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## Vacuum Choices and the Predictions of Inflation

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In the presence of a short-distance cutoff, the choice of a vacuum state in an inflating, non-de Sitter universe is unavoidably ambiguous. The ambiguity is related to the time at which initial conditions for the mode functions are specified and to the way the expansion of the universe affects those initial conditions. In this paper we study the imprint of these uncertainties on the predictions of inflation. We parametrize the most general set of possible vacuum initial conditions by two phenomenological variables. We find that the generated power spectrum receives oscillatory corrections whose amplitude is proportional to the Hubble parameter over the cutoff scale. In order to further constrain the phenomenological parameters that characterize the vacuum definition, we study gravitational particle production during different cosmological epochs.

### I. INTRODUCTION

Inflation [\[1](#page-9-0)] causally explains the origin of the superhorizon density perturbations that seed the structures we observe in the universe. During inflation, the physical size of any given perturbation mode grows faster than the Hubble radius. In particular, observationally relevant modes start well within the Hubble radius, cross it and "freeze" till they reenter the Hubble radius and develop into galaxies, clusters, etc. [\[2\]](#page-9-1). Causality within the Hubble radius naturally allows us to determine their initial amplitude by postulating that perturbations start in their vacuum state.

In Minkowski space there exists a well-defined, unique, vacuum state, but in any expanding universe—and in particular, during inflation— the notion of a vacuum is ambiguous [\[3](#page-9-2)]. In de Sitter space there exists a concrete set of vacuum states invariant under the symmetry group of the spacetime. Such vacua, the Bunch-Davies vacuum and the  $\alpha$ -vacua, have received widespread attention in the recent literature [\[4](#page-9-3)]. However, strictly speaking, an inflating spacetime is *not* de Sitter spacetime. de Sitter space admits a time-like Killing vector field, whereas the non-existence of a time-like Killing vector field is what singles out cosmological spacetimes. A Friedmann-Robertson-Walker universe whose scale factor grows quadratically in cosmic time  $(a \propto t^2)$  is an inflating spacetime, and it is far from obvious why de Sitter spacetime, where a grows exponentially with time  $(a \propto e^{Ht})$ shall be a good description of such a spacetime. More importantly, in de Sitter space scalar cosmological perturbations are "ill-defined" [\[5](#page-9-4)], as signaled for instance by the divergence of the power spectrum in the de Sitter limit. Thus, during cosmic inflation one still has to face

the problem of defining a vacuum state in an expanding universe that does not admit any particular additional symmetry.

Recent advances in the formulation of quantum field theory in curved spacetimes [\[6\]](#page-9-5) suggest that such a preferred vacuum state might not exist. Whereas one can construct mathematically well-defined quantum fieldtheories in globally hyperbolic spacetimes, they do not single out any particular quantum state. Allowed physical states only have to satisfy the Hadamard condition, which is a condition on the ultraviolet  $(k \to \infty)$  behavior of two-point functions. In this work we assume physics to be unknown above cutoff energies  $\Lambda$ . The presence of this ultraviolet cutoff thus renders the Hadamard condition inapplicable. Therefore, i) in curved spacetimes there is no single preferred quantum state and ii) even though there is a class of preferred states, in the presence of an ultraviolet cutoff  $\Lambda$  the condition that singles out those states is not applicable.

Nevertheless, it is still possible to single out a set of "reasonable" vacuum states by appealing to the flatness of an expanding universe at short distances. In the limit where the physical length  $\lambda$  of a mode is infinitely smaller than the Hubble radius  $H^{-1}$ , the expansion is completely negligible. Therefore, in the conventional treatments of inflation, the vacuum for a particular mode is chosen when  $\lambda/H^{-1} \to 0$ , i.e. when the vacuum state agrees with the Minkowski vacuum. However, if physical laws are unknown below certain cutoff length  $\Lambda^{-1}$ , the limit  $\lambda \to 0$  leads into a region where physics is unknown [\[7\]](#page-9-6). In the presence of a cutoff, in order to minimize the ambiguity related to the expansion of the universe, and in order to avoid the region of unknown physics, the best one can do is to define the vacuum at the time the physical length  $\lambda$  of the mode equals the fundamental length scale of the theory,  $\Lambda^{-1}$  [\[8\]](#page-9-7). In that case, the conventional predictions of inflation get modified due to the finite effects of the expansion of the universe [\[9\]](#page-9-8). These corrections can be expanded as a series in  $H/\Lambda$ . Let us

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stress though, that the corrections we are talking about have little to do with trans-Planckian physics (see [\[10](#page-9-9)] for a review). Rather, they arise from the uncertainties related to the definition of vacuum in an expanding universe. If we knew how to uniquely define the vacuum of a field in an expanding universe, there would not be any uncertainty at all. In fact, in the limit of no expansion,  $H \to 0$ , all vacuum prescriptions we consider here agree, i.e. to zeroth order in  $H/\Lambda$  all of them yield the same "conventional" power spectrum prediction.

The precise nature of the small  $H/\Lambda$  corrections is not a question of academic interest only. In some inflationary models,  $H/\Lambda$  might be large enough in order for linear corrections to leave an observable imprint on the CMB spectrum [\[11,](#page-9-10) [12\]](#page-9-11), whereas quadratic corrections are expected to be unobservable [\[13\]](#page-9-12). In addition, the definition of a vacuum also directly affects the number of particles produced due to the expansion of the universe. By imposing observational constraints on the amount of the gravitationally produced particles one can thus gain information about the realized vacuum [\[3,](#page-9-2) [14\]](#page-9-13).

The goal of this paper is not to assess which vacuum choice is the correct one, as we have argued that there might be no answer for that question. Our goal is rather to take a phenomenological approach and find out what is a reasonable set of possible vacua, and how and to what extent these possibly different vacua alter the conventional predictions of inflation. Then, instead of relying on theoretical arguments to single out the vacuum that was realized during inflation, we shall rely on observations to put constraints on possibly realized vacua.

