rho_\varphi + p_\varphi = \varphi'^2/a^2 \) and that the effective “velocity” field in the case of a scalar field is \( V = \chi/\varphi' \). Making now use of Eq. (2.6) into Eq. (2.5), Eq. (2.20) can be expressed as
where the last equality follows from Eq. (2.2).

From Eq. (2.21), it also follows that

\[ \pi_{\mathcal{R}} = z^2 \mathcal{R}' \equiv -6a^2 \mathcal{H} \epsilon_m, \]  

(2.22)

where Eq. (2.21) has been used together with the expression of \( \mathcal{R}' \) coming from (2.10). Hence, in this description, while the canonical field is the curvature fluctuations on co-moving spatial hypersurfaces, the canonical momentum is the density contrast on the same hypersurfaces.

In order to bring the second-order action in the simple form (2.16) various (non-covariant) total derivatives have been dropped [22]. Hence, there is always the freedom of redefining the canonical fields through time-dependent functions of the background geometry. In particular, introducing

\[ v = -z \mathcal{R} = a \chi + z \Psi, \]  

(2.23)

the following action can be obtained

\[ S^{(2)} = \frac{1}{2} \int d^4x \left[ v'^2 - 2z' vv' - (\partial_i v)^2 + \left( \frac{z'}{z} \right)^2 v^2 \right], \]

(2.24)

whose related Hamiltonian and canonical momentum are, respectively

\[ H^{(2)}(\eta) = \frac{1}{2} \int d^3x \left[ \pi_v^2 + 2\pi_v v + (\partial_i v)^2 \right], \quad \text{and} \quad \pi = v' - \frac{z'}{z} v. \]

(2.25)

In Eq. (2.24) a further total derivative term can be dropped, leading to another action:

\[ S^{(3)} = \frac{1}{2} \int d^4x \left[ v'^2 - (\partial_i v)^2 + \frac{z''}{z} v^2 \right], \]

(2.26)

and another Hamiltonian

\[ H^{(3)}(\eta) = \frac{1}{2} \int d^3x \left[ \pi_v^2 + (\partial_i v)^2 - \frac{z''}{z} v^2 \right]. \]

(2.27)
where $\pi = v'$. The Hamiltonians obtained in Eqs. (2.17), (2.25) and (2.27) are related by canonical transformation and an example is provided in the Appendix, where a swift derivation of the analogous Hamiltonians is presented in the case of the tensor modes of the geometry. Thus Hamilton’s equations derived from the Hamiltonians (2.17), (2.25 and (2.27) will all have the same dynamical content. However, in spite of the dynamical equivalence of the descriptions, the quantum-mechanical states minimizing the different Hamiltonians will be different.

III. POWER SPECTRA OF CURVATURE FLUCTUATIONS

In the present section the main “observable” to be computed is the two-point function of curvature fluctuations for different spatial points but at the same time. This calculation will be consistently done in the case of the three examples discussed in the previous section, i.e. (2.17), (2.25) and (2.27). The quantum mechanical-normalization will be imposed at the same finite value of the conformal time $\eta_0$.

Consider the situation when a given quantum mechanical fluctuation is inside the horizon at a given time $\eta_0$. Suppose then to give initial conditions for the evolution of the quantum mechanical operators at $\eta_0$ and adopt, for concreteness, the Heisenberg description. The condition

$$k/a(\eta_0) = \Lambda, \quad (3.1)$$

defines the time $\eta_0$ at which a given physical scale crosses the NPH, i.e. the time at which the quantum mechanical initial conditions are assigned. In order to make the calculations explicit, the case of exponential potentials

$$V = V_0 e^{-\sqrt{\frac{p}{2} \dot{\phi}a}}, \quad \dot{\phi} = \frac{\sqrt{2pM_P}}{t},$$

$$z(t) = \frac{\sqrt{\frac{2}{p}}M_P a(t)}{t} \quad (3.2)$$

will be studied. In Eqs. (3.2) the dot denotes a derivation with respect to the cosmic time $t$.  

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This set-up is sufficiently general to illustrate the different corrections arising in the case of different Hamiltonians. In particular notice that the slow-roll parameters**

$$\epsilon = \frac{M_P^2}{2} \left( \frac{\partial \ln V}{\partial \varphi} \right)^2, \quad \sigma = -\frac{M_P^2}{2} \left( \frac{\partial \ln V}{\partial \varphi} \right)^2 + \frac{M_P^2 \partial^2 V}{V} \frac{\partial^2}{\partial \varphi^2}$$

(3.3)

are all equal, i.e. $\epsilon = \sigma = 1/p$. This case can easily be generalized to the situation where the slow-roll parameters are different (as in the case of polynomial potentials).

**A. The Hamiltonian for gauge-invariant curvature fluctuations**

In this case the canonical field is $\mathcal{R}$, i.e. the curvature perturbation of Eq. (2.9). The canonical momentum is the density contrast as discussed in Eq. (2.22). The relevant Hamiltonian is given by (2.17). The classical fields $\mathcal{R}$ and $\pi_\mathcal{R}$ can now be promoted to quantum-mechanical operators, obeying equal-time commutation relations

$$[\hat{\mathcal{R}}(\vec{x}, \eta), \hat{\pi}_\mathcal{R}(\vec{y}, \eta)] = i\delta^{(3)}(\vec{x} - \vec{y}),$$

(3.4)

so that the Hamiltonian operator will be

$$\hat{H}(\eta) = \frac{1}{2} \int d^3x \left[ \frac{\hat{\pi}_\mathcal{R}^2(\vec{x})}{z^2} + z^2 (\partial_i \hat{\mathcal{R}})^2 \right].$$

(3.5)

Going to Fourier space

$$\hat{\mathcal{R}}(\vec{x}, \eta) = \frac{1}{2(2\pi)^{3/2}} \int d^3k \left[ \hat{\mathcal{R}}_k e^{-ik \cdot \vec{x}} + \hat{\mathcal{R}}_k^\dagger e^{ik \cdot \vec{x}} \right],$$

$$\hat{\pi}_\mathcal{R}(\vec{x}, \eta) = \frac{1}{2(2\pi)^{3/2}} \int d^3k \left[ \hat{\pi}_k e^{-ik \cdot \vec{x}} + \hat{\pi}_k^\dagger e^{ik \cdot \vec{x}} \right],$$

