JHEP

PUBLISHED BY INSTITUTE OF PHYSICS PUBLISHING FOR SISSA

RECEIVED: March 2, 2006 ACCEPTED: April 11, 2006 PUBLISHED: April 28, 2006

Universal correction to the inflationary vacuum

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ABSTRACT: The Bunch-Davies state appears precisely thermal to a free-falling observer in de Sitter space. However, precise thermality is unphysical because it violates energy conservation. Instead, the true spectrum must take a certain different form, with the Boltzmann factor $\exp(-\beta\omega_k)$ replaced by $\exp(\Delta S)$, where S is the entropy of the de Sitter horizon. The deviation from precise thermality can be regarded as an explicitly calculable correction to the Bunch-Davies state. This correction is mandatory in that it relies only on energy conservation. The modified Bunch-Davies state leads, in turn, to an $\mathcal{O}(H/M_p)^2$ modification of the primordial power spectrum of inflationary perturbations, which we determine.

KEYWORDS: Cosmology of Theories beyond the SM, Classical Theories of Gravity.

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1. Introduction

One of the most satisfying aspects of the inflationary paradigm is that the enormous structures in the present universe actually arose out of minuscule quantum fluctuations in the far past. As the spacetime geometry of the universe during inflation was, to excellent approximation, that of de Sitter space, this means that the large-scale structure visible today is intimately tied to the expectation value, $\langle \phi^2 \rangle$, of quantum fields in de Sitter space. Moreover, through observations of the cosmic microwave background and through galaxy surveys, we are able to indirectly probe the initial state of the universe.

Traditionally, the initial state in which the expectation values are calculated is assumed to be the Bunch-Davies state, $|BD\rangle$. This state is chosen, firstly, because the corresponding Green's function resembles that of the Poincaré-invariant vacuum at short distances and, secondly, because (for a massive scalar field) the Bunch-Davies state is invariant under the full de Sitter isometry group. Furthermore, the expectation value of the inflaton in the Bunch-Davies state, $\langle BD | \phi^2 | BD \rangle$, leads to the familiar, and observationally corroborated, scale-invariant primordial power spectrum of scalar density perturbations.

However, the assumption of the Bunch-Davies state as the initial state has recently been questioned [1-9]. Several plausible alternatives for the initial state have been suggested based on the anticipated behavior of quantum fields at Planckian energies [10-18]. Because the initial state is modified, these alternatives lead to slightly different predictions for the primordial power spectrum. This is an exciting possibility because the signatures of the modified initial state may be within the realm of observational investigation [19-25]. Nevertheless, one drawback so far has been that the assumed behavior of the fields at Planckian energies remains model-dependent.

In this paper, we take a different approach. We use the fact that energy must be conserved. Energy conservation does not break down in string theory and it would be surprising if we could not assume it during inflation. This suggests a modification of the Bunch-Davies state, as we now argue. It is well known that an inertial observer in de Sitter space is immersed in a bath of de Sitter radiation emanating from the de Sitter horizon [26]. The spectrum of this radiation (not to be confused with the primordial power spectrum) is, to first approximation, thermal. Indeed, it can be shown that, in the Bunch-Davies state, the spectrum is *precisely* the thermal Planck distribution characterized by the de Sitter temperature.

In fact, however, the true spectrum cannot be precisely thermal. Instead, as is known from parallel work on black hole radiation, implementing energy conservation modifies the spectrum in a definite way [27, 28]. One can regard the de Sitter radiation, whose origin is quantum-mechanical, as emerging out of virtual pairs of particles, one member of which has materialized by tunneling across the horizon. The probability of emission of a quantum of energy ω_k is then roughly

$$\Gamma_k \approx \exp(-\beta \omega_k) \,. \tag{1.1}$$

That is, it is roughly thermal. However, it is not exactly thermal because the horizon suffers a back-reaction when a particle is emitted, as a consequence of energy conservation. In a derivation in which energy conservation is taken into account [29], the effect is that the thermal Boltzmann factor is replaced by $\exp(\Delta S)$:

$$\exp(-\beta\omega_k) \to \exp(\Delta S(\omega_k)) , \qquad (1.2)$$

where S is the Bekenstein-Hawking entropy of the de Sitter horizon, and $\Delta S(\omega_k)$ is the change in the entropy when a quantum of radiation with energy ω_k is emitted. Since the Bunch-Davies state resulted in a perfectly thermal spectrum, we may regard this new modified spectrum as a consequence of a small modification of the initial state:

$$|BD\rangle \to |BD'\rangle$$
 . (1.3)

In turn, we are led to a robust and explicitly calculable modification to the primordial power spectrum of inflationary perturbations:

$$\frac{2\pi^2}{k^3} P(k) = \int d^3x \ e^{-i\vec{k}\cdot\vec{x}} \ \langle BD'|\phi(\vec{x})\phi(0)|BD'\rangle \ . \tag{1.4}$$

The modification to the primordial power spectrum thus arises unavoidably by energy conservation via a correction to the Bunch-Davies state.

This paper proceeds as follows. In section 2, we review the different vacuum choices in de Sitter space. We also substantiate the following interesting suggestion: the Bunch-Davies state actually appears empty, rather than thermal, to a hypothetical lightlike observer. In section 3, we state the results of the tunneling derivation of de Sitter radiation. In section 4, we present a formalism for obtaining the modification to the Bunch-Davies state from the modification to the thermal spectrum. In section 5, we compute the primordial power spectrum in this modified initial state. The result, a correction of order $(H/M_p)^2$, while small, is universal; as such, it is a model-independent signature of quantum gravity in the sky.

2. Vacuum states in de Sitter space

A well known feature of quantum field theory, and one that makes itself particularly manifest in curved spacetime backgrounds, is that the very definition of a particle excitation and hence of a thermal state depends sensitively on the choice of vacuum state. In a general curved spacetime, there is no canonical or even preferred vacuum state. However, if a spacetime admits isometries, and, in particular, a timelike Killing vector field, then this provides a natural means of partitioning modes into positive and negative frequency categories and then, in line with the standard procedure in Minkowski space, associating these with annihilation and creation operators. A vacuum state can then be defined by imposing the condition that the state be annihilated by all the annihilation operators.

In the absence of an everywhere timelike Killing vector, there is no natural choice of vacuum state. In that case, one can apply different criteria to motivate particular choices of vacuum. A simple choice, where possible, might be to restrict one's interest to a region of spacetime for which a timelike Killing vector does exist, and to use the corresponding vacuum state. Similarly, if the spacetime admits an asymptotically Minkowskian region, another possibility is to use the natural Poincaré vacuum in that region. Alternatively, one could demand that the vacuum be annihilated by the generators of some symmetry group. A vacuum state can also be deemed unphysical if it fails to satisfy certain criteria. For example, if the expectation value of the stress tensor diverges at a nonsingular point in spacetime, such as at a horizon, one would consider this grounds to reject the underlying vacuum state. In our case, we will require a certain universal form for the particle spectrum detected by an inertial observer, a form dictated by the conservation of energy.

In this section, we review some of the important vacua of de Sitter space, as well as some affiliated coordinate systems.