### II. FORMALISM

For completeness, we shortly review in this section the formalism of the generation of perturbations in an inflating spacetime. The reader might want to skip to the next section and eventually refer back for notational details. We also summarize our notation in Table [I.](#page-3-0)

We consider in the following power-law inflation in a spatially flat FRW universe,

<span id="page-2-4"></span>
$$
ds^{2} = a^{2}(\eta)(d\eta^{2} - d\vec{x}^{2}).
$$
 (1)

Power-law inflation is simple enough to allow a straightforward treatment of the equations of motion of the perturbations, and it is general enough to accommodate a wide realistic class of inflationary behaviors. During power law inflation the scale factor is given by

<span id="page-2-0"></span>
$$
a \propto |\eta|^{\frac{p}{1-p}},\tag{2}
$$

where  $p > 1$ . In the limit  $p \to \infty$  one recovers de Sitter space,  $a \propto -1/\eta$ . Note that conformal time is negative during inflation  $(p > 1)$ . Equation [\(2\)](#page-2-0) also applies to any stage of power-law expansion  $(0 \leq p < 1)$ , when conformal time is positive. For  $p = 0$  one recovers Minkowski space.

The behavior of scalar and tensor perturbations during inflation driven by a single scalar field can be described in terms of a single scalar variable  $v(\eta, \vec{x})$  [\[2](#page-9-1), [15\]](#page-9-14). For scalar perturbations the variable  $v$  is a particular combination of metric and scalar field perturbations, whereas in the case of tensor perturbations, the variable  $v$  is simply proportional to the amplitude of the gravitational waves. The dynamics of v are determined by the quadratic La $grangian<sup>1</sup>$ 

<span id="page-2-1"></span>
$$
L = \frac{1}{2} \int d^3x \left[ v'^2 - \delta^{ij} \frac{\partial v}{\partial x^i} \frac{\partial v}{\partial x^j} + \frac{a''}{a} v^2 \right],\qquad(3)
$$

where a prime denotes a derivative with respect to conformal time and  $i, j$  run from 1 to 3.

The classical variable  $v$  can be quantized following the standard rules  $[2]$ . Upon quantization, v turns into an operator  $\hat{v}$ , which can be expanded in Fourier modes,

$$
\hat{v} = \frac{1}{\sqrt{2}} \int \frac{d^3k}{(2\pi)^{3/2}} \left( v_k(\eta) e^{i\vec{k}\cdot\vec{x}} \hat{a}_k + v_k^*(\eta) e^{-i\vec{k}\cdot\vec{x}} \hat{a}_k^{\dagger} \right). (4)
$$

The mode functions  $v_k(\eta)$  obey the differential equation

<span id="page-2-3"></span><span id="page-2-2"></span>
$$
v_k'' + \left(k^2 - \frac{a''}{a}\right)v_k = 0,\tag{5}
$$

<span id="page-2-5"></span>and the operators  $a_k$  can be interpreted as annihilation operators,  $[a_k, a_{k'}^{\dagger}] = \delta(\vec{k} - \vec{k'})$ , if the  $v_k$  satisfy the normalization condition

$$
v'_k v^*_k - v'^*_k v_k = -2i.
$$
 (6)

<span id="page-2-7"></span>In terms of creation and annihilation operators, the Hamiltonian of the system [\(3\)](#page-2-1) is given by

$$
\hat{\mathcal{H}} = \frac{1}{4} \int d^3k \left[ (v_k^{\prime 2} + \omega_k^2 v_k^2) a_k a_{-k} + (|v_k^{\prime}|^2 + \omega_k^2 |v_k|^2) a_k^{\dagger} a_k + h.c. \right],
$$
\n(7)

where we have defined the squared frequency

<span id="page-2-6"></span>
$$
\omega_k^2 = k^2 - \frac{a''}{a}.\tag{8}
$$

Given a mode expansion, i.e. given a particular set of annihilation operators  $a_k$ , the vacuum of the field  $|0\rangle$ is implicitly defined by the condition  $a_k|0\rangle = 0$ . Since, in the absence of further requirements Eq. [\(5\)](#page-2-2) does not suffice alone to uniquely determine the mode functions  $v_k$ , infinitely many definitions of vacuum are possible [\[3\]](#page-9-2). In the next section we shall formulate additional criteria that constrain the possible vacuum state choices.

 $1$  For scalar perturbations the quoted Lagrangian only applies during a stage of power-law inflation. See [\[2](#page-9-1)], Eq. (11.1), for the correct expression in an arbitrary background.

Once a vacuum state has been determined, it is possible to study the imprint of the vacuum upon observable quantities, such as temperature anisotropies in the cosmic microwave background. For scalar perturbations, the amplitude of such fluctuations can be characterized by the power spectrum of the Bardeen variable [\[2](#page-9-1)]

<span id="page-3-1"></span>
$$
\zeta = \frac{\sqrt{4\pi p}}{M_{Pl}} \frac{v}{a},\tag{9}
$$

where  $M_{Pl}$  is the Planck mass  $M_{Pl}^2 = G^{-1}$ . The power spectrum  $P$  is then implicitly defined by the correlation function of the  $\zeta$  variable,

<span id="page-3-4"></span>
$$
\langle 0|\hat{\zeta}^{\dagger}(\eta,\vec{x})\hat{\zeta}(\eta,\vec{x}+\vec{r})|0\rangle \equiv \int \frac{dk}{k} \frac{\sin(kr)}{kr} \mathcal{P}_k. \tag{10}
$$

<span id="page-3-7"></span>Substituting the mode expansion [\(4\)](#page-2-3) into the last definitions one arrives at the following expression for the power spectrum,

$$
\mathcal{P}_k = \frac{p}{\pi M_{Pl}^2} \frac{k^3 |v_k|^2}{a^2}.
$$
 (11)

The value of the power spectrum for a given  $k$  is a measure of the mean square fluctuations of the variable  $v$ over *comoving* distances  $r \approx 1/k$  [\[2\]](#page-9-1). Hence, the physical extent of a field fluctuation labeled by k is

<span id="page-3-3"></span>
$$
\lambda = \frac{a}{k},\tag{12}
$$

<span id="page-3-2"></span>which depends on time for fixed  $k$ . In an expanding universe there is a natural physical distance scale given by the Hubble radius  $H^{-1}$ , where  $H \equiv a'/a^2$  is the Hubble parameter. We denote by  $\theta$  the (dimensionless) ratio of the physical distance associated to a given mode  $k$  and the Hubble radius,

$$
\theta \equiv \frac{\lambda}{H^{-1}} = \frac{p}{1 - p} \frac{1}{k \eta}.
$$
 (13)

In the limit of no expansion,  $p \to 0$ ,  $\theta$  tends to zero. The parameter  $\theta$  will play a crucial role in our further discussions.

