Initial state of matter fields and trans-Planckian physics: Can CMB observations disentangle the two?

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The standard, scale-invariant, inflationary perturbation spectrum will be modified if the effects of trans-Planckian physics are incorporated into the dynamics of the matter field in a phenomenological manner, say, by the modification of the dispersion relation. The spectrum also changes if we retain the standard dynamics but modify the initial quantum state of the matter field. We show that, given any spectrum of perturbations, it is possible to choose a class of initial quantum states which can exactly reproduce this spectrum with the standard dynamics. We provide an explicit construction of the quantum state which will produce the given spectrum. We find that the various modified spectra that have been recently obtained from 'trans-Planckian considerations' can be constructed from suitable squeezed states above the Bunch-Davies vacuum in the standard theory. Hence, the CMB observations can, at most, be useful in determining the initial state of the matter field in the standard theory, but it can not help us to discriminate between the various Planck scale models of matter fields. We study the problem in the Schrödinger picture, clarify various conceptual issues and determine the criterion for negligible back reaction due to modified initial conditions.

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I. THE TANGLED WEB

The inflationary scenario [1–3] is at present the most attractive paradigm for generating the initial small scale inhomogeneities [4, 5]. These perturbations leave their imprints as anisotropies in the Cosmic Microwave Background (CMB) [6] and later evolve, due to gravitational instability, into the large-scale structures that we see around us today. While there is no natural particle physics candidate for generating the inflationary phase, a single (or a few) 'inflaton' field(s), with fine-tuned designer couplings, is (are) often introduced in order to reproduce the observed magnitude and shape of the perturbation spectrum.

In many of the models of inflation [3], the period of acceleration lasts sufficiently long so that length scales that are of cosmological interest today would have emerged from sub-Planckian length scales at the beginning of inflation. This suggests that physics at the very high energy scales can, in principle, modify the primordial perturbation spectrum [7] and these modifications can—in turn—leave their signatures on the CMB [8]. This has led to a considerable interest in understanding the effects of Planck scale physics on the inflationary perturbation spectrum [7]–[20] and the CMB [21–23].

Metric fluctuations during the inflationary epoch can be modeled by a quantized, massless and minimally coupled scalar field [4, 5, 24]. In the absence of a workable quantum theory of gravity, the Planck scale effects on the perturbation spectrum have to be studied by phenomenologically modifying the dynamics of the scalar field to take into account the quantum gravitational effects (for an early attempt in this direction, see Ref. [7]). The high energy models of the quantum scalar field that have been popular in the literature either introduce new features in the dispersion relation [8–12] or modify the standard uncertainty principle [13, 14] or assume that the spacetime coordinates are non-commutative [15]. (For other approaches, see Refs. [16–19] and, for a recent review of many of these approaches, see Ref. [20]). Some of these models have been utilized to evaluate not only the Planckian corrections to the standard, scale-invariant perturbation spectrum, but also the resulting signatures on the CMB [21–23]. This suggests the possibility that sufficiently accurate measurements of the CMB anisotropies can help us understand physics beyond the Planck scale.

There is, however, one serious difficulty with this approach, which we shall now briefly describe.

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$$\psi_{\mathbf{k}}(q_{\mathbf{k}},t) = \int d\bar{q}_{\mathbf{k}} K[q_{\mathbf{k}},t; \ \bar{q}_{\mathbf{k}},t_i(\mathbf{k})] \ \psi_{\mathbf{k}}[\bar{q}_{\mathbf{k}},t_i(\mathbf{k})], \tag{1}$$

where $K(q_{\mathbf{k}}, t; \bar{q}_{\mathbf{k}}, t_i)$ is the (path integral) kernel for an oscillator with time dependent parameters, which can be written down in terms of the classical solution (see, for e.g., Ref. [25]). To keep our discussion general, we have allowed for the possibility that the initial quantum state of each of the oscillators is specified at different times so that t_i can depend on \mathbf{k} . For instance, one may choose to specify the quantum state of each oscillator when the proper wavelength of that mode is equal to the Planck length [16, 26]. Of course, when the initial state of all the modes are specified at a given time, $t_i(\mathbf{k}) = t_i$ will be independent of \mathbf{k} . The *dynamics* of the system is completely specified by the kernel K.

It is obvious that the mathematics of a free scalar field in a Friedmann universe is trivial and is no more complicated than that of an oscillator with time dependent parameters. The perennial interest in this problem (allowing so many e-prints to be written!) arises from two conceptual issues:

- 1. To make any predictions, we need to know $\psi_{\mathbf{k}}(q_{\mathbf{k}}, t)$, which, in turn, requires knowing $\psi_{\mathbf{k}}[\bar{q}_{\mathbf{k}}, t_i(\mathbf{k})]$. We have absolutely no idea what to use for $\psi_{\mathbf{k}}[\bar{q}_{\mathbf{k}}, t_i(\mathbf{k})]$ and so different choices (usually called 'vacuum states', which is only a manner of speaking) can be investigated.
- 2. There are infinite number of such oscillators, leading to the standard, unresolved, issues of regularization in quantum field theory.

To make any progress, we need to make an assumption regarding $\psi_{\mathbf{k}}[\bar{q}_{\mathbf{k}}, t_i(\mathbf{k})]$ and our results are only as valid as this assumption.

If we now further modify the dynamics (due to a phenomenological input regarding trans-Planckian physics), we will be changing the form of the kernel K. But, since we can only observe the integrated effect of K and $\psi_{\mathbf{k}}[\bar{q}_{\mathbf{k}}, t_i(\mathbf{k})]$, the observations can tell us something about the K (and trans-Planckian physics) only if we assume something about $\psi_{\mathbf{k}}[\bar{q}_{\mathbf{k}}, t_i(\mathbf{k})]$. The usual assumption is to consider the initial quantum state to be the Bunch-Davies vacuum [27], but it is only an assumption. The crucial question is whether the effect of trans-Planckian physics can be mimicked by a different choice of the initial state other than the Bunch-Davies vacuum.

We shall show that any (modified) spectrum of fluctuations can be obtained from a suitably chosen initial state $\psi_{\mathbf{k}}[\bar{q}_{\mathbf{k}}, t_i(\mathbf{k})]$, which will prove to be a squeezed state above the Bunch-Davies vacuum in the standard theory. We shall provide an explicit construction of the state for any given spectrum of perturbations that is observed. So, if some specific deviation from the standard scale invariant spectrum is seen in the CMB, a conservative interpretation will be to attribute it to a deviation from the standard initial state of the theory. Unless this possibility is ruled out, one cannot claim that the observation supports, say, a particular model of trans-Planckian phenomenology. Motivated by this result, we argue that the CMB can at most help us identify the quantum state of the scalar field in the standard theory, but it can *not* aid us in discriminating between the various Planck scale models of matter fields.

The remainder of this paper is organized as follows. In Section II, we set up the formalism and study the evolution of a Gaussian quantum state in a Friedmann universe. We apply this formalism to power law inflation in Section III. In Section IV, we show that any modified spectrum can be reproduced from a suitable squeezed state above the Bunch-Davies vacuum in the standard theory. We explicitly discuss four modified spectra that have recently been considered in the literature. In Section V, we evaluate the energy density in these excited states and examine whether these modified spectra also lead to a large back reaction on the inflating background. Finally, in Section VI, we conclude with a discussion on the wider implications of our analysis.

Our conventions and notations are as follows. We shall set $\hbar = c = 1$ and the metric signature we shall adopt is (+, -, -, -).

II. EVOLUTION OF THE QUANTUM STATE: GENERAL FORMALISM

Consider a flat Friedmann universe described by the line-element

$$ds^{2} = dt^{2} - a^{2}(t) \, d\mathbf{x}^{2} = a^{2}(\eta) \left(d\eta^{2} - d\mathbf{x}^{2} \right), \tag{2}$$

where t is the cosmic time, a(t) is the scale factor and η denotes the conformal time with $d\eta = dt/a(t)$. The scalar as well as the tensor perturbations during the inflationary epoch can be modeled by a massless and minimally coupled,

real scalar field, say, Φ , governed by the action [1, 2, 4, 5, 24, 28]

$$S[\Phi] = \frac{1}{2} \int d^4x \sqrt{-g} \,\partial_\mu \Phi \,\partial^\mu \Phi. \tag{3}$$

The homogeneity and isotropy of the Friedmann metric (2) allows us to decompose the scalar field Φ as

$$\Phi(x) = \int \frac{d^3 \mathbf{k}}{(2\pi)^{3/2}} \,\bar{q}_{\mathbf{k}}(\eta) \,e^{i\mathbf{k}\cdot\mathbf{x}} \tag{4}$$