The Bunch-Davies state

The Bunch-Davies vacuum state, $|BD\rangle$, is usually defined using planar coordinates,

$$ds^{2} = -dt^{2} + e^{2Ht}dx^{2} = \frac{1}{(H\eta)^{2}} \left(-d\eta^{2} + d\rho^{2} + \rho^{2}d\Omega^{2} \right) , \qquad (2.1)$$

where $\eta = -e^{-Ht}/H$ is conformal time. See figure 1. The mode solutions to the massless scalar field wave equation,

$$u_k(\eta, \vec{x}) = N_k (1 + ik\eta) e^{-ik\eta + ik \cdot \vec{x}} , \qquad (2.2)$$



Figure 1: Penrose diagram for de Sitter space. Planar coordinates cover the shaded region. The curves are sections of constant η and constant ρ .

are termed positive frequency modes because they satisfy

$$\frac{\partial}{\partial \eta} u_k(\eta, \vec{x}) = -iku_k(\eta, \vec{x}) \tag{2.3}$$

in the infinite past i.e. in the $\eta \to -\infty$ limit. An off-cited motivation for this boundary condition is that, in this limit, the physical wavelength of any given mode is arbitrarily short compared to the Hubble length, and hence any distinction between de Sitter space and Minkowski space should be suppressed. The boundary condition (2.3) is recognized as the standard Minkowski space boundary condition, written in de Sitter space.

Another distinguishing property of the collection of modes (2.2) is that, under an arbitrary SO(4, 1) de Sitter transformation, the positive frequency modes each mix amongst themselves, the negative frequency modes mix amongst themselves, but these two classes of modes do not mix among each other. This implies, in particular, that the Bunch-Davies vacuum state is de Sitter invariant¹.

Even so, it is well known that the Bunch-Davies vacuum is not uniquely de Sitter invariant; for massive scalar fields, there is a one-parameter family of de Sitter-invariant vacua called α -vacua. These are related to the Bunch-Davies vacuum by choosing the positive frequency modes to be

$$u_k^{\alpha}(\eta, \vec{x}) = A \, u_k(\eta, \vec{x}) + B \, u_{-k}^*(\eta, \vec{x}) \,, \tag{2.4}$$

with A, B parameterized according to $A = \frac{1}{\sqrt{(1-e^{\alpha+\alpha^*})}}$ and $B = e^{\alpha}A$. Here, α is a complex number labeling the α -vacuum; the Bunch-Davies modes correspond to B = 0 i.e. to $\alpha = -\infty$. A somewhat more transparent expression of the α modes is to introduce the antipodal map $(\eta, \vec{x}) \to (-\eta, \vec{x}) \equiv (\overline{x})$ in terms of which (2.4) can be written

$$u_k^{\alpha}(x) = A \, u_k(x) + B \, u_{-k}(\overline{x}) \,.$$
 (2.5)

¹Even though, formally, no de Sitter-invariant vacuum exists for a massless scalar field [30], by assuming a tiny but nonzero mass, we can ignore this subtlety.



Figure 2: Penrose diagram for de Sitter space. Static coordinates cover the shaded region. The curves are sections of constant t and constant r.

Under an arbitrary de Sitter transformation, the positive and negative frequency u_k^{α} don't mix, and hence an α -vacuum state, defined by the condition that it lies in the kernel of all annhibition operators, is also de Sitter invariant.

The static state

Another important state in de Sitter space is the static vacuum, $|S\rangle$. Consider de Sitter space in static coordinates:

$$ds^{2} = -(1 - H^{2}r^{2})dt^{2} + (1 - H^{2}r^{2})^{-1}dr^{2} + r^{2}d\Omega^{2}.$$
(2.6)

See figure 2. The time coordinate here is the proper time of a static geodesic observer at the origin and $r = H^{-1}$ corresponds to the horizon in de Sitter space.

Using this time coordinate to define positive and negative frequencies leads to the static vacuum, so called because the generator of time translations, ∂_t , is a Killing vector. The physical significance of the static vacuum is that the particular geodesic observer resting at r = 0 sees it as empty: $b_k |S\rangle = 0$ for all k. Of course there is nothing special about this observer, and, indeed, there exists a corresponding vacuum state for each of the infinitely many freely falling observers that crisscross de Sitter space. The static vacuum is invariant under $SO(3) \times R$, i.e. under rotations and time translations, but not under the entire de Sitter isometry group, SO(4, 1). What seems to disqualify the static vacuum as a consistent state in de Sitter space is that the expectation value of the energy-momentum tensor blows up as one approaches the de Sitter horizon [31].

Relation between the Bunch-Davies state and the static state

It can be shown that the Bunch-Davies state appears precisely thermal to the static observer with temperature

$$T = \frac{H}{2\pi} . \tag{2.7}$$

The easiest way to see this is to consider the Bunch-Davies Green's function, G(x, x'). One sets $x(\tau)$ and $x'(\tau')$ to lie along a timelike geodesic with proper time τ ; the observer moving along such a geodesic registers a thermal spectrum if two conditions hold. First, the Green's function needs to be periodic under a shift $\tau \to \tau + i\beta$ (where $\beta = T^{-1}$), and second, the singularities of the two-point Green's function must allow for contour integrals that are consistent with detailed balance. In this way, it can be shown that the Bunch-Davies state appears thermal to the static observer, and, indeed, by de Sitter symmetry, to all timelike geodesic observers.

While the Bunch-Davies vacuum is a thermal state, the same is not true of any of the α -vacua for $\alpha \neq -\infty$. For $B \neq 0$, the combination in (2.5) introduces additional singularities for the two-point Green function in the complex plane, which in turn spoils the thermality of the state. The α -vacua deviations from a thermal spectrum can be calculated by properly accounting for the extra singularities [32–34], or by using a Bogolubov approach as illustrated in the appendix.

Perhaps, then, the best way to characterize the Bunch-Davies vacuum is its being the unique de Sitter-invariant state that appears thermal to a freely falling observer. Indeed, this is an accurate characterization of the Bunch-Davies state, but what is less widely appreciated is that there are an infinity of other states that fail to meet this very same set of criteria in the most mild of ways.

Here is what we mean. Consider a freely falling observer in de Sitter space, using static coordinates. Since ∂_t is a manifest Killing vector in these coordinates, we know that

$$u_0 = -(1 - H^2 r^2) \frac{dt_s}{d\tau}$$
(2.8)

is conserved along geodesics. Here τ is the proper time and u^{μ} are the components of the velocity four-vector (which should not be confused with mode functions). Let's call the value of this conserved quantity -E. Since $u^2 = -1$ we also have

$$\left(\frac{dr}{d\tau}\right)^2 = E^2 - (1 - H^2 r^2) .$$
(2.9)

Solving (2.8) and (2.9) subject to the boundary conditions $t_s(\tau = 0) = 0, r(\tau = 0) = 0$ we find

$$r(\tau) = \frac{1}{H}\sqrt{(E^2 - 1)}\sinh(H\tau)$$

$$t_s(\tau) = \frac{1}{H}\tanh^{-1}(E\tanh(H\tau)). \qquad (2.10)$$

When E = 1, we find that $r(\tau) = 0$ and $t_s(\tau) = \tau$, which parameterizes the worldline of the static observer who stays put at r = 0. In contrast, notice that for any $E \neq 1$, t_s is invariant under $\tau \to \tau + \pi i H^{-1}$ while r is invariant under $\tau \to \tau + 2\pi i H^{-1}$.