## III. VACUUM CHOICE

Several vacuum choices have been proposed in the literature, and we discuss some of them in the Appendix. Here we shall pursue however a different approach. Instead of declaring one of the several different vacua to be the correct one, we shall abstract the property all the different vacua share and use that property to define a general class of "sensible" vacuum states.

Specifying a set of mode functions  $v_k(\eta)$  is tantamount to choosing a vacuum state  $|0\rangle$ . Because  $v_k$  is determined by the equation of motion [\(5\)](#page-2-2), all that has to be done to define a vacuum is to specify initial conditions for  $v_k$ . We

<span id="page-3-0"></span>TABLE I: Summary of notation

Symbol	Meaning	Equation
$\beta$ and $\alpha$	Bogolubov coefficients	(30)
	Bardeen variable	(9)
$\eta$	Conformal time	(1)
Ĥ	Mode length over Hubble radius	(13)
Λ	High energy cutoff	
$\lambda$	Physical size of a mode	(12)
$\boldsymbol{\nu}$	Index of Hankel function	(20)
$\alpha$	Scale factor	(1)
$\kappa$	Labels a perturbation mode	
$\cal P$	Power spectrum	(10)
$\boldsymbol{p}$	Power-law expansion exponent	(2)
$\boldsymbol{\eta}$	The quantization variable	(3)
$v_k$	Mode function	(4)
$X$ and $Y$	Vacuum parameters	(17)
Subscript 0	Initial time	
	$d/d\eta$	

shall require of any vacuum state that in the limit where the physical length of the perturbation is much smaller than the Hubble radius ( $\theta \ll 1$ ), the mode functions approach the ones in Minkowski space  $v_k \approx e^{-ik\eta}/\sqrt{k}$ . In fact, in such a limit cosmic expansion should be irrelevant. In other words, when  $\theta \to 0$  the values of  $v_k$  and its time derivative respectively approach (up to an irrelevant phase)

$$
v_k = \frac{1}{\sqrt{k}} \quad \text{and} \quad v'_k = -i\sqrt{k}.\tag{14}
$$

<span id="page-3-6"></span>All the vacuum choices we discuss in the appendix share this property. However, in an inflating universe (where  $H$  remains finite) physics is not well defined in the limit  $\theta \rightarrow 0$ . In that limit the physical length of the perturbation is infinitely smaller than the Planck length. Hence, one cannot rely on our conventional understanding of physics in that regime<sup>2</sup>. Thus, for a given mode  $k$ , the best one can do is pick a vacuum by prescribing the values of  $v_k$  and  $v'_k$  at a finite time  $\eta_0$  such that the physical length of the mode is much smaller than the Hubble radius (in order for the expansion to be "unimportant"), but much larger than the Planck scale (in order for trans-Planckian effects to be negligible). We shall take  $\eta_0$  to be the time when the physical length of the mode equals a given (fixed) length scale  $\Lambda^{-1}$ ,

<span id="page-3-5"></span>
$$
\frac{a(\eta_0)}{k} = \Lambda^{-1}.\tag{15}
$$

<sup>2</sup> In Pre-Big Bang [\[16\]](#page-9-15) and Epkyrotic/Cyclic [\[17\]](#page-9-16) scenarios, the universe contracts from Minkowski space at past infinity. In that case the limit  $\theta \to 0$  is physically well defined. For those models, the ambiguities we are considering in this work can be avoided.

The scale  $\Lambda$  is the highest possible scale where we can trust our understanding of physics. Conventionally it is assumed that  $\Lambda$  is the Planck scale  $\Lambda = M_{Pl} \approx 10^{19} \text{ GeV}$ , although the cutoff could be as low as  $\Lambda \approx 1$  TeV [\[18\]](#page-10-0). Note that the time of cutoff crossing  $\eta_0$  is k-dependent.

According to Eq. [\(15\)](#page-3-5), initial conditions for each mode are prescribed at the same physical length  $\Lambda^{-1}$ . Hence, the hypersurface where initial conditions are chosen is timelike. For comparison, it is going to be useful to consider an additional hypersurface where initial conditions for the modes are specified. We shall choose this hypersurface to be the constant time spatial section where the Hubble parameter equals the cutoff  $\Lambda$ ,

<span id="page-4-7"></span>
$$
H(\eta_0) = \Lambda. \tag{16}
$$

In this case  $\eta_0$  does not depend on k. Note that in the latter case, observationally relevant modes might be trans-Planckian at the time initial conditions are fixed [\[7](#page-9-6)].

Because initial conditions for the mode functions are fixed at a finite time rather that at  $\eta_0 = -\infty$ , one expects corrections to Eqs. [\(14\)](#page-3-6) due to the expansion of the universe. The only dimensionless quantity one can construct from the two scales that appear to be relevant in the problem—the physical length of the mode  $\lambda$  and the Hubble radius  $H^{-1}$ —is their ratio  $\theta$ . Hence, those corrections are expected to be a function of  $\theta_0$ , the value of  $\theta$  evaluated at the time initial conditions are imposed. Since we assume  $\theta_0$  to be small at that time, and because those corrections should vanish in the limit  $\theta_0 \rightarrow 0$ , we can expand them in a power series around  $\theta_0 = 0$ . We shall concentrate on the lowest order corrections (first order), i.e. we impose [\[2\]](#page-9-1)

<span id="page-4-1"></span>
$$
v_k(\eta_0) = \frac{e^{i\phi_1}}{\sqrt{k}} \left[ 1 + \frac{X+Y}{2} \theta_0 + \mathcal{O}(\theta_0^2) \right]
$$
 (17a)

$$
v'_{k}(\eta_0) = -i\sqrt{k}e^{i\phi_2} \left[1 + \frac{Y - X}{2} \theta_0 + \mathcal{O}(\theta_0^2)\right] (17b)
$$