The $\bar{q}_{\mathbf{k}}$ is complex and for each \mathbf{k} gives two degrees of freedom in the real and imaginary parts of $\bar{q}_{\mathbf{k}} = A_{\mathbf{k}} + iB_{\mathbf{k}}$. But since Φ is a real scalar field, we can relate the variables for \mathbf{k} to that for $-\mathbf{k}$ by $A_{\mathbf{k}}^* = A_{-\mathbf{k}}, B_{\mathbf{k}}^* = -B_{-\mathbf{k}}$ and only half the modes are independent degrees of freedom. Therefore, we can work with new set of the real modes $q_{\mathbf{k}}$ for all values of \mathbf{k} with suitable redefinition, say, by taking $q_{\mathbf{k}} = A_{\mathbf{k}}$ for one half of \mathbf{k} vectors and $q_{-\mathbf{k}} = B_{\mathbf{k}}$ for the other half. In terms of real variables $q_{\mathbf{k}}$, the action (3) can be expressed as follows:

$$S[\Phi] = \frac{1}{2} \int d^3 \mathbf{k} \int d\eta \ a^2 \left(q_{\mathbf{k}}^{\prime 2} - k^2 \ q_{\mathbf{k}}^2 \right), \tag{5}$$

where the primes denote differentiation with respect to the conformal time η and $k = |\mathbf{k}|$. The action (5) describes a collection of independent oscillators with time dependent mass a^2 and frequencies k. (It is sometimes useful to keep track of the real and imaginary parts of the $\bar{q}_{\mathbf{k}}$ separately. In our case, this is unnecessary and we can define our system in terms of real $q_{\mathbf{k}}$. Our approach is completely equivalent to the conventional one. Also, note that, in the literature, one usually finds the Fourier decomposition in Eq. (4) expressed in terms of $(q_{\mathbf{k}}/a)$ rather than with just $q_{\mathbf{k}}$. Such a decomposition will lead to oscillators that have a unit mass, but a time-dependent frequency, say, $\omega_{\mathbf{k}}^2$, which can become negative at super Hubble scales. In our description—which is, again, equivalent to the conventional one—the mass varies as a^2 , but the frequency is constant.)

In the Schrödinger picture, the scalar field Φ can be quantized by quantizing each independent oscillator $q_{\mathbf{k}}$. The Hamiltonian corresponding to the k-th oscillator is given by

$$\mathsf{H}_{\mathbf{k}} = \frac{p_{\mathbf{k}}^2}{2\,a^2} + \frac{1}{2}\,a^2k^2q_{\mathbf{k}}^2,\tag{6}$$

where $p_{\mathbf{k}}$ is the momentum conjugate to the coordinate $q_{\mathbf{k}}$. Therefore, each of the oscillators satisfy the Schrödinger equation

$$i\frac{\partial\psi_{\mathbf{k}}}{\partial\eta} = -\frac{1}{2a^2}\frac{\partial^2\psi_{\mathbf{k}}}{\partial q_{\mathbf{k}}^2} + \frac{1}{2}a^2k^2q_{\mathbf{k}}^2\psi_{\mathbf{k}}$$
(7)

and the complete quantum state of the field is described by a wave function that is a product of $\psi_{\mathbf{k}}$ for all \mathbf{k} . Equivalently, the time evolution of the wave function can be described by Eq. (1) in terms of the kernel $K[q_{\mathbf{k}}, t; \bar{q}_{\mathbf{k}}, t_i(\mathbf{k})]$.

As we do not expect a large scale, spatially inhomogeneous classical scalar field to be present in the universe, it is conventional to assume that the expectation value $\langle \psi_{\mathbf{k}} | \hat{q}_{\mathbf{k}} | \psi_{\mathbf{k}} \rangle$ vanishes in the quantum state of the field for $\mathbf{k} \neq 0$. (Since $\langle \psi_{\mathbf{k}} | \hat{q}_{\mathbf{k}} | \psi_{\mathbf{k}} \rangle$ satisfies the classical equations of motion, this condition can be satisfied at all times if suitable initial conditions are imposed at an early epoch.) When the mean value vanishes, the power spectrum as well as the statistical properties of the perturbations are completely characterized by the two-point functions of the quantum field. Therefore, the power spectrum of the perturbations per logarithmic interval, viz. $[k^3 \mathcal{P}_{\Phi}(k)]$, is given by (see, for instance, Ref. [28])

$$k^{3} \mathcal{P}_{\Phi}(k) = \frac{k^{3}}{2\pi^{2}} \int_{-\infty}^{\infty} dq_{\mathbf{k}} |\psi_{\mathbf{k}}(q_{\mathbf{k}}, \eta)|^{2} q_{\mathbf{k}}^{2}.$$
(8)

Though this result is fairly well established in literature, there are a couple of subtleties we would like to mention.

The quantity on the right hand side of the above equation depends on the time η and one needs to settle at what epoch it has to be evaluated. In classical perturbation theory, one evaluates the perturbation at Hubble exit, i.e. when the physical wavelength $(k/a)^{-1}$ of the mode corresponding to the wavenumber **k** is comparable to the Hubble radius H^{-1} , where $H = (a'/a^2)$. In other words, the spectrum is to be evaluated when, say, (k/a) = (z H), where z is a number of the order of unity. This is a thumb rule which accounts for the differences in the evolutionary history of the mode when its proper wavelength is smaller than the Hubble radius as compared to the situation when it is

larger than the Hubble radius. There is no simple way of deciding whether one should evaluate the expression when z = 1 or when, say, $z = (2\pi)$. In the literature, one also finds the perturbation spectrum evaluated at super Hubble scales (i.e. when $(k/aH) \rightarrow 0$) which corresponds to the limit $z \rightarrow 0$. Even for the simplest case of exponential inflation with the Bunch-Davies vacuum for the initial state, these results differ by a numerical factor. In this case, we will find that, $[k^3 \mathcal{P}_{\Phi}(k)] = [C(z) (H^2/2\pi^2)]$, where $C(z) = [(1+z^2)/2]$ (see Eq. (47) below). It is sometimes claimed erroneously in the literature, that evaluating the spectrum as $z \to 0$ leads to the same result as evaluating it at z = 1. (See, for instance, Ref. [2], pp. 182–183. Notice that, in this reference, Eq. (7.87) is wrong by a factor 2 and the claim after Eq. (7.98) that Eqs. (7.98) and (7.87) are "in agreement" is incorrect. This can be trivially verified from equations (7.96) and (7.98).) In this particular case (i.e. exponential inflation with the Bunch-Davies vacuum for the initial state), this discrepancy is not of great importance since it only changes the amplitude by a numerical factor, since C(1) = 1, $C(2\pi) = \left[\left(1 + 4\pi^2 \right)/2 \right]$ and C(0) = (1/2). But when one considers the power spectrum in a more general context, these choices will lead to a more complicated difference, as we shall see. Of course, if one first approximates the wave function $\psi_{\mathbf{k}}(q_{\mathbf{k}},\eta)$ with an assumption such as $z \to 0$ (when the expressions do simplify) and then evaluate it at $z \simeq 1$, one is being inconsistent. This may sound rather elementary but we were surprised to find papers in the literature which do this. Any result which crucially depends on one specific choice for z in computing the power spectrum is suspect. In what follows, we shall usually assume that the expressions are evaluated for z = 1(i.e. when (k/a) = H) when the choice of z is not of much consequence and will comment on the results which depend crucially on this choice.

Let us now consider the problem of determining the wave function $\psi_{\mathbf{k}}(q_{\mathbf{k}},\eta)$. For a time dependent oscillator, there is no concept of a unique ground ('vacuum') state unless the parameters describing the oscillator go to a constant value asymptotically—which, in general, it does not, for the Friedmann universe. There is, however, a class of solutions to the time dependent harmonic oscillator which are *form invariant* in the sense that the $q_{\mathbf{k}}$ dependence of the wave function $\psi_{\mathbf{k}}(q_{\mathbf{k}},\eta)$ is the same at all η . One can show that the most general state having this property is an exponential of a quadratic function of $q_{\mathbf{k}}$ and such states have been extensively investigated in the past in different contexts (see, for instance, Refs. [29, 30]). When $\langle \psi_{\mathbf{k}} | \hat{q}_{\mathbf{k}} | \psi_{\mathbf{k}} \rangle = 0$, the mean value of the Gaussian vanishes and the quantum state of the mode can be described by the wave function [28–30]

$$\psi_{\mathbf{k}}\left(q_{\mathbf{k}},\eta\right) = N_{k}(\eta) \exp\left[R_{k}(\eta) q_{\mathbf{k}}^{2}\right],\tag{9}$$

where $N_k(\eta)$ and $R_k(\eta)$ are complex quantities. The normalization condition on the wave function then relates N_k and R_k as follows:

$$|N_k|^2 = \left(\frac{R_k + R_k^*}{\pi}\right)^{1/2}.$$
 (10)

Therefore, the only non trivial aspect of the quantum state is encoded in the time dependence of the function $R_k(\eta)$. It can be shown that (for details, see Appendix A), if we introduce a function $\mu_k(\eta)$ through the relation $R_k = -(i a^2/2) (\mu'_k/\mu_k)$, then μ_k satisfies the differential equation

$$\mu_k'' + 2\frac{a'}{a}\mu_k' + k^2\mu_k = 0 \tag{11}$$

which is the same as the classical equation of motion satisfied by the oscillator variable $q_{\mathbf{k}}$. We find that the perturbation spectrum (8) corresponding to the wave function (9) can be expressed as (see Appendix A)

$$k^{3} \mathcal{P}_{\Phi}(k) = \frac{k^{3}}{2\pi^{2}} \left(\frac{|\mu_{k}|^{2}}{W(k)} \right), \tag{12}$$

where W(k) is a k-dependent constant determined by the Wronskian condition for μ_k [cf. Eq. (A5)].

