Non-linear inflationary perturbations

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We present a method by which cosmological perturbations can be quantitatively studied in single and multi-field inflationary models beyond linear perturbation theory. A non-linear generalization of the gauge-invariant Sasaki-Mukhanov variables is used in a long-wavelength approximation. These generalized variables remain invariant under time slicing changes on long wavelengths. The equations they obey are relatively simple and can be formulated for a number of time slicing choices. Initial conditions are set after horizon crossing and the subsequent evolution is fully non-linear. We briefly discuss how these methods can be implemented numerically to the study of non-Gaussian signatures from specific inflationary models.

I. INTRODUCTION

Our current understanding of the universe on large scales inevitably leads to questions regarding its earliest moments. The patterns seen in the distribution of matter on such scales and the fluctuations in the temperature of the CMB, point to mechanisms in the early universe that could have imprinted the initial conditions for such patterns on the otherwise homogeneous primordial universe. Recent data on CMB anisotropies\textsuperscript{[1]} leave no doubt that initial fluctuations existed on scales much larger than the causal horizon at the time of recombination. Inflation\textsuperscript{[2]} is a concept which can explain the origin of such fluctuations\textsuperscript{[3, 4]} as well as many other special features of the cosmos.

Even though the inflationary paradigm has been developing for over twenty years now, there is currently no agreed upon model of the inflationary epoch. Almost all models of inflation invoke one or more scalar fields to drive an initial phase of accelerated expansion. The latter is capable of producing fluctuations in the energy density by amplifying the quantum fluctuations of any light scalar field present during inflation. These fluctuations are usually represented as linearized deviations from a homogeneous evolution and are therefore described by non-interacting quantum fields living in the expanding spacetime. Linearity, along with the additional assumption that the initial state is the vacuum (as defined on scales much smaller than the Hubble radius), lead to the prediction that inflation creates Gaussian fluctuations.\textsuperscript{[2, 4]} The smallness of the observed CMB anisotropy certainly justifies the use of linear perturbation theory as a first approximation. However, some non-linearity will always be present in inflation due to the non-linear nature of gravity and the fact that the potential responsible for inflation may be interacting. Another property that is usually attributed to inflation is that it produces adiabatic fluctuations. This is strictly true only for single-field models. When more scalar fields are present, there is also a possibility for isocurvature perturbations. It has been suggested in the past that the interplay of isocurvature perturbations and non-linearity can lead to enhancement of the non-Gaussianity of primordial fluctuations. Reference\textsuperscript{[5]} is an example of this; the curvaton paradigm\textsuperscript{[6]} provides another possibility\textsuperscript{[5]}.

In this paper we present a method for studying the evolution of perturbations in an arbitrary scalar-field-driven inflationary model. The equations are valid in the long wavelength regime (scales larger than the Hubble radius) and allow for the calculation of non-linear effects. Scalar metric perturbations are taken into account and the scheme can in principle be formulated with an arbitrary time slicing. However, we find the use of a particular choice of time more convenient. The main variables of this formalism are non-perturbative generalizations of the useful Sasaki-Mukhanov variables of linear theory and are invariant under time slicing changes on long wavelengths; one can say that they are gauge invariant beyond perturbation theory. Initial conditions are provided after horizon crossing from linear perturbation theory. We argue that this is enough and any observable non-linearity will be produced by the subsequent evolution.

The outline of the paper is as follows: In section 2 we provide a framework for the analysis of the long-wavelength evolution of perturbations in single and multi-field models. The equations are valid in the long wavelength regime (scales larger than the Hubble radius) and allow for the calculation of non-linear effects. Scalar metric perturbations are taken into account and the scheme can in principle be formulated with an arbitrary time slicing. However, we find the use of a particular choice of time more convenient. The main variables of this formalism are non-perturbative generalizations of the useful Sasaki-Mukhanov variables of linear theory and are invariant under time slicing changes on long wavelengths; one can say that they are gauge invariant beyond perturbation theory. Initial conditions are provided after horizon crossing from linear perturbation theory. We argue that this is enough and any observable non-linearity will be produced by the subsequent evolution.

\textsuperscript{1}In contrast, topological defects cannot be described as a smooth linear deviation from a homogeneous background and hence are intrinsically non-Gaussian.
dynamics for a general inhomogeneous inflationary model. The approach goes beyond perturbation theory and allows for a treatment of all possible non-linearities. It is technically much simpler than higher order perturbation approaches \[^{[8]}\]. In section 3 we supplement the long-wavelength equations by stochastic terms which set the initial conditions after horizon crossing. Although formulated for a general time slicing, we find that a particular choice of time is most convenient. In section 4 we discuss progress towards a numerical implementation of these methods and the future prospects.