Consider now the two-point Green's function for a scalar field, making use of the static vacuum, i.e. the zero-particle state as seen by a given E = 1 observer. Since this two-point Green's function when evaluated along a geodesic is a function of $(t(\tau), r(\tau))$, we see that the Green's function is invariant under $\tau \to \tau + 2\pi i H^{-1}$. Moreover, since in this analysis

we have not modified the static patch Green function – we have only evaluated it along a particular curve – we can be sure that no new singularities have been introduced (in contrast to the case with α -vacua). Thus the periodicity of the Green's function implies that any freely falling observer (except for the sole such observer with E = 1) measures a thermal spectrum of particle excitations.

In other words, the static state as defined by the static (E = 1) observer, appears to be a thermal state for all other freely falling observers. The only freely falling observer who does not see a thermal spectrum is the static observer at r = 0, for whom this is the vacuum. Of course, nothing is special about this observer in our analysis; we can do the same analysis for every other freely falling observer. Doing so, we conclude that any freely falling observer can define a vacuum state with respect to which his or her "Unruh" particle detector will fail to detect any particles. The Unruh detectors of *all* other freely falling observers, however, will measure a thermal spectrum with the same temperature.

There is an intuitive way to understand this. Recall that, for black holes, the state that seems empty to the infalling observer looks thermal to the outside observer. Since the derivations are identical, this implies that, in de Sitter space, the state that seems empty to an observer who falls through another observer's horizon will seem thermal to the other observer. It follows by de Sitter symmetry that the static vacuum of any observer looks thermal to all other observers.

From the perspective of thermality, therefore, the distinction between the Bunch-Davies vacuum and the static patch vacua just described is simply this: All freely falling observers see the Bunch-Davies vacuum as a thermal state. All but one freely falling observer sees a given static patch vacuum state as thermal. That one special observer, of course, is the observer with respect to which the static vacuum is defined.

Heuristically, this suggests thinking about the Bunch-Davies vacuum state in the following way. All observers moving along timelike geodesics see the Bunch-Davies vacuum state as thermal. As above, all but one observer sees a given static patch vacuum state as thermal. If this one special observer should actually be moving along a lightlike trajectory, then the odd man out – the one observer who does not see the static patch vacuum state as thermal – would not be among the timelike observers. This suggests that one might think of the Bunch-Davies vacuum as that state which appears empty to an observer moving on a lightlike trajectory, but which appears thermal to all observers moving on timelike trajectories. From this perspective, the Bunch-Davies vacuum and the static patch vacua are all part of a single class of vacuum states, each appearing empty to one observer and thermal to everyone else.

One clue that this heuristic picture is correct is that the light ray emanating from r = 0in the limit $\eta \to -\infty$ actually travels along the $\eta \to -\infty$ time slice. But as $\eta \to -\infty$, the Bunch-Davies state becomes the ordinary vacuum of Minkowski space. Now, it is known that, in Minkowski space, the Poincaré-invariant vacuum is the same as the light-cone vacuum i.e. the vacuum with respect to the Hamiltonian generating lightlike translations. Thus the Bunch-Davies state is the same as the vacuum state for a lightlike observer. To make this more explicit, we note that the Bunch-Davies modes become plane waves in the far past. Picking an arbitrary spatial direction x, one expands the field operator in the $\eta \to -\infty$ limit as

$$\phi(\eta, x, \vec{x}) = \int_0^\infty \frac{dk_x}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{d^2 k_T}{2\pi} \frac{1}{\sqrt{2\omega_k}} \left\{ \left(a_{k_x, \vec{k}_T} e^{-i\omega_k \eta + ik_x x + i\vec{k}_T \cdot \vec{x}_T} + \text{h.c.} \right) + \left(a_{-k_x, \vec{k}_T} e^{-i\omega_k \eta - ik_x x + i\vec{k}_T \cdot \vec{x}_T} + \text{h.c.} \right) \right\}, \quad (2.11)$$

where x_T and k_T are the transverse position and wave number. The Bunch-Davies state is defined by $a_{k_x,\vec{k}_T}|BD\rangle = a_{-k_x,\vec{k}_T}|BD\rangle = 0$. But now these modes can be written in light cone coordinates $x^{\pm} = \eta \pm x$:

$$\phi(x^{\pm}, \vec{x}) = \int_0^\infty \frac{dk_x}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{d^2k_T}{2\pi} \frac{1}{\sqrt{2\omega_k}} \left\{ \left(a_{k_x, \vec{k}_T} e^{-i[(\omega_k - k_x)x^+ + (\omega_k + k_x)x^-] + i\vec{k}_T \cdot \vec{x}_T} + \text{h.c.} \right) + \left(a_{-k_x, \vec{k}_T} e^{-i[(\omega_k + k_x)x^+ + (\omega_k - k_x)x^-] + i\vec{k}_T \cdot \vec{x}_T} + \text{h.c.} \right) \right\}. (2.12)$$

Since $(\omega_k \pm k_x) \ge 0$, the positive frequency modes defining the Bunch-Davies vacuum also correspond to the positive frequency modes defining the light-cone vacuum. Accordingly, since one of the light-cone coordinates x^{\pm} corresponds to the affine parameter along a lightlike trajectory, the Bunch-Davies vacuum, being equivalent to the light-cone vacuum, also appears empty with respect to a fiducial observer traveling along a lightlike trajectory.

Formally, we can regard the transformation that takes a timelike observer into a lightlike observer as an infinite boost. Infinite boosts are not contained in the de Sitter group, which is noncompact, but one can include them by extending the de Sitter group to include its one-point compactification. Under the de Sitter group, the Bunch-Davies state is special in that it is thermal to all geodesic observers. But under the compactified de Sitter group the Bunch-Davies state is merely in the same class of states as the static vacua.

Painlevé coordinates

Painlevé coordinates [29] are a particularly useful coordinate system. The line element is

$$ds^{2} = -(1 - H^{2}r^{2}) dt^{2} - 2Hr dr dt + dr^{2} + r^{2} d\Omega^{2}. \qquad (2.13)$$

These coordinates resemble static coordinates, but have the advantage that the components of the metric and its inverse are finite at the horizon. Moreover, constant-time slices correspond to flat Euclidean space. In fact, the time slices are equivalent to the constanttime slices using planar coordinates. See figure 3. Indeed, Painlevé coordinates are a hybrid of static and planar coordinates, sharing the radial coordinate of the former but the time coordinate of the latter:

$$t_{\text{Painleve}} = t_{\text{planar}} = t_{\text{static}} + \frac{1}{2H} \ln(1 - H^2 r^2)$$

$$r_{\text{Painleve}} = r_{\text{static}} = \rho_{\text{planar}} e^{Ht}.$$
 (2.14)

Physically, Painlevé time is the proper time of comoving observers, as Painlevé time is the same as planar time.



Figure 3: Penrose diagram for de Sitter space. Painlevé coordinates cover the shaded region. The curves are sections of constant t and constant r. Also shown is a constant-time slice split into two.

What is the vacuum associated with Painlevé time? Because of the off-diagonal metric component, the time translation vector ∂_t is different from the normal vector, n, to surfaces of constant t. Should one consider modes to be positive frequency if they have positive eigenvalues with respect to ∂_t or with respect to n? The answer follows immediately from the Klein-Gordon inner product,

$$(\phi_1, \phi_2) = i \int_{\Sigma} d\Sigma^a (\phi_1^* \overleftrightarrow{\partial_a} \phi_2) . \qquad (2.15)$$

In this expression, $d\Sigma^a = n^a d\Sigma$ is the oriented volume element of a spatial slice, Σ . The inner product defines positive norm modes, and, since these are paired with annihilation operators, also defines the vacuum state. As the above expression shows, positive frequency should be defined with respect to the normal vector, n, not ∂_t . But Painlevé time and planar time are the same, and hence, so are their time-slices. It follows that the Painlevé vacuum is precisely the Bunch-Davies state. This is important because the derivation of the approximately thermal spectrum in the next section will imply a back-reaction modification to the Painlevé state. So it must mean that the Bunch-Davies state is modified.