Since the differential equation (11) has real coefficients, if s_k is a solution, so is s_k^* and the general solution is a linear superposition of the form, say, $\mu_k = [\mathcal{A}(k) s_k + \mathcal{B}(k) s_k^*]$. The quantum state $\psi_{\mathbf{k}}(q_{\mathbf{k}}, \eta)$, however, depends only on R_k which is independent of the overall scaling of μ_k . This feature translates into the power spectrum (12) as well; a global scaling of μ_k also changes the Wronskian W(k) leaving $[|\mu_k|^2/W(k)]$ invariant. Hence, we can ignore the overall scaling in μ_k . We shall set $\mathcal{A}(k)$ to unity and choose the Wronskian W(k) to be

$$W(k) = 1 - |\mathcal{B}(k)|^2.$$
(13)

Then, the power spectrum (12) reduces to

$$k^{3} \mathcal{P}_{\Phi}(k) = \frac{k^{3}}{2\pi^{2}} \left(\frac{\left[1 + |\mathcal{B}(k)|^{2}\right] |s_{k}|^{2} + 2 \operatorname{Re.} \left[\mathcal{B}(k) s_{k}^{*2}\right]}{1 - |\mathcal{B}(k)|^{2}} \right).$$
(14)

(In the Heisenberg picture, one usually introduces the Bogoliubov coefficients $\alpha(k)$ and $\beta(k)$. These coefficients are related to $\mathcal{B}(k)$ through the relation: $\mathcal{B}(k) = [\beta(k)/\alpha(k)]$. In terms of $\alpha(k)$ and $\beta(k)$, the Wronskian condition (13) reduces to the standard normalization condition, viz. $(|\alpha(k)|^2 - |\beta(k)|^2) = 1$.) The dynamics imposes no restrictions on the form of $\mathcal{B}(k)$, which is related to the choice of the quantum state at any specified time. The spectrum evidently depends on $\mathcal{B}(k)$ and with a suitable choice for $\mathcal{B}(k)$ we can generate any, given, reasonable spectrum.

A. Squeezing and instantaneous particle content of the quantum state

We shall see concrete examples of this result and its consequences for the case of power law inflation in the following sections. But, before we do that, let us try and understand what the wave function (9) implies. The wave function (9), in general, describes what is referred to in the literature as a squeezed state (see, for e.g., Refs. [30]). Squeezed states for a given mode $q_{\mathbf{k}}$ are described by two parameters, say, r_k and φ_k and the quantity R_k can be related to these two parameters as follows [30]:

$$R_k = \left(\frac{k a^2}{2}\right) \left(\frac{\cosh r_k + e^{2i\varphi_k} \sinh r_k}{\cosh r_k - e^{2i\varphi_k} \sinh r_k}\right).$$
(15)

This, however, does not lead to any deeper insight in this particular case.

An alternative procedure, which is physically better motivated, is to compare the quantum state (9) with the instantaneous ground state at any given time. We recall that the oscillators have the frequency k and a time dependent mass $a^2(\eta)$. The ground state of a harmonic oscillator with the frequency k and mass $a^2(\eta)$ will depend on $q_{\mathbf{k}}$ as $\exp -[(k/2) a^2 q_{\mathbf{k}}^2]$. Suppose we are given a specific quantum state determined by the function $R_k(\eta)$. We can attempt to solve the equation $R_k(\eta) = [k a^2(\eta)/2]$ for η determining a function, say, $\bar{\eta}(k)$. If such a real solution can be obtained, then we can interpret our quantum state as the ground state for the mode $q_{\mathbf{k}}$ at the moment of time $\bar{\eta}(k)$. In general, however, this will not be possible since $R_k(\eta)$ is complex. (One exception is in the adiabatic approximation, in which the mode μ_k is chosen such that that $R_k \approx (k a^2/2)$ so that this condition is identically satisfied; as to be expected, the state evolves as an adiabatic vacuum in this case.)

More generally, one can expand our quantum state in terms of the instantaneous states of the harmonic oscillator at any given time η , thereby identifying its particle content. At any given time η , the *instantaneous* ground and excited states of the oscillators $q_{\mathbf{k}}$ can be described by the wave functions

$$\phi_n (q_{\mathbf{k}}, \eta) = (2^n n!)^{-1/2} \left(\frac{k a^2}{\pi}\right)^{1/4} H_n \left(\sqrt{k} a q_{\mathbf{k}}\right) \exp \left(\frac{k}{2} a^2 q_{\mathbf{k}}^2 + iE_n \eta\right), \tag{16}$$

where H_n are the Hermite polynomials, $E_n = [(n + (1/2))k]$ and n = 0, 1, 2, ... We can now decompose the actual wave function $\psi_{\mathbf{k}}(q_{\mathbf{k}}, \eta)$ in terms of the above instantaneous wave functions as follows:

$$\psi_{\mathbf{k}}\left(q_{\mathbf{k}},\eta\right) = \sum_{n=0}^{\infty} c_n(k,\eta) \,\phi_n\left(q_{\mathbf{k}},\eta\right) \,e^{iE_n\eta},\tag{17}$$

where the decomposition amplitude c_n is given by the integral

$$c_n(k,\eta) = \int_{-\infty}^{\infty} dq_{\mathbf{k}} \ \psi_{\mathbf{k}}(q_{\mathbf{k}},\eta) \ \phi_n^*(q_{\mathbf{k}},\eta).$$
(18)

On evaluating this integral, we find that the amplitude c_n corresponding to the odd n's vanish, while the amplitude for the even n's are given by

$$c_{(2n)}(k,\eta) = \Delta_k \left(\frac{\sqrt{(2n)!}}{2^n n!}\right) \Gamma_k^n,\tag{19}$$

where

$$\Delta_k = N_k \left(\frac{k a^2}{\pi}\right)^{1/4} \left(\frac{2\pi i \mu_k / a^2}{\mu'_k + i k \, \mu_k}\right)^{1/2} \tag{20}$$

is a n-independent normalization and

$$\Gamma_k = -\left(\frac{\mu'_k - ik\,\mu_k}{\mu'_k + ik\,\mu_k}\right).\tag{21}$$

The probability $P_k(n)$ for our quantum state to be in the (2n)-th excited state of the instantaneous harmonic oscillator mode can be thought of as the probability for existence of n pairs of particles at the time η . This is given by

$$P_k(n) \equiv |c_{(2n)}(k,\eta)|^2 = P_k(0) \left(\frac{(2n)!}{n!^2}\right) \left(\frac{|\Gamma_k|^2}{4}\right)^n$$
(22)

and the generating function $\mathcal{G}_k(\sigma)$ for this pair creation probability can be expressed in closed form as follows:

$$\mathcal{G}_k(\sigma) \equiv \sum_{n=0}^{\infty} P_k(n) \, \mu^n = \frac{P_k(0)}{\left(1 - \sigma \, |\Gamma_k|^2\right)^{1/2}} = \left(\frac{1 - |\Gamma_k|^2}{1 - \sigma \, |\Gamma_k|^2}\right)^{1/2}.$$
(23)

The last equation follows from explicitly calculating $P_k(0)$ or—more simply—by noticing that $P_k(n)$ is normalized and hence $\mathcal{G}_k(1) = 1$. Given this generating function one can compute various moments of the created particles. In particular, the mean number of *particles*, which are present at the time η (obtained by doubling the mean number of pairs) is given by

$$\langle n_k \rangle = \frac{|\Gamma_k|^2}{1 - |\Gamma_k|^2}.$$
(24)

These equations exhibit the time dependent particle content of our quantum state and it can be computed once the function $\mu_k(\eta)$ is specified. Though, $\langle n_k \rangle$ can not be interpreted as particles with respect to the in-vacuum at late times, it is related in a simple manner to the energy density. The expectation value of the Hamiltonian operator corresponding to the oscillator $q_{\mathbf{k}}$, say, \mathcal{E}_k , can be evaluated using the wave function (9). We obtain that

$$\mathcal{E}_{k} = \left(\frac{a^{2}}{2W(k)}\right) \left(|\mu_{k}'|^{2} + k^{2} |\mu_{k}|^{2}\right)$$
(25)

and, on using the expressions (21), (24) and (25), we find that \mathcal{E}_k and $\langle n_k \rangle$ are related as follows:

$$\mathcal{E}_k = \left(\langle n_k \rangle + \frac{1}{2} \right) \, k. \tag{26}$$

The energy density of the quantum scalar field is then given by

$$\rho = \frac{1}{2\pi^2 a^4} \int_0^\infty dk \; k^2 \, \mathcal{E}_k = \frac{1}{2\pi^2 a^4} \int_0^\infty dk \; k^3 \left(\langle n_k \rangle + \frac{1}{2} \right). \tag{27}$$

We will require these results while discussing the issue of back reaction due to the modified initial conditions.

