The general solution at large scale for second order perturbations in a scalar field dominated universe

Claes Uggla\textsuperscript{a} and John Wainwright\textsuperscript{b}

\textsuperscript{a}Department of Physics, Karlstad University, S-651 88 Karlstad, Sweden
\textsuperscript{b}Department of Applied Mathematics, University of Waterloo, Waterloo, ON, N2L 3G1, Canada

E-mail: claes.uggla@kau.se, jwainwri@uwaterloo.ca

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Abstract. In this paper we consider second order perturbations of a flat Friedmann-Lemaître universe whose stress-energy content is a single minimally coupled scalar field with an arbitrary potential. We derive the general solution of the perturbed Einstein equations in explicit form for this class of models when the perturbations are in the super-horizon regime. As a by-product we obtain a new conserved quantity for long wavelength perturbations of a single scalar field at second order.

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1 Introduction

Cosmological perturbation theory plays a central role in confronting theories of the early universe with observations. The increasing accuracy of the observations, however, has made it necessary to extend the theory from linear to second order (i.e. nonlinear) perturbations, which presents various technical challenges. This paper is a contribution to this effort, focusing on long wavelength perturbations of a flat Friedmann-Lemaître (FL) universe whose stress-energy content is a single minimally coupled scalar field with an arbitrary potential. For this class of models we derive the general solution of the perturbed Einstein equations at second order when the perturbations are in the super-horizon regime, including both the growing and decaying modes. This paper relies on three of our previous papers on cosmological perturbation theory which we shall refer to as UW1 [23] (a unified and simplified formulation of change of gauge formulas at second order), UW2 [21] (five ready-to-use systems of governing equations for second order perturbations) and UW3 [22] (conserved quantities and the general solution of the perturbed Einstein equations for adiabatic long wavelength perturbations).

Our method is to apply the general solution in the total matter gauge given in UW3 [22] to the case of a scalar field and then transform to the uniform curvature gauge. The scalar field perturbations at first and second order are algebraically related to the metric perturbations, and we show that in the uniform curvature gauge, denoted by a subscript \( c \), they have the following form:

\[
\begin{align*}
\varphi_c^{(1)} & \approx (\varphi_0')^{(1)} C, \\
\varphi_c^{(2)} & \approx (\varphi_0')^{(2)} C - (\varphi_0'')^{(1)} C^2,
\end{align*}
\]

(1.1)

where \( \varphi_0 = \varphi_0(N) \) is the background scalar field and \( ' \) denotes the derivative\(^2\) with respect to e-fold time \( N = \ln x = \ln(a/a_{\text{init}}) \). The background scalar field is determined by the

\(^1\)Experience has shown that for these models the uniform curvature gauge is the best choice to represent the perturbations of the scalar field. See, for example, Hwang (1994) [9] (remarks in the Discussion), Liddle and Lyth (2000) [10] (page 93).

\(^2\)We note that in cosmological perturbation theory a \( ' \), in contrast to the present paper, is often used to denote differentiation with respect to conformal time.
background Klein-Gordon equation:

\[ \phi''_0 + \frac{1}{2}(6 - (\phi'_0)^2) (\phi'_0 + V_r / V) = 0, \]  

(1.2)

where \( V_r \) is the derivative of the potential \( V(\phi_0) \) with respect to \( \phi_0 \). The arbitrary spatial functions \( (1)C \) and \( (2)C \) in equation (1.1) are related to the comoving curvature perturbation \( (r)R, r = 1, 2 \), according to

\[ (1)C = (1)R, \quad (2)C = (2)R + 2(1)R^2. \]  

(1.3)

Note that we have not imposed the slow-roll approximation in obtaining this solution, and have not had to solve the perturbed Klein-Gordon equation. As a by-product we obtain a new conserved quantity for long wavelength perturbations of a single scalar field at second order.

The outline of the paper is as follows. In section 2 we present the main results, first the new conserved quantity at second order for a perturbed scalar field, and then give explicit expressions for the scalar field perturbations up to second order. In section 3 we derive a new form of the perturbed Klein-Gordon equation which makes explicit the existence of the conserved quantities at first and second order. In appendix A we introduce the necessary background material concerning scalar field perturbations.