(3.6)

the Hamiltonian will have the form

$$\hat{H}(\eta) = \frac{1}{4} \int d^3k \left[ \frac{1}{z^2} (\hat{\pi}_k \hat{\pi}_k^\dagger + \hat{\pi}_k^\dagger \hat{\pi}_k) + k^2 z^2 (\hat{\mathcal{R}}_k \hat{\mathcal{R}}_k^\dagger + \hat{\mathcal{R}}_k^\dagger \hat{\mathcal{R}}_k) \right].$$

(3.7)

**We denoted with $\epsilon$ and $\sigma$ the parameters related to the slow-roll of the curvature and of the scalar field $\varphi$. Usually $\sigma$ is denoted by $\eta$, which would have generated confusion since this letter is already used, in the present notation, for the conformal time coordinate.**
Defining
\[ \hat{Q}_k(\eta_0) = \frac{1}{\sqrt{2k}} \left[ \hat{\pi}_k(\eta_0) - iz(\eta_0)k\hat{R}_k(\eta_0) \right], \] (3.8)

Eq. (3.7) can be expressed as
\[ \hat{H}(\eta_0) = \frac{1}{4} \int d^3k \left[ \hat{Q}_k^+ \hat{Q}_k + \hat{Q}_k^+ \hat{Q}_k - \hat{Q}_k^+ \hat{Q}_k^+ - \hat{Q}_k \hat{Q}_k^+ \hat{Q}_k \right], \] (3.9)

while canonical commutation relations between conjugate field operators imply \[ [\hat{Q}_k, \hat{Q}_k^+] = \delta^{(3)}(\vec{k} - \vec{p}) \]. Consequently, the state minimizing (3.7) at \( \eta_0 \) is the one annihilated by \( \hat{Q}_k \), i.e.
\[ \hat{Q}_k(\eta_0)|0^{(1)}\rangle = 0, \quad \hat{Q}_{-k}(\eta_0)|0^{(1)}\rangle = 0. \] (3.10)

The specific relation between field operators dictated by (3.10) provides initial conditions for the Heisenberg equations
\[ i\hat{\mathcal{R}}' = [\hat{\mathcal{R}}, \hat{H}], \quad i\hat{\pi}'_R = [\hat{\pi}_R, \hat{H}]. \] (3.11)

The full solution of this equation can be written as
\[ \hat{\mathcal{R}}_k(\eta) = \hat{a}_k(\eta_0)f_k(\eta) + \hat{a}_{-k}^+(\eta_0)f_k^\ast(\eta), \] (3.12)
\[ \hat{\pi}_k(\eta) = \hat{a}_k(\eta_0)g_k(\eta) + \hat{a}_{-k}^+(\eta_0)g_k^\ast(\eta), \] (3.13)

where, recalling the explicit solution of the equations in the case of the exponential potential (3.2) and defining \( x = k\eta \)
\[ f_k(\eta) = \frac{\sqrt{\pi}e^{\frac{1}{2}(\mu+1/2)\pi}}{4z(\eta)\sqrt{k}} \sqrt{-x}H^{(1)}_\nu(-x), \quad \nu = \frac{3p - 1}{2(p - 1)}, \]
\[ g_k(\eta) = -\frac{\sqrt{\pi}e^{\frac{1}{2}(\mu+1/2)\pi}z(\eta)\sqrt{k}}{2\sqrt{-x}H^{(1)}_{\nu - 1}(-x)}, \] (3.14)

satisfy the Wronskian normalization condition
\[ f_k(\eta)g_k^\ast(\eta) - f_k^\ast(\eta)g_k(\eta) = i. \] (3.15)

The creation and annihilation operators appearing in (3.13) are defined as
\[
\hat{a}_k(\eta_0) = \frac{1}{z_0 \sqrt{2k}} \{ [g_k^\ast(\eta_0) + i k z_0^2 f_k^\ast(\eta_0)] \hat{Q}_k(\eta_0) - [g_k^\ast(\eta_0) - i k z_0^2 f_k^\ast(\eta_0)] \hat{Q}_{-k}(\eta_0) ,
\]
\[
\hat{a}_{-k}^\dagger(\eta_0) = \frac{1}{z_0 \sqrt{2k}} \{ [g_k(\eta_0) - i k z_0^2 f_k(\eta_0)] \hat{Q}_{-k}^\dagger(\eta_0) - [g_k(\eta_0) + i k z_0^2 f_k(\eta_0)] \hat{Q}_k(\eta_0) .
\] (3.16)

So far two sets of creation and annihilation operators have been introduced: the operators \( \hat{Q}_k(\eta_0) \) and the operators \( \hat{a}_k \). The state annihilated by \( \hat{Q}_k(\eta_0) \) minimizes the Hamiltonian at \( \eta_0 \) while the state annihilated by \( \hat{a}(\eta_0) \) does not minimize the Hamiltonian at \( \eta_0 \). The state annihilated by \( \hat{a}_k(\eta_0) \) is the result of the unitary evolution of the fluctuations from \( \eta = -\infty \) up to \( \eta_0 \). It is relevant to introduce these operators not so much for the calculation of the two-point function but for the subsequent applications to the back-reaction effects. In fact, in the standard approach to the initial value problem for the quantum mechanical fluctuations, the initial state is chosen to be the one annihilated by \( \hat{a}_k(\eta_0) \) for \( \eta_0 \to -\infty \).