B. Wigner function

Another possible way of understanding the physical content of a quantum state, especially its classicality, is through the Wigner function (see, for e.g., Ref. [31]). Given a wave function $\psi_{\mathbf{k}}(q_{\mathbf{k}}, \eta)$, the Wigner function $\mathcal{W}_k(q_{\mathbf{k}}, p_{\mathbf{k}}, \eta)$ is defined as [31]

$$\mathcal{W}_k\left(q_{\mathbf{k}}, p_{\mathbf{k}}, \eta\right) = \frac{1}{2\pi} \int_{-\infty}^{\infty} du_{\mathbf{k}} \psi_{\mathbf{k}}^* \left[\left(q_{\mathbf{k}} + \frac{1}{2}u_{\mathbf{k}}\right), \eta \right] \psi_{\mathbf{k}} \left[\left(q_{\mathbf{k}} - \frac{1}{2}u_{\mathbf{k}}\right), \eta \right] e^{ip_{\mathbf{k}}u_{\mathbf{k}}}.$$
(28)

The Wigner function corresponding to the Gaussian wave function (9) can be expressed as

$$\mathcal{W}_k\left(q_{\mathbf{k}}, p_{\mathbf{k}}, \eta\right) = \frac{1}{\pi} \exp\left[\frac{q_{\mathbf{k}}^2}{\sigma_k^2(\eta)} + \sigma_k^2(\eta) \left(p_{\mathbf{k}} - \mathcal{J}_k(\eta) q_{\mathbf{k}}\right)^2\right],\tag{29}$$

where σ_k and \mathcal{J}_k are given by

$$\sigma_k^2 = (R_k + R_k^*)^{-1}$$
 and $\mathcal{J}_k = i (R_k - R_k^*).$ (30)

On using the relations (A3) and (A5), we find that the quantities σ_k and \mathcal{J}_k can be written in terms of the function μ_k and the Wronskian W(k) as follows:

$$\sigma_k^2 = \left(\frac{2\,|\mu_k|^2}{W(k)}\right); \qquad \mathcal{J}_k = \left(\frac{a^2}{2}\right) \frac{d\,\ln|\mu_k|^2}{d\eta}. \tag{31}$$

The quantum versus classical nature of the wave function depends on the evolutionary behaviour of $\sigma_k(\eta)$ and $\mathcal{J}_k(\eta)$. It is possible for evolution to lead to a Wigner function sharply peaked around some region in the phase space, starting from a Wigner function which is uncorrelated in phase space [32]. For example, in the case of exponential inflation and the Bunch-Davies vacuum for the initial state which we will discuss later on (see Eqs. (43) and (55)), we we will find that

$$\sigma_k^2 = \left(\frac{H^2}{k^3}\right) \left(1 + k^2 \eta^2\right); \qquad \mathcal{J}_k = \left(\frac{k^2}{H^2 \eta}\right) \left(1 + k^2 \eta^2\right)^{-1}. \tag{32}$$

In such a case, $\mathcal{J}_k(\eta) \to 0, \sigma_k^2 \to \infty$ at early times $(\eta \to -\infty)$ which corresponds to a state sharply peaked around the *q*-axis. At late times $(\eta \to 0)$, however, we have $\mathcal{J}_k(\eta) \to \infty$ with a finite σ_k^2 which corresponds to a state sharply peaked around the *p*-axis. In fact, whenever $k\eta \to 0$ (corresponding to super Hubble scales), the Wigner function gets peaked around a classical trajectory. This can be verified more explicitly by studying the classical solution for our problem. Classically, for the case of exponential inflation, we can write the general solution for $q_{\mathbf{k}}$ as:

$$q_{\mathbf{k}} = 2\operatorname{Re}\left[-\mathcal{L}H\eta\left(1+\frac{i}{k\eta}\right)e^{ik\eta}\right]$$
(33)

where $\mathcal{L}(k)$ is an arbitrary complex number. Writing $\mathcal{L}(k) = L(k) e^{i l(k)}$, this solution becomes

$$q_{\mathbf{k}} = -2L \, H\eta \, \cos\left[k\eta + l(k)\right] + \frac{2L \, H}{k} \, \sin\left[k\eta + l(k)\right]. \tag{34}$$

The conjugate momentum $p_{\mathbf{k}} = (a^2 q'_{\mathbf{k}})$ corresponding to the above $q_{\mathbf{k}}$ is then given by

$$p_{\mathbf{k}} = -\left(2L\,k/H\eta\right)\,\sin\left[k\eta + l(k)\right].\tag{35}$$

The trajectory of the system in the phase space is given by

$$\frac{q_{\mathbf{k}}}{L} = \frac{H^2 \eta}{k^2 L} p_{\mathbf{k}} \pm 2H\eta \left(1 - \frac{H^2 \eta^2}{4L^2 k^2} p_{\mathbf{k}}^2\right)^{1/2}$$
(36)

At late times (when $\eta \to 0$) or at super Hubble scales, we have $(q_{\mathbf{k}}/p_{\mathbf{k}}) \to 0$ indicating a trajectory along the vertical p axis, which is precisely what we get from the Wigner function. On the other hand, one cannot naively take the early time limit (when $\eta \to -\infty$) with finite $q_{\mathbf{k}}, p_{\mathbf{k}}$ in the trajectory in Eq.(36) since $q_{\mathbf{k}}$ becomes imaginary. One can, however, take the limit of $\eta \to -\infty, p_{\mathbf{k}} \to 0$ keeping $\eta p_{\mathbf{k}}$ constant; in this limit, we obviously get a trajectory along the horizontal $p_{\mathbf{k}} = 0$ axis, which matches with the analysis based on the Wigner function. Incidentally, notice that the Hamiltonian for our system has a kinetic energy term $K \propto p^2/a^2 \propto (p\eta)^2$ and a potential energy term $U \propto a^2 q^2 \propto (q/\eta)^2$. At late times, potential energy dominates over kinetic energy leading to near classical behaviour peaked around q = 0; on the other hand, at early times if we let $\eta \to -\infty$ keeping $(p\eta)$ fixed, the kinetic energy remains finite and dominates over the potential energy. This is the quantum regime. (We plan to explore these ideas in detail in a separate publication).

III. POWER LAW AND EXPONENTIAL INFLATION

A. Standard initial conditions

Let us now apply the above formalism to the case of power law inflation. Power law inflation corresponds to the situation wherein the scale factor a(t) grows with t as

$$a(t) = a_0 t^p, (37)$$

where p > 1. In terms of the conformal time η , this scale factor can be written as

$$a(\eta) = \left(-\mathcal{H}\,\eta\right)^{(\gamma+1)},\tag{38}$$

where γ and \mathcal{H} are given by

$$\gamma = -\left(\frac{2p-1}{p-1}\right) \quad \text{and} \quad \mathcal{H} = (p-1) a_0^{1/p}. \tag{39}$$

Note that $\gamma \leq -2$ with $\gamma = -2$ corresponding to exponential inflation. Also, the quantity \mathcal{H} denotes the characteristic energy scale associated with inflation and, in the case of exponential inflation, it exactly matches the Hubble scale.

On writing $\mu_k = (f_k/a)$ in the differential equation (11), we find that f_k satisfies the following equation:

$$f_k'' + \left[k^2 - \left(\frac{a''}{a}\right)\right] f_k = 0.$$

$$\tag{40}$$

In a Friedmann universe described by the scale factor (38), the general solution to this differential equation can be written as (see, for e.g., Ref. [33], p. 362)

$$f_k(\eta) = \frac{\sqrt{\pi\eta}}{2} \left(e^{-(i\pi\gamma/2)} H^{(1)}_{-(\gamma+\frac{1}{2})}(k\eta) + \mathcal{B}(k) e^{(i\pi\gamma/2)} H^{(2)}_{-(\gamma+\frac{1}{2})}(k\eta) \right), \tag{41}$$

where $H_{\nu}^{(1)}$ and $H_{\nu}^{(2)}$ are the Hankel functions of the first and the second kind, respectively. The k-dependent constant $\mathcal{B}(k)$ is to be fixed by choosing suitable initial conditions for each of the modes. For the above solution, it can be easily shown that the Wronskian condition (A5) leads to the relation (13) between $\mathcal{B}(k)$ and W(k).

Let us first briefly review the standard theory (see, for e.g., Ref. [28]) in which the initial conditions are imposed on sub-Hubble scales, i.e. when the physical wavelengths $(k/a)^{-1}$ of the modes are much smaller than the Hubble radius H^{-1} . A natural choice for the initial condition will be the one in which each of the oscillators $q_{\mathbf{k}}$ is in its ground state at sub-Hubble scales. This condition implies that the wave function (9) has the following asymptotic form:

$$\lim_{(k/aH)\to\infty} \psi_{\mathbf{k}}\left(q_{\mathbf{k}},\eta\right) \to \left(\frac{k\,a^2}{\pi}\right)^{1/4} \,\exp\left(\frac{k\,a^2}{2}\,q_{\mathbf{k}}^2 + i\frac{k}{2}\eta\right) \tag{42}$$

which, in turn, requires that, as $(k/aH) \to \infty$, we need to have $R_k \to (k a^2/2)$ and $N_k \to (k a^2/\pi)^{1/4} e^{-ik\eta/2}$. These conditions can be satisfied provided $f_k \to (e^{ik\eta}/\sqrt{2k})$ as $(k/aH) \to \infty$ [cf. Eqs. (A3), (A4) and (A6)]. This can be achieved by setting $\mathcal{B}(k) = 0$ in Eq. (41), so that we have

$$f_k(\eta) = \left(\frac{\sqrt{\pi\eta}}{2}\right) e^{-(i\gamma\pi/2)} H^{(1)}_{-(\gamma+\frac{1}{2})}(k\eta)$$
(43)

and this choice corresponds to what is known as the Bunch-Davies vacuum [27]. Note that, according to the Eq. (13), $\mathcal{B}(k) = 0$ implies W(k) = 1. Therefore, on substituting the above f_k in Eq. (12) and imposing the condition of Hubble exit, viz. that (k/a) = (zH), we obtain the spectrum of perturbations to be (for a recent discussion, see, for e.g., Ref. [34])

$$k^{3} \mathcal{P}_{\Phi}(k) = C(z) \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left(\frac{k}{\mathcal{H}}\right)^{2(\gamma+2)},\tag{44}$$

where C(z) is given by

$$C(z) = \left(\frac{\pi}{4}\right) \left| H^{(1)}_{-\left(\gamma + \frac{1}{2}\right)} \left[(\gamma + 1) z \right] \right|^2 \left| (\gamma + 1) z \right|^{-(2\gamma + 1)}.$$
(45)