2 Long wavelength perturbations

We consider second order scalar perturbations of a flat FL universe with a single minimally coupled scalar field as matter. Since we are going to specialize the general framework developed in UW2 [21] to this situation we begin by briefly introducing the notation used in [21], referring to that paper for further details. We write the perturbed metric in the form

\[ ds^2 = a^2 \left( -(1 + 2\phi)d\eta^2 + D_i B d\eta dx^i + (1 - 2\psi)\delta_{ij} dx^i dx^j \right), \]  

(2.1)

where \( \eta \) is conformal time, the \( x^i \) are Cartesian background coordinates and \( D_i = \partial / \partial x^i \). The background geometry is described by the scale factor \( a \) which determines the conformal Hubble scalar \( H = a'/a \), where in this specific situation \( ' \) denotes differentiation with respect to \( \eta \). By expanding the functions \( \phi, B, \psi \) in a perturbation series\(^4\) we obtain the following metric perturbations up to second order: \( (r)\phi, (r)B, (r)\psi, r = 1, 2 \), where the factor of \( H \) ensures that the \( B \)-perturbation is dimensionless, see UW1 [23] and UW2 [21]. We use a perfect fluid stress-energy tensor (A.1b) to describe the matter-energy content, with the matter perturbations described by the variables \( (r)\delta, (r)V, (r)T, r = 1, 2 \), where \( (r)\delta = (r)\rho / (\rho_0 + p_0) \) is the density perturbation, \( (r)V \) is the scalar velocity perturbation, defined by writing\(^5\) \( au_i = D_i V \), and \( (r)T \) is the non-adiabatic pressure perturbation.

The scalar field will be denoted by \( \varphi \) with background field \( \varphi_0 \) and perturbations \( (r)\varphi, r = 1, 2 \), and the potential will be denoted by \( V(\varphi_0) \). As is well known, the stress-energy tensor of a minimally coupled scalar field (A.1a) in a cosmological setting can be written in

\(^3\)The scalar perturbations at first order will generate vector and tensor perturbations at second order, but we do not give these perturbation variables since we will not consider these modes in this paper.

\(^4\)A perturbation series for a variable \( f \) is a Taylor series in a perturbation parameter \( \epsilon \), of the form \( f = f_0 + \epsilon (1)f + \frac{1}{2}\epsilon^2 (2)f + \ldots \).

\(^5\)UW2 [21], section IIC. We note that \( V \) is the customary notation for the potential of a scalar field, which we will also use in this paper. The context will eliminate possible confusion.
the form of a perfect fluid, which means that we can apply the above framework. Using the relation between the two stress-energy tensors the matter perturbations can be expressed in terms of the scalar field perturbations and the metric perturbations. We give the technical details in appendix A.2. In this paper at the outset we need the relation between $H(r)\psi$ and $(r)\varphi$ given by equations (A.8c) and (A.9c) and the simplified expressions for $(r)T$ given by (A.13).

In this section, since we are considering long wavelength perturbations, we will rely heavily on the results of UW3 [22].

2.1 A new conserved quantity

When analyzing perturbed inflationary universes two useful and complementary sets of variables are the gauge invariants $(r)\varphi_c$, $r = 1, 2$, the perturbations of the scalar field in the uniform curvature gauge which are sometimes referred to as the Sasaki-Mukhanov variables\footnote{See for example Malik (2005) [12], equations (3.14) and (3.21).} and the gauge invariants $(r)\psi_{sc}$, $r = 1, 2$, the curvature perturbations in the uniform field gauge.\footnote{See for example, Maldacena (2003) [11], section 3, in which both descriptions are used and compared.} Our analysis in this section will rely to a large extent on these variables.

At the outset we note that we will primarily use $e$-fold time $N$ as the time variable. We will write $\partial N f = \partial f / \partial N$ for brevity, and when $f$ is a background quantity we will use a $'$ as in the introduction, for example $\partial_N \varphi_0 \equiv \varphi_0'$. We will also use the factor $l$, given by

$$l := -(\varphi_0')^{-1},$$

as a shorthand notation to represent the frequent divisions by $\varphi_0'$ that occur in the equations involved in the study of perturbations of scalar fields.

