Inflationary perturbations near horizon crossing

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We study the behaviour of inflationary density perturbations in the vicinity of horizon crossing, using numerical evolution of the relevant mode equations. We explore two specific scenarios. In one, inflation is temporarily ended because a portion of the potential is too steep to support inflation. We find that perturbations on super-horizon scales can be modified, usually leading to a large amplification, because of entropy perturbations in the scalar field. This leads to a broad feature in the power spectrum, and the slow-roll and Stewart–Lyth approximations, which assume the perturbations reach an asymptotic regime well outside the horizon, can fail by many orders of magnitude in this regime. In the second scenario we consider perturbations generated right at the end of inflation, which re-enter shortly after inflation ends — such perturbations can be relevant for primordial black hole formation.

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I. INTRODUCTION

The inflationary cosmology remains the leading candidate theory for the origin of structure (see Refs. [1,2] for reviews). Considerable attention has been focussed on producing highly accurate calculations of the perturbations produced during inflation [3], which ultimately may be measured at the percent level via the microwave anisotropies they induce [4]. Special interest has been given to the simplest case, where there is only a single scalar field degree of freedom during inflation, and we will focus exclusively on that case in this paper.

In considering how a perturbation might evolve, a crucial quantity is the comparison of the inverse wavenumber with the Hubble length, given by the ratio $aH/k$. By definition inflation corresponds to a decreasing comoving Hubble length, $\frac{d(aH)}{dt} > 0$; consequently when modes of a given wavenumber are considered, they begin their evolution well inside the horizon and cross outside during inflation. At early times, flat space-time quantum field theory can be used to fix the initial normalization of the perturbations. Around the epoch of horizon crossing, the perturbation becomes frozen in, corresponding to a constant curvature perturbation once the mode is well outside the horizon. This leads to standard expressions for the spectrum of density perturbations such as

$$P_R^{1/2}(k) = \frac{1}{2\pi} \left. \frac{H^2}{|\dot{\phi}|} \right|_{k=aH},$$

(1)

where $P_R$ is the power spectrum of the curvature perturbation $R$, using the notation of Refs. [1,2]. This expression gives the amplitude of the perturbations in terms of the values of the Hubble parameter $H$ and scalar field velocity $\dot{\phi}$ at the time the mode crossed the horizon, i.e. when $k = aH$. A similar expression holds for the gravitational wave amplitude, and more sophisticated higher-order versions have also been derived.

Eq. (1) gives the impression that the amplitude of perturbations is being quoted at the instant of horizon crossing. However, it is important to realize that that is not in fact the case. The value quoted is the perturbation amplitude attained in the asymptotic limit $k/aH \to 0$ when the perturbation is well outside the horizon; it just happens to be written in terms of the values the background parameters had at the instant of horizon crossing. In fact the value of the curvature perturbation at the instant of horizon crossing typically differs by a significant factor from the asymptotic value.

Bearing that in mind, in this paper we consider two circumstances where the standard formula for the perturbation amplitude may not be valid, due to a failure to reach the asymptotic limit. In each case, this is because inflation ends before the true asymptotic regime has been reached. In our first scenario, we consider a temporary interruption to inflation, where the field driving inflation has a region where the potential is too steep to sustain inflation. We will see that this can lead to significant modifications to the standard results, and indeed that even modes significantly outside the horizon can receive a large change in amplitude due to entropy perturbations in the scalar field. In the second scenario, we consider perturbations produced at the end of inflation, where their amplitude on re-entry has relevance to the production of primordial black holes.