II. LONG WAVELENGTH DYNAMICS

A key characteristic of the inflationary era is the behaviour of the comoving Hubble radius \((aH)^{-1}\) which shrinks quasi-exponentially. This behaviour is unlike what happens during the radiation and matter eras where this scale grows. This feature allows inflation to answer a number of puzzling facts about the universe and also provides a mechanism for the quantum generation of fluctuations \[^{[3, 4]}\]. All of the astrophysically relevant scales start their lives subhorizon but eventually they are stretched to superhorizon sizes. In this paper we will focus on the superhorizon regime. Hence, a long-wavelength approximation along with a way to set initial conditions suffices for our purposes. The long-wavelength approximation we employ consists of dropping from the equations all terms containing second order spatial gradients \[^{[9, 10, 11]}\]. Then, spacetime can be described by the metric

\[
ds^2 = -N^2(t, \mathbf{x}) dt^2 + a^2(t, \mathbf{x}) h_{ij}(\mathbf{x}) dx^i dx^j,
\]

where \(N\) is the lapse function, \(a\) is a local scale factor and \(h_{ij}\) is a local spatial metric with unit determinant. In linear perturbation language, the latter contains one scalar degree of freedom (d.o.f), which enters as a second order spatial gradient and hence can be ignored, vector and tensor d.o.f’s. It can be shown quite generally that \(h_{ij}\) freezes on superhorizon scales \[^{[9]}\]. The local scale factor \(a\) contains the other scalar d.o.f that carries the dynamics on these scales. \(N\) can be chosen freely and corresponds to a choice of time slicing.

It turns out that under the above long-wavelength approximation the equations of motion are reduced to those of a homogeneous Friedmann-Lemaitre-Robertson-Walker (FLRW) cosmology, applied locally, plus a gradient constraint linking spatial gradients in matter and geometry. Hence, each point evolves as an independent universe with its own value for the matter fields, Hubble rate and scale factor, provided initial conditions which satisfy the gradient constraint have been specified \[^{[9, 11]}\]. In particular, after dropping a decaying mode \[^{[9, 11]}\], the evolution equations become

\[
\frac{dH}{dt} = -\frac{4\pi}{m_{pl}^2} N \left( \mathcal{E} + \frac{1}{3} S \right),
\]

\[
\frac{d\mathcal{E}}{dt} = -3NH \left( \mathcal{E} + \frac{1}{3} S \right),
\]

and are supplemented by two constraints

\[
H^2 = \frac{8\pi}{3m_{pl}^2} \mathcal{E}, \quad \partial_i H = \frac{4\pi}{m_{pl}^2} \mathcal{J}_i.
\]

Here, matter is described by the energy momentum tensor \(T_{\mu\nu}\). We have defined the energy density, momentum density and stress tensor

\[
\mathcal{E} \equiv N^{-2} T_{00}, \quad \mathcal{J}_i \equiv -N^{-1} T_{0i}, \quad S_{ij} \equiv T_{ij},
\]

and the local expansion rate

\[
H \equiv \frac{1}{N} \frac{d}{dt} (\ln a).
\]

A vertical bar denotes a covariant derivative with respect to the spatial metric. The above system is consistent only if \(S_{ij} = \frac{1}{3} S \delta_{ij}\) which is expected to be true on long wavelengths.

\[^2\] We restrict attention to metrics with zero shift \(N_i = 0\).
We now focus on an inflationary era driven by $n$ scalar fields with the energy momentum tensor

$$T_{\mu\nu} = G_{AB} \partial_\mu \phi^A \partial_\nu \phi^B - g_{\mu\nu} \left( \frac{1}{2} G_{AB} \partial^A \phi^A \partial^B + V \right), \quad (7)$$

so that

$$\mathcal{E} \simeq \frac{1}{2} G_{AB} \Pi^A \Pi^B + V(\phi), \quad (8)$$

$$\mathcal{J}_i = - G_{AB} \Pi^A \partial_i \phi^B, \quad (9)$$

$$S_{ij} \simeq a^2 h_{ij} \left( \frac{1}{2} G_{AB} \Pi^A \Pi^B - V \right), \quad (10)$$

where the approximate equality indicates second order spatial gradients dropped. We defined the field momentum as

$$\Pi^A = \frac{\dot{\phi}^A}{N}. \quad (11)$$

Then, the long-wavelength equations of motion for this system are

$$\frac{dH}{dt} = - \frac{4\pi}{m_{pl}^2} N \Pi_B \Pi^B, \quad \quad (12)$$

$$\mathcal{D}_i \Pi^A = - 3NH \Pi^A - N G^{AB} \Pi_B, \quad \quad (13)$$

$$H^2 = \frac{8\pi}{3m_{pl}^2} \left( \frac{1}{2} \Pi_B \Pi^B + V \right), \quad \quad (14)$$