Here, Y and X are two complex parameters, and  $\phi_1$ and  $\phi_2$  are two arbitrary real phases. The normalization condition [\(6\)](#page-2-5) implies that the phases are the same,  $\phi_1 = \phi_2$ . Because the power spectrum [\(11\)](#page-3-7) is invariant under  $v_k \to e^{i\phi} v_k$  we shall drop the phases,  $\phi_1 = \phi_2 = 0$ . In the same way, Eq.  $(6)$  constraints the values of Y,

$$
Re(Y) = 0.
$$
 (18)

<span id="page-4-6"></span>The variables  $X$  and  $Y$  are two phenomenological parameters that characterize the choice of vacuum to first order in  $\theta_0$ . Our approach could be generalized to higher orders by including additional parameters, but for our purposes it will suffice to consider the lowest order corrections. All the sensible vacuum prescriptions we are aware of can be cast in the form [\(17\)](#page-4-1). In fact, our point is that any vacuum prescription that can be cast in the form [\(17\)](#page-4-1) is a sensible vacuum choice. The specific values of X and Y for the particular vacuum prescriptions that have been considered in the literature are listed in Table

TABLE II: Properties of different vacuum prescriptions

<span id="page-4-2"></span>

Vacuum prescription		
Conventional	O	$i(1-2p)/(1-p)$
Adiabatic $> 1st$ order		
Hamiltonian diagonalization		
Danielsson		

[II](#page-4-2) (see the Appendix for details). If X and Y were  $p$ independent, one could use the information about vacua in spacetimes other than Minkowski to restrict the values of  $X$  and  $Y$ . For instance, if it turned out that the Bunch-Davies vacuum is the only consistent vacuum in de Sitter spacetime [\[4\]](#page-9-3), one could directly compute the values of  $X$  and  $Y$  for de Sitter and apply them to non-de Sitter spacetimes. However, at a phenomenological level  $X$  and  $Y$  could be  $p$ -dependent, as happens for instance in the "conventional" vacuum prescription.

Our next task is to implement the "generalized" vacuum prescription [\(17\)](#page-4-1) during a stage of power-law inflation. In a power-law expanding, not necessarily inflating universe the general solution of Eq. [\(5\)](#page-2-2) is

<span id="page-4-3"></span>
$$
v_k(\eta) = |\eta|^{1/2} \left[ A_k H_\nu(|k\eta|) + B_k H_\nu^*(|k\eta|) \right],\tag{19}
$$

<span id="page-4-0"></span>where the  $H_{\nu}$  is the Hankel function [\[19](#page-10-1)] of the first kind if conformal time is negative  $(p > 1)$  and of the second kind if conformal time is positive  $(p < 1)$ . The index  $\nu$ is given by

$$
\nu = \frac{3}{2} + \frac{1}{p - 1}.\tag{20}
$$

We shall determine the values of the time-independent complex coefficients  $A_k$  and  $B_k$  by imposing the conditions [\(17\)](#page-4-1) on the exact solution [\(19\)](#page-4-3). For large values of  $|k\eta|$  the Hankel function  $H_{\nu}$  has the expansion

<span id="page-4-4"></span>
$$
H_{\nu}(|k\eta|) \approx \sqrt{\frac{2}{\pi |k\eta|}} \left[ 1 - i \frac{4\nu^2 - 1}{8k\eta} + \mathcal{O}(\theta^2) \right] \times (21)
$$

$$
\times \exp\left[ -ik\eta \mp i\pi \left( \frac{\nu}{2} + \frac{1}{4} \right) \right],
$$

which is valid for both  $p > 1$  (upper sign) and  $p < 1$ (lower sign). Plugging the expansion [\(21\)](#page-4-4) into [\(19\)](#page-4-3) and matching to Eqs. [\(17\)](#page-4-1) we find (to first order in  $\theta_0$ )

<span id="page-4-5"></span>
$$
A_k = \sqrt{\frac{\pi}{2}} \left[ 1 + Y \frac{\theta_0}{2} - \frac{i}{2} \frac{1 - 2p}{1 - p} \theta_0 \right] e^{i\varphi}, \quad (22a)
$$

$$
B_k = \sqrt{\frac{\pi}{2}} X \frac{\theta_0}{2} e^{-i\varphi}, \qquad (22b)
$$

$$
\varphi = \frac{p}{1-p} \theta_0^{-1} \pm \frac{\pi}{2} \left( \frac{1-2p}{1-p} \right). \tag{22c}
$$

For  $\theta_0 = 0$ ,  $A_k = \sqrt{\pi/2}$  and  $B_k = 0$ . These are the values one conventionally chooses when computing inflationary

spectra [\[2\]](#page-9-1). For finite  $\theta_0$  one hence obtains corrections to these "conventional" results.

Let us emphasize again that the corrections in powers of  $\theta_0$  we consider here are not directly related to trans-Planckian effects. Our corrections become large on length scales of the Hubble radius. Their origin can be ultimately traced back to the ambiguity in defining the notion of a particle in an expanding universe, when the Compton wavelength has a size comparable to the Hubble radius [\[3](#page-9-2)]. Unknown trans-Planckian physics only enter our discussion by preventing us from taking the limit  $\theta_0 \rightarrow 0$ , making those corrections finite (but still small) rather than zero.

## IV. IMPRINT ON THE POWER SPECTRUM

The power spectrum [\(10\)](#page-3-4) is defined through the vacuum expectation value of the two-point function of the Bardeen variable  $\zeta$ . Hence, the choice of vacuum directly affects the power spectrum.