In the limit of $z \to 0$, this expression simplifies to [34]

$$C(0) = \left(\frac{2^{-2(\gamma+1)}}{2\pi}\right) \left|\Gamma\left[-\left(\gamma+\frac{1}{2}\right)\right]\right|^2.$$
(46)

In the case of exponential inflation, corresponding to $\gamma = -2$, the perturbation spectrum in Eq. (44) reduces to

$$k^3 \mathcal{P}_{\Phi}(k) = \left(\frac{1+z^2}{2}\right) \frac{\mathcal{H}^2}{2\pi^2} \tag{47}$$

which is a spectrum that is exactly scale invariant. (Note that, for exponential inflation, $\mathcal{H} = H$.) As we pointed out before, the numerical value of the amplitude depends on whether we evaluate the expression at $z = 1, z = (2\pi)$ or as $z \to 0$.

Let us now consider a more general situation with $\mathcal{B}(k) \neq 0$. It is convenient to write

$$\mathcal{B}(k) = B(k) \exp\left[i \, b(k)\right],\tag{48}$$

so that the resulting power spectrum can be expressed as [on assuming that Hubble exit occurs at (k/a) = (zH)]

$$k^{3} \mathcal{P}_{\Phi}(k) = C(z) \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left(\frac{k}{\mathcal{H}}\right)^{2(\gamma+2)} \left[1 - B^{2}(k)\right]^{-1} \left(1 + B^{2}(k) + 2B(k)\cos\left[b(k) + \pi\gamma - 2\theta\right]\right), \tag{49}$$

where θ is the phase of the Hankel function $H_{\nu}^{(1)}$ at Hubble exit, given by the relation

$$H^{(1)}_{-\left(\gamma+\frac{1}{2}\right)}[(\gamma+1)z] = \left| H^{(1)}_{-\left(\gamma+\frac{1}{2}\right)}[(\gamma+1)z] \right| e^{i\theta}.$$
(50)

If we write $\cos[b(k) + \pi\gamma - 2\theta] = d(k)$, then, the power spectrum (49) reduces to

$$k^{3} \mathcal{P}_{\Phi}(k) = C(z) \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left(\frac{k}{\mathcal{H}}\right)^{2(\gamma+2)} \left(\frac{1+B^{2}(k)+2B(k)d(k)}{1-B^{2}(k)}\right),$$
(51)

where $-1 \leq d(k) \leq 1$.

At super-Hubble scales (i.e. as $z \to 0$), the above power spectrum bears a simple relation to the mean number of particles $\langle n_k \rangle$ as given by Eq. (24). We find that they are related as follows:

$$k^{3} \mathcal{P}_{\Phi}(k) \simeq \left(\frac{\mathcal{H}^{2}}{\pi^{2}}\right) \left(\langle n_{k} \rangle \left[(\gamma+1) z \right]^{2} \right) \left(\frac{k}{\mathcal{H}(\gamma+1) z} \right)^{2(\gamma+2)}.$$
(52)

This relation can be easily obtained by using the expression (25) for \mathcal{E}_k and Eq. (26) which relates \mathcal{E}_k to $\langle n_k \rangle$. At super-Hubble scales (i.e. as $(k\eta) \to 0$), the general solution for f_k as given by Eq. (41) reduces to

$$f_k(\eta) \propto \frac{1}{\sqrt{k}} (k\eta)^{(\gamma+1)}.$$
(53)

On using this expression, it is straightforward to show that $\mu'_k = (f_k/a)'$ is sub-dominant to μ_k at super-Hubble scales. Then, from Eqs. (25) and (26), we have

$$\mathcal{E}_k \simeq \frac{k^2 a^2}{2} \left(\frac{|\mu_k|^2}{W(k)} \right) \simeq \langle n_k \rangle \, k. \tag{54}$$

It is then evident from the definition (12) that the power spectrum will be proportional to the mean number of particles at super Hubble scales. On using the above result, one can easily arrive at the relation (52), by first imposing the condition for Hubble exit [viz. that (k/a) = (zH)] and then taking the limit $z \to 0$. In the limit of exponential inflation (i.e. as $\gamma \to -2$), we find that $[k^3 \mathcal{P}_{\Phi}(k)] \simeq (H^2 \langle n_k \rangle z^2 / \pi^2)$ at super-Hubble scales.

In the next section, we shall show that any modified spectrum obtained from a high energy model can be constructed in the standard theory by simply choosing suitable forms for the functions B(k) and b(k). But, before we do that, we shall discuss an alternative procedure for imposing the initial conditions wherein the initial condition for different modes are imposed at different times.

B. Specifying initial conditions when $[k/a(\eta_k)] \simeq L_{\rm P}^{-1}$

In the last section, we chose the quantum state by imposing a condition as $(k/aH) \rightarrow \infty$ and one may question whether we are sure of the short distance, sub-Planck scale physics well enough to make this choice. An alternative procedure, discussed extensively in the literature [16], attempts to address this question by choosing to impose the initial conditions for the different oscillators at different times. Specifically, one chooses the initial condition for the oscillator $q_{\mathbf{k}}$ at a time η_k such that $[k/a(\eta_k)] \simeq L_{\mathbf{P}}^{-1}$, where $L_{\mathbf{P}}$ is the Planck length. The initial state of the oscillator uniquely determines the function $\mathcal{B}(k)$ and the corresponding power spectrum can then be constructed using Eq. (49). However, it should be emphasized here that, apart from the fact that it has to be consistent with the observations, there exists no restrictions on the initial state to be chosen at η_k .

To illustrate the point, let us consider the case of exponential expansion for which $a(\eta) = (-\mathcal{H}\eta)^{-1}$. Let us assume that the oscillator $q_{\mathbf{k}}$ is in the ground state at a given time, say, η_i , which then requires that, at this instant, $R_k = -(i a^2/2) (\mu'_k/\mu_k) = (k a^2/2)$. For the case of exponential expansion, the general solution for f_k as given by Eq. (41) can be expressed in terms of simple functions as follows (see, for instance, Ref. [33], pp. 437–438):

$$f_k(\eta) = \frac{1}{\sqrt{2k}} \left[\left(1 + \frac{i}{k\eta} \right) e^{ik\eta} + \mathcal{B}(k) \left(1 - \frac{i}{k\eta} \right) e^{-ik\eta} \right].$$
(55)

On imposing the condition $R_k = (k a^2/2)$ at η_i , we can determine the function $\mathcal{B}(k)$ to be

$$\mathcal{B}(k) = (1 + 2i \, k\eta_i)^{-1} \, e^{2ik\eta_i}.$$
(56)

Our original choice of the Bunch-Davies vacuum corresponds to assuming $\eta_i \to -\infty$ so that $\mathcal{B}(k)$ vanishes for all k. The modified procedure will be to choose η_i differently for different k by imposing the initial condition at, say, $[k/a(\eta_k)] = L_{\rm P}^{-1}$. For exponential inflation, this translates to $(k \eta_k) = -(\mathcal{H} L_{\rm P})^{-1} \equiv -\xi^{-1}$, a constant. For $\eta_i = \eta_k$, the $\mathcal{B}(k)$ above reduces to [16, 20]

$$\mathcal{B}(k) = [1 - (2i/\xi)]^{-1} e^{-(2i/\xi)}$$
(57)

which is a constant independent of k. Thus the k-dependence of the power spectrum remains unchanged when the initial condition on the k-th oscillator is imposed at a time such that $[k/a(\eta_k)] = \text{constant}$. The amplitude of the power spectrum, of course, gets scaled by a k-independent factor; this is of no observable consequence since we do not know how to obtain the amplitude from a first principle theory anyway.