$$\partial_i H = - \frac{4\pi}{m_{pl}^2} \Pi_B \partial_i \phi^B, \quad \quad (15)$$

where $V_B \equiv \partial_B V$ and the symbol $\mathcal{D}_i$ appearing in (13) will be defined shortly. Note that we have taken a general field metric $G_{AB}$ and all the equations below will be valid for such an arbitrary metric. We thus view the dynamics as taking place on a general $n$-dimensional field manifold where $\phi^A$ are just a set of $n$ functions parameterizing it. Hence, it makes sense to define covariant derivatives when considering the spatial or temporal dependence of various quantities. For a spacetime dependent quantity $L^A(t, x)$ which transforms as a vector in field space, we define the covariant derivatives

$$\mathcal{D}_i L^A = \partial_i L^A + \Gamma^A_{BC} \partial_i \phi^B L^C, \quad \quad (16)$$

with $\Gamma^A_{BC}$ the symmetric connection formed from $G_{AB}$. The quantities $\partial_i \phi^B$ and $N \Pi_B$ transform as vectors in field space but $\phi^B$ does not.

As mentioned above, the system of eqs (12) - (14) is exactly the same as the equations of FLRW cosmology applied locally. However, equation (14) gives an additional constraint which is obviously absent in the homogeneous case. If one drops the $\Pi^2$ term from the Friedmann equation (14) and the $\mathcal{D}_i \Pi^A$ term from eq (13), eqs (14) and (15) are equivalent. This assumption is implicit in the "separate universe" picture of non-linear evolution which is a simple way to view the long wavelength dynamics (see eg. [7] and references therein). However, in the case of several fields certain components of $\mathcal{D}_i \Pi^A$ may be important even though slow-roll inflation is still valid [12], and ignoring them may miss the relevant effects. No such assumption needs to be made for the formalism we develop here.

A natural way to parameterize inhomogeneity beyond perturbation theory is to use spatial gradients of various quantities of interest. This is similar in spirit to the approach first advocated in [13]. In general, the value of any spatial gradient will depend on the chosen time-slicing and by an appropriate choice of time slices the inhomogenous part of any spacetime scalar can be made to vanish. However, one can form combinations of spatial gradients, including the gradient of the integrated expansion (the local scale factor), which are invariant under long wavelength changes of time slicing. They can be constructed similarly to those of linear perturbation theory. One such variable is

$$Q^A_i = a \left( \partial_i \phi^A - \frac{\Pi^A}{H} X_i \right), \quad \quad (17)$$

with $X_i \equiv \partial_i \ln a$. Such combinations were first introduced in [11] and it can be checked explicitly that they are invariant under $t \rightarrow T(t, x)$ transformations on long wavelengths. More recently, such variables were considered by
the authors of [14] in a more geometric framework who also showed explicitly that they reproduce previously introduced gauge-invariant perturbations at second order. Note that when linearized around a homogeneous background, \( Q^A_i \) is just the gradient of the well known Sasaki-Mukhanov variable [15]

\[
\delta q^A = a \left( \delta \phi^A - \frac{\dot{\phi}^A}{NH} \Psi \right),
\]

where \( \Psi = \delta a/a \) is the perturbation in the trace of the spatial metric. In our notation, the linear version of \( X_i \) is just \( \partial_i (\delta a/a) = \partial_i \Psi \). A similar gauge-invariant variable is [11]

\[
\zeta_i = X_i - \frac{NH}{H} \partial_i \mathcal{E}
\]

which, using eqs (15) and (17), (19) can also be written as

\[
\zeta_i = \frac{4\pi m_{\text{pl}}^2}{\rho_a} \frac{1}{H} \Pi A Q_i^A.
\]

This is a non-linear generalization of the well known linear curvature variable \( \zeta \).