Our first goal is to derive a general relation between the scalar field perturbations $(r)\varphi$, $r = 1, 2$, and the metric perturbations, specifically the curvature perturbations $(r)\psi$, $r = 1, 2$. We begin by performing a change of gauge from the uniform field gauge, defined by $(r)\varphi = 0$, $r = 1, 2$, to an arbitrary gauge using the formula (42e) in UW1 [23] with $\Box = \psi$:

$$(1)\psi_{sc} = (1)\psi - (1)\varphi,$$  
$$(2)\hat{\psi}_{sc} = (2)\hat{\psi} - (2)\hat{\varphi} + 2(1)\varphi \partial_N (1)\psi_{sc} - D_2 (1)B_{sc} + D_2 (1)B,$$  

where $D_2$, the so-called Newtonian spatial operator,\footnote{See UW1 [23], appendix B. The specific form of $D_2(\bullet)$ does not concern us here.} is a spatial differential operator of order 2 in $D_j$ and hence negligible in the super-horizon regime. The hatted variables are given by (see UW1 [23], equations (37)):

$$(2)\hat{\psi} := (2)\psi + 2(1)\psi^2,$$  
$$l(2)\hat{\varphi} := l(2)\varphi + \frac{3}{2}(w - c_s^2)(l(1)\varphi)^2,$$

where $w - c_s^2$ is related to $\varphi_0$ and its derivatives by equation (A.5) in appendix A.1.

It is helpful to use the fact that the uniform field gauge is equivalent to the total matter gauge, defined by $(r)V = 0$, $r = 1, 2$, since equations (A.8c) and (A.9c) show that $(r)\varphi = 0 \iff (r)V = 0$, $r = 1, 2$. This means that the various gauge invariants in the two gauges are equal. For example, for the curvature perturbation we have

$$(r)\psi_{sc} = (r)\psi_v, \quad r = 1, 2.$$
By solving for the $\varphi$-perturbation in equations (2.3) and using equation (2.5) we obtain

\begin{align}
  l^{(1)}\varphi &= (1)^{\psi} - (1)^{\psi_v}, \\
  l^{(2)}\tilde{\varphi} &= (2)^{\psi} - (2)^{\psi_v} + 2(1)^{\psi} - (1)^{\psi_v})\partial_N(1)^{\psi_v} - D_2(1)^{B_v} + D_2(1)^B,
\end{align}

which determine the scalar field perturbations in any gauge in terms of the metric perturbations.

At this stage we need two general properties of long wavelength perturbations:\(^9\)

(i) The density perturbations in the total matter gauge satisfy,

\begin{equation}
  (1)\delta_v \approx 0, \quad (2)\delta_v \approx 0.
\end{equation}

(ii) If the perturbations are adiabatic the curvature perturbations in the total matter gauge satisfy,

\begin{equation}
  \partial_N(1)^{\psi_v} \approx 0, \quad \partial_N(2)^{\psi_v} \approx 0.
\end{equation}

In addition we need to determine the non-adiabatic pressure perturbations for a scalar field. In appendix A.2 we have shown that the \(^{(r)T_r, r=1, 2}\) depend linearly on \(^{(r)\delta_v, r=1, 2}\), with source terms at second order depending on \(^{(1)\delta_v\), as in equation (A.13). It thus follows from equation (2.7) that

\begin{equation}
  (1)^{\Gamma} \approx 0, \quad (2)^{\Gamma} \approx 0, \quad (2.9)
\end{equation}

i.e. long wavelength scalar field perturbations are adiabatic.\(^10\) Thus (2.8) holds, which implies that for long wavelength perturbations equations (2.6) reduce to

\begin{equation}
  l^{(1)}\varphi = (1)^{\psi} - (1)^{\psi_v}, \quad l^{(2)}\tilde{\varphi} \approx (2)^{\psi} - (2)^{\psi_v}.
\end{equation}

In other words, when using the hatted variables the first order relation generalizes to second order.

We now choose the arbitrary gauge in these equations to be the uniform curvature gauge, which gives

\begin{equation}
  l^{(1)}\tilde{\varphi}_c = -(1)^{\psi_v}, \quad l^{(2)}\tilde{\varphi}_c \approx -(2)^{\psi_v}.
\end{equation}

Since (2.8) holds the first equation in (2.11) gives the known result\(^11\) that at first order \(l^{(1)}\tilde{\varphi}_c\) is a conserved quantity while the second equation gives the new result that at second order

\begin{equation}
  l^{(2)}\tilde{\varphi}_c := l^{(2)}\varphi_c + 3\frac{1}{2}(w_\varphi - c^2_\varphi)(l^{(1)}\varphi_c)^2,
\end{equation}

is a conserved quantity for long wavelength perturbations of a single field inflationary universe. We note that the relation (2.12) is obtained by choosing the uniform curvature gauge in (2.4b).