The power spectrum corresponding to the above $\mathcal{B}(k)$ when evaluated at Hubble exit, say, when (k/a) = (z H), is given by

$$k^{3} \mathcal{P}_{\Phi}(k) = \left(\frac{1+z^{2}}{2}\right) \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left[1 + \frac{\xi^{2}}{2} + \left(\frac{(z^{2}-1)\xi^{2} - 4z\xi}{2(1+z^{2})}\right) \cos\left(\frac{2}{\xi} - 2z\right) + \left(\frac{(z^{2}-1)\xi + z\xi^{2}}{1+z^{2}}\right) \sin\left(\frac{2}{\xi} - 2z\right)\right].$$
(58)

This expression is exact and shows that the spectrum is strictly scale invariant, but is modified from the original result [viz. Eq. (47)] by a multiplicative factor independent of k. This factor depends on two parameters: (i) $\xi = (\mathcal{H} L_{\rm P})$ which measures the energy scale of inflation relative to the Planck scale and (ii) z which is the ratio of the Hubble radius and the physical wavelength of the perturbation. As we explained before, we can evaluate the power spectrum either at z = 1 or at $z = (2\pi)$. For z = 1, the spectrum (58) reduces to

$$k^{3} \mathcal{P}_{\Phi}(k) = \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left[1 + \frac{\xi^{2}}{2} - \xi \cos\left(\frac{2}{\xi} - 2\right) + \frac{\xi^{2}}{2} \sin\left(\frac{2}{\xi} - 2\right)\right],$$
(59)

while, for $z = (2\pi)$, we get

$$k^{3} \mathcal{P}_{\Phi}(k) = \left(\frac{1+4\pi^{2}}{2}\right) \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left[1 + \frac{\xi^{2}}{2} + \left(\frac{(4\pi^{2}-1)\xi^{2} - 8\pi\xi}{2(1+4\pi^{2})}\right) \cos\left(\frac{2}{\xi}\right) + \left(\frac{(4\pi^{2}-1)\xi + 2\pi\xi^{2}}{1+4\pi^{2}}\right) \sin\left(\frac{2}{\xi}\right)\right]. \tag{60}$$

The numerical value of these modified amplitudes will depend on the parameter ξ which is expected to be very small compared to unity for GUT scale inflation. For $\xi \ll 1$, one can easily obtain the leading order terms of polynomial expressions involving ξ , but determining $\cos(1/\xi)$ and $\sin(1/\xi)$ for $\xi \ll 1$ requires care. Since, one can easily replace $(1/\xi)$ by, say, $[(1/\xi) + (\pi/2)]$, in the arguments of trigonometric functions to the leading order, these expressions are intrinsically ambiguous. For $\xi \ll 1$ and z = 1, we get

$$k^{3} \mathcal{P}_{\Phi}(k) \simeq \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left[1 - \xi F\left(2/\xi\right)\right],\tag{61}$$

where F is a rapidly oscillating cosine function. (Note that, if one evaluates the spectrum at super Hubble scales, i.e. as $z \to 0$, then, instead of the cosine, one gets a sine function [16].) Similarly, when $\xi \ll 1$, for $z = (2\pi)$, we have

$$k^{3} \mathcal{P}_{\Phi}(k) \simeq \left(\frac{1+4\pi^{2}}{2}\right) \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left[1 - \left(\frac{4\pi\xi}{1+4\pi^{2}}\right) F(2/\xi) + \left(\frac{(4\pi^{2}-1)\xi}{1+4\pi^{2}}\right) G(2/\xi)\right],\tag{62}$$

where G is a sine function and F, as above, is a cosine function. In each of these cases, a different choice for the sub-leading phase in the argument of the trigonometric function can make cosine into sine and vice versa. Hence, only the profile of the oscillating functions are of relevance in the limit of $\xi \ll 1$, though the full expressions are often quoted in literature.

Note that the quantum state with the choice of $\mathcal{B}(k)$ in Eq. (57) is a state with the initial condition for all the oscillators specified at a given moment of time. Thus the above analysis maps the prescription of specifying the quantum state for different oscillators at different times to specifying the initial condition at a given time. We can now explore the physical content of this quantum state at any given η in terms of, for e.g., the mean occupation number $\langle n_k \rangle$ in the instantaneous harmonic oscillator states. On using the expressions (21), (24), (55) and (57), we find the particle content of this quantum state to be

$$\langle n_k \rangle = \left(\frac{1}{4k^2\eta^2}\right) \left[1 + \frac{\xi^2}{2} + \xi^2 k^2 \eta^2 - \frac{\xi}{2} \left(\xi - 4k\eta\right) \cos\left(\frac{2}{\xi} + 2k\eta\right) - \xi \left(1 + \xi k\eta\right) \sin\left(\frac{2}{\xi} + 2k\eta\right)\right].$$
(63)

This expression has several interesting features.

First, let us consider very early times (i.e. as $\eta \to -\infty$) or very short wavelengths (i.e. as $k \to \infty$). It is precisely this limit which was considered uncertain due to trans-Planckian effects which motivated imposing the initial condition for different modes at different times; therefore, it is this limit which is of some interest to explore, to understand what kind of *effective* quantum state at $\eta = \text{constant} \to -\infty$ will lead to the vacuum state for the k-th mode when $(k\eta) = -\xi^{-1}$. We see from Eq. (63) that the mean occupation number has two sets of contributions. The first three terms in Eq. (63) is secular, while the last two terms are oscillatory. The secular term increases monotonically from $\langle n_k \rangle = (\xi^2/4)$ at $\eta = -\infty$. Thus, in the trans-Planckian limit (i.e. as $\eta \to -\infty$ or as $k \to \infty$) all the modes have the same mean excitation $(\xi^2/4)$. (The oscillatory terms do not contribute in this limit.)

Second, we do know that $\langle n_k \rangle$ must vanish for $(k\eta) = -\xi^{-1}$, since this is the condition we used to choose this state. As can be directly verified, this is indeed true for the expression in Eq. (63), but occurs because of a cancellation between the secular and the oscillatory terms. At later times, the secular terms dominate the oscillatory terms and $\langle n_k \rangle$ increases on the average with superimposed oscillations. (We stress the fact that $\langle n_k \rangle$ is computed in terms of the instantaneous harmonic oscillator modes; one should not think of them as particles which are produced with respect to the in-out states.) Thus, for each of the modes, we start with $\langle n_k \rangle = (\xi^2/4)$ as $\eta \to -\infty$, evolve to $\langle n_k \rangle = 0$ at $(k\eta) = -\xi^{-1}$ and grow to

$$\langle n_k \rangle = \left(\frac{1}{4z^2}\right) \left[1 + \frac{\xi^2}{2} + \xi^2 z^2 - \frac{\xi}{2} \left(\xi + 4z\right) \cos\left(\frac{2}{\xi} - 2z\right) - \xi \left(1 - \xi z\right) \sin\left(\frac{2}{\xi} - 2z\right) \right]$$
(64)

at Hubble exit. We see that the alternative prescription of specifying the initial condition when the physical wavelength of the mode is comparable to the Planck length (which sounds reasonable at first sight) is equivalent to assuming a quantum state at a η = constant hypersurface, with very specific properties. It can be realized only if unknown physical effects of the trans-Planckian sector acts in a particular manner to populate the modes with a specific prescription. It is far from clear whether this will be possible in a generic context.

IV. MIMICKING THE TRANS-PLANCKIAN EFFECTS

We shall now turn to the question of choosing an initial state such that a given power spectrum of perturbations is reproduced. Let us assume that, in the case of power-law inflation, a 'trans-Planckian' theory leads to the following spectrum:

$$\left[k^3 \mathcal{P}_{\Phi}(k)\right]_{\mathrm{M}} = C(z) \left(\frac{\mathcal{H}^2}{2\pi^2}\right) \left(\frac{k}{\mathcal{H}}\right)^{2(\gamma+2)} M(k), \tag{65}$$

where M(k) is the modification factor with, of course, $M(k) \ge 0$ for all k. (Alternatively, let us suppose that a future CMB observation leads to such a spectrum, starting a hectic flurry of theoretical activity to explain it!) Evidently, the modified spectrum (65) can be constructed from the spectrum (51) in the standard theory, provided we can find a positive definite function B(k) that satisfies the condition

$$\left[1 + B^{2}(k) + 2B(k)d(k)\right] = \left[1 - B^{2}(k)\right]M(k).$$
(66)

This is a quadratic equation in B(k) for each value of k and, if we choose $d(k) = \pm 1$, then, we find that the non trivial and positive definite roots for B(k) can be expressed in terms of M(k) as follows:

$$B(k) = \frac{|M(k) - 1|}{M(k) + 1}.$$
(67)

Given a M(k), this expression then allows us to reproduce the modified spectrum in the standard theory. However, note that the B(k) we have constructed above is not unique as it corresponds to a particular value of the phase b(k) in Eq. (48) such that $d(k) = \pm 1$. Clearly, a whole *class* of such functions can be constructed, with different choices for d(k), but, as we shall see, this particular choice is sufficient for our purpose.

As we had mentioned in Section I, the Planck scale modifications to the standard inflationary perturbation spectrum have been obtained in the literature by considering various high energy models for the scalar field [7]–[20]. Most of these modified spectra deviate from the standard scale invariant spectrum at the ultra-violet end. On the other hand, the lower power in the quadrupole and the octopole moments of the CMB as measured by WMAP [6]—if it survives further releases of WMAP data!—requires a suppression of power in the infra-red end of the spectrum [35, 36]. Such spectra have also been obtained in certain high energy models of the scalar field [19, 22]. It is interesting to determine how these different modified spectra can be constructed by choosing suitable initial conditions on the scalar field in the standard theory.

In the following subsections, we shall explicitly construct the function B(k) for four modified power spectra that have either been proposed to fit the observational data or have been obtained from a high energy model of the scalar field.