The \( Q^A_i \)'s obey relatively simple equations of motion which can be derived by taking spatial derivatives of equations (12) - (14) and using (15). Details of the derivation can be found in Appendix A. It is convenient to define a set of slow-roll parameters for the multi-field model (see [12] for a discussion in the framework of linear perturbation theory):

\[
\tilde{\epsilon} = -\frac{\dot{H}}{NH^2} = \frac{4\pi \Pi^2}{m_{\text{pl}}^2 H^2}, \quad \tilde{\eta}^A = \frac{1}{N} \frac{D_i \Pi^A}{H \Pi},
\]

which are usually assumed to be much smaller than unity during inflation. It will also be useful to define

\[
\omega^A = \sqrt{\tilde{\epsilon}} \frac{\Pi^A}{\Pi}.
\]

Then, the following equations of motion can be derived for the \( Q_i^A \)'s (see Appendix A)

\[
D_i^2 Q_i^A = \left( \frac{\tilde{\epsilon}}{N} - NH \right) D_i Q_i^A + \Omega^A_B Q_i^B = 0
\]

with the “mass matrix”

\[
\Omega^A_B = N^2 V^A_B - \frac{m_{\text{pl}}^2}{4\pi} (NH)^2 R_{FCB} \omega^F \omega^C - (NH)^2 \left[ \left( 2 - \tilde{\epsilon} \right) \delta^A_B + 2 \left( 3 + \tilde{\epsilon} \right) \omega^A \omega_B + 2 \sqrt{\tilde{\epsilon}} \left( \tilde{\eta}_B \omega^A + \tilde{\eta}_A \omega_B \right) \right],
\]

\( V^A_B = D_B V^A \) and \( R_{FCB} \) the curvature tensor of the field manifold. These are formally the same equations as those of linear perturbation theory for the Sasaki-Mukhanov variables with the \( k^2 \) terms dropped [12]. Note that although equation (23) appears to be linear in the \( Q_i^A \)'s, it incorporates the full non-linear dynamics on large scales since its coefficients are spatially varying functions. They depend implicitly on the \( Q_i^A \)'s via a set of relations which express various local quantities in terms of them. Hence, the \( Q_i^A \)'s can be seen as master variables encoding all the d.o.f's of the inhomogeneous system. Expressing \( \partial_i \phi^A \) in terms of \( Q_i^A \), using (15) and noting that \( D_i (\partial_i \phi^A) = D_i (N \Pi^A) \), we get

\[
\partial_i (\ln H) = -\frac{1}{a} \left( \frac{4\pi}{m_{\text{pl}}^2} \right)^\frac{1}{2} \omega_A Q_i^A - \tilde{\epsilon} X_i,
\]

\[
\partial_i \phi^A = \frac{1}{a} Q_i^A + \left( \frac{m_{\text{pl}}^2}{4\pi} \right)^\frac{1}{2} \omega^A X_i,
\]

3 We note here that the following equations, although expressed in terms of the slow roll parameters, are exact, i.e. no assumption has been made about the smallness of the latter.
and
\[
D_i \Pi^A = \frac{1}{aN} D_i Q^A_i - \frac{H}{a} \left[ \delta^A C + \omega^A \omega_C \right] Q^C_i + H \left( \frac{m^2_{\text{pl}}}{4\pi} \right)^{\frac{1}{2}} \sqrt{\epsilon^A} X_i. \tag{27}
\]

The right hand sides of Eqs (25) - (27) are given in terms of gauge invariant variables, apart from the terms involving \(X_i\). The latter cannot be expressed via a similar relation of the form \(X_i = f_A Q^A_i\). For a general choice of time, (28) can also be written as
\[
\dot{X}_i = -NH\dot{\epsilon}X_i + H\partial_i N - \left( \frac{4\pi}{m^2_{\text{pl}}} \right)^{\frac{1}{2}} \frac{NH}{a} \omega_A Q^A_i. \tag{28}
\]

Note that \(X_i\) is not considered as an independent d.o.f. since it is gauge-dependent. All physical d.o.f's describing inhomogeneity are encoded in the \(Q^A\)’s. Hence, a natural choice is to have \(X_i = 0\) if, at all times, \(Q^A_i = 0\) and \(\dot{Q}^A_i = 0\). Such a choice simply means setting \(X_i(t_{\text{init}}) = 0\) initially and making \(N\) some function of \(H, \phi^A, \Pi^A\) and \(a\). This ensures that \(\partial_i N = f_A Q^A_i + g_A \dot{Q}^A_i + hX_i\) with \(f_A, g_A\) and \(h\) arbitrary functions.