The Fourier transform of the two-point function,
\[
\langle 0^{(1)}, \eta_0 | \hat{R}(\vec{x}, \eta) \hat{R}(\vec{y}, \eta) | \eta_0, 0^{(1)} \rangle = \int \frac{dk}{k} \mathcal{P}_R \frac{\sin kr}{kr}, \quad r = |\vec{x} - \vec{y}|,
\] (3.17)
can now be computed, and the result is
\[
\mathcal{P}_R = \frac{k^2}{2\pi^2} \left\{ \left| f_k(\eta) \right|^2 \left[ \frac{\left| g_k(\eta_0) \right|^2}{z(\eta_0)^2} + k^2 z(\eta_0)^2 \right] f_k^\ast(\eta_0)^2 - \frac{f_k(\eta_0)^2}{2} \left[ \frac{\left| g_k^\ast(\eta_0) \right|^2}{z(\eta_0)^2} + k^2 z(\eta_0)^2 f_k^\ast(\eta_0)^2 \right] \right\}.
\] (3.18)

To derive Eq. (3.18) it is useful to recall that, from (3.16):
\[
\langle \eta_0, 0^{(1)} | \hat{a}_k(\eta_0) \hat{a}_p(\eta_0) | 0^{(1)}, \eta_0 \rangle = - \left[ \frac{z(\eta_0)^2 k}{2} f_k^\ast(\eta_0)^2 + \frac{1}{2 k z(\eta_0)^2} |g_k(\eta_0)|^2 \right] \delta^{(3)}(\tilde{k} + \tilde{p}),
\]
\[
\langle \eta_0, 0^{(1)} | \hat{a}_k^\dagger(\eta_0) \hat{a}_p(\eta_0) | 0^{(1)}, \eta_0 \rangle = \left[ \frac{k z(\eta_0)^2}{2} |f_k(\eta_0)|^2 + \frac{1}{2 k z(\eta_0)^2} |g_k(\eta_0)|^2 \right]
- \left[ \frac{i}{2} \left( f_k(\eta_0)^* g_p(\eta_0) - g_k(\eta_0)^* f_p(\eta_0) \right) \right] \delta^{(3)}(\tilde{k} - \tilde{p}),
\] (3.19)

and similarly for the correlators of the Hermitian conjugates operator products.

To make contact with the standard notation, scalar and tensor power spectra can be written as
\[ \mathcal{P}_R = \frac{25}{4} A_S^2, \]
\[ \mathcal{P}_h = 25 A_T^2. \]

The explicit form of \( A_S \) and \( A_T \) can be obtained by inserting Eqs. (3.14) into Eq. (3.18). The results should be expanded for \(|x| = k\eta \ll 1\) and for \(|x_0| = k\eta_0 \gg 1\). While \(|k\eta|\) measures how much a given mode is outside the horizon,

\[ |x_0| = |k\eta_0| \simeq \frac{\Lambda}{H(t_0(k))} = \frac{\Lambda}{H_{\text{ex}}}, \]

defines the moment at which the given mode exits \(^{††}\). In more explicit terms, the following relation holds

\[ \eta_0(k) = -\eta_1 \left( \frac{\Lambda}{k} \right)^{1-\frac{1}{p}}. \]

As already pointed out, within the present approach, the time at which the quantum-mechanical normalization is implemented, depends on the comoving wavelength. In the case of ordinary inflationary models the initial time \( \eta_0(\lambda) \) is directly proportional to a (positive) power of the comoving wavelength. This means that, for the same inflationary curvature scale, larger comoving wavelengths exit the NPH earlier than the small ones.

The final result of the double expansion then is

\[ A_S = \sqrt{p} C(p) \left( \frac{H_1}{M_P} \right) \left( \frac{k}{k_1} \right)^{\frac{1}{p-1}} \left[ 1 + \frac{p}{2(p-1)} \sin \frac{2x_0 + p\pi/(p-1)}{x_0} \right], \]
\[ C(p) = \frac{1}{5 \sqrt{2} \pi^{3/2}} \left( \frac{p}{p-1} \right)^{-\frac{3}{2(p-1)}} \Gamma \left( \frac{3p-1}{2(p-1)} \right), \]
\[ A_T = A_S / \sqrt{p}. \]

The result of Eq. (3.24) (valid for the tensor modes of the geometry) is obtained by comparing Eq. (3.23) with the result for the correlator of the tensor fluctuations (see [8]). In (3.23) \( H_1 \) is the Hubble parameter at the end of inflation and \( k_1 = H_1 \) is the corresponding

\(^{††}\)In this equation we denoted by \( H(t_0(k)) \) the moment at which a given mode exits the NPH.
comoving frequency. Since, in the present case, \( \epsilon(\varphi) = \sigma(\varphi) = 1/p \) (see Eq. (3.3, Eqs. (3.23) and (3.24) imply \( A_T = \sqrt{\epsilon} A_S \), which is the usual relation.

In Eqs. (3.23) and (3.24), on top of the standard (leading) terms there is a correction that goes, roughly, as \( 1/x_0 \sim H_{ex}/\Lambda \) where, as discussed in Eq. (3.21), \( H_{ex} \) denotes the Hubble parameter evaluated at the moment the given scale exits the NPH. If \( \Lambda \sim M_P \), \( H_{ex}/\Lambda \sim 10^{-6} \). This is the correction that would apply in the scalar power spectrum if quantum mechanical initial conditions were assigned in such a way that the initial state minimizes (2.17). As will be shown in a moment, if a different Hamiltonian is minimized, the correction will be much smaller.

### B. Hamiltonians for the canonical variable

Having discussed in detail the results for the case of (2.17) the attention will now be turned to the case of (2.25). Following the same procedure discussed as previous case, commutation relations are imposed for the canonically conjugate fields

\[
[\hat{v}(\vec{x}, \eta), \hat{\pi}_v(\vec{y}, \eta)] = i\delta^{(3)}(\vec{x} - \vec{y}),
\]

and the resulting Hamiltonian becomes \( \dagger\dagger \):

\[
\hat{H}(\eta) = \frac{1}{4} \int d^3k \left[ (\hat{\pi}_k \hat{\pi}^\dagger_k + \hat{\pi}_k^\dagger \hat{\pi}_k) + k^2 (\hat{v}_k \hat{v}^\dagger_k + \hat{v}^\dagger_k \hat{v}_k) + \frac{z'}{z} (\hat{\pi}_k \hat{v}^\dagger_k + \hat{\pi}_k^\dagger \hat{v}_k + \hat{v}_k \hat{\pi}_k^\dagger + \hat{v}^\dagger_k \hat{\pi}_k) \right].
\]  