Substituting the mode function [\(19\)](#page-4-3) into Eq. [\(11\)](#page-3-7), using the values of the coefficients [\(22\)](#page-4-5) and taking Eq. [\(18\)](#page-4-6) into account one easily finds in the long-wavelength limit  $(k\eta \ll 1)$ 

<span id="page-5-0"></span>
$$
\mathcal{P} = \mathcal{P}_C \Big[ 1 - \text{Re}(X) \theta_0 \cos\left(\frac{2p\theta_0^{-1} + \pi(1 - 2p)}{1 - p}\right) - \frac{1}{2} \text{Im}(X) \theta_0 \sin\left(\frac{2p\theta_0^{-1} + \pi(1 - 2p)}{1 - p}\right) + \mathcal{O}(\theta_0^2) \Big], (23)
$$

where  $P_C$  is the conventional power spectrum generated during power-law inflation,

$$
\mathcal{P}_C = \left[ \frac{|\Gamma(\nu)|^2}{\pi^2} \left( \frac{2(p-1)}{p} \right)^{\frac{2p}{p-1}} \left( \frac{H_*}{\Lambda} \right)^{\frac{2}{p-1}} \right] \times \times p \frac{H_*^2}{M_{Pl}^2} \left( \frac{k}{k_*} \right)^{-\frac{2}{p-1}}.
$$
 (24)

In the last formula,  $H_*$  denotes the value of the Hubble parameter when the particular reference mode crosses the cutoff  $\Lambda$ . The spectral index  $n<sub>S</sub>$  of the conventional power spectrum is directly related to  $p$  by the equation

$$
n_S = 1 - \frac{2}{p - 1}.\tag{25}
$$

Current observations [\[20](#page-10-2), [21\]](#page-10-3) set the lower limit  $n_S > 0.9$ , which implies  $p > 21$ . Notice that in the limit  $p \to \infty$ , the conventional power spectrum diverges,  $\mathcal{P}_C \propto p$ . In de Sitter space the theory of scalar cosmological perturbations is not well-defined [\[5\]](#page-9-4).

The value of  $\theta_0$  depends on the hypersurface at which initial conditions are chosen. If the initial time is chosen to be cutoff-crossing, Eq. [\(15\)](#page-3-5),  $\theta_0$  is given by

<span id="page-5-2"></span>
$$
\theta_0 = \frac{H_*}{\Lambda} \left(\frac{k}{k_*}\right)^{-1/p}.\tag{26}
$$

On the other hand, if the time is chosen to be the same for all modes, Eq. [\(16\)](#page-4-7),  $\theta_0$  is given by

<span id="page-5-3"></span>
$$
\theta_0 = \left(\frac{H_*}{\Lambda}\right)^p \frac{k_*}{k}.\tag{27}
$$

In both formulas  $H_*$  is again the value of H at the time a comoving reference mode  $k_{\ast}$  crosses the cutoff.

<span id="page-5-1"></span>The term in the square bracket of Eq. [\(23\)](#page-5-0) contains the corrections to the standard predictions of inflation due to the ambiguity in the choice of vacuum. For arbitrary values of  $X$  these corrections are oscillatory, with amplitude  $\theta_0$ . First order  $\theta_0$  corrections are absent if and only if

$$
X = 0.\t(28)
$$

Taking into account the constraint [\(18\)](#page-4-6), our generalized vacuum choice spans a 3-dimensional space parametrized by, say, Im $(Y)$ , Re $(X)$  and Im $(X)$ . Equation [\(28\)](#page-5-1) just says that the set of parameters for which there are no linear corrections is a two-dimensional plane, i.e. it is of zero measure in parameter space.

If the vacuum is chosen at cutoff crossing, Eq. [\(26\)](#page-5-2), corrections are hence generically linear in  $H_*/\Lambda$  [\[9,](#page-9-8) [22\]](#page-10-4). For large values of  $p$ , the frequency of the oscillations  $\omega_{osc}$  [as a function of  $\log(k/k_*)$ ] is mildly k-dependent. To lowest order in  $1/p$ , it is given by

$$
\omega_{osc} = \frac{2}{p-1} \left(\frac{H_*}{\Lambda}\right)^{-1}.
$$
\n(29)

In the de Sitter limit,  $p \to \infty$ , there are no oscillations. A plot of both the conventional and the corrected power spectrum is shown in Figure [1.](#page-6-1)

If the vacuum for each mode is chosen at the time when the Hubble parameter equals the cutoff, Eq. [\(27\)](#page-5-3) the amplitude of the corrections is proportional to  $(H_*/\Lambda)^p$ . Therefore, unless  $H_* \approx \Lambda$  those corrections are highly suppressed, since for reasonable values of the spectral index, p is large.

In the Appendix we discuss many of the vacuum prescriptions that have been proposed in the literature and how they translate into specific values of  $X$  and  $Y$ . The results are summarized in Table [II.](#page-4-2) Inspection of that table shows that only for the Danielsson prescription corrections to the power spectrum are linear in  $H/\Lambda$ . For the remaining prescriptions, the adiabatic vacuum (of order bigger than one) and Hamiltonian diagonalization [\[23,](#page-10-5) [26\]](#page-10-6), the lowest order corrections are at the most quadratic<sup>3</sup> . Let us note however that in our opinion, no strong theoretical argument singles out any of the different vacuum choices.

<sup>3</sup> This conclusion is in agreement with [\[23](#page-10-5)], although the adiabatic vacuum we discuss here is not the "adiabatic vacuum" considered by those authors.



<span id="page-6-1"></span>FIG. 1: A plot—in arbitrary units—of the conventional (dashed) and the corrected power spectra (solid) log( $k/k_*$ ). The values of the parameters are  $p = 50$  (uncorrected  $n_S = 0.96$ ,  $H_*/\Lambda = 10^{-2}$  and  $\theta = -4 + 8i$ .

## V. PARTICLE PRODUCTION

Given the ambiguities in the definition of a vacuum state in an expanding universe, one might take a phenomenological approach to constrain plausible vacua. In general, one expects particles to be produced due to the changing gravitational field in an expanding universe. The amount of particles produced depends on the way the vacuum is defined. Hence, by requiring the rate of particle production to be negligible, one can put constraints on the vacuum choice [\[14](#page-9-13)].