The above equations are obviously valid for any choice of \(N\) and, as emphasized above, \(Q^A_i\) is gauge invariant. During inflation however, it is natural to use the logarithm of the local value of the Hubble radius as the time variable \(t\)

\[
t = \ln(aH) \iff t = \int H(1 - \dot{\epsilon})dT,
\]

with \(T\) being proper time. For such a gauge choice we get
\[
N^{-1} = \frac{dt}{dT} = H(1 - \dot{\epsilon}). \tag{30}
\]

Since \(\partial_i t = 0\) by definition on surfaces of constant time, we have
\[
X_i = -\partial_i (\ln H), \tag{31}
\]

and (28) is automatically satisfied. In this gauge the constraints simplify:
\[
\begin{align*}
X_i &= \left( \frac{4\pi}{m^2_{\text{pl}}} \right)^{\frac{1}{2}} \frac{1}{a(1 - \dot{\epsilon})} \omega_A Q^A_i = -\partial_i (\ln H), \tag{32} \\
\partial_i \phi^A &= \frac{1}{a} \left[ \delta^A B + \frac{\omega^A \omega_B}{(1 - \dot{\epsilon})} \right] Q^B_i, \tag{33}
\end{align*}
\]

and
\[
D_i \Pi^A = \frac{H}{a} (1 - \dot{\epsilon}) D_i Q^A_i - \frac{H}{a} \left[ \delta^A C + \omega^A \omega_C - \sqrt{\epsilon^A} \frac{\omega_C}{(1 - \dot{\epsilon})} \right] Q^C_i. \tag{34}
\]

Another advantage of (28) will be discussed in the next section. Equations (29) - (33) specify the gradients of the local quantities that appear in the coefficients of (28) in terms of the \(Q^A_i\)’s. Note that in this slicing, for quasi-exponential expansion, \(t\) is monotonic. The validity of such a time variable extends only up to the end of inflation when the comoving horizon starts growing again.

Before closing this section we would like to make one final remark. By taking the time derivative of equation (16) we can derive the following relation between \(D_i Q^A_i\) and \(\dot{Q}^A_i\)
\[
\Pi_A D_i Q^A_i = NH [(1 + \dot{\epsilon}) \Pi_A + \Pi \dot{\eta}_A] Q^A_i. \tag{35}
\]

Since \(D_i Q^A_i\) is related to \(\dot{Q}^A_i\), there is an apparent reduction of order for projections of the perturbations along the \(\Pi^A\) direction in field space. In particular, for the single-field case the full dynamics on long wavelengths can be simply written as a first order equation
\[
d_t \dot{Q}_i = NH (1 + \dot{\epsilon} + \dot{\eta}) Q_i. \tag{36}
\]
From (36) we can obtain a non-linear conservation law [11] (see also [14]) in the single field case. For

\[ \zeta_i \equiv -\left(\frac{4\pi}{m_{pl}}\right)^\frac{1}{2} \frac{1}{a\sqrt{\epsilon}} Q_i, \]  

(37)

given that

\[ \dot{\epsilon} = 2NH\epsilon \left(\dot{\epsilon} + \tilde{\eta}_i B_i \Pi_B \right), \]  

(38)

it straightforward to calculate that \( \zeta_i \) is conserved,

\[ \dot{\zeta}_i = 0. \]  

(39)

### III. INITIAL CONDITIONS

In the previous section we derived a set of equations describing the long wavelength evolution of fully non-linear gauge-invariant variables. These equations are exact, as long as the long wavelength approximation we employed is valid, and are free of any slow roll assumptions. Of course, one still needs a recipe for providing initial conditions for the \( Q_i \) variables. We propose to use linear theory for calculating their values after horizon crossing. Any further non-linearity is introduced via the non-linear evolution. We comment below on whether this is good enough, at least for the cases where interesting effects may arise.

When linearized, the spatial vectors \( Q_i \) are simply the gradients of the well known Sasaki-Mukhanov variables. These are the proper fields to be quantized during inflation [3, 15] and we will assume that they are the appropriate variables for setting up initial conditions. One way of proceeding would be to just take

\[ Q_i(t_{in}, x) = \partial_i \delta q^A = \int_V \frac{d^3k}{(2\pi)^3} \sqrt{2} \frac{1}{\sqrt{2}} \left[ Q^A_B(t_{in}, k) \alpha^B(k) e^{ikx} + c.c. \right], \]  

(40)

where c.c. stands for the complex conjugate. We have taken a finite region in \( k \)-space, denoted by \( V \), which includes the scales of interest and we have defined \( n \) constant complex stochastic quantities \( \alpha^A \) with \( n \) being the number of scalar fields, \( A = 1 \ldots n \). The classical random field exhibits the same correlations as the quantum field if the stochastic constants \( \alpha^A \) satisfy

\[ \langle \alpha^A(k) \alpha^B(k') \rangle = \delta^A_B \delta(k - k'), \quad \langle \alpha^A(k) \alpha_B(k') \rangle = 0 \]  