\(^9\) These results are part of the folklore of perturbation theory, but derivations at second order are not easy to find. We have given simple derivations in UW3 [22], equations (20) and (26a).

\(^10\) This result has been given by Vernizzi (2005) [24].

\(^11\) Sasaki (1986) [20] (see equation (2.33)) introduced the quantity \((1)^{\psi_v} - l^{(1)}\tilde{\varphi}_v\) in our notation, and stated that it is constant on large scales provided that the entropy and spatial anisotropy perturbations are negligible.
2.2 Explicit form of the scalar field perturbations

In a recent paper UW3 [22] we gave the general solution of the perturbed Einstein equations at second order for long wavelength adiabatic perturbations of a FL universe, with stress-energy tensor of the perfect fluid form (A.1b). We solved the equations for the metric perturbations in the total matter gauge, giving the general solution, i.e. including the decaying mode. At first order the solution is

\[ \phi_v \approx 0, \quad \psi_v \approx C, \quad H(B_v) \approx \left(1 - g(a)\right)C + \left(H/a^2\right)C^*, \]

where the perturbation evolution function \( g(a) \) is defined by

\[ g(a) = 1 - H(a) \int_0^a \frac{\dd \bar{a}}{H(\bar{a})}. \]

At second order the solution is:

\[ \phi_v \approx 0, \quad \hat{\psi}_v \approx C, \quad H(B_v) \approx \left(1 - g(a)\right)\left(2C - 2D_0(1C)\right) + \left(H/a^2\right)C^*. \]

We identify the spatial functions \( C(x^i) \) and \( C^*(x^i) \) as the conserved quantities at first and second order, while \( C^*(x^i) \) describes the decaying mode. If we apply this solution in the case of a scalar field the Hubble scalar \( H(a) \) is determined explicitly in terms of the background scalar field and the scalar field potential by equation (A.3a), which then determines the function \( g(a) \) through (2.14).

In the total matter gauge it follows from (2.10) that the scalar field perturbations are zero \( (r)\varphi_v = 0, \ r = 1, 2 \). In effect, in this gauge the perturbations of the scalar field are hidden in the metric perturbations. On the other hand, in the uniform curvature gauge it follows from (2.11) that the scalar field perturbations are given by

\[ l(\varphi_c) = -(1)\psi_v \approx -(1)C, \quad l(\varphi_c) \approx -(2)\hat{\psi}_v \approx -(2)C, \]

the last step following from (2.13a) and (2.15a). To obtain an explicit expression for \( \varphi_c \) we use the definition (2.12) of \( \varphi_c \) and \( l = -1/(\varphi_0^0) \) which yields:

\[ \varphi_c \approx \varphi_0^0(1)C, \quad \varphi_c \approx \varphi_0^0 \left(2C + \frac{3}{2}(w_\varphi - c_\varphi^2)(1)C^2\right), \]

where \( w_\varphi - c_\varphi^2 \) is given by equation (A.5) in appendix A.1, which we also give here:

\[ w_\varphi - c_\varphi^2 = \frac{2}{3} \left(\frac{\varphi''_0}{\varphi_0}\right). \]

Substituting this result into (2.17) yields the expression (1.1) for \( \varphi_c \) in the introduction. The scalar field \( \varphi_0(N) \) is determined by the background Klein-Gordon equation (1.2).

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12 We refer to UW3 [22] for this name, and for its history and properties (see appendix C in [22]).

13 The spatial differential operator \( D_0 \) is defined by \( D_0(C) := S^{ij}(D_i(C)D_j(C)) \), where the scalar mode extraction operator \( S^{ij} \) is defined by \( S^{ij} = \frac{2}{3}(D^{-2})^{ij} \). Here \( D^{-2} \) is the inverse spatial Laplacian and \( D_{ij} := D_i(D_j) - \frac{1}{3}\delta_{ij}D^2 \). Spatial indices are raised with \( \delta^{ij} \).
We now calculate the scalar field perturbation in the Poisson gauge by choosing the Poisson gauge in equation (2.10) which yields:

\[ l^{(1)} \phi_p = (1) \psi_p - (1) \psi_v, \quad l^{(2)} \phi_p \approx (2) \hat{\psi} - (2) \hat{\psi}_v. \]  

(2.19)