Consider a graviton (or a massless scalar field) propagating in a fixed expanding universe. The amplitude  $h$ of any of the two polarization states of the graviton is described by the action [\(3\)](#page-2-1), where  $v = h/a$ . Hence, we can use our previous results to define a vacuum state for gravitational waves. Let us focus on a single comoving k-mode (we drop in the following the subscript  $k$ ). It is reasonable to expect that the vacuum prescription for gravitons and scalars are the same. Hence, we shall assume that the quantum state of the field is the vacuum defined by Eq. [\(17\)](#page-4-1) at the time of cutoff crossing, Eq. [\(15\)](#page-3-5). The prescription [\(17\)](#page-4-1) fixes the initial conditions for the mode functions  $v_{\text{in}}$ , and hence uniquely determines the annihilation operators  $a_{\text{in}}$ . We shall call such a vacuum the "in-vacuum",  $a_{\text{in}}| \text{in} \rangle = 0$ . At an arbitrary later moment of time  $\eta_{\text{out}}$ , an observer would use the same prescription  $(17)$  (with the same values of the parameters X and Y i to define a new vacuum  $|$ out  $\rangle$ . He would use a constant time hypersurface to define a vacuum state at that moment. Because  $\theta$  changes with time, such a prescription yields a different set of modes  $v_{\text{out}}$  and hence, a set of different annihilation operators  $a_{\text{out}}$ . Let us call the latter vacuum the out-vacuum,  $a_{\text{out}}|_{\text{out}} \rangle = 0$ . In general the in-vacuum and out-vacuum are different. In particular, the in-vacuum contains particles of the out-vacuum. It is easy to show that if the out-modes are expressed in terms of the in-modes,

<span id="page-6-0"></span>
$$
v_{\rm in} = \alpha \, v_{\rm out} + \beta \, v_{\rm out}^* \tag{30}
$$

the number of out-particles  $N_{\text{out}} = a_{\text{out}}^{\dagger} a_{\text{out}}$  contained in the in-vacuum is

<span id="page-6-3"></span>
$$
\langle \text{in} | N_{\text{out}} | \text{in} \rangle = |\beta|^2. \tag{31}
$$

This phenomenon is known as gravitational particle production. Using Eq. [\(30\)](#page-6-0) and the solution [\(19\)](#page-4-3) one can easily compute the Bogolubov coefficient  $\beta$ ,

$$
\beta = \frac{2}{\pi} (A_{\text{out}} B_{\text{in}} - B_{\text{out}} A_{\text{in}}).
$$
 (32)

Here,  $A$  and  $B$  are the coefficients  $(22)$  evaluated at the corresponding time: at cutoff crossing for the "in" subscript, and at  $\eta_{\text{out}}$  for the "out" subscript. Note that the Bogolubov coefficient vanishes if  $\eta_{\text{out}}$  is taken to be the time of cutoff crossing; the mode is indeed in the vacuum at cutoff crossing.

The number of particles in each k-mode can be used to estimate the total energy density of particles produced by the gravitational field at any arbitrary moment of time  $\eta_{\text{out}}$ . The differential particle density dn is (we restore the  $k$ -subindex in the following)

$$
dn = \frac{1}{4\pi^2} \frac{|\beta_k|^2}{a^3} k^2 dk.
$$
 (33)

Since we are working to lowest order in  $\theta$  we can assume the energy of the graviton to be given by  $E = k/a$ . Thus, the differential energy density of produced particles is

<span id="page-6-2"></span>
$$
d\rho = \frac{1}{4\pi^2} \frac{|\beta_k|^2}{a^4} k^3 dk. \tag{34}
$$

The total energy density contributed by the created particles is obtained by integrating Eq. [\(34\)](#page-6-2) over a suitable range of modes. At any given moment of time  $\eta_{\text{out}}$ , the maximum value of  $k$  is determined by the cutoff,  $k_{\text{max}} = a(\eta_{\text{out}})$ Λ. Because our vacuum prescription [\(17\)](#page-4-1) only makes sense for modes well-inside the Hubble radius, we shall take  $k_{\text{min}}$  to be determined by the size of the Hubble radius at time  $\eta_{\text{out}}$ ,  $k_{\text{min}} = a(\eta_{\text{out}})H_{\text{out}}$ . Substituting Eq. [\(32\)](#page-6-3) into Eq. [\(34\)](#page-6-2) and integrating between  $k_{\text{min}}$  and  $k_{\text{max}}$  one obtains to lowest order

<span id="page-6-4"></span>
$$
\rho = \frac{H_{\text{out}}^4}{16\pi^2} \left(\frac{H_{\text{out}}}{\Lambda}\right)^{-2} |X|^2 \cdot I\left(\frac{H_{\text{out}}}{\Lambda}\right),\tag{35}
$$

where  $I(r)$  is the integral

$$
I(r) = \int_{r}^{1} \left\{ x^{3-2/p} + x - \right. \left. (36)
$$

$$
- 2x^{2-1/p} \cos \left[ \frac{p}{1-p} \frac{\Lambda}{H_{\text{out}}} \left( x^{1/p} - x \right) \right] \right\} dx.
$$

For large values of  $\Lambda/H_{\text{out}}$  the oscillatory term in the integral averages out. Then, for  $p > 1/2$  the integral I is dominated by the upper limit  $(x = 1)$ , i.e. by the high momentum modes, and the integral is of order one. For values of  $p$  smaller or equal  $1/2$  the integral is dominated by the lower limit  $(x = H_{\text{out}}/\Lambda)$ , i.e. by the modes close to the horizon. Because for those modes our vacuum prescription breaks down, and because horizon size modes at that time crossed the cutoff during inflation, we shall restrict our attention to  $p > 1/2$  (matter domination or cosmic acceleration).