(41)

where \( \langle \ldots \rangle \) denotes an ensemble average. We have of course implicitly assumed that on long wavelengths quantum fields can be considered as classical stochastic fields with the same correlation properties [16, 17, 18]. The matrix \( Q^A_B(k, t) \) is the solution to the linear equation of motion [12]

\[ D_t^2 Q^A_B - \left(\frac{\dot{N}}{N} - NH\right) D_t Q^A_B + \left(\frac{Nk}{a} \right)^2 \delta^A_C \Omega^2_B = 0. \]  

(42)

The initial conditions for \( Q^A_B \) are in turn set up when the relevant mode is deep inside the horizon \( ((k/a) \gg H) \) using the properly normalized WKB solutions of (42) in that regime

\[ Q^A_B(k, t) = \frac{1}{\sqrt{2k}} \exp \left[ -i k \int_{t_0}^t \frac{N dt'}{a(t')} \right] \delta^A_B. \]  

(43)

A more dynamic way of setting up the \( Q^A \) after horizon crossing involves using source terms on the r.h.s. of (23) which continuously update the values of \( Q^A \) as more modes enter the long wavelength system. In this sense these sources also set up “initial conditions”, albeit in a continuous manner. A heuristic argument for the derivation of such terms, which is exact at the linear level, is as follows: Start from linear theory and the full equation of motion for \( \delta q^A \)

\[ D_t^2 \delta q^A - \left(\frac{\dot{N}}{N} - NH\right) D_t \delta q^A + \left(\frac{Nk}{a} \right)^2 \delta^A_C + \Omega^2 q^A \]  

(44)
Since we are interested in the long-wavelength semi-classical dynamics, we can coarse-grain $\delta q^A$ thus defining a long wavelength linear field

$$\delta \bar{q}^A(x) = \int d^3x' \delta q^A(x') W \left( \frac{|x-x'|}{R} \right), \quad (45)$$

where $R$ is an appropriate smoothing scale and the window function $W$ is normalised to unity

$$(2\pi)^{-3/2} \int d^3x' W \left( \frac{|x-x'|}{R} \right) = 1. \quad (46)$$

From the convolution theorem the Fourier transform of $\delta \bar{q}^A(x)$ reads

$$\delta \bar{q}^A(k) = \delta q^A(k) W(k), \quad (47)$$

where $W(k)$ is the Fourier transform of the window function $W$. From $(47)$ we can now derive an equation of motion for $\delta \bar{q}^A(k)$. It is easily seen to be

$$D_t^2 \delta \bar{q}^A(k) - \left( \frac{\dot{N}}{N} - NH \right) D_i \delta \bar{q}^A(k) + \Omega^A_B \delta \bar{q}^B(k) = \xi^A(k), \quad (48)$$

with

$$\xi^A(k) = \delta q^A(k) W(k) + \left[ 2D_i \delta q^A(k) - \left( \frac{\dot{N}}{N} - NH \right) \delta q^A(k) \right] W(k) - \left( \frac{Nk}{a} \right)^2 W(k) \delta q^A(k). \quad (49)$$

In $(49)$, $\delta q^A(k)$ refers to the solution of the full linear equation $(44)$ with subhorizon initial conditions $(43)$. The real space version of $(48)$ reads

$$D_t^2 \delta \bar{q}^A(x) - \left( \frac{\dot{N}}{N} - NH \right) D_i \delta \bar{q}^A(x) + \Omega^A_B \delta \bar{q}^B(x) = \int \frac{d^3k}{(2\pi)^2} \xi^A(k) e^{ikx} + \text{c.c.}. \quad (50)$$

The gradient of the l.h.s of $(50)$ is the linear version of $(48)$. We will therefore postulate that a suitable equation for the study of the long wavelength non-linear dynamics of the system with initial conditions provided from subhorizon scales by linear theory is

$$D_t^2 Q_i^A - \left( \frac{\dot{N}}{N} - NH \right) D_i Q_i^A + \Omega^A_i Q_i^B = \int \frac{d^3k}{(2\pi)^2} i k_i \xi^A(k) e^{ikx} + \text{c.c.}, \quad (51)$$

where now all coefficients depend on the full non-linear $Q_i^A$. Since $\xi^A$ is stochastic, equation $(51)$ is a non-linear Langevin equation for the long wavelength system.

Equation $(51)$ is the main result of this section. We can use it along with $(32)$ - $(34)$ to generate non-linear simulations of inflationary perturbations. Note that the choice of time $(29)$ has one more advantage when used in conjunction with stochastic noise. The scale that separates the long-wavelength from the short-wavelength regime for linear perturbations is the comoving Hubble radius. For this reason we will choose our smoothing scale $R$ to be a multiple of $(aH)^{-1}$:

$$R = \frac{c}{aH}, \quad (52)$$

with $c > 1$. For the gauge choice $(26)$ the split between long and short wavelengths is homogeneous throughout all of space since $aH$ is homogeneous. For other choices of time parameter, the ‘time’ when a mode is added to the long wavelength system differs from point to point. It seems conceptually more appealing to have the noise added simultaneously everywhere and that is exactly what a $\partial_i \ln(aH) = 0$ gauge does. The same conclusion for slightly different reasons was reached in $(16)$.