Solving the evolution in the Heisenberg picture, the mode functions can be written as

\[
f_k(\eta) = \frac{\sqrt{\pi}}{4} \frac{e^{\frac{(\nu + \frac{1}{2})\pi}{4}}}{\sqrt{k}} \sqrt{-x} H^{(1)}_{\nu}(\nu) \sim -x, \quad (3.27)
\]

\[
g_k(\eta) = -e^{\frac{(\nu + \frac{1}{2})\pi}{4}} \sqrt{\pi} \sqrt{k} \sqrt{-x} H^{(1)}_{\nu-1}(\nu) \sim -x, \quad (3.28)
\]

where, as in the previous case, \( 2\nu = (3p - 1)/(p - 1) \). The quantum-mechanical state minimizing (3.26) at the initial time \( \eta_0 \), i.e. \( |0^{(2)}\rangle \), is the one annihilated by \( \hat{Q}_k \) whose definition is now

\( \dagger\dagger \)The Fourier transform of the momentum operator \( \hat{\pi}_v \) will be denoted, again, by \( \hat{\pi}_k \).
\[
\hat{Q}_\vec{k}(\eta_0) = \frac{1}{\sqrt{2k}} \left[ e^{-i\alpha_0} \hat{\pi}_\vec{k}(\eta_0) - ie^{i\alpha_0} k \hat{\psi}_\vec{k}(\eta_0) \right], \\
\hat{Q}_\vec{k}|0^{(2)}\rangle = 0, \quad \hat{Q}_{-\vec{k}}|0^{(2)}\rangle = 0,
\]
(3.29)

where \( \alpha_0 = \alpha(\eta_0) \), i.e.
\[
\sin 2\alpha_0 = \left. \frac{z'}{kz} \right|_{\eta_0}.
\]
(3.30)

The canonical commutation relations Eq. (3.4) now imply \([\hat{Q}_\vec{k}, \hat{Q}^\dagger_{\vec{p}}] = \cos 2\alpha_0 \delta^{(3)}(\vec{k} - \vec{p})\). In terms of (3.29) the Hamiltonian (3.26) has again the form (3.9) but, obviously, the meaning of \( \hat{Q}_\vec{k} \) is different.

The wave-functional of the initial state has a Gaussian form:
\[
\psi[v_\vec{k}] = N \exp \left( -\sum_k \frac{k}{2} (v_\vec{k}^* v_\vec{k}) e^{-2i\alpha_0} \right).
\]
(3.31)

This state is normalizable provided \( |\alpha_0| < \pi/4 \). We see that \( |\alpha_0| = \pi/4 \) corresponds to a time \( \eta_0 \) for which \( |k\eta_0| \sim 1 \) (recall that \( z'/z \) goes as \( 1/\eta \)), which is basically equivalent to the condition of (standard) horizon crossing. Consequently, provided the modes of the field are inside the horizon at the “initial” time \( \eta_0 \), the state (3.31) is normalizable.

The two-point function of the curvature fluctuations can now be computed, with the difference that, now, the state minimizing (3.26) at \( \eta_0 \) is the one annihilated by (3.29), i.e.
\[
\langle 0^{(2)}, \eta_0 | \mathcal{R}(\vec{x}, \eta) \hat{\mathcal{R}}(\vec{y}, \eta) | \eta_0, 0^{(2)} \rangle = \int \frac{dk}{k} p R \sin kr \frac{kr}{kr}, \quad r = |\vec{x} - \vec{y}|,
\]
(3.32)

The result of this calculation follows the same steps as outlined before and, recalling the definitions (3.20), the results are
\[
A_S = \sqrt{p} \, C(p) \left( \frac{H_1}{M_p} \right) \left( \frac{k}{k_1} \right)^{\frac{1}{2}p} \left[ 1 - \frac{p}{4(p-1)} \cos \frac{2\alpha_0}{x_0} \right], \\
A_T = A_S/\sqrt{p},
\]
(3.33)

where \( C(p) \) is the same as in (3.23). A comparison of Eqs. (3.24) and (3.33) shows two important facts. The first is that the leading term of the spectrum is \textit{the same in both cases}. Furthermore, it will be shown that this is true even if (2.27) is used. This phenomenon simply
reflects the fact that different Hamiltonians, connected by canonical transformations, must lead to the same evolution and to the same leading term in the power spectra. The second fact to be noticed is that the correction to the power spectrum goes as $1/x^2_0$ in the case of (3.33). This correction is then much smaller than the one appearing in (3.24). If $\Lambda \sim M_P$ then the correction will be $O(10^{-12})$, i.e. six orders of magnitude smaller than in the case of (3.24).

Finally the case of the Hamiltonian (2.27) will be examined. Equation (2.27) can be minimized following the same procedure as already discussed in the case of Eqs. (2.17) and (2.25). Defining the function
\[ \omega^2(x) = \left( 1 - \frac{1}{k^2} \frac{a''}{a} \right), \] (3.34)
and recalling that $\bar{\pi}_v = \nu'$, the Hamiltonian (3.35) can be written in the simple form
\[ \hat{H}(\eta) = \frac{1}{4} \int d^3k \left[ (\hat{\pi}^-_k \hat{\pi}^+_k + \hat{\pi}^+_k \hat{\pi}^-_k) + k^2 \omega^2(x)(\hat{v}^+_k \hat{v}^-_k + \hat{v}^-_k \hat{v}^+_k) \right]. \] (3.35)
Defining now the operator
\[ \hat{Q}_k(\eta_0) = \frac{1}{\sqrt{2k}} \left[ \hat{\pi}^-_k(\eta_0) - ik\omega(\eta_0)\hat{v}^-_k(\eta_0) \right], \] (3.36)
the Hamiltonian can again be expressed, at $\eta_0$ in the same form as previously discussed, namely, the one given by Eq. (3.9), with the caveat that now the operator (3.36), if compared with that defined in Eq. (3.29), has a different expression in terms of the canonical fields. The commutation relations now are $[\hat{Q}_k(\eta_0), \hat{Q}^+_p(\eta_0)] = \omega_0 \delta^{(3)}(k - p)$. The mode functions $f_k(\eta)$ are the same as those given in Eq. (3.27), while $g_k$ is given by
\[ g_k(\eta) = -\frac{\sqrt{\pi}}{4} e^{(\nu + \frac{1}{2})\pi} \sqrt{k} \sqrt{-x} \left[ H^{(1)}_{\nu-1}(-x) + \frac{1 - 2\nu}{2(-x)} H^{(1)}_{\nu}(-x) \right], \] (3.37)
Repeating the steps used in the previous two cases the two-point function
\[ \langle 0^{(3)}, \eta_0| \hat{R}(\vec{x}, \eta) \hat{R}(\vec{y}, \eta)| \eta_0, 0^{(3)} \rangle \] (3.38)
can be computed recalling that $|0^{(3)}\rangle$ is the state annihilated by (3.36). The following power spectra are then obtained
\[ A_S = \sqrt{p} C(p) \left( \frac{H_{1p}}{M_p} \right) \left( \frac{k}{k_1} \right)^{p - 1} \left[ 1 + \frac{p(2p - 1) \sin \left[ 2x_0 + \frac{p\pi}{(p - 1)} \right]}{(p - 1) 4x_0^3} \right], \]  