A. Modified spectrum I

Recently, the following spectrum was obtained in a power law inflationary scenario using a Lorentz invariant modified theory [19]:

$$\left[k^{3} \mathcal{P}_{\Phi}(k)\right]_{\mathrm{M}} = C(1) \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left(\frac{k}{\mathcal{H}}\right)^{2(\gamma+2)} \left[1 - \bar{C} \left(\frac{\mathcal{H}}{k_{c}}\right) \left(\frac{k}{\mathcal{H}}\right)^{(\gamma+2)}\right],\tag{68}$$

where $k_{\rm c}$ denotes the high energy scale, \bar{C} is given by

$$\bar{C} = \left[2C(1) (\gamma + 1)^{3(\gamma+1)}\right]^{-1}$$
(69)

and it is assumed that $10^{-5} \leq (\mathcal{H}/k_c) \leq 10^{-3}$. (However, it should be mentioned here that this spectrum is not valid for arbitrarily small values of k [19].) In fact, a similar spectrum have also been obtained in non-commutative models of inflation [15, 22]. These spectra exhibit a suppression of power at the large scales, a feature that could be relevant to the low quadrupole moment observed in the CMB [35]. It is straightforward to see that, for z = 1, the function B(k) corresponding to the modified spectrum (68) is given by

$$B(k) = \left[\left(\frac{2}{\bar{C}}\right) \left(\frac{\mathcal{H}}{k_c}\right)^{-1} \left(\frac{k}{\mathcal{H}}\right)^{-(\gamma+2)} - 1 \right]^{-1}.$$
(70)

For $\gamma < -2$, we have $B \to k^{(\gamma+2)} \to 0$ as $k \to \infty$. This implies that, while, towards the infra-red end, the initial state is different from the Bunch-Davies vacuum, the Bunch-Davies vacuum structure is retained at the ultraviolet end.

B. Modified spectrum II

Another modified primordial spectrum that has been *proposed* (see, for e.g., Refs. [36]) in order to account for the low quadrupole moment observed in the CMB, is the following:

$$\left[k^{3} \mathcal{P}_{\Phi}(k)\right]_{M} = A k^{(n_{s}-1)} \left[1 - e^{-(k/k_{1})^{\alpha}}\right],$$
(71)

where A and n_s are the scalar amplitude and index of the standard spectrum. The pivot scale k_1 and the constant α (which turns out to be a positive number of the order of unity) are chosen to fit the CMB data. If we now assume that amplitude A and the index n_s of the above modified spectrum are the same as those in the case of power-law inflation in the standard theory [cf. Eq. (44)], then, we find that B(k) is given by

$$B(k) = \left[2 e^{(k/k_1)^{\alpha}} - 1\right]^{-1}.$$
(72)

Note that $B(k) \to 1$ as $k \to 0$ and $B_k \simeq e^{-(k/k_1)^{\alpha}} \to 0$ for large k. Once again, the vacuum structure at the ultraviolet end is not modified.

C. Modified spectrum III

Another modified spectrum whose effects on the CMB has also been analyzed is the following spectrum [21]

$$\left[k^{3} \mathcal{P}_{\Phi}(k)\right]_{\mathrm{M}} = \left(\frac{\mathcal{H}^{2}}{2\pi^{2}}\right) \left(1 - \xi \left(\frac{k}{k_{2}}\right)^{-\epsilon} \sin\left[\frac{2}{\xi}\left(\frac{k}{k_{2}}\right)^{\epsilon}\right]\right),\tag{73}$$

where $\xi \simeq 10^{-3}$, $\epsilon \simeq 10^{-2}$ and k_2 is a pivot scale. In order to match the leading term in the spectrum, let us assume that the inflating background undergoes exponential expansion and that the spectrum is evaluated at z = 1. It is then straightforward to construct B(k) for the above spectrum and it is given by

$$B(k) = \left(\frac{\xi (k/k_2)^{-\epsilon} |\sin[(2/\xi) (k/k_2)^{\epsilon}]|}{2 - \xi (k/k_2)^{-\epsilon} \sin[(2/\xi) (k/k_2)^{\epsilon}]}\right).$$
(74)

D. Modified spectrum IV

A more general modification of spectrum one can envisage is a spectrum which has corrections at both the infra-red and the ultra-violet ends. If we now assume that the standard spectrum is modified in the infra-red as in Eq. (71) and has the same correction at the ultra-violet end as in Eq. (73), then the complete spectrum will be given by

$$\left[k^{3} \mathcal{P}_{\Phi}(k)\right]_{M} = A k^{(n_{s}-1)} \left(1 - e^{-(k/k_{1})^{\alpha}} - \xi \left(\frac{k}{k_{2}}\right)^{-\epsilon} \sin\left[\frac{2}{\xi} \left(\frac{k}{k_{2}}\right)^{\epsilon}\right]\right),$$
(75)

where A and n_s are the scalar amplitude and index of the standard spectrum and k_1 and k_2 are pivot scales such that $k_1 \ll k_2$. Also, as in the earlier case, let α be a positive constant of the order of unity. The corresponding B(k) can be easily obtained to be

$$B(k) = \left(\frac{\left|e^{-(k/k_1)^{\alpha}} + \xi (k/k_2)^{-\epsilon} \sin\left[(2/\xi)(k/k_2)^{\epsilon}\right]\right|}{2 - e^{-(k/k_1)^{\alpha}} - \xi (k/k_2)^{-\epsilon} \sin\left[(2/\xi)(k/k_2)^{\epsilon}\right]}\right).$$
(76)

These examples demonstrate the fact that the modification of the spectrum due to 'trans-Planckian considerations' is degenerate with the choice of the initial quantum state. Without further input, such as an assumption for the choice of initial quantum state, observations cannot distinguish between these two physical effects.

V. MODIFIED SPECTRA AND BACK REACTION

An issue that remains unresolved in obtaining the modified spectra is whether the conditions that lead to modifications of the standard spectrum will also lead to a large back reaction on the inflating background. In particular, will the energy in the quantum field dominate the inflaton energy thereby, possibly, terminating inflation? The approach we have adopted here allows us to address this issue along the following manner.

Since the modified spectra from a high energy theory can be obtained from the standard theory with a suitable choice of initial conditions on the modes, we are probably justified in using these modes to evaluate the energy density of the quantum scalar field (for an earlier discussion on this point, see the first reference listed under Ref. [12]). In what follows, we shall show that the energy density of the quantum scalar field *above* the Bunch-Davies vacuum is finite only if |M(k) - 1| decays faster than k^{-2} for large k and M(k) goes as k^{λ} with $-2 < \lambda < 2$ for small k. Also, we shall restrict our attention to the easily tractable case of exponential inflation.

Recall that the energy density of the quantum scalar field is given by Eq. (27) with the quantity \mathcal{E}_k to be evaluated using Eq. (25). In the case of exponential inflation, as we had mentioned earlier, the general solution for f_k can be expressed in terms of simple functions [cf. Eq. (55)]. On substituting the solution (55) in the expression (25), we find that the energy density per mode of the quantum field is given by

$$\mathcal{E}_{k} = \left(\frac{1}{4k\eta^{2}}\right) \left[1 - B^{2}(k)\right]^{-1} \left(\left[1 + B^{2}(k)\right] \left(1 + 2k^{2}\eta^{2}\right) - 2B(k)\cos[b(k) - 2k\eta] + 4B(k)\left(k\eta\right)\sin[b(k) - 2k\eta]\right).$$
(77)

In the Bunch-Davies vacuum, which corresponds to $\mathcal{B}(k) = 0$, this expression for \mathcal{E}_k reduces to

$$\mathcal{E}_k^{\rm BD} = \frac{k}{2} + \frac{1}{2k\eta^2} \tag{78}$$

and it known that the corresponding energy density (when regularized by point-splitting) is given by [27, 37]

$$\rho_{\rm BD} = -\left(\frac{29}{960\,\pi^2}\right)\,\mathcal{H}^4.\tag{79}$$

This energy density is much smaller than the energy density in the classical field that drives inflation. The energy density of the scalar field *above* the Bunch-Davies vacuum is then given by Eq. (27) with \mathcal{E}_k replaced by $\bar{\mathcal{E}}_k$, where

$$\bar{\mathcal{E}}_{k} = \mathcal{E}_{k} - \mathcal{E}_{k}^{\mathrm{BD}} = \left(\frac{1}{2k\eta^{2}}\right) \left[1 - B^{2}(k)\right]^{-1} \left(B^{2}(k)\left(1 + 2k^{2}\eta^{2}\right) - B(k)\cos[b(k) - 2k\eta] + 2B(k)(k\eta)\sin[b(k) - 2k\eta]\right).$$
(80)

In order to understand the behavior of the above $\overline{\mathcal{E}}_k$ for large k, we can ignore the terms containing the sine and the cosine functions as they will oscillate rapidly in this limit. On neglecting these terms and, on making use of the relation (67) between B(k) and M(k), we find that, for large k, the above expression for $\overline{\mathcal{E}}_k$ can be written in terms of M(k) as follows:

$$\bar{\mathcal{E}}_k \simeq \left(\frac{\left[M(k) - 1\right]^2}{4\,M(k)}\right)\,k.\tag{81}$$

For the energy density ρ corresponding to this $\overline{\mathcal{E}}_k$ to be finite in the ultraviolet limit, the integral of $(k^2 \overline{\mathcal{E}}_k)$ over k should converge at large k. It is easy to see that this condition cannot be satisfied if $M(k) \propto k^{\nu}$ for any value of ν . For all values of ν , this expression varies as $k^{(3+\nu)}$ at large k and hence the integral is divergent. To obtain a finite result, we need $M(k) \to 1$ at large k. If we now assume that $M(k) \propto (1 \pm k^{-\delta})$ for large k, it is then clear that the energy density corresponding to the above $\overline{\mathcal{E}}_k$ will converge only if $\delta > 2$. Thus, the deviations from the standard spectra should die down faster than k^{-2} for large k.