3. Deviations from thermality

In inflationary cosmology, the initial state of the universe is usually taken to be the Bunch-Davies state. As explained above, the motivation for this choice of state is two-fold: the state is de Sitter invariant and the corresponding Green's function has a short-distance behavior appropriate to Minkowski space. Now, the Bunch-Davies state is a thermal state; an Unruh detector for a free-falling observer registers a precisely Planckian spectrum with temperature $H/2\pi$. However, there exist quite general reasons why the initial state cannot be strictly thermal; the Bunch-Davies state is not physical because it violates energy conservation. To see this, consider the closely analogous background of a Schwarzschild black hole.

At first sight, the spectrum of a black hole's Hawking radiation is also Planckian. Yet, for a variety of reasons, the true spectrum actually departs from pure thermality. First, a purely thermal spectrum would have a tail extending out to infinitely high energies. But a black hole obviously cannot emit a quantum with more energy than its own mass. Thus there is a high-energy cut-off to the spectrum. Moreover, even at energies significantly lower than this cut-off, the spectrum must deviate from strict thermality. This is because the "temperature" of a black hole is a function of the mass – but the mass is different before and after emission.

Parallel arguments apply to de Sitter space. De Sitter space has a horizon of radius H^{-1} . This puts an upper bound on the energy of any quantum in de Sitter space: it cannot exceed the mass of the "Nariai black hole," the largest black hole that can fit inside the de Sitter horizon. Moreover, as we will see, when the de Sitter horizon emits a quantum of energy, it shrinks, much as a black horizon does. The horizon temperature is thus affected by the emission of the quantum so that the spectrum has small deviations from thermality even at lower energies. This effect become more prominent at higher energies.

Finally, there is also a more fundamental reason why, in a gravitational setting, one does not have a well-defined notion of temperature. Recall that to define a temperature for a system, one formally places the system in contact with an infinite reservoir. But, in the presence of gravity, no such reservoir exists: any system larger than the Jeans length will collapse. One should therefore more properly consider the microcanonical ensemble – in which energy is fixed – rather than the canonical ensemble (for which the temperature is fixed).

The above arguments indicate that the Bunch-Davies state, by virtue of being precisely thermal, cannot be quite the right state. Rather, the correct state is the one that yields the spectrum appropriate to the microcanonical ensemble. Once we have this spectrum, we will, in the next section, determine the state that gives rise to it; we will then calculate the modification to the power spectrum of primordial density perturbations.

Fortunately, there already exists a treatment of de Sitter radiation [29] in a microcanonical framework. In this picture, de Sitter radiation arises because a virtual pair is created on the other side of the horizon. The positive-energy member of the pair is forbidden outside the horizon, because, in static coordinates, the t - t component of the metric has the opposite sign there. This positive-energy particle then tunnels across the horizon towards the observer where, because of the flip in the sign of the metric, it becomes classically allowed. This picture of radiation as a tunneling phenomenon naturally incorporates energy conservation because the barrier across which the particle tunnels is determined by the change in the horizon radius. One finds [29, 35] that the probability of emission is

$$\Gamma \sim \exp(\Delta S) = \exp\left[\frac{\pi}{G}(r_f^2 - r_i^2)\right] , \qquad (3.1)$$

where ΔS is the change in the entropy of the horizon, and r_i and r_f are the initial and final positions of the horizon. As we will see, at low energies (3.1) approximates a thermal Boltzmann factor. We note that the form of the expression, as anticipated in [36], is exactly the same as for black holes [28, 37]. Another appealing aspect of this result in that context is that it is consistent with an underlying unitary quantum theory [38].²

To see that r_i differs from r_f , consider a single particle emitted by the de Sitter horizon. Before emission, the spacetime is empty and is described by the line element of de Sitter space, (2.6). Thus the initial horizon radius is simply

$$r_i = H^{-1} . (3.3)$$

After emission, the spacetime is not pure de Sitter space because it contains a quantum of energy ω . For simplicity, consider emission in the s-wave so that the particle is really a spherical shell. The spherically-symmetric spacetime with energy ω is Schwarzschild-de Sitter space. This has the line element

$$ds^{2} = -(1 - H^{2}r^{2} - 2G\omega/r)dt^{2} + (1 - H^{2}r^{2} - 2G\omega/r)^{-1}dr^{2} + r^{2}d\Omega^{2}.$$
 (3.4)

The final location of the horizon is determined by setting g^{rr} to zero and solving the resulting cubic equation for its largest root. We find

$$r_f = \frac{2}{H\sqrt{3}} \cos\left(\frac{1}{3}\arctan\left(\frac{\sqrt{\frac{1}{27} - (G\omega H)^2}}{-G\omega H}\right)\right) , \qquad (3.5)$$

where the arctan takes values between $\pi/2$ and π . Equation (3.1) then implies an emission rate of

$$\Gamma \sim \exp\left[\frac{\pi}{H^2 G} \left(\frac{4}{3} \cos^2\left(\frac{1}{3} \arctan\left(\frac{\sqrt{\frac{1}{27}} - (G\omega H)^2}{-G\omega H}\right)\right) - 1\right)\right] . \tag{3.6}$$

This expression can be rendered more tractable by considering the low-energy limit $G\omega H \ll$ 1. Then

$$\Gamma \approx \exp\left[-\frac{2\pi}{H}\omega\left(1+\frac{\omega H}{8\pi M_p^2}\right)\right],$$
(3.7)

where we have expressed Newton's constant in terms of the Planck mass: $M_p^{-2} = 8\pi G$. If we neglect the $\omega H/(8\pi M_p^2)$ correction, we find a probability that is precisely the Boltzmann factor for emission at temperature $H/2\pi$. Had there been no correction term, elementary statistical mechanics would then have implied a spectrum with Planckian occupation numbers, precisely the spectrum detected by a free-falling Unruh detector in the Bunch-Davies state.

The correction term can be regarded as a consequence of self-gravitation or, equivalently, of back-reaction or energy conservation [27, 37]. In the next section, we will infer

$$\Gamma = |\text{amplitude}|^2 \times (\text{phase space factor}) \sim \frac{e^{S_{\text{final}}}}{e^{S_{\text{initial}}}} = \exp(\Delta S) , \qquad (3.2)$$

in accord with our expression.

²Were there a description of de Sitter radiation in a unitary theory of quantum gravity, one would expect the emission rate to be given by the square of the amplitude times the phase space factor. The latter is given by summing over the $e^{S_{\text{final}}}$ final states and averaging over the $e^{S_{\text{initial}}}$ initial states. Thus we would expect

the corrected initial state that corresponds to the corrected spectrum. Note that we can already anticipate a modification to the primordial power spectrum. From (3.7), we can attribute an effective temperature

$$T_{\rm eff} \approx \frac{H}{2\pi} \left(1 - \frac{\omega H}{8\pi M_p^2} \right) ,$$
 (3.8)

so that, at typical energies, $\omega \sim H$, we have a modification of order $(H/M_p)^2$, whereas at Planckian energies we find a modification of order H/M_p .