(3.39)

\[ A_T = A_S / \sqrt{p}. \]  

(3.40)

In Eqs. (3.39) and (3.40) the correction arising from the initial state goes as \(1/x_0^3\) and, again, if \(\Lambda \sim M_p\) it is \(\mathcal{O}(10^{-18})\), i.e. 12 orders of magnitude smaller than in the case discussed in Eqs. (3.23) and (3.24).

IV. RESOLVING THE AMBIGUITY: BACK-REACTION EFFECTS

In order to select the correct Hamiltonian in a way compatible with the idea of assigning initial conditions on the NPH, it is desirable to address the issue of back-reaction effects. The energetic content of the quantum-mechanical state minimizing the given Hamiltonian should be estimated and compared with the energy density of the background geometry. The back-reaction effects of the different quantum-mechanical states minimizing the Hamiltonians will now be computed. Without loss of generality, the attention will be focused on the tensor modes of the geometry. In the appendix it is shown, the same Hamiltonians as were discussed for the scalar modes of the geometry can also be defined in the case of the tensors. Moreover, there is one-to-one correspondence between scalar and tensor Hamiltonians. The advantage of discussing the gravitons is that they do not couple to the sources and, therefore, the form of the energy-momentum pseudo-tensor is simpler than in the case of the scalar modes [17].

The appropriate energy-momentum tensor of the fluctuations of the geometry will be averaged over the state minimizing a given Hamiltonian at \(\eta_0\) and the result compared with the energy density of the background geometry. The energy density of the fluctuations cannot exceed that of the background geometry.

The energy density of the gravitational waves can be computed from the energy-momentum pseudo-tensor [17], written, for simplicity, for one of the two traceless and divergenceless polarizations (i.e. \(h_i^i = 0\) and \(\partial_i h_j^i = 0\)):

\[ \langle \tilde{T}^0_0 \rangle = \frac{\mathcal{H}}{2a^2} \langle (\hat{h}' \hat{h} + \hat{h} \hat{h}') \rangle + \frac{1}{8a^2} \langle [\hat{h}^2 + (\partial_i \hat{h}^i)^2] \rangle, \]  

(4.1)

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where \( \langle \ldots \rangle \) denotes the expectation value with respect to a quantum mechanical state minimizing a given Hamiltonian and \( \hat{h} \) denotes the field operator corresponding to a single tensor polarization of the geometry.

In the appendix we swiftly recall the main quantities that are required in order to discuss the minimization of the Hamiltonians of the tensor modes of the geometry. This notation will be followed here too. Consider, to begin with, the first Hamiltonian, i.e. (A.3). The quantity

\[
\rho_{GW}^{(1)}(\eta, \eta_0) = \langle 0^{(1)}(\eta) | \hat{T}_0^0(\eta) | \eta_0, 0^{(1)} \rangle, \tag{4.2}
\]

should be computed. Here \( |\eta_0, 0^{(1)} \rangle \) is the state minimizing the first Hamiltonian, i.e. the state annihilated by

\[
\hat{Q}_k(\eta_0) = \frac{1}{\sqrt{2k}} \left[ \hat{\Pi}_k(\eta_0) a(\eta_0) - i a(\eta_0) k \hat{h}_k(\eta_0) \right]. \tag{4.3}
\]

As illustrated in the case of the scalar modes of the geometry, the evolution equations in the Heisenberg description can be solved in terms on the values of the field operators at the initial time \( \eta_0 \). Using repeatedly the action of the operators (4.3),

\[
\rho_{GW}^{(1)}(\eta, \eta_0) = \frac{H^4}{32\pi^2} \int \frac{dk}{k} x^4 \left[ \frac{a^2(\eta)}{a^2(\eta_0)} A_k^{(1)}(\eta, \eta_0)^2 + \frac{a^2(\eta_0)}{a^2(\eta)} D_k^{(1)}(\eta, \eta_0)^2 \right. \\
+ \left. \frac{C_k^{(1)}(\eta, \eta_0)^2}{k^2a^2(\eta_0)a^2(\eta)} + k^2a^2(\eta)a^2(\eta_0)B_k^{(1)}(\eta, \eta_0)^2 \right. \\
+ \left. 8\mathcal{H} \frac{A_k^{(1)}(\eta, \eta_0)C_k^{(1)}(\eta, \eta_0)}{k^2a^2(\eta_0)} + 8\mathcal{H}a(\eta_0)^2D_k^{(1)}(\eta, \eta_0)B_k^{(1)}(\eta, \eta_0) \right], \tag{4.4}
\]

where, defining \( \Delta x = x - x_0 \),

\[
A_k^{(1)}(\eta, \eta_0) = \frac{x \cos \Delta x - \sin \Delta x}{x_0}, \\
B_k^{(1)}(\eta, \eta_0) = \frac{H^2 [(-x + x_0) \cos \Delta x + (1 + x x_0) \sin \Delta x]}{k^3}, \\
C_k^{(1)}(\eta, \eta_0) = -\left( \frac{k^3 \sin \Delta x}{H^2 x x_0} \right), \\
D_k^{(1)}(\eta, \eta_0) = \frac{x_0 \cos \Delta x + \sin \Delta x}{x}. \tag{4.5}
\]