One can use Eq. [\(35\)](#page-6-4) and the Friedmann equation  $H^2 = 8\pi \rho_{\text{crit}}/(3M_{Pl}^2)$  to compute the ratio of produced particles to the total energy density in a flat universe. As an example, we shall consider our recent past, where the universe has been mostly matter dominated  $(p = 2/3)$ . Then,  $I(r) \approx 3/2$  and we find

$$
\frac{\rho}{\rho_{\rm crit}} \approx \frac{1}{4\pi} \left(\frac{\Lambda}{M_{Pl}}\right)^2 |X|^2. \tag{37}
$$

Presently, several cosmological probes constrain the contributions of the different universe constituents to the critical energy density [\[20](#page-10-2)]. The uncertainties in those contributions are within 10%. Thus, requiring the energy density of the produced particles to be less than 1/10 of the critical density, we find

<span id="page-7-0"></span>
$$
|X|^2 \le 1.3 \left(\frac{\Lambda}{M_{Pl}}\right)^{-2}.\tag{38}
$$

If one sets  $\Lambda = M_{Pl}$  one finds  $|X| \leq 1.1$ , which is still consistent with the Danielsson prescription. For lower values of the cutoff, condition [\(38\)](#page-7-0) is even laxer. Similar limits apply during inflation, since the inflaton has to remain the dominant energy component during that epoch.

## VI. SUMMARY AND CONCLUSIONS

Due to the ambiguity in the choice of a vacuum state during inflation, we have followed a phenomenological approach to characterize different possible vacuum choices. The vacuum ambiguity has two sources. The first one is the time at which the vacuum is defined. We have considered two alternatives: cutoff crossing and constant H. The second source consists on the way a particular vacuum is chosen at the specified time. We have parametrized any possible vacuum by a set of two complex parameters  $X$  and  $Y$ , subject to the constraint [\(18\)](#page-4-6). These parameters characterize the departures from Minkowski vacuum due to the expansion to first order in a properly chosen expansion parameter: the ratio of physical length of the mode to the Hubble radius.

To first order, only the parameter  $X$  enters the predicted power spectra generated during a stage of inflation. Generically, if initial conditions are chosen at cutoff crossing, corrections to the conventional predictions of inflation have the form of oscillations with an amplitude proportional to  $H/\Lambda$ , Eq. [\(23\)](#page-5-0). By "generically" we mean that the set of  $X$  values that yield no linear corrections is of zero measure in parameter space. Nevertheless, for the particular vacuum choices that have been

traditionally discussed in the literature (adiabatic vacuum and Hamiltonian diagonalization), corrections are at most quadratic. If initial conditions are specified at a constant time, the amplitude of the oscillations is proportional to a large power of  $H/\Lambda$ , i.e. it is highly suppressed.

Since theoretical arguments might not be able to constrain  $X$  and  $Y$ , we have attempted to set limits on their values by studying graviton creation in an expanding universe. By requiring the energy density of the produced gravitons to be less than ten per cent of the critical energy density today we obtain a constraint on the value of  $X$ , Eq. [\(38\)](#page-7-0). Even if the cutoff is chosen to be the Planck energy, the Danielsson prescription is still allowed by observations. For lower values of the cutoff, our observational constraint is not significant.

We conclude that, at the level of our analysis, the issue about the choice of vacuum is observational, rather than theoretical. This does not mean however that inflation is not predictive. All the vacuum choices we have discussed yield the same results at zeroth order in our expansion parameter. The first order corrections are "Planck"-suppressed, i.e. they are proportional to  $H/\Lambda$ . Thus, these corrections are always small, albeit in some cases they might be big enough to be detectable.

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## APPENDIX A: VACUUM PRESCRIPTIONS

We discuss in the following most of the different vacuum choices that have been proposed in the literature. They are based on imposing different conditions on the vacuum state. Up to what we shall call the "conventional" choice, they all share the same ambiguity related to the time where initial conditions for the mode functions shall be set.

#### 1. Adiabatic vacua

The adiabatic vacuum [\[24,](#page-10-7) [25\]](#page-10-8) has been claimed to be the best available notion of vacuum in a spacetime that has no static regions [\[3\]](#page-9-2) or any further additional symmetry. The notion of adiabatic vacuum is slightly technical, and has been the origin of some confusion in the literature. We hence review here the presentation of [\[3\]](#page-9-2).

The first ingredient of the adiabatic vacuum prescription is the exact, formal "positive frequency" WKB solution of the equation of motion [\(5\)](#page-2-2),

<span id="page-8-0"></span>
$$
v_k = \frac{1}{\sqrt{W_k}} \exp\left(-i \int^{\eta} W_k(\tilde{\eta}) d\tilde{\eta}\right), \quad (A1)
$$

where  $W_k$  is implicitly defined by the equation

<span id="page-8-3"></span>
$$
W_k^2 = \omega_k^2 - \frac{1}{2} \left( \frac{W_k''}{W_k} - \frac{3}{2} \frac{W_k'^2}{W_k^2} \right), \tag{A2}
$$

and  $\omega_k$  is given by Eq. [\(8\)](#page-2-6),

$$
\omega_k^2 = k^2 \left( 1 - \frac{2p - 1}{p} \theta^2 \right). \tag{A3}
$$

The reader can easily verify that the function [\(A1\)](#page-8-0) satisfies the normalization condition [\(6\)](#page-2-5).

In the limit where the expansion of the universe is "slow", one expects an expansion in the number of derivatives to be a good approximation to solve for  $W_k$ . To perform such an expansion one formally replaces  $\eta$  by  $\eta T$  and expands all quantities in a power series in  $T^{-1}$ . To *n*th adiabatic order, only powers up to  $T^{-n}$  are kept. Such an expansion is the second ingredient of the adiabatic prescription. It can be easily verified that to lowest and first adiabatic order  $\omega_k = k$  and  $W_k = \omega_k = k$ . Nontrivial time-dependent corrections do not show up until 2nd order.

If one substitutes the nth order adiabatic approximation to  $W_k$  into [\(A1\)](#page-8-0), one obtains the *n*th order adiabatic mode  $v_k^{(n)}$  $\binom{n}{k}$ . Note however that this *n*th order approximation is not an exact solution of the mode equation [\(5\)](#page-2-2) anymore. The third step of the adiabatic prescription consists of matching the nth order adiabatic approximation  $v_k^{(n)}$  $\kappa_k^{(n)}$  to the exact mode solutions of Eq. [\(5\)](#page-2-2) at an arbitrary time  $\eta_0$ . In other words, the *n*th adiabatic approximation is used to prescribe the values of  $v_k$  and  $v'_k$ at time  $\eta_0$ ,

<span id="page-8-1"></span>
$$
v_k(\eta_0) = v_k^{(n)}(\eta_0), \quad v'_k(\eta_0) = v'_k^{(n)}(\eta_0). \tag{A4}
$$

Because the WKB solution has been expanded only to nth adiabatic order, the matching of the two functions has to be carried only to that same order, i.e. only terms containing up to n powers of  $1/T$  have to be matched. Conditions [\(A4\)](#page-8-1) then uniquely define the mode function  $v_k$ . By construction,  $v_k$  is an exact solution of Eq. [\(5\)](#page-2-2), with initial conditions determined by the "distorted" adiabatic modes  $v_k^{(n)}$  $\binom{n}{k}$  at time  $\eta_0$ .