4. Determining the correction to the Bunch-Davies state

We will now interpret the corrections to the thermal spectrum in terms of a small modification of the initial state. Let us first explain the setup. In canonical language, the probability for pair creation of quanta of energy ω_k is

$$\Gamma_{k} = \left| \frac{\langle \operatorname{out} | b_{k} b_{-k} | \operatorname{in} \rangle}{\langle \operatorname{out} | \operatorname{in} \rangle} \right|^{2} , \qquad (4.1)$$

where the operators b_k annihilate the out-vacuum, i.e. $b_k |\text{out}\rangle = 0$. We need to determine what $|\text{in}\rangle$ and $|\text{out}\rangle$ refer to in the tunneling calculation. Now, that calculation was performed using Painlevé coordinates³ [29, 35]. The tunneling probability is the probability to go from empty de Sitter space to a spacetime containing a pair of particles, one on either side of the horizon, only one of which is detected as de Sitter radiation by the observer at r = 0. This suggests that the out-state should be related to the static vacuum $|S\rangle$, as defined by an r = 0 observer. But, more precisely, because Painlevé coordinates cover the full planar patch, the out-state actually splits (see Figure 3) into a tensor product:

$$|\text{out}\rangle = |\text{I}\rangle \otimes |\text{II}\rangle, \qquad (4.2)$$

with the state in the static region I corresponding to the static vacuum, $|I\rangle \sim |S\rangle$. That $|I\rangle$ corresponds to the static vacuum can be seen in a couple of ways. First, it is suggested by the near-thermal result of the path integral. And second, in region I, the timelike Killing vectors $\partial_{t_{\text{static}}}$ and $\partial_{t_{\text{Painleve}}}$ agree, by $(2.14)^4$. Then since the quanta in the out-state have to be created in pairs, and because only one member of the pair ends up on each side of the horizon, only one of the creation operators acts on the static vacuum. The other one acts on II, on the other side of the horizon. That is, the amplitude is for the transition $|in\rangle \rightarrow b_k^{(I)\dagger} b_{-k}^{(II)\dagger} |out\rangle$. Thus the probability of creating two particles in the out-state is the same as the probability of detecting one particle in the static vacuum.

Furthermore, the in-state is, to first approximation, just the Painlevé vacuum. We argued in section 2 that that was just the Bunch-Davies state, $|BD\rangle$. However, were the instate really the Bunch-Davies state, we would have obtained a precisely thermal spectrum.

³See [27] for earlier work incorporating back-reaction using a Hamiltonian formalism.

⁴In principle one should be able to determine the structure of the $|out\rangle$ -state unambiguously from the path integral derivation; it would be nice to show this formally.

The not-quite thermal spectrum suggests instead that the in-state is a slightly modified Bunch-Davies state, $|BD'\rangle$. Indeed, the effective geometry seen by a self-gravitating shell is not pure de Sitter space, but rather Schwarzschild-de Sitter space, (3.4). This has a slightly different Painlevé metric and is therefore associated with a slightly different state.

In summary, we have three states: $|out\rangle$, $|BD\rangle$, and $|BD'\rangle$. Moreover,

$$\left|\frac{\langle \operatorname{out} | b_k b_{-k} | \operatorname{BD} \rangle}{\langle \operatorname{out} | \operatorname{BD} \rangle}\right|^2 = e^{-\beta\omega_k}$$
$$\left|\frac{\langle \operatorname{out} | b_k b_{-k} | \operatorname{BD}' \rangle}{\langle \operatorname{out} | \operatorname{BD}' \rangle}\right|^2 = e^{\Delta S(\omega_k)}, \qquad (4.3)$$

where the first expectation value is the standard thermal expression, and the second expectation value was derived through the tunneling calculation. Let us now use these expressions to determine the precise relationship between the Bunch-Davies state and the modified state in terms of Bogolubov coefficients.

4.1 A general Bogolubov approach

Consider a real quantum scalar field in the planar patch of de Sitter space. Expand the scalar field in a complete set of orthonormal momentum eigenmodes:

$$\phi(x) = \sum_{k} \phi_k(x) , \qquad (4.4)$$

with $k \equiv |\vec{k}|$. The time coordinate is assumed to be Painlevé time (2.13), which itself is equivalent to planar time. Define three different expansions of the same quantum field:

$$\phi_k(x) = a_k \ u_k(x) + a^{\dagger}_{-k} \ u^*_{-k}(x)$$

= $a'_k \ u'_k(x) + a'^{\dagger}_{-k} \ u'^*_{-k}(x)$
= $b_k \ v_k(x) + b^{\dagger}_{-k} \ v^*_{-k}(x)$. (4.5)

Also define three different vacuum states, each corresponding to an "empty" state in terms of the associated annihilation operators:

$$a_k |BD\rangle = 0$$
, $a'_k |BD'\rangle = 0$, $b_k |\text{out}\rangle = 0$. (4.6)

We have in mind that these three states are the Bunch-Davies state, the modified Bunch-Davies state, and the out-state. As in (4.2), the out-state can be written as a tensor product of states in regions I and II; the vacuum state in region I is just the static vacuum.

The particle content of our three states will generally be nonzero with respect to each other; Bogolubov transformations mix up the positive and negative frequency modes. Expressing the linear decomposition for the mode functions $v_k(x)$ in terms of $u_k(x)$ or $u'_k(x)$ we have

$$v_{k}(x) = \sum_{j} \left[\tilde{\alpha}_{jk} \ u_{j}(x) + \tilde{\beta}_{jk} \ u_{-j}(x)^{*} \right]$$

=
$$\sum_{i} \left[\tilde{\alpha}'_{ik} \ u'_{i}(x) + \tilde{\beta}'_{ik} \ u'_{-i}(x)^{*} \right] .$$
(4.7)

Similarly, the different creation and annihilation operators are related via

$$b_{k} = \sum_{j} \left[\tilde{\alpha}_{jk}^{*} a_{j} - \tilde{\beta}_{jk}^{*} a_{-j}^{\dagger} \right]$$
$$= \sum_{i} \left[\tilde{\alpha}_{ik}^{\prime *} a_{i}^{\prime} - \tilde{\beta}_{ik}^{\prime *} a_{-i}^{\prime \dagger} \right] .$$
(4.8)

Proper normalization of the scalar field requires that

$$\sum_{k} \left(\tilde{\alpha}_{ik} \, \tilde{\alpha}_{jk}^{*} - \tilde{\beta}_{ik} \, \tilde{\beta}_{jk}^{*} \right) = \sum_{k} \left(\tilde{\alpha}_{ik}^{\prime} \, \tilde{\alpha}_{jk}^{\prime *} - \tilde{\beta}_{ik}^{\prime} \, \tilde{\beta}_{jk}^{\prime *} \right) = \delta_{ij}$$
$$\sum_{k} \left(\tilde{\alpha}_{ik} \, \tilde{\beta}_{jk} - \tilde{\beta}_{ik} \, \tilde{\alpha}_{jk} \right) = \sum_{k} \left(\tilde{\alpha}_{ik}^{\prime} \, \tilde{\beta}_{jk}^{\prime} - \tilde{\beta}_{ik}^{\prime} \, \tilde{\alpha}_{jk}^{\prime} \right) = 0 \,. \tag{4.9}$$