In our previous paper UW3 [22] we used a change of gauge formula to calculate the curvature \( \psi_p \) determined by the solution (2.13) and (2.15). The results are:

\[ \psi_p \approx g C - \left( \frac{H}{a^2} \right) C_s, \]  

(2.20a)

\[ (2) \hat{\psi}_p \approx g (2) C + \left( \frac{3}{2} (1 + c^2) (1 - g) \right) C^2 + 4 g D_0 (C). \]  

(2.20b)

where we note that for brevity have not included the decaying mode at second order. We substitute these expressions into (2.19) and use (2.13a) and (2.15a). The final expressions for the scalar field perturbations, using the unhatted variable and excluding the decaying mode at second order, are as follows:\(^{14}\)

\[ l^{(1)} \phi_p \approx -(1 - g) (1) C - \left( \frac{H}{a^2} \right) (1) C_s, \]  

(2.21a)

\[ l^{(2)} \phi_p \approx (1 - g) \left[ -(2) C + \left( \frac{3}{2} (1 + c^2) (1 - g) \right) C^2 + 4 g D_0 (C) \right]. \]  

(2.21b)

The linear solution is well known but is usually found by solving the Bardeen equation or the perturbed Klein-Gordon equation.\(^{15}\) The second order solution is new. Note that the decaying mode appears in the scalar field perturbations in the Poisson gauge, in contrast to the situation in the uniform curvature gauge in equation (2.17).\(^{16}\)

We end this section with a comment on multiple scalar fields. We note that perturbations of universes with multiple scalar fields (see for example, Malik and Wands (2005) [15], for linear perturbations and Malik (2005) [12] for second order perturbations) have been studied using the uniform curvature gauge. However, since large scale perturbations of multiple scalar fields are not adiabatic, our explicit large scale solution for a single scalar field cannot be generalized to multiple fields.

3 The perturbed Klein-Gordon equation

Although the Klein-Gordon equation plays a central role in governing scalar field perturbations, we have obtained simple expressions for these perturbations to second order on super-horizon scale and have obtained conserved quantities, using only some of the perturbed Einstein equations. On inspecting the form of the perturbed Klein-Gordon equation at first and second order as given in the literature\(^{17}\) it is clear that our results are unexpected,
since it is not obvious that the equation admits conserved quantities or that the explicit expressions for \((1)\varphi_c\) and \((2)\varphi_c\), as given by equation (1.1), are in fact solutions of the equation on super-horizon scale.

There are two standard ways to derive the perturbed Klein-Gordon equation. The first is to use the perturbed energy conservation equation to obtain an expression for the second time derivative of \(\varphi_c\) and then use (some of) the perturbed Einstein equations to express the metric perturbations that appear in this equation in terms of the scalar field perturbations. The second is to use the variation of the Einstein action coupled to the scalar field. We refer to Malik et al. (2008) [14] for a comparison of the two approaches.

In this section we give a new way of deriving the perturbed Klein-Gordon equation, leading to a simpler form of the equation with \(l = -1/(\varphi_0')\) acting as a scale factor for the perturbation, which by inspection admits a conserved quantity at first and second order. We begin with the perturbed Einstein equations in the uniform curvature gauge as given in our earlier paper UW2 [21], see section IVB.1. These equations, which determine the metric perturbations \(\varphi_c\) and \(B_c\) at first order, read

\[
\partial_N((1 + q)^{-1}(1)\varphi_c) = -c_s^2(1 + q)^{-1}H^{-2}D^2(H^{(1)}B_c) + (1)\Gamma, \quad (3.1a)
\]
\[
\partial_N(a^2(1)B_c) = -a^2H^{-1}(1)\varphi_c. \quad (3.1b)
\]

Here \(q\) denotes the background deceleration parameter which is defined by

\[
1 + q = -H'/H, \quad \Leftrightarrow \quad q = \mathcal{H}'/\mathcal{H}, \quad (3.2)
\]

where \(H\) is the background Hubble scalar, \(\mathcal{H} = aH\) and ‘\( denotes differentiation with respect to \(N\). The velocity perturbation and density perturbation are given by

\[
\mathcal{H}^{(1)}V_c = -(1 + q)^{-1}(1)\varphi_c, \quad (3.3a)
\]
\[
(1)\delta_v = -(1 + q)^{-1}H^{-2}D^2(H^{(1)}B_c). \quad (3.3b)
\]