II. FORMALISM

The scalar perturbations are best followed using the variable $u = a \delta \phi$ [3,4], and the equation satisfied by its
Fourier modes $u_k$ is

$$u_k'' + \left( k^2 - \frac{z''}{z} \right) u_k = 0,$$  \hspace{1cm} (2)

where primes denote differentiation with respect to conformal time, $z \equiv a \dot{\phi}/H$, and

$$\frac{z''}{z} = 2a^2 H^2 \left[ 1 + \epsilon - \frac{3}{2} \eta + \epsilon^2 - 2\epsilon \eta + \frac{1}{2} \eta^2 + \frac{1}{2} \xi^2 \right],$$  \hspace{1cm} (3)

where we define the Hubble slow-roll parameters \cite{7} as

$$\epsilon \equiv \frac{m_{	ext{Pl}}^2}{4\pi} \left( \frac{H \phi}{H} \right)^2 = 3 \frac{\dot{\phi}^2}{V + \dot{\phi}^2/2};$$  \hspace{1cm} (4)

$$\eta \equiv \frac{m_{	ext{Pl}}^2}{4\pi} \frac{H \dot{\phi} \phi}{H^2} = -3 \frac{\ddot{\phi}}{3H \phi};$$  \hspace{1cm} (5)

$$\xi^2 \equiv \frac{m_{	ext{Pl}}^4}{16\pi^2} \frac{H \phi H \dot{\phi} \phi}{H^2} = 3(\epsilon + \eta) - \eta^2 - \frac{V_{,\phi\phi}}{H^2},$$  \hspace{1cm} (6)

where $\dot{\cdot}, \ddot{\cdot}$ denotes differentiation with respect to $\phi$. Mode equation (2) has two asymptotic regimes characterized by the relative sizes of $k^2$ and $z''/z$. Only in the slow-roll limit, where $\epsilon, |\eta|, |\xi^2| \ll 1$, will this necessarily be the same as comparing $k$ and $aH$. Bearing this in mind, well within the horizon in the limit of $aH/k \to 0$ each mode behaves like a free field

$$u_k \to \frac{1}{\sqrt{2k}} e^{-ik\tau},$$  \hspace{1cm} (7)

while in the limit $k^2 \ll z''/z$ we have a growing mode solution

$$u_k \propto z,$$  \hspace{1cm} (8)

which means that the curvature perturbation, $|\mathcal{R}_k| = |u_k/z|$, remains constant on superhorizon scales. The quantity $z$ is sometimes described as the pump field for scalar perturbations.

To calculate the constant of proportionality of Eq. (3) it is generally assumed that $\epsilon$ and $\eta$ are slowly varying at around horizon crossing, which will be a valid approximation as long as these parameters are small, since

$$\frac{\epsilon'}{aH} = 2(\epsilon - \eta); \quad \frac{\eta'}{aH} = \epsilon \eta - \xi^2.$$  \hspace{1cm} (9)

The expression for conformal time $\tau$ then takes on a simple form

$$\tau \equiv \int \frac{dt}{a} \approx -\frac{1}{aH} \ln \frac{1}{1 - \epsilon},$$  \hspace{1cm} (10)

and Eq. (2) reduces to a Bessel equation leading to the Stewart–Lyth result for the power spectrum \cite{8}

$$\mathcal{P}_\mathcal{R}^{1/2} \simeq \left[ 1 - (2C + 1)\epsilon - C\eta \right] \frac{1}{2\pi} \left| \frac{H^2}{|\phi|} \right|_{k=aH},$$  \hspace{1cm} (11)

where $C \simeq -0.73$ is a numerical constant.

In fact, the constancy of $\mathcal{R}_k$ depends on $\epsilon$ and $\eta$ doing nothing dramatic even after horizon crossing, which can be seen if we rewrite Eq. (2) in terms of $\mathcal{R}_k$

$$\mathcal{R}_k'' + \frac{2}{{z'}} \mathcal{R}_k' + k^2 \mathcal{R}_k = 0,$$  \hspace{1cm} (12)

where

$$\frac{z''}{z} = aH \left[ 1 + \epsilon - \eta \right].$$  \hspace{1cm} (13)

Initially $\mathcal{R}_k$, like $u_k$, will be oscillating, although we are only interested in the envelope of this oscillation, $|\mathcal{R}_k|$, because only the envelope contributes to the value of the real space curvature perturbation, $\mathcal{R}$. Mode equation (12) is of the form of a damped harmonic oscillator. In the slow-roll limit, at around horizon crossing the system becomes dominated by the exponentially growing friction term proportional to $\mathcal{R}_k'$, and the solution to Eq. (12) soon becomes well approximated by the form

$$\mathcal{R}_k(\tau) = \text{const}; \quad \frac{\mathcal{R}_k'(\tau)}{aH} \simeq \text{const} \times \exp (-2N),$$  \hspace{1cm} (14)

where $N$ is the number of $\epsilon$-folds after horizon crossing.