Inserting Eqs. (4.5) into Eq. (4.4) the following expression can be obtained:
$$\rho_{GW}^{(1)}(\eta, \eta_0) = \frac{H^4}{64\pi^2} \int \frac{dk}{k} \left( \frac{x}{x_0} \right)^2 \left\{ (2x_0^2 + 1)(2x^2 - 7) + (12xx_0 + 7) \cos 2\Delta x 
+ 2(3x - 7x_0) \sin 2\Delta x \right\}. \tag{4.6}$$

where the explicit parametrisation of de Sitter space has been used, namely, $a(\eta) = (-H\eta)^{-1}.$

In curved space-times, it is often mandatory to implement a suitable renormalization procedure, which amounts, in some cases, to subtracting the appropriate counter terms which can in turn be expressed as known geometrical quantities. Instead of looking immediately at this problem from a formal point of view, it is useful to see what physics suggests. Let us go back to the logic behind the present exercise. We want to assign quantum-mechanical initial conditions for the field operators at a finite value of the conformal time, as soon as the physical wavelength becomes sub-Planckian. Following this logic, the energy-density present for $\eta_0 \to -\infty$ has no meaning since, in this limit, all the physical wavelength will go to 0, i.e. will be much smaller than the Planck length. Let us then take the limit of Eq. (4.6) for $\eta_0 \to -\infty$:

$$\lim_{\eta_0 \to -\infty} \rho_{GW}^{(1)} = \frac{H^4}{64\pi^2} \int \frac{dk}{k} 2x^2(2x^2 - 7) \equiv \langle \hat{T}_0^0 \rangle_{BD}. \tag{4.7}$$

This quantity, as can be checked from the other expectation values presented later in this section, is the same for all three Hamiltonians. The result of Eq. (4.7) has a simple interpretation: it is the expectation value of the energy-momentum pseudo-tensor over the Bunch–Davies vacuum for $\eta \to -\infty$. In fact $\langle \hat{T}_0^0 \rangle_{BD}$ can be obtained by averaging each of the Hamiltonians discussed in the present section over the state annihilated by the corresponding operators $\hat{a}_\vec{k}$ and $\hat{a}_{-\vec{k}}$. These operators have been discussed in Eqs. (3.12) and (3.13) in the case of the first class of scalar Hamiltonians. There it was noticed that when $\eta_0$ is finite, the state annihilated by $\hat{a}_\vec{k}$ and $\hat{a}_{-\vec{k}}$ does not minimize any Hamiltonian. Clearly the same set of operators can be defined, with the appropriate differences, for all the Hamiltonians discussed in the present investigation. In [23] it was suggested that a sensible renormalization procedure amounts to subtracting the energy density of the Bunch-Davies...
vacuum.

The renormalized energy density can then be defined as

\[
\bar{\rho}^{(1)}_{GW}(\eta, \eta_0) = \rho^{(1)}_{GW}(\eta, \eta_0) - \langle T^0_0 \rangle_{BD} = \frac{H^4}{64\pi^2} \int \frac{dk}{k} \left( x_{\eta_0} \right)^2 \left\{ (2x_{\eta_0}^2 - 7) + (12x_{\eta_0} + 7) \cos 2\Delta x + 2(3x_{\eta_0} - 7) \sin 2\Delta x \right\}. \tag{4.8}
\]

Recall now that \( x = k\eta \). Then integrating between \( |x| \sim 1 \) and \( |x| \sim x_0 \), and keeping only the leading terms for \( x_0 \gg 1 \), we have the following result:

\[
\bar{\rho}^{(1)}_{GW}(\eta, \eta_0) \sim \frac{H^4}{64\pi^2} \left[ x_0^2 + O\left( \frac{1}{x_0} \right) \right] \approx \frac{H^4}{64\pi^2} \left( \frac{\Lambda}{H} \right)^2 \left[ 1 + O\left( \frac{H^2}{\Lambda^2} \right) \right]. \tag{4.9}
\]

It can be checked numerically that the agreement of (4.9) with the exact result of the integral is excellent. Since, as already discussed, \( |x_0| = \Lambda/H \gg 1 \), in the case of de Sitter space, the back-reaction effects related to the state minimizing the first Hamiltonian are then large. Recall, in fact, that the energy density of the background geometry is \( O(H^2M_P^2) \). Hence, if \( \Lambda \sim M_P \) the energy density of the fluctuations will be of the same order as that of the background geometry, which is not acceptable since, if this is the case, inflation could not even start.

Let us now turn our attention to the case of the state minimizing the second Hamiltonian,

The expectation value of the energy-momentum pseudo-tensor

\[
\rho^{(2)}_{GW}(\eta, \eta_0) = \langle 0^{(2)}, \eta_0 | \tilde{T}^0_0(\eta) | \eta_0, 0^{(2)} \rangle \\
= \frac{H^4}{64\pi^2} \int \frac{dk}{k} x^4 \left\{ A_k^{(2)}(\eta, \eta_0)^2 + \frac{C_k^{(2)}(\eta, \eta_0)^2}{k^2} + 8\mathcal{H}D_k^{(2)}(\eta, \eta_0)B_k^{(2)}(\eta, \eta_0) \right. \\
+ 8\mathcal{H}A_k^{(2)}(\eta, \eta_0)C_k^{(2)}(\eta, \eta_0) + D_k^{(2)}(\eta, \eta_0)^2 + k^2B_k^{(2)}(\eta, \eta_0)^2 \right. \\
- \left. \frac{2}{k} \sin 2\alpha_0 \left[ C_k^{(2)}(\eta, \eta_0)D_k^{(2)}(\eta, \eta_0) + k^2B_k^{(2)}(\eta, \eta_0)A_k^{(2)}(\eta, \eta_0) \right. \\
- \left. 4\mathcal{H} \left( A_k^{(2)}(\eta, \eta_0)D_k^{(2)}(\eta, \eta_0) + B_k^{(2)}(\eta, \eta_0)C_k^{(2)}(\eta, \eta_0) \right) \right] \right\} \tag{4.10}
\]