In a universe with a single scalar field equations (A.8c) and (A.13a) in appendix A.2 give

\[
\mathcal{H}^{(1)}\varphi_c = l^{(1)}\varphi_c, \quad (1)\Gamma = (1 - c_s^2)(1)\delta_v, \quad (3.3c)
\]

where \(l = -1/(\varphi_0')\). Using equations (3.3), which show that

\[
(1 + q)^{-1}(1)\varphi_c = -l^{(1)}\varphi_c, \quad (3.4)
\]

we can write equations (3.1) as a coupled system for \(\varphi_c\) and \(B_c\):

\[
(1 + q)\partial_N(l^{(1)}\varphi_c) = \mathcal{H}^{-2}D^2(H^{(1)}B_c), \quad (3.5a)
\]
\[
\partial_N(a^2(1)B_c) = a^2\mathcal{H}^{-1}(1 + q)l^{(1)}\varphi_c. \quad (3.5b)
\]

We now eliminate the metric perturbation \((1)B_c\) by applying \(D^2\) to (3.5b) and substituting for \(D^2(HB_c)\) from (3.5a). This leads to

\[
\left(\partial_N^2 + 2\frac{H'}{H}\partial_N - \mathcal{H}^{-2}D^2\right)(l^{(1)}\varphi_c) = 0, \quad (3.6)
\]
where $h = h(N)$ is a background scalar given by $^{18} h^2 = 2a^2H(1+q)$, and $h' \equiv \partial_N h$. By differentiating this expression and using equations (3.2), (A.4) and (A.6) one can express the coefficient $h'/h$ in (3.6) in terms of the scalar field potential $V(\varphi_0)$, as follows:

$$
\frac{h'}{h} = \frac{(2V_\varphi - V)}{2H^2},
$$

(3.7)

with $H$ given by (A.3a) in appendix A.1.

Equation (3.6) with (3.7) is the desired new form of the perturbed Klein-Gordon equation at first order. By inspection it is clear that in the super-horizon regime $l^{(1)}\varphi_c \approx C$, where $C$ is a spatial function, is a solution of this equation as expected. However, since (3.6) is a second order differential equation, it will have two independent solutions, and the general solution in the super-horizon regime can be written in the form

$$
l^{(1)}\varphi_c \approx C_1 + C_2 \int_{N_{\text{init}}}^{N} \frac{d\bar{N}}{h(\bar{N})^2},
$$

(3.8)

which at first sight contradicts the earlier result $^{20} l^{(1)}\varphi_c \approx C$ is the general solution of the perturbation equations in the super-horizon regime. It follows that the spatial function $C_2$ must be of order $O(D^2)$, making the second term negligible in the super-horizon regime.

Although (3.6) can be solved explicitly in the super-horizon regime as above and also in the special case of power-law inflation and in the slow-roll approximation $^{19}$ there is a restriction as regards its overall applicability. On recalling that $l = -1/(\varphi_0')$, it follows that the coefficient (3.7) will be singular whenever $\partial_N \varphi_0 = 0$. For example, during the period of reheating that occurs at the end of inflation the scalar field $\varphi_0$ oscillates, which means that $\partial_N \varphi_0$ will be zero repeatedly. In order to avoid this singularity one can use $^{(1)}\varphi_c$ as dependent variable. The alternative form of the Klein-Gordon equation is given in appendix A.3.

One can also use the above procedure to derive the perturbed Klein-Gordon equation at second order. The leading order terms in equations (3.1) and (3.3c) will be the same as at first order, but the equations will also have source terms that are quadratic in the first order perturbations $\phi_c, B_c$ and $\varphi_c$. $^{21}$ At the first stage equations (3.5) will have the form

$$
(1+q)\partial_N(l^{(2)}\varphi_c) = H^{-2}D^2(\mathcal{H}^{(2)}B_c) + (1+q)S_\varphi,
$$

(3.9a)

$$
\partial_N(a^{2(2)}B_c) = a^2H^{-1}(1+q)l^{(2)}\varphi_c + S_B,
$$

(3.9b)

where we have chosen to use $^{(2)}\varphi_c$ instead of $^{(2)}\varphi_c$ since this simplifies the source term $S_\varphi$ so that it has the property

$$
S_\varphi = O(D^2).
$$

(3.10)

This can be confirmed by inspecting the various terms that contribute to $S_\varphi$. Here we note that we have used (3.4) to replace $^{(1)}\phi_c$ by $^{(1)}\varphi_c$ in the source terms so that they depend only

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$^{18}$We use $h^2$ instead of $h$ in order to have a simple link with the commonly used Mukhanov-Sasaki form of the perturbed Klein-Gordon equation, as in equations (A.18) and (A.20) in appendix A.3.