The rapid freezing in of the curvature perturbation is apparent from Eq. (14), which measures the rate of change of $\mathcal{R}$ per Hubble time. We will examine the properties of the late-time solution in more detail later in the paper.

In this paper we are interested in a more dramatic situation, arising through a failure of slow-roll. If at any time after horizon crossing the friction term in Eq. (12) changes sign and becomes a negative driving term, then we can expect dramatic effects on modes which have recently left the horizon. This change of sign will occur whenever $z$ reaches a local maximum, or equivalently whenever

$$1 + \epsilon - \eta = 0.$$  \hspace{1cm} (15)

As $\epsilon$ is always positive, $\eta$ must be at least one for this to happen, which implies that a turn around in $z$ can occur only during a transition to fast-roll inflation or to a non-inflationary period.

Before progressing to specific applications of the above, we note that no such interesting effects can occur for gravitational waves. Their mode equation is given by

$$v_k'' + \left( k^2 - \frac{a''}{a} \right) v_k = 0,$$  \hspace{1cm} (16)

where

$$\frac{a''}{a} = 2a^2 H^2 \left[ 1 - \frac{1}{2} \frac{\epsilon'}{aH} \right].$$  \hspace{1cm} (17)

In analogy with the above, Eq. (16) can be written as

$$V_k'' + 2aHV_k' + k^2 V_k = 0,$$  \hspace{1cm} (18)
The evolution of the quantity $1+\epsilon - \eta$ for some time after inflation restarts. It is during this latter period that scalar modes which have recently left the horizon feel the effect of the driving term in Eq. (12). We set the correspondence of scales such that $k = 1$ corresponds to the scale which equals the horizon at the time when inflation stops. This correspondence is arbitrary, depending on the mechanism for ending inflation and in particular the value of $\phi$ at which inflation ends.

The evolution of perturbations on a particular scale $k$, again for $B = 0.55$, is shown in Fig. 2 obtained numerically using the approach of Ref. [10]. Even though this particular mode left the horizon around 7 e-folds before $z'/z$ turns negative, the residual $R_k'$ given by Eq. (14) is quickly blown up by the exponentially growing driving term. After some time the exponential growth becomes important and it drives $|R_k|$ through zero and on to a much larger amplitude. Although the mode is well outside the horizon at this time, its amplitude is enhanced by a factor of around a hundred; we will discuss the physical interpretation of this further later. Once $z'/z$ becomes positive again normal friction domination resumes, freezing out $|R_k|$ at the enhanced amplitude. The standard approximations therefore fail by a factor of around a hundred in this case, which as we will see is by no means the worst. The tensor amplitude is unchanged, so the tensor-to-scalar ratio is suppressed.

In Fig. 2 we consider two other modes, this time tracking the evolution of $|u_k|$. One mode crosses the horizon during the epoch when $z'/z < 0$. Clearly Eq. (10) does not depend explicitly on $z'/z$, and so the transition from the oscillating regime still occurs when $k^2 = z^4/z$. Scalar modes that leave the horizon after $z'/z$ turns positive again, as is the case in the second mode shown in Fig. 3, asymptote to a value that is independent of the influence of $z'/z$ turning negative. This is to be expected,
FIG. 3. The evolution of two scalar modes, \( |u_k| \), as in Fig. 2. The arrows again indicate horizon crossing for each mode. For the first mode, \( k_1 \), horizon crossing occurs while \( z'/z < 0 \), while for the second it occurs after \( z'/z \) becomes positive again. Both modes asymptote to approximately the same amplitude.

since sub-horizon modes do not feel the influence of any background quantities.