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4 The values $c \sim 3 - 5$ will do for safely neglecting the $k^2$ term in $\xi^A$. 
The use of linear theory for setting up initial conditions for the $Q^4_i$, or constructing the noise term completely ignores non-linearities from sub-horizon scales for these variables. One might question whether such an approximation misses out important effects before and around horizon crossing. Although this question cannot be answered within the framework described above, explicit calculations using this methodology prove that such effects are actually unimportant. In the case of both single and multiple-field inflation perturbative calculations at tree level (see also for a consideration of loop effects) show that non-Gaussianity at the time of horizon crossing is suppressed by slow-roll factors. This is considered too low to be observable in any future experiment. This result is actually reproduced in a simple way using the methods outlined above. However, as shown in subsequent non-linear evolution in certain models can enhance non-Gaussianity, making initial non-linearities subdominant. If this non-Gaussianity is observable, the scheme proposed above can safely be used to calculate it.

IV. DISCUSSION AND FUTURE PROSPECTS

The system of stochastic inflation equations presented here provides a concrete and self-consistent realization for simulating the generation and evolution of perturbations in the long wavelength approximation. The method can be applied to arbitrary single or multi-field inflationary models producing both adiabatic and isocurvature fluctuations and does not depend on the slow-roll approximation. Moreover, this approach incorporates the non-linearities inherent in the Einstein equations from the point the perturbations leave the cosmological horizon until the end of inflation. The method is, therefore, very relevant to the study of non-Gaussianity in inflation, which may prove to be a key litmus test of specific realistic models. Indeed, the limits on non-Gaussianity are set to improve substantially over the next few years with forthcoming CMB experiments and so this may prove to be an important confrontation with observation. An extension of the ideas presented here as well as analytic and numerical approaches for calculating this non-Gaussianity will appear in forthcoming publications.

The aim is to estimate the amount of non-Gaussianity generated and check whether it can be used as a further discriminant between models. Since this method can provide the real space non-Gaussian fluctuations, the possibility opens up for applying non-Gaussian tests both in real and Fourier space and determining which one is the optimal given a particular model. Such simulations therefore would be an important advance towards making quantitative predictions for realistic inflation models which can be tested against observational data, notably forthcoming CMB experiments.

Here, we shall only briefly describe the numerical implementation of these methods, leaving a detailed discussion for a much longer paper. The development of a large and complex stochastic inflation code is well-advanced but is still undergoing rigorous testing in specific cases on a parallel supercomputer (COSMOS). There are basically five key stages to the implementation: (i) homogeneous (background) solution, (ii) linear perturbation evolution, (iii) stochastic inflation generation and initial nonlinear evolution, (iv) subsequent long wavelength or separate universe evolution and, finally, (v) the end of inflation and a determination of the resulting (nongaussian) adiabatic and isocurvature fluctuations, corresponding to the initial conditions for standard large-scale structure and CMB analysis. Both (i) and (iv) are straightforward and essentially identical, solving and although the separate universe evolution is for a large grid of $N^3$ universes with perturbed initial conditions and so it is computationally intensive. Step (ii) entails the solution of the linear mode matrix equations for a general single or multi-field inflation model. The next stage (iii) is the most complex and computationally intensive when we solve for the $Q_i$'s in the key nonlinear perturbation equations while adding stochastic noise from the linear perturbation evolution as in. At each timestep in this evolution, this entails the iterative correction of the separate universe variables to incorporate the new stochastic fluctuations in the $Q_i$'s. There are several constraint equations which are monitored to ensure that this occurs self-consistently and that the evolution does not drift away from the correct nonlinear solution. This expensive evolution is only undertaken while the window function for the stochastic evolution is such that significant new fluctuations are being added to the numerical grid, before switching to the more efficient separate universe evolution (iv). Finally, at the end of inflation (v) we only implement fairly rudimentary ‘instantaneous’ reheating to obtain a set of gauge-invariant perturbations suitable for subsequent perturbation evolution. We are then using the final data products of nongaussian adiabatic and isocurvature perturbations as input in a full Boltzmann evolution code to create full-sky and high resolution CMB realizations for analysis and comparison with observation.