A general Bogolubov transformation, viewed as a matrix, can have nonvanishing offdiagonal components. However, for our present situation, because the spatial modefunctions are defined on the same spatial slice for all three states (4.4), we can choose an orthonormal basis such that the Bogolubov coefficients are diagonal in k:

$$\tilde{\alpha}_{kl} \equiv \tilde{\alpha}_k \delta_{kl}, \quad \beta_{kj} \equiv \beta_k \delta_{kj}, \quad |\tilde{\alpha}_k|^2 - |\beta_k|^2 = 1$$

$$\tilde{\alpha}'_{kl} \equiv \tilde{\alpha}'_k \delta_{kl}, \quad \tilde{\beta}'_{kj} \equiv \tilde{\beta}'_k \delta_{kj}, \quad |\tilde{\alpha}'_k|^2 - |\tilde{\beta}'_k|^2 = 1.$$
(4.10)

We are interested in solving the following problem: Suppose we know the Bogolubov coefficients $\tilde{\alpha}_k$, $\tilde{\beta}_k$ and $\tilde{\alpha}'_k$, $\tilde{\beta}'_k$, relating the $|BD\rangle$ and $|BD'\rangle$ states to the $|\text{out}\rangle$ state. How do we then determine the Bogolubov coefficients between the $|BD\rangle$ and $|BD'\rangle$ states? In other words, we want to express the Bogolubov coefficients α_k and β_k , defined by

$$a'_{k} = \alpha_{k}^{*} a_{k} - \beta_{k}^{*} a_{-k}^{\dagger}$$
(4.11)

in terms of the coefficients $\tilde{\alpha}_k$, $\tilde{\beta}_k$ and $\tilde{\alpha}'_k$ and $\tilde{\beta}'_k$. Since the final result will be important for the rest of the paper, let us be as explicit as possible. Multiplying (4.8), by $\tilde{\alpha}'^*_k$ and its complex conjugate by $\tilde{\beta}'_k$, and subtracting, we see that

$$a'_k = \tilde{\alpha}'_k \ b_k + \tilde{\beta}'^*_k \ b^{\dagger}_{-k} \ . \tag{4.12}$$

Using (4.8), we find

$$a'_{k} = \left(\tilde{\alpha}'_{k}\tilde{\alpha}^{*}_{k} - \tilde{\beta}'^{*}_{k}\tilde{\beta}_{k}\right) a_{k} + \left(-\tilde{\alpha}'_{k}\tilde{\beta}^{*}_{k} + \tilde{\beta}'^{*}_{k}\tilde{\alpha}_{k}\right) a^{\dagger}_{-k} , \qquad (4.13)$$

so that, by (4.11),

$$\alpha_k^* = \tilde{\alpha}_k' \tilde{\alpha}_k^* - \tilde{\beta}_k'^* \tilde{\beta}_k$$

$$-\beta_k^* = -\tilde{\alpha}_k' \tilde{\beta}_k^* + \tilde{\beta}_k'^* \tilde{\alpha}_k . \qquad (4.14)$$

As a check, note that when $|BD\rangle = |BD'\rangle$ the Bogolubov coefficients α_k and β_k become trivial. Once the Bogolubov coefficients $\tilde{\alpha}'_k$, $\tilde{\beta}'_k$, $\tilde{\alpha}_k$ and $\tilde{\beta}_k$ are known, these expressions allow us to immediately determine the Bogolubov coefficients relating the $|BD\rangle$ the $|BD'\rangle$ state.

4.2 Relating the two in-states

The Bogolubov transformation guarantees that both the $|BD\rangle$ and the $|BD'\rangle$ in-state can be realized as squeezed out-states:

$$|BD\rangle = \tilde{S} |\text{out}\rangle \quad , \quad |BD'\rangle = \tilde{S}' |\text{out}\rangle \; , \tag{4.15}$$

where \tilde{S} and \tilde{S}' are unitary squeezing operators:

$$\tilde{S} = \prod_{k} \left(1 - |\tilde{\gamma}_{k}|^{2} \right)^{\frac{1}{4}} \exp\left(\frac{1}{2} \tilde{\gamma}_{k} b_{k}^{\dagger} b_{-k}^{\dagger} \right) \,. \tag{4.16}$$

The other squeezing operator \tilde{S}' is obtained by replacing $\tilde{\gamma}_k$ with $\tilde{\gamma}'_k$. Demanding (4.6) and expressing the annihilation operators for $|BD\rangle$ and $|BD'\rangle$ in terms of b_k and b_k^{\dagger} , we find

$$\tilde{\gamma}_k \equiv -\frac{\tilde{\beta}_k^*}{\tilde{\alpha}_k} \quad , \quad \tilde{\gamma}'_k \equiv -\frac{\tilde{\beta}'^*_k}{\tilde{\alpha}'_k} \,.$$
(4.17)

This is easiest to show by writing b_k as $\frac{d}{db_k^{\dagger}}$ in the Bogolubov transformations. We can also show (see for instance [39, 40]) that

$$\tilde{\gamma}_{k} = \frac{\langle \text{out} | b_{k} b_{-k} | \text{BD} \rangle}{\langle \text{out} | \text{BD} \rangle}$$
$$\tilde{\gamma}_{k}' = \frac{\langle \text{out} | b_{k} b_{-k} | \text{BD}' \rangle}{\langle \text{out} | \text{BD}' \rangle} .$$
(4.18)

In words: the two $\tilde{\gamma}_k$'s are the probability amplitudes for pair-creation in the Bunch-Davies and modified Bunch-Davies state.

Now recall that we defined the Bunch-Davies and modified Bunch-Davies state through the absolute value of exactly these squared expectation values in (4.3). As a consequence the absolute values squared of the Bogolubov ratios $\tilde{\gamma}_k$ and $\tilde{\gamma}'_k$ are

$$|\tilde{\gamma}_k|^2 = e^{-\beta\omega_k} \quad , \quad |\tilde{\gamma}'_k|^2 = e^{\Delta S(\omega_k)} \ . \tag{4.19}$$

Given these expressions for $\tilde{\gamma}_k$ and $\tilde{\gamma}'_k$ we are now in a position to calculate $\gamma_k \equiv -\frac{\beta_k^*}{\alpha_k}$, using (4.14). We find

$$\gamma_k = \tilde{\gamma}_k \frac{\tilde{\alpha}'_k}{\tilde{\alpha}'^*_k} \frac{1 - \tilde{\gamma}'_k / \tilde{\gamma}_k}{1 - \tilde{\gamma}_k \tilde{\gamma}'^*_k} \,. \tag{4.20}$$

Now, multiplying one set of operators, say $\{b_k\}$, by overall phases clearly does not affect the choice of state. We can use this rescaling freedom to make $\tilde{\alpha}'_k$ real. (Indeed, by further rescalings, we can also force $\tilde{\alpha}_k$ to be real.) But to proceed, we also need to know something about the phase of $\tilde{\gamma}'_k$. In fact, it turns out that neither $\tilde{\gamma}'_k$ nor $\tilde{\gamma}_k$ have any nontrivial phases; they are both real and positive. There are a couple of ways to see this. Generally, probability amplitudes for tunneling — which is what the $\tilde{\gamma}_k$'s represent — are real. For example, in nonrelativistic quantum mechanics, the probability amplitude for a particle to tunnel across a potential barrier V(x) is

$$\frac{\psi(x_{II})}{\psi(x_I)} = \exp\left(i\int_{x_I}^{x_{II}} p \ dx\right) \ , \tag{4.21}$$

where the momentum, p, is purely imaginary: $p = \sqrt{2m(E - V(x))}$. Thus there is no nontrivial phase in the amplitude.