The overall result is that an extremely broad feature arises in the scalar power spectrum. This is shown in Fig. 4, where the spectrum for two different choices of \( B \) has been computed mode by mode, interpolating between the two different epochs of inflation. For comparison we plot the amplitude predicted by the slow-roll and Stewart–Lyth formulae, where we use the background values and slow-roll parameters derived from the numerical evolution. For a small range of scales near \( k = aH|_{\text{end}} \) there is some ambiguity as to when the formulae should be applied, since these modes leave the horizon twice. We plot both possible values. The slow-roll and Stewart–Lyth predictions fail by orders of magnitude for many \( e \)-folds (potentially enough to encompass all scales accessible to large-scale structure observations in the \( B = 0 \) case), resuming their usual good agreement with the numerical results soon after \( z'/z \) turns positive again.

An intriguing feature of the spectrum for \( B = 0.55 \) is the very flat portion on the right, which arises even though the disagreement with the slow-roll prediction indicates that we are nowhere near the slow-roll limit. In fact, this is a realization of the more general circumstance for a scale-invariant spectrum uncovered by Wands [11] using duality arguments. During this epoch, the field is fast-rolling along a relatively flat section of the potential, obeying

\[
\ddot{\phi} + 3H\dot{\phi} + V_{,\phi} \simeq \ddot{\phi} + 3H\dot{\phi} = 0. \tag{21}
\]

The solution is \( \dot{\phi} \propto a^{-3} \), giving \( z \propto \tau^2 \) rather than the \( z \propto \tau^{-1} \) typical of slow-roll inflation. Nevertheless, this relation between \( z \) and \( \tau \) leads to a scale-invariant spectrum of scalar perturbations [11], just as in the slow-roll limit. This decaying solution of \( \dot{\phi} \) is always present but is usually neglected. Seto et al. [12] have shown that in extreme cases, when \( \dot{\phi} \) becomes equal to zero, the slow-roll amplitude of the density perturbation as written in Eq. (1) will completely fail unless \( \dot{\phi} \) is replaced by the corresponding slow-roll velocity \( \dot{\phi}_s = -V_{,\phi}/3H \).

As the field slows down, one might have expected a feature to be produced. However, as long as \( \epsilon \) is small, a necessary and sufficient condition for a scale-invariant spectrum is that the entire square-bracketted term in Eq. (3) remains constant in time, which taking \( \epsilon \ll 1 \) reduces to

\[
\xi^2 + \eta^2 - 3\eta = \text{constant}. \tag{22}
\]

This encompasses both slow-roll (\( |\eta| \ll 1 \)) and fast-roll (\( \eta \gtrsim 1 \)) inflation, as well as any smooth transition between the two. This condition will be automatically
satisfied as long as the inflaton is effectively massless, allowing us to neglect the last term of Eq. (1). However obtaining the flat portion required significant fine-tuning of $B$; notice that with $B = 0.3$ the potential is much less flat in the corresponding region, though still flatter than the slow-roll formulae predict.

In the limit of an instantaneous transition from slow-roll to fast-roll behaviour, inflation is no longer suspended and we arrive at Starobinsky’s model [13]. In this case the inflaton potential is characterized by a sudden gradient discontinuity and the power spectrum takes on a similar step-like form, but with superimposed oscillations on the upper plateau.

We now return to the physical interpretation of the change in the curvature perturbation on super-horizon scales. Although ordinarily a single scalar field is associated with purely adiabatic perturbations, it can in fact support entropy perturbations if its velocity perturbation does not obey a generalized adiabatic condition with respect to the field perturbation [14]. Under quite general circumstances, however, single field inflation does only generate adiabatic perturbations [15], with the entropy perturbation $S$ associated with a general scalar field perturbation being non-zero but becoming highly suppressed, $S \sim \epsilon^{-2N}$, once the mode becomes frozen in upon leaving the horizon [14]. The constancy of the curvature perturbation on super-horizon scales in the absence of entropy perturbations holds under extremely general circumstances [14].