is taken over the state minimizing the second Hamiltonian, i.e. the state annihilated by

\[
\hat{Q}^\dagger_{\bar{k}}(\eta_0) = \frac{1}{\sqrt{2k}} \left[ e^{-i\alpha_0} \hat{\pi}^\dagger_{\bar{k}}(\eta_0) - ie^{i\alpha_0} k\hat{\mu}^\dagger_{\bar{k}}(\eta_0) \right]. \tag{4.11}
\]
Recall that, in Eq. (4.10), \( \sin 2\alpha_0 = -1/x_0 \) and \( \mathcal{H}_0 = -1/\eta_0 \). Taking into account the explicit form of the coefficients

\[
\begin{align*}
A_k^{(2)}(\eta, \eta_0) &= \cos \Delta x - \frac{\sin \Delta x}{x}, \\
B_k^{(2)}(\eta, \eta_0) &= \frac{(1 + x x_0) \sin \Delta x - \Delta x \cos \Delta x}{k x_0}, \\
C_k^{(2)}(\eta, \eta_0) &= -k \sin \Delta x, \\
D_k^{(2)}(\eta, \eta_0) &= \cos \Delta x + \frac{\sin \Delta x}{x_0},
\end{align*}
\]

(4.12)

the renormalized energy-momentum pseudo-tensor becomes:

\[
\rho_{GW}^{(2)}(\eta, \eta_0) = \frac{H^4}{64\pi^2} \int \frac{dk}{k} \left( \frac{x}{x_0} \right)^2 \frac{1}{\cos 2\alpha_0} \left\{ (2x^2 - 7)[2x_0^2 - 1 - 2x_0^2 \cos 2\alpha_0] \right\} \\
- 7 \cos 2\Delta x - 6 \sin 2\Delta x.
\]

(4.13)

Applying the procedure described above and performing the integral over all the modes inside the horizon, but below the cut-off \( \Lambda \), we have

\[
\rho_{GW}^{(2)}(\eta, \eta_0) \simeq -\frac{25}{512\pi^2} H^4 \left[ 1 + O\left( \frac{H^2}{\Lambda^2} \right) \right].
\]

(4.14)

In this case the energy density is smaller, by a factor of \((H/\Lambda)^2\), than the energy density obtained in (4.9). If we took \( \Lambda \sim M_P \), this result would be acceptable except for the sign of the averaged energy density, which is negative. The fact that negative energy densities could be obtained, by averaging the energy density over a specific quantum state was noted long ago by Ford and Kuo [24] (see also [25]). In [24] it was actually noticed that the averaged energy density becomes negative whenever the fluctuations of the energy momentum tensor itself are large.

Finally, in the third and last case, the state minimizing the Hamiltonian (A.7) is the one annihilated by

\[
\hat{Q}_k^{(2)}(\eta_0) = \frac{1}{\sqrt{2k}} \left[ \hat{\pi}_k(\eta_0) - i\omega_0 \hat{\mu}_k(\eta_0) \right],
\]

(4.15)

where
\[ \omega_0 = \sqrt{1 - \frac{(\mathcal{H}_0^2 + \mathcal{H}'_0)}{k^2}} = \sqrt{1 - \frac{2}{x_0^2}}. \] (4.16)

The average of the energy-momentum pseudo-tensor over this state leads to the following expression

\[
\rho^{(3)}_{\text{GW}}(\eta, \eta_0) = \langle 0^{(3)}(\eta_0) | \hat{T}_0^{(0)}(\eta) | 0^{(3)} \rangle = \frac{H^4}{32\pi^2} \int \frac{dk x^4}{k \omega_0} \left\{ \left(1 - \frac{7H}{k^2}\right) \left[A_k^{(3)}(\eta, \eta_0)^2 + k^2 \omega_0^2 B_k^{(3)}(\eta, \eta_0)^2\right] \right.
\]
\[ + \frac{6H}{k^2} \left[ A_k^{(3)}(\eta, \eta_0) C_k^{(3)}(\eta, \eta_0) + k^2 \omega_0^2 B_k^{(3)}(\eta, \eta_0) D_k^{(3)}(\eta, \eta_0) \right] \left. + \frac{1}{k^2} \left[ C_k^{(3)}(\eta, \eta_0)^2 + k^2 \omega_0^2 D_k^{(3)}(\eta, \eta_0)^2 \right] \right\}. \] (4.17)

Recalling that

\[
A_k^{(3)}(\eta, \eta_0) = \frac{(x_0 + x (x_0^2 - 1)) \cos \Delta x + (1 + (x - x_0) x_0) \sin \Delta x}{x x_0^2},
\]
\[
B_k^{(3)}(\eta, \eta_0) = \frac{(-x + x_0) \cos \Delta x + (1 + x x_0) \sin \Delta x}{k x x_0},
\]
\[
C_k^{(3)}(\eta, \eta_0) = -\frac{k \left[ (x_0 - x^2 x_0 + x (x_0^2 - 1)) \cos \Delta x + (1 + x x_0 - x_0^2 + x^2 (x_0^2 - 1)) \sin \Delta x \right]}{x^2 x_0^2},
\]
\[
D_k^{(3)}(\eta, \eta_0) = \frac{(x - x_0 + x^2 x_0) \cos \Delta x + (1 + x^2 - x x_0) \sin \Delta x}{x^2 x_0}, \] (4.18)

we arrive at the following final expression

\[
\rho^{(3)}_{\text{GW}}(\eta, \eta_0) = \frac{H^4}{64\pi^2} \int \frac{dk x^2}{k \omega_0} \left\{ \left(2x_0^2 - 7\right)\left(2x_0^4 - 2x_0^2 - 1 - 2x_0^4\omega_0^2\right) \right.
\]
\[ - \left(12x x_0 + 7\right) \cos 2\Delta x + 2\left(7x_0 - 3x\right) \sin 2\Delta x \right\}. \] (4.19)

Applying the same procedure as described above and integrating over \( k \), we have

\[
\rho^{(3)}_{\text{GW}}(\eta, \eta_0) \simeq \frac{27}{256\pi^2} H^4 \left(\frac{H}{\Lambda}\right)^2 \left[1 + \mathcal{O}\left(\frac{H^4}{\Lambda^4}\right)\right], \] (4.20)

i.e. even smaller than the result discussed in the case of the second Hamiltonian. In this case, the averaged energy density is much smaller than that of the background, and it is positive.