Moreover, one can show that if $\tilde{\gamma}_k$ is real and positive, then $\tilde{\gamma}'_k$ must be real and positive as well. That is, if the amplitude for tunneling without back-reaction has no phase, then neither does the amplitude when back-reaction is incorporated. To see this, imagine the particle or shell of energy ω_k being made up of a large number, N, of smaller noninteracting sub-shells, each of energy ω_k/N . As N becomes infinite, the constituent shells have negligible energy and Hawking's thermal formula, which neglected back-reaction, becomes exact. The probability amplitude for emitting one of these sub-shells is then $\exp(-\frac{1}{2}\beta\omega_k/N)$, where β is the inverse de Sitter temperature. But now the probability amplitude for the finite shell is just the product of the probability amplitudes for the sub-shells, taking into account that β changes infinitesimally with each emission. Hence

$$\tilde{\gamma}'_k = \prod^N e^{-\frac{1}{2}\beta\omega_k/N} = e^{-\frac{1}{2}\sum\beta\omega_k/N} \to e^{-\frac{1}{2}\int\beta d\omega} .$$
(4.22)

Writing $dM = -d\omega_k$ and invoking the first law of thermodynamics, $\beta dM = dS$, we obtain

$$\tilde{\gamma}_k' = e^{\frac{1}{2}\Delta S(\omega_k)} . \tag{4.23}$$

This is perhaps the easiest way to see that the tunneling probability had to take the form $\exp(\Delta S)$. But in addition one learns that, since the infinitesimal probability amplitudes had no phase, $\tilde{\gamma}'_k$ is real and positive. As a final check, we confirm explicitly that these arguments are borne out by considering the particle spectrum of the α -states, for which the result is known. This is done in the appendix. We indeed find that $\tilde{\gamma}_k$ has no nontrivial phase. Then, by the above arguments, neither does $\tilde{\gamma}'_k$.

Thus we can write (4.20) as

$$\gamma_k = \frac{\tilde{\gamma}_k - \tilde{\gamma}'_k}{1 - \tilde{\gamma}_k \tilde{\gamma}'_k} \,. \tag{4.24}$$

Plugging in (4.19) yields

$$\gamma_k = \frac{e^{-\frac{1}{2}\beta\omega_k} - e^{\frac{1}{2}\Delta S(\omega_k)}}{1 - e^{-\frac{1}{2}\beta\omega_k}e^{\frac{1}{2}\Delta S(\omega_k)}} \,. \tag{4.25}$$

As a check, we note that γ_k vanishes in the limit $\Delta S(\omega_k) = -\beta \omega_k$, i.e. the corrections due to back-reaction vanish when $\frac{\omega_k}{M_n} \to 0$.

In (3.7) we found that

$$\Delta S(\omega_k) \approx -\beta \omega_k \left(1 + \frac{\omega_k H}{8\pi M_p^2} \right) . \tag{4.26}$$

Expanding the exponential in (4.25) to lowest order in ω_k/M_p , and using $\beta = 2\pi/H$, we find that

$$\gamma_k \approx \frac{e^{\pi \frac{\omega_k}{H}}}{e^{2\pi \frac{\omega_k}{H}} - 1} \frac{\omega_k H}{8M_p^2} \,. \tag{4.27}$$

The energy ω_k corresponds to the physical energy of the emitted quantum as measured by a static observer at r = 0. In terms of comoving momentum, which is the natural momentum label in planar coordinates, the physical energy ω_k is related to comoving momentum by the scale factor: $\omega_k \propto \frac{k}{a(t)}$. We will need this relation in the next section, when we calculate the primordial spectrum of inflationary perturbations using the modified Bunch-Davies state.

5. Primordial spectrum of inflationary perturbations

We have argued that the standard Bunch-Davies vacuum state needs to be modified because it is inconsistent with energy conservation. Rather, the spectrum of perturbations should be calculated instead in the modified state $|BD'\rangle$. Now, the standard primordial power spectrum of inflationary perturbations is directly proportional to the massless scalar field spectrum; the results we obtain for the scalar field therefore also pertain to the spectrum of inflationary density perturbations, as is usual in such calculations.

Consider then an arbitrary vacuum state $|X\rangle$. Let $|X\rangle$ be annihilated by all the annihilation operators a'_k , and call the corresponding Fourier-transformed mode functions $u'_k(\eta)$. The equal-time variance of the scalar field in $|X\rangle$,

$$\langle X | \phi(\vec{x}) \phi(\vec{y}) | X \rangle = \int \frac{d^3k}{(2\pi)^3} \, |u'_k|^2 \, e^{i\vec{k}(\vec{x}-\vec{y})} \,, \tag{5.1}$$

defines the power spectrum, $\langle X | \phi^2 | X \rangle \equiv \int d \ln k P(k)$, of scalar field perturbations:

$$\frac{2\pi^2}{k^3} P(k) = \int d^3x \, e^{-i\vec{k}\cdot\vec{x}} \, \langle X|\phi(\vec{x})\phi(0)|X\rangle = |u'_k|^2 \,. \tag{5.2}$$

The well-known scale-invariant result arises when the variance is computed in the Bunch-Davies state: $|X\rangle = |BD\rangle$. We denote this by $P_{BD} \equiv \frac{k^3}{2\pi^2} |u_k|^2$. Now let $|X\rangle = |BD'\rangle$, and call P(k) the power spectrum in the modified state. From the Bogolubov transformation

$$u_k'(\eta) = \alpha_k u_k(\eta) + \beta_k u_k^*(\eta) , \qquad (5.3)$$

it is straightforward to find the relation between the two power spectra. We know that we can set α_k to be real. Moreover, in the previous section we showed that $\gamma_k \equiv -\beta_k^*/\alpha_k$ is real. Also, write $u_k = |u_k|e^{i\delta}$. Then we conclude that

$$P(k) = \frac{1}{1 - \gamma_k^2} \left(1 - 2\gamma_k \cos(2\delta) + \gamma_k^2 \right) P_{BD} .$$
 (5.4)

When calculating the power spectrum of inflationary perturbations one is usually instructed to evaluate the spectrum for different k at the time of horizon crossing, corresponding to k = a(t)H. The reason this gives the right answer is that, after horizon crossing, the mode-function very quickly approaches a constant. Furthermore, the Bunch-Davis modefunctions also have the property that the phase δ is fixed and independent of k, after imposing k = aH. We can determine δ from the expression for the Bunch-Davies modes, (2.2). Also, since $\gamma_k \ll 1$, we can write

$$P(k) \approx \left(1 - 2\gamma_k \cos(2\delta)\right)|_{k=aH} P_{BD} .$$
(5.5)

Now we simply plug in the expression for γ_k , (4.27), to find the leading correction to the primordial power spectrum from picking the modified Bunch-Davies vacuum $|BD'\rangle$. We also have to impose the condition k = aH (which leads to $\cos(2\delta) \approx -1$). As noted above, this condition tells us to evaluate the expression for the power spectrum at the time the physical momentum equals the Hubble scale H. Since the expression for γ_k is in terms of the physical energy scale, ω_k , we must set $\omega_k = H$. Thus we find

$$P(k) \approx P_{BD} \left[1 + \frac{1}{4e^{\pi}} \left(\frac{H(k)}{M_p} \right)^2 \right] .$$
(5.6)

This is our final result. We have introduced a k-dependence because, in a generic slowroll inflationary model, H depends on k. The deviation from unity of the term in brackets represents the contribution of the most universal quantum gravity effect – back-reaction due to energy conservation – to the primordial power spectrum of inflationary perturbations.