$^{19}$This involves using conformal time $\eta$ instead of $e$-fold time $N$. See appendix A.3 for the resulting alternative forms of the Klein-Gordon equation.

$^{20}$Some implications of this singularity have been discussed by Finelli and Brandenberger (1999) $[^4]$.

$^{21}$The detailed expressions can be obtained from the equations in UW2 $^{[21]}$. We do not give them because in this paper we are just interested in the overall structure of the equations.
on the spatial derivatives of $B_c$ and $\phi_c$. Eliminating $B_c$ in equations (3.9) as in the linear case leads to
\[
\left(\partial_N^2 + 2\frac{h'}{h}\partial_N - \mathcal{H}^2 \mathcal{D}^2\right) (l(2)\hat{\phi}_c) = \partial_N (h^2 S_\phi) + \mathcal{H}^2 \mathcal{D}^2 S_B, \tag{3.11}
\]
where $h'/h$ is given by (3.7). Equation (3.11) is a new version of the perturbed Klein-Gordon equation at second order. We note that there is one complication as regards the source term in (3.11). Since it depends on both $\phi_c$ and $B_c$ one has to express $B_c$ in terms of $\phi_c$ using (3.5a) in order to make (3.11) a closed equation,\(^{22}\) and this involves using the inverse Laplacian operator $D^{-2}$.

An important property of equation (3.11) is that the total source term on the right side of the equation is $O(D^2)$ on account of (3.10), and this is due to using the hatted variable $(2)\hat{\phi}_c$ instead of $(2)\phi_c$. Thus in the super-horizon regime, equation (3.11) reduces to the DE
\[
\left(\partial_N^2 + 2\frac{h'}{h}\partial_N\right) (l(2)\hat{\phi}_c) \approx 0, \tag{3.12}
\]
in complete analogy with equation (3.6), which means that the general solution has the same form as (3.8) with $l(2)\hat{\phi}_c$ replacing $l(1)\phi_c$. Since equation (2.16) shows that $l(2)\hat{\phi}_c$ is a conserved quantity in general the second term in the solution must be negligible in the super-horizon regime, as in the first order case. Another similarity is that the changes of variable made on the first order equation (3.6) as in equations (A18)–(A22), which affect only the terms on the left side of the equation, can performed on equation (3.11) in an identical manner. On the other hand changing from $(2)\hat{\phi}_c$ to $(2)\phi_c$ as the dependent variable using (2.4b) will complicate the equation (3.11) significantly by introducing additional source terms that are non-zero in the super-horizon regime.

Equations (3.9) or (3.11), when transformed to Fourier space both provide an algorithm for calculating $l(2)\hat{\phi}_c$ numerically.\(^{23}\) Using (3.9) would have two advantages. First there is no need to eliminate $B_c$ thereby avoiding the introduction of the inverse Laplacian in the source terms, and second the output directly determines two other quantities of physical interest, namely the Bardeen potential $\psi_p$ and the density perturbation $\delta_v$, via the equations $\psi_p = -\mathcal{H}B_c$ and $\delta_v = -\partial_N (l\phi_c)$, generalized to second order with source terms.

4 Discussion

In this paper we have considered second order perturbations of a flat Friedmann-Lemaître universe whose stress-energy content is a single minimally coupled scalar field. We have derived the general solution of the perturbed Einstein equations in explicit form for this class of models when the perturbations are in the super-horizon regime. We assumed an arbitrary potential and made no use of the slow-roll approximation. We also showed that the Einstein equations in the uniform curvature gauge lead to a new form of the perturbed Klein-Gordon equation for linear perturbations using $l\phi_c$ as dependent variable, which we generalize to second order.

\(^{22}\)See for example, Malik et al. 2008 [14] for an explicit example of this process: the second order differential equation that arises from the conservation of energy equation is equation (3.5) which becomes equation (3.22) after the metric terms have been eliminated, in the slow-roll approximation.