If one carries over the program described above, one obtains expressions for  $A_k$  and  $B_k$  as a power series in  $1/(T_{\eta_0})$ . To nth adiabatic order only terms up to order  $1/(T\eta_0)^n$  are significant. Hence, if we are interested in determining  $A_k$  and  $B_k$  to first order in  $\theta_0 \propto 1/(T\eta_0)$ , it hence suffices to consider the 1st order adiabatic vacuum; higher order adiabatic vacua only yield higher order corrections. Because to first adiabatic order  $W_k = k$ , the matching condition [\(A4\)](#page-8-1) to that same adiabatic order reads, up to an irrelevant common phase,

$$
v_k(\eta_0) = \frac{1}{\sqrt{k}}, \quad v'_k(\eta_0) = -i\sqrt{k}.
$$
 (A5)

By comparison with Eqs. [\(17\)](#page-4-1) we thus find

$$
Y = 0, \quad X = 0. \tag{A6}
$$

#### 2. The conventional choice

<span id="page-8-2"></span>Conventionally, the vacuum is chosen by requiring that the mode functions  $v_k$  reduce to the Minkowski ones in the limit  $\eta \rightarrow -\infty$ ,

$$
v_k(-\infty) = \frac{1}{\sqrt{k}}, \quad v'_k(-\infty) = -i\sqrt{k}.\tag{A7}
$$

Using the expansion [\(21\)](#page-4-4) one can directly find the values of the coefficients  $A_k$  and  $B_k$  for which the mode function [\(19\)](#page-4-3) satisfies Eqs. [\(A7\)](#page-8-2),

$$
A_k = \sqrt{\frac{\pi}{2}}, \quad B_k = 0.
$$
 (A8)

Once these coefficients are known one can then determine X and Y by comparing them Eqs.  $(22)$ ,

$$
X = 0, \quad Y = i \frac{1 - 2p}{1 - p}.
$$
 (A9)

The conventional vacuum is sometimes called the adiabatic vacuum, since it agrees with the adiabatic vacuum (of any order) in the limit  $\eta \to -\infty$ . One should bear in mind however that the conventional vacuum is only a particular adiabatic vacuum in the infinite set of adiabatic vacua parametrized by  $\eta_0$ . Let us note in addition that all the vacuum prescriptions we discuss here also yield the adiabatic vacuum in the limit  $\eta_0 \to -\infty$ .

### 3. Hamiltonian diagonalization

The Hamiltonian diagonalization vacuum<sup>4</sup> is the state that diagonalizes the field Hamiltonian [\(7\)](#page-2-7) at a given moment of time  $\eta_0$  [\[2](#page-9-1), [3\]](#page-9-2). Alternatively, it can be shown that the Hamiltonian diagonalization vacuum is the state that minimizes the energy  $E = \langle 0|\mathcal{H}|0\rangle$  at  $\eta_0$ . It directly follows from the Hamiltonian [\(7\)](#page-2-7) and the normalization condition [\(6\)](#page-2-5) that the diagonalization prescription amounts

<sup>4</sup> During the preparation of this work the preprint [\[26\]](#page-10-6) appeared, which discusses how the choice of different Hamiltonians affects the state of minimal energy.

to imposing the initial conditions

<span id="page-9-17"></span>
$$
v_k(\eta_0) = \frac{1}{\sqrt{\omega_k(\eta_0)}}, \quad v'_k(\eta_0) = -i\sqrt{\omega_k(\eta_0)}, \quad \text{(A10)}
$$

where  $\omega_k$  is the frequency [\(8\)](#page-2-6). Note that it is only possible to diagonalize the Hamiltonian for a particular subset of field modes.

The squared frequency [\(A3\)](#page-8-3) is quadratic in  $\eta_0$ . Hence the expansion of the square roots in Eq. [\(A10\)](#page-9-17) in a power series in  $\theta_0$  does not contain linear terms ( $\propto \theta_0$ ). Therefore, we immediately find

$$
X = 0, \quad Y = 0. \tag{A11}
$$

In the absence of a cutoff, Hamiltonian diagonalization has has been criticized on the grounds of excessive particle production [\[3\]](#page-9-2). Note that the Hamiltonian diagonalization and 1st order adiabatic vacua are the same.

#### 4. Danielsson prescription

According to Danielsson [\[9](#page-9-8), [22\]](#page-10-4), the vacuum shall be chosen by imposing the following condition on the mode

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<span id="page-9-18"></span>functions,

$$
\left(\frac{v_k}{a}\right)'(\eta_0) = -ik\frac{v_k}{a}(\eta_0). \tag{A12}
$$

<span id="page-9-19"></span>Using the normalization condition [\(6\)](#page-2-5), Eq. [\(A12\)](#page-9-18) implies the following relations (up to a common irrelevant phase)

$$
v_k(\eta_0) = \frac{1}{\sqrt{k}}, \quad v'_k(\eta_0) = -i\sqrt{k}(1 + i\theta_0).
$$
 (A13)

Therefore, by comparing Eqs. [\(17\)](#page-4-1) with Eqs. [\(A13\)](#page-9-19) it follows

$$
X = -i, \quad Y = i. \tag{A14}
$$

The Danielsson vacuum is a state of minimal uncertainty [\[27](#page-10-9)], but not the only one. It is not the state of minimal energy either, in the sense that it minimizes the Hamiltonian [\(7\)](#page-2-7) (see also [\[26\]](#page-10-6)). Nevertheless, at this stage the prescription [\(A13\)](#page-9-19) is as valid as any other.

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