Our situation is an exception to this. An entropy perturbation is the only source of super-Hubble growth [13, 14], and during the phase where $z$ decreases the entropy perturbation grows until it becomes significant enough to source the curvature perturbation. The further above the Hubble length a scale is, the more the entropy has been suppressed and hence more time is needed for the entropy to become significant, so the effect does not extend up to arbitrarily large scales. After slow-roll resumes the entropy dies away and the perturbations become purely adiabatic, remaining so thereafter but retaining the shift in amplitude. The influence of the scalar field entropy can be studied using the definitions of Ref. [14], where the entropy is given by

$$S = \frac{2V}{3\dot{\phi}^2 \left(3H\dot{\phi} + V_{\phi}\right)} \left[\ddot{\phi} \left(\delta\phi - \dot{\phi}A\right) - \dot{\phi} \delta\phi\right], \quad (23)$$

where $A$ is the perturbation to the metric lapse function which is related to the curvature perturbation via the constraint equation $A = 4\pi\dot{\phi}^2 R / m_{Pl}^2 H^2$ [14]. The entropy measures the failure of the perturbed velocity to match the generalized adiabatic condition with respect to the field perturbation itself. It allows Eq. (12) to be rewritten as two first-order equations

$$\frac{\mathcal{R}'}{aH} = \frac{3}{2} \frac{3 - 2\eta}{3 - \eta} S; \quad (24)$$

Even in the slow-roll case, care is required in deriving the late-time evolution of the entropy, because its suppression is strong enough that the effect of the $\mathcal{R}$ term does not become negligible despite its $k^2/a^2 H^2$ prefactor. If we were able to neglect that term, and taking the slow-roll limit, one would find $S'/aH \approx -3S$ implying $S \sim \epsilon^{-3N}$, but we see that this does fall off faster than the last term. The self-consistent solution therefore has late-time behavior $S \sim \epsilon^{-2N}$, and indeed is what we see in our numerical simulations.

During fast-roll the situation is very different, because $S$ is able to grow and so the influence of the final term in Eq. (25) becomes negligible. Making the false vacuum ($\epsilon \ll 1$) and massless ($V_{\phi} \ll H^2$) assumptions, Eq. (25) can then be written as

$$\frac{S'}{aH} \approx \left[2\eta - 3 + \frac{3\eta}{2\eta - 3}\right] S; \quad (26)$$

During fast-roll $\eta \approx 3$, and the entropy can swiftly grow $\sim \epsilon^{3N}$ until it becomes large enough to have a significant impact on $\mathcal{R}$. Once fast-roll ends the $k^2 \mathcal{R}$ term in Eq. (25) is initially small giving the $S \sim \epsilon^{-3N}$ behaviour, but soon after the curvature terms re-asserts itself restoring the $S \sim \epsilon^{-2N}$ late-time behaviour. However this transition is not of any particular physical significance since the curvature perturbation itself has long since approached its asymptotic value.

One might wonder whether the entropy perturbations in the scalar field could survive as such after inflation, but that does not seem to be possible. Either fast-roll is followed by slow-roll as just discussed, or it is followed by inflation ending through decay of the inflaton. That decay will lead to a purely radiation-dominated universe, which is unable to support non-adiabatic perturbations. The process of decay of the inflaton would therefore remove the entropy source term. Note also that considerable fine-tuning is required to stay in the fast-roll regime for a prolonged period; in order to have inflation the initial kinetic energy can at most be of order of the potential energy, but then the kinetic energy falls off very quickly, and yet for fast-roll to be sustained its contribution to the scalar wave equation must remain larger than that from the slope of the potential.