Thus, by taking the average of the energy-momentum pseudo-tensor, we were able to give an intrinsic characterization of the back-reaction effects that arise when quantum-mechanical
initial condition are assigned at a finite time and for all the physical wavelength in excess of a given fundamental scale $\Lambda^{-1}$.

V. CONCLUDING REMARKS

If quantum-mechanical initial conditions are assigned at a finite time $\eta_0$ during inflation and in excess of a given physical wavelength, ambiguities may arise. The presence of a cut-off $\Lambda$ in the physical momenta $k/a(\eta)$, by itself, does not specify any corrections in the late-time observables. In order to predict quantitatively the corrections in the scalar and tensor power spectra, it is mandatory to give a prescription for assigning the quantum mechanical normalization of the fluctuations. In general terms, the answer to this question is that quantum-mechanical fluctuations should minimize at $\eta_0$ a given Hamiltonian. However, since the problem is time-dependent, canonical transformations can change the form of the Hamiltonian. Different Hamiltonians, related by canonical transformations, lead to the same evolution of the fluctuations. However, since the initial state differs for each of the selected Hamiltonians, the power spectra of scalar and tensor modes will inherit computable corrections. Examples of this phenomenon were given in the present paper. Various, rather natural, Hamiltonians can be defined in the analysis of cosmological perturbations. It has been shown that the most adiabatic Hamiltonians lead to the smallest corrections, not only for the tensor modes of the geometry [8] but also for the scalar modes.

The criteria used to select one prescription or the other cannot be related only to “achievable” magnitude of the corrections in the two-point functions. On the contrary, it is important to estimate the energetic content of the initial states by minimizing the different Hamiltonians. The energy density of the quantum fluctuations should then be compared with that of the background geometry. This procedure provides a way of discarding initial states on the basis of excessive back-reaction effects. This exercise has been performed in detail, making use of the energy-momentum pseudo-tensor which is a common tool in the analysis of back-reaction effects of metric fluctuations.
If non-adiabatic Hamiltonians are minimized at $\eta_0$, the corrections to the tensor power spectrum can be as large as $10^{-6}$. However, the energy density of the initial state is, in this case, comparable with the energy density of the background geometry if $\Lambda \sim M_P$. On the contrary, if adiabatic Hamiltonians are minimized at $\eta_0$, the energy density of the fluctuations is always smaller than that of the background geometry by 12 or 24 orders of magnitude making then negligible back-reactiuon effects.

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APPENDIX A: TENSOR MODES OF THE GEOMETRY

In this appendix the explicit results concerning the tensor modes of the geometry will be swiftly recalled in view of the applications related to the back-reaction effects. The quadratic action for the tensor modes of the geometry can be written as

\[ S_{GW} = \frac{1}{64\pi G} \int d^4x a^2 \partial_\alpha h^i_j \partial_\beta h^i_j \eta^{\alpha\beta}, \]  
(A.1)

where \( \eta_{\alpha\beta} \) is the Minkowski metric and where \( \partial_i h^i_j = h^i_i = 0 \). In this gauge-invariant splitting of the degrees of freedom of the perturbed metric, the gravitational wave is a rank 2 tensor in three spatial dimensions, which is symmetric, traceless and divergenceless. If we then consider the action of a single polarization and redefine, accordingly, the tensor amplitude in order to include the Planck mass, we will see that the action is given by

\[ S^{(1)}_{GW} = \frac{1}{2} \int d^4x \partial^2 h \partial_\alpha h \eta^{\alpha\beta}, \]  
(A.2)

whose canonical momentum is simply given by \( \Pi = a^2 h' \) and whose associated Hamiltonian is

\[ H^{(1)}_{GW}(\eta) = \frac{1}{2} \int d^3x \left[ \Pi^2 + a^2 (\partial_i h)^2 \right]. \]  
(A.3)

Since this Hamiltonian is time-dependent, it is always possible to perform time-dependent canonical transformations, leading to a different Hamiltonian. In particular, if we define the rescaled field, \( \mu = ah \), the corresponding action will become

\[ S^{(2)}_{GW} = \frac{1}{2} \int d^4x \left[ \mu^2 - 2H\mu\mu' + H^2 \mu^2 + (\partial_i \mu)^2 \right], \]  
(A.4)

while the associated Hamiltonian can be written as

\[ H^{(2)}_{GW}(\eta) = \int d^3x \left[ \pi^2 + 2H\mu\pi + (\partial_i \mu)^2 \right], \]  
(A.5)

in terms of \( \mu \) and of the canonically conjugate momentum \( \pi = \mu' - H\mu \). Finally, a further canonical transformation can be performed starting from (A.5). Defining the generating functional in terms of the old fields \( \mu \) and of the new momenta \( \tilde{\pi} \),
\[ \mathcal{F}_{2\rightarrow 3}(\mu, \tilde{\pi}, \eta) = \int d^3 x \left( \mu \tilde{\pi}, -\frac{\mathcal{H}}{2} \mu^2 \right), \]  
(A.6)

the new Hamiltonian can be obtained by taking the partial (time) derivative of (A.6), with the result

\[ H_{gw}^{(3)}(\eta) = \frac{1}{2} \int d^3 x \left[ \tilde{\pi}^2 + (\partial_i \mu)^2 - \left( \mathcal{H}^2 + \mathcal{H}' \right) \mu^2 \right], \]  
(A.7)

where, recalling the definition of \( \pi \), from (A.6) we have \( \tilde{\pi} = \mu' \).

It is clear from the comparison of these results with the ones reported in Section II and III that there is a one-to-one correspondence between the Hamiltonians (and the actions) written in the case of tensor modes and those obtained in the case of scalar modes. In particular, Eqs. (A.3) and (A.5) will have their scalar counterpart in Eqs. (2.17) and (2.25), while (A.7) corresponds to (2.27).
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