6. Discussion

Our calculation shows that the inclusion of back-reaction results in a mild breaking of de Sitter invariance with a corresponding mild effect on the CMB power spectrum. This can be seen by noting that the Bogolubov coefficients relating the modified Bunch-Davies state to the standard de Sitter invariant vacuum depend on the momentum scale ω_k . Because the set of all de Sitter invariant states is paramerized by k-independent Bogolubov coefficients (the α -vacua) this necessarily implies that the modified Bunch-Davies state breaks de Sitter invariance. Moreover, as the conservation of energy is mandatory, this observation could perhaps have other important consequences, such as for the stability of de Sitter space.

The correction we computed can intuitively be understood as coming from a slightly modified effective de Sitter temperature. By instead regarding the effect as a modification of the Bunch-Davies vacuum we were able to compute the exact coefficient of the correction. Generically, modifications to the initial state during inflation, as studied in [5, 6, 16], give rise to a quite specific modification to the power spectrum: an oscillatory correction with amplitude on the order of (H/M) where M is the scale at which the modification is implemented. The fact that the power spectrum correction we compute here is not of that form, but is instead a shift of order (H^2/M_p^2) – exactly what one expects from including higher order operators in a bulk effective field theory [41] – suggests that there may be a bulk effective field theory description of the modification we've studied. In particular, a correction of this magnitude generically arises from a Planck-scale-suppressed dimension 6 irrelevant operator; it would be interesting to study the exact details and the interpretation in effective field theory of the operator responsible for this gravitational correction. Our final formula, (5.6), obviously implies a tiny correction, already highly constrained by $H/M_p \leq 10^{-5}$. Nevertheless, the result is interesting for a couple of reasons. First, it is unavoidable, originating as it does in energy conservation. And second, the correction can be calculated explicitly without requiring any knowledge of new Planck scale physics. In that sense, it is a universal imprint of quantum gravity in the large-scale structure of the universe.

Acknowledgments

We thank Daniel Kabat for several valuable discussions. The authors are supported in part by DOE grant DE-FG02-92ER40699. M. P. is a Columbia University Frontiers of Science Fellow.

A. Particle spectrum in the α -states

Rather than choosing the Bunch-Davies state, which gives rise to a thermal spectrum for a free-falling timelike observer, one could just as well have picked one of the de Sitter-invariant α -states instead. As an illustration of our general Bogolubov method we shall calculate here the spectrum detected by an inertial observer in an α -state. We will reproduce the known result [32–34], a result usually obtained by carefully analyzing the singularity structure of the Wightman Green's function.

Now, by definition, the operators, a'_k , that annihilate an α -state are obtained from the Bunch-Davies operators, a_k , by a Bogolubov transformation,

$$a'_k = \alpha_k^* \ a_k - \beta_k^* \ a_{-k}^\dagger , \qquad (A.1)$$

where the Bogolubov coefficients are k-independent:

$$\alpha_k = \frac{1}{\sqrt{1 - e^{\alpha + \alpha^*}}}$$

$$\beta_k = \frac{e^{\alpha}}{\sqrt{1 - e^{\alpha + \alpha^*}}}.$$
 (A.2)

Here α is a complex number, with $\operatorname{Re}(\alpha) < 0$, that labels the α -state (and is not to be confused with the Bogolubov coefficient α_k); $\operatorname{Re}(\alpha) = -\infty$ corresponds to the Bunch-Davies state.

The operators, b_k , that annihilate the out-state are themselves related by a Bogolubov transformation to the Bunch-Davies creation and annihilation operators:

$$b_k = \tilde{\alpha}_k^* a_k - \tilde{\beta}_k^* a_{-k}^{\dagger} . \tag{A.3}$$

Now, multiplying b_k by an overall phase obviously does not affect the choice of vacuum state. Use this freedom to fix the phase so that $\tilde{\alpha}_k$ is real. Next, express these operators in terms of the α -state operators:

$$b_{k} = \tilde{\alpha}_{k}^{\prime *} a_{k}^{\prime} - \tilde{\beta}_{k}^{\prime *} a_{-k}^{\prime \dagger} .$$
 (A.4)

Then, by inverting (A.1),

$$a_k = \alpha_k \ a'_k + \beta_k^* \ a'_{-k}^{\dagger} , \qquad (A.5)$$

and substituting into (A.3), we conclude that

$$\tilde{\alpha}_k^{\prime *} = \tilde{\alpha}_k^* \alpha_k - \tilde{\beta}_k^* \beta_k$$
$$\tilde{\beta}_k^{\prime *} = \tilde{\beta}_k^* \alpha_k^* - \tilde{\alpha}_k^* \beta_k^* .$$
(A.6)

Or, using (A.2),

$$\tilde{\alpha}_{k}^{\prime*} = \frac{1}{\sqrt{1 - e^{\alpha + \alpha^{*}}}} \left[\tilde{\alpha}_{k}^{*} - e^{\alpha} \tilde{\beta}_{k}^{*} \right]$$
$$\tilde{\beta}_{k}^{\prime*} = \frac{1}{\sqrt{1 - e^{\alpha + \alpha^{*}}}} \left[\tilde{\beta}_{k}^{*} - e^{\alpha^{*}} \tilde{\alpha}_{k}^{*} \right] .$$
(A.7)

The spectrum is controlled by the absolute value of the parameter $\tilde{\gamma}'_k \equiv -\frac{\hat{\beta}^*_k}{\tilde{\alpha}'_k}$. Now we use the fact that, for the thermal Bunch-Davies state, $|\tilde{\gamma}_k|^2 = e^{-\beta\omega_k}$. Then a little algebra yields

$$|\tilde{\gamma}_{k}'|^{2} = e^{-\beta\omega_{k}} \left| \frac{1 + e^{\alpha^{*}} \tilde{\gamma}_{k}^{-1}}{1 + e^{\alpha^{*}} \tilde{\gamma}_{k}^{*}} \right|^{2} .$$
(A.8)

In section 4.2, we argued that, on general grounds, $\tilde{\gamma}_k$ is purely real. This allows us to write $\tilde{\gamma}_k = \exp\left(-\frac{1}{2}\beta\omega_k\right)$, and we obtain

$$|\tilde{\gamma}_k'|^2 = e^{-\beta\omega_k} \left| \frac{1 + e^{\alpha + \frac{1}{2}\beta\omega_k}}{1 + e^{\alpha - \frac{1}{2}\beta\omega_k}} \right|^2 , \qquad (A.9)$$

in perfect agreement with previously derived results [33]. (Had we not known that $\tilde{\gamma}_k$ was purely real, we would have learned that by matching our result with that in the literature.) Note incidentally that, for $\operatorname{Re}(\alpha) \neq -\infty$, the spectrum is not thermal; in the limit $\frac{\omega_k}{H} \to \infty$, for instance, we find $|\bar{\gamma}_k|^2 = e^{\alpha + \alpha^*}$, corresponding to constant occupation numbers.

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