**IV. PERTURBATIONS AT THE END OF INFLATION**

A second scenario where the standard equations cannot be directly applied is at the true end of inflation. This is an important regime because such short-scale perturbations can lead to the formation of primordial black holes,
which gives the most important constraint on the late stages of inflation. There are two standard mechanisms for ending inflation, one being the hybrid method of an instability in another direction in field space and the second being the breakdown of slow-roll (see Ref. [2] for a review). A particularly relevant case is in hybrid inflation models such as the running-mass model [16], where the slow-roll approximation is only well respected over a limited range of scales. In the running-mass model slow-roll inflation comes to an end due to $\eta$ growing, but inflation may continue in the fast-roll regime until an instability is reached.

Typically the standard formulae for the perturbations will break down near the end of inflation, because of a failure to reach the asymptotic limit (see e.g. Ref. [17]) and often because the slow-roll approximation is not accurate. For example, in the running-mass model Eq. (15) becomes

$$1 - \eta \simeq 0, \quad (27)$$

and so $\eta = 1$ is the last point at which constraints based on the shape and size of a blue inflationary power spectrum can be reliably applied without resorting to mode-by-mode integration of the power spectrum [18].

We are not able to study the hybrid case due to the complexity of the multi-field dynamics (though see Ref. [14] for a general formalism for doing so), so we restrict our attention to single-field models ending by violation of slow-roll. This is not in fact the most interesting case as typically such models have a red spectrum where small-scale perturbations are not very significant, but illustrates the main physics. For simplicity we study the quadratic chaotic inflation model $V(\phi) \propto \phi^2$.

In Fig. 5 we plot the scalar power spectrum for the last few $e$-folds of modes to leave the horizon before inflation ends. Because the asymptotic regime is not adequately reached at any stage, there is no preferred choice as to when to plot the amplitude, and we evaluate it at three stages: horizon crossing during inflation, at the end of inflation, and at horizon re-entry after inflation once the background field begins oscillating. Notice that the amplitude at horizon exit is typically much greater than the value at the end of inflation, and that the slow-roll and Stewart–Lyth approximations indeed resemble the latter rather than the former.

We see that the slow-roll and Stewart–Lyth formulae underpredict the asymptotic and re-entry amplitudes of perturbations which exited the horizon close to the end of inflation. One therefore expects an enhancement of primordial black hole production, though a detailed calculation would need to track the derivative of the curvature perturbation at re-entry as well as its amplitude. This result suggests that normally quoted constraints are on the conservative side, though typically the correction would not be large. We mention additionally that for perturbations which do not reach the asymptotic regime there are questions as to how the quantum-to-classical transition might take place (see e.g. Ref. [19]); we will not however attempt to address this here.

V. DISCUSSION

The accuracy of the usual analytic expressions for the inflationary power spectrum depends on scales evolving smoothly through horizon crossing and into the asymptotic regime $k^2 \ll z''/z$. In this paper, we have investigated two situations where this is not achieved, one being a temporary end to inflation and the other the true end. In the former case we have seen that the modes can have a very complicated evolution, including the possibility of amplification on super-horizon scales via an exponential driving term corresponding to an entropy perturbation in the scalar field. Such behaviour can be traced to the complicated evolution of the scalar pump field $z$, which no longer grows monotonically. The net effect is the insertion of a broad feature into the power spectrum that can only be computed by mode-by-mode integration, and which can differ wildly from the slow-roll and Stewart–Lyth approximations. Typically the features are sufficiently non-scale-invariant to be excluded already on astrophysical scales, but we have also seen that a very flat spectrum can be obtained while far from slow-roll, confirming an analytic analysis by Wands [1].

The second scenario we studied was the true end of inflation, where the failure to reach an asymptotic regime means that perturbations re-enter the horizon with a higher amplitude. The most interesting physical consequence of such modes is in primordial black hole formation, and this result indicates that earlier treatments assuming the slow-roll formulae are somewhat conservative, as the mode equation solutions indicate that these
formulae underestimate the perturbation amplitude at horizon re-entry.

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