We finish by emphasising the key advantages of this new approach to the study of nonlinear inflationary fluctuations, while also pointing out areas for further development of these ideas. First, although the discussion of stochastic inflation and the separate universe approach now has a substantial history in most previous work it has usually been applied to the field perturbation sector without self-consistently solving the constraints for the metric perturbations or, in exceptional cases, that has been achieved only for very specific single-field models. Here, the method has been applied to both field and metric perturbations in generic inflation models with all the constraints satisfied in the long wavelength approximation. Secondly, ‘generic’ includes multi-field models which are believed to
be much more likely to produce significant non-Gaussianity; indeed, most recent realistic inflation model-building entails several fields. Thirdly, the methods presented here allow for the nonlinear evolution of the perturbations from the time at which each mode leaves the horizon. This takes into account the effect of the long wavelength modes on the subsequent shorter wavelength noise. Fourthly, unlike previous work, this long wavelength framework allows for general choices of time-slicing with the relevant perturbation variables always remaining invariant. Finally, the separate universe approach considered here corresponds to the lowest order terms of a gradient expansion of the full nonlinear Hamilton-Jacobi equations [25]. This seems to the authors likely to be a more fruitful and elegant approach than the technically much more complicated alternative of applying higher order perturbation theory to the original Einstein equations [8]. Of course, other improvements can be made to the methods discussed here, such as including the subdominant effects of vector and tensor modes and a more rigorous justification of the quantum noise. Nevertheless, we believe the present work constitutes an important step forward since it enables the quantitative calculation of nonlinear effects in generic inflationary models.

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APPENDIX A: DERIVATION OF EQUATION [25]

In this appendix we outline the derivation of equations [25]. Taking the covariant time derivative of $Q^A_i$ we get

$$D_t Q^A_i = NH Q^A_i + a D_i (NP)^A_i - a \partial_i (NH) \frac{\Pi^A_i}{H} - a X_i D_t \left( \frac{\Pi^A_i}{H} \right),$$

(A1)

where we have used that $D_t \partial_i \phi^A = D_i (NP)^A_i$. We then take the second time derivative. Most of the calculation is straightforward and we will not reproduce it here since it leads to long expressions. We only discuss non-trivial points. In calculating $D_t^2 Q^A_i$ we encounter the term $D_t D_i \Pi^A$. Using the definitions [16] we readily see that

$$D_t D_i \Pi^A = D_t D_i \Pi^A + N R^A_{FCB} \Pi^F_i \Pi^C_i \partial_i \phi^B_i
= D_t D_i \Pi^A + N a R^A_{FCB} \Pi^F_i \Pi^C_i \dot{Q}^B_i.$$  

(A2)

Here, $R^A_{FCB}$ is the curvature tensor of the field manifold and in deriving the last equality we used the antisymmetry properties of its last two indices. Now we can readily evaluate the $D_t D_i \Pi^A$ term by taking a covariant spatial derivative of [13] so we have

$$D_t D_i \Pi^A = -3NH D_i \Pi^A - 3N\Pi^A \partial_i H - 3\partial_i NH \Pi^A - \partial_i N V^A - N V^A B \partial_i Q^B + \frac{N}{a} R^A_{FCB} \Pi^F_i \Pi^C_i \dot{Q}^B_i.$$  

(A3)

We can now replace $D_t \Pi^A$ wherever it occurs by

$$D_t \Pi^A = \frac{1}{N} D_t \left( \frac{1}{a} Q^A_i \right) + X_i \frac{\Pi^A_i}{H} - \frac{1}{N} \Pi^A \partial_i N,$$

(A4)

and substitute $\partial_i H$ from

$$\partial_i H = \frac{4\pi}{m_{pl}^2} \Pi^B_i \left( \frac{1}{a} Q^B_i + \frac{\Pi^B_i}{H} X_i \right).$$  

(A5)

Another term that needs to be dealt with is $\partial_i \dot{H}$. By differentiating [12] we get

$$\partial_i \dot{H} = -\frac{4\pi}{m_{pl}^2} \partial_i N \dot{\Pi}^2 - \frac{8\pi}{m_{pl}^2} N \Pi^B D_i \dot{\Pi}^B.$$  

(A6)
The second term on the r.h.s can be obtained from the differentiation of (14) along with the use of (15). It reads
\[
\Pi_B D_i \Pi^B = - \frac{1}{a} \left( 3H \Pi_C + V_C \right) Q_i^C - \left( 3H^2 + \frac{V_C \Pi_C}{H} \right) X_i.
\] (A7)

Putting everything together and using eq. (28) we see that the terms involving \( X_i \) and \( \partial_i N \) cancel out and we are left with eq. (23).