One can also investigate the infrared limit in a similar fashion. As $k \to 0$, we find that the leading divergence arises due to the first term in the expression (80) for $\bar{\mathcal{E}}_k$ so that, in this limit, we have

$$\bar{\mathcal{E}}_k \propto \left(\frac{[M(k)-1]^2}{M(k)k}\right). \tag{82}$$

If we now assume that $M(k) \propto k^{\lambda}$ as $k \to 0$, then the finiteness of the energy density ρ corresponding to this $\bar{\mathcal{E}}_k$ requires that $-2 < \lambda < 2$. It is therefore possible to enhance or reduce power in the infrared limit within a range and still maintain finite energy density. Modifications of the form $[M(k) - 1] \propto k^{\varepsilon}$ with $\varepsilon > 0$ are also allowed and there are no restrictions on ε in this case. (We stress that the finiteness of ρ is a necessary condition for ignoring back reaction, but it is not sufficient. The latter will require comparing the energy density in the quantum field with the background energy density which is difficult to do without assuming a specific model.) Clearly, amongst the four modified spectra that we have considered in the last section, only the second spectrum (provided $\alpha < 2$) will lead to a finite energy density for the case of exponential inflation.

Our expression in Eq. (81) shows that a constant M(k) independent of k leads to a divergent energy density above the Bunch-Davies vacuum. In particular, the state obtained by giving initial conditions for each of the modes at $[k/a(\eta_k)]$ =constant (leading to a $\mathcal{B}(k)$ that is independent of k), produces a divergent contribution to the energy density and hence is suspect as a valid quantum state. It is sometimes argued in the literature that this state has the same energy density as the Bunch-Davies vacuum along the following lines: When \mathcal{B} is independent of k, we are dealing with mode functions of the form $(f_k + \mathcal{B} f_k^*)$, with f_k given by Eq. (55), which belong the set of so called α -vacua [38]. It is possible to construct a regularization scheme such that the divergences which arise at the coincidence limit of the Greens function in this case, is the same as that in the case of $\mathcal{B} = 0$. Such a subtraction will lead to $\rho = \rho_{BD}$ for these states. In our approach, this is equivalent to ignoring the contributions in Eq. (81) when $M(k) = M_0$ is a constant different from unity. Since this leads to $\bar{\mathcal{E}}_k \propto k$, one can think of M_0 as the (constant) occupation number $\langle n_k \rangle$ for all k; the regularization involves ignoring all these 'particles' in measuring the energy density.

We believe this argument is spurious for two reasons. Firstly, a transparent and direct discussion in terms of harmonic oscillators presented above gives a different result showing that $M(k) = M_0 = \text{constant}$ leads to a divergent energy density. So, at the least, the results depend on the explicit regularization procedure adopted. Secondly, in a realistic model, we will have to deal with a weak dependence of \mathcal{B} on k rather than no dependence. Then, the argument based on α -vacua will no longer hold, irrespective of how weak this dependence is. The analysis given above, however, is completely transparent and clear.

VI. DISCUSSION

The fact that the measurements of the CMB anisotropies strongly indicate a primordial spectrum that is nearly scale invariant already implies that the initial state of the quantum scalar field is a state that is 'very close' to the Bunch-Davies vacuum. Clearly, sufficiently precise measurements of the anisotropies in the CMB can provide us with the form the inflationary perturbation spectrum to a good accuracy. However, this information can at most help us determine the initial state of the quantum scalar field in the standard theory and it is not sufficient to aid us in discriminating between the various Planck scale models of matter fields. The reason being that, given a perturbation spectrum, we should be able obtain the spectrum from *any* high energy model of the matter field by simply choosing a suitable state in the modified theory just as we had done in the standard theory.

The above result can be obtained either in the Heisenberg picture or in the Schrodinger picture since these descriptions are mathematically equivalent. We have, however, adapted the Schrodinger picture since the problem we are discussing is essentially that of a harmonic oscillator with a time dependent frequency for which the intuition available in the Schrodinger picture is of some value. Our discussion clearly shows that virtually any power spectrum which is either observed in future or suggested by phenomenological models, can be reproduced by a suitable choice of the quantum state. Evidently, without additional assumptions one cannot disentangle the dynamics from the initial conditions and, hence, the CMB observations alone cannot act as a discriminator between different theoretical models.

There are several possible avenues for future work arising from this discussion. One particularly interesting question will be the evolution of the quantum state of the universe into the future. Several recent observations [39] (as well as not so recent observations, see Refs. [40]) suggest that the universe has just entered an accelerating phase dominated by dark energy with an equation of state $P \approx -\rho$. While the nature of this dark energy is unclear, it seems likely that at least at sufficiently large scales it will act like a cosmological constant leading to a late time de Sitter phase [41]. It will be interesting to study the late time evolution of the quantum wave function of the scalar field. The de Sitter phase in the future should lead to its own thermal fluctuations with a characteristic temperature and it will be interesting to see how that can emerge.

Another issue of interest is the study of correlations across the horizon in the case of de Sitter spacetime. It has been shown that the quantum entanglement of modes across the horizon can lead to a holographic description of gravity [42]. The effects of this entanglement are easy to calculate when de Sitter spacetime is described in the static coordinates. On the other hand, the time dependent Gaussian state used in this paper is more naturally tuned to the Friedmann coordinates of the de Sitter spacetime. It will be worthwhile to relate these two descriptions and understand how the correlations across the horizon arises in the time dependent background.

Finally, the description in terms of the wave function can be easily translated to one in terms of the path integral kernel using the Feynman-Kac formula. This will allow one to provide a purely path integral derivation of the results presented in this paper. All these issues are currently under investigation.

APPENDIX A: EVALUATING THE POWER SPECTRUM

Recall that the quantum state $\psi_{\mathbf{k}}$ of the time dependent oscillator $q_{\mathbf{k}}$ was described by the Gaussian wave function (9). On substituting the wave function (9) in the Schrödinger equation (7) and equating the coefficients of $q_{\mathbf{k}}$ and $q_{\mathbf{k}}^2$, we find that N_k and R_k satisfy the following differential equations:

$$i N_k' = \frac{R_k N_k}{a^2},\tag{A1}$$

$$i R'_k = \frac{2R_k^2}{a^2} - \frac{k^2 a^2}{2},$$
 (A2)

where the prime, as before, denotes differentiation with respect to η . Let us now introduce a new quantity $\mu_k(\eta)$ through the relation [28–30]

$$R_k = -\left(\frac{i\,a^2}{2}\right)\,\left(\frac{\mu'_k}{\mu_k}\right).\tag{A3}$$

On substituting this expression in the above differential equation for R_k , we find that μ_k satisfies the differential equation (11) which is the same as the classical equation of motion satisfied by the classical oscillator variable q_k . Also, in terms of μ_k , the differential equation (A1) can be integrated to obtain

$$N_k = \left(\frac{D(k)}{\sqrt{\mu_k}}\right),\tag{A4}$$

where D(k) is a k-dependent constant determined by the normalization condition (10). Note that the differential equation satisfied by μ_k [viz. Eq. (11)] implies the Wronskian condition

$$\left(\mu_k \,\mu'_k^{*} - \mu'_k \,\mu_k^{*}\right) = -\left[i \,W(k)/a^2\right],\tag{A5}$$

where W(k) is a k-dependent constant. The relations (A3) and (A4) along with the above Wronskian condition and the normalization condition (10) determine D(k) to be

$$D(k) = \left(\frac{W(k)}{2\pi}\right)^{1/4}.$$
(A6)

Thus, the solution to classical equation of motion allows us to construct the wave function for the corresponding quantum problem [25, 28–30]. However, it should be pointed out here that, while $q_{\mathbf{k}}$ is real, μ_k , in general, is a complex quantity.

The power spectrum of the perturbations (8) is given by

$$k^{3} \mathcal{P}_{\Phi}(k) = \frac{k^{3}}{2\pi^{2}} \int_{-\infty}^{\infty} dq_{\mathbf{k}} |\psi_{\mathbf{k}}|^{2} q_{\mathbf{k}}^{2} = \frac{k^{3} |N_{k}|^{2}}{2\pi^{2}} \int_{-\infty}^{\infty} dq_{\mathbf{k}} q_{\mathbf{k}}^{2} e^{-\left[(R_{k} + R_{k}^{*})q_{\mathbf{k}}^{2}\right]}, \tag{A7}$$

where we have substituted the expression (9) for the wave function $\psi_{\mathbf{k}}$. On carrying out the integral over $q_{\mathbf{k}}$ in the above equation and making use of the relation (10) and the Wronskian condition (A5), we obtain the power spectrum to be

$$k^{3} \mathcal{P}_{\Phi}(k) = \frac{k^{3}}{2\pi^{2}} \left(\frac{|\mu_{k}|^{2}}{W(k)} \right)$$
(A8)

which is expression (12) we have quoted in the text.

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