\(^{23}\)Numerical procedures for determining second order scalar perturbations using the perturbed Klein-Gordon equation with $(2)\phi_c$ rather than $(2)\hat{\phi}_c$ as the dependent variable have been given by Huston and Malik (2009) [7] using the slow-roll approximation, and by Huston and Malik (2011) [8] in general.
The perturbations of the scalar field have a simple form in the uniform curvature gauge, which reflects the fact that the perturbations admit a conserved quantity. Although second order perturbations of scalar fields minimally coupled to gravity have been studied extensively during the past fifteen years in connection with inflation, starting with Acquaviva et al. (2003) [1] and Maldacena (2003) [11] (see also, for example, Finelli et al. [5, 6], Malik (2005) [12] and Vernizzi (2005) [24]), the conserved quantity \( l^{(2)} \phi_c \) given by (2.12) and the general solution for \( (2) \phi_c \) in equation (1.1) have not been given previously, to the best of our knowledge. However, we note that Finelli et al. (2004) [5] have derived an approximate solution for \( (2) \phi_c \) using the perturbed Klein-Gordon equation at second order (their equation (28)). They impose the slow-roll approximation and use the potential \( V = \frac{1}{2} m^2 \varphi^2_0 \) that corresponds to chaotic inflation. We have not been able to relate their solution which is described in equations (53)–(57) in [5] to our general result. In addition, some of the change of variable formulas that we use in section 2.1 have been given previously but in a more complicated form. For example equation (8) in Finelli et al. (2006) [6] corresponds to our equation (2.3b), while equations (3.3)–(3.4) in Maldacena (2003) [11] correspond to the special case of our equation (2.3b) when the gauge on the right side is chosen to be the uniform curvature gauge.

A Cosmological scalar fields as perfect fluids

We are considering a flat FL universe in which the matter-energy content is a single minimally coupled scalar field \( \varphi \). The stress-energy tensor is of the form

\[
T^a_b = \nabla^a \varphi \nabla_b \varphi - \left[ \frac{1}{2} \nabla^c \varphi \nabla_c \varphi + V(\varphi) \right] \delta^a_b, \tag{A.1a}
\]

and the conservation equation leads to the Klein-Gordon equation \( \nabla^c \nabla_c \varphi - V(\varphi) = 0 \), where the potential \( V(\varphi) \) has to be specified. In cosmology this stress-energy tensor has the perfect fluid form

\[
T^a_b = (\rho + p) u^a u_b + p \delta^a_b, \tag{A.1b}
\]

with \( \rho + p = -\nabla^a \varphi \nabla_a \varphi \), \( \rho - p = 2V(\varphi) \), \( u_a = \frac{\nabla_a \varphi}{\sqrt{-\nabla^c \varphi \nabla_c \varphi}} \). \tag{A.1c}

A.1 Background equations

In a spatially flat background the Friedmann equation\(^{24}\) and the conservation of energy equation read\(^{25}\)

\[
3H^2 = \rho_0, \quad \dot{\rho}_0 = -3(\rho_0 + p_0), \tag{A.2a}
\]

where \( H \) is the background Hubble variable while \( \rho_0 \) and \( p_0 \) are the background energy density and pressure, respectively. We introduce the standard matter variables \( w = p_0/\rho_0 \) and \( c_s^2 = p_0/\rho_0 \). Using these equations and the definition \( 1 + q = -H'/H \) it follows that

\[
3(1 + w) = 2(1 + q), \quad w' = 3(1 + w)(w - c_s^2). \tag{A.2b}
\]

When evaluated on the FL background, equation (A.1c) leads to

\[
\rho_0 + p_0 = H^2 (\varphi'_0)^2, \quad \rho_0 - p_0 = 2V(\varphi_0). \tag{A.2c}
\]

\(^{24}\)We use units with \( c = \hbar = 1 \) and \( 8\pi G = 1/(M_{Pl})^2 = 1 \), where \( M_{Pl} \) is the reduced Planck mass and \( G \) the gravitational constant.

\(^{25}\)We remind the reader that a ’ denotes the derivative with respect to \( N \).
We can use equations (A.2) to express $H^2$, $w$ and $c_\phi^2$ in terms of $\varphi_0$ and $V(\varphi_0)$. To indicate that $w$ and $c_\phi^2$ describe a scalar field we will label them as $w_\varphi$ and $c_\phi^2$. The resulting expressions are as follows:

\begin{align}
H^2 &= \frac{2V(\varphi_0)}{6 - (\varphi_0')^2}, \\
w_\varphi &= -1 + \frac{1}{3}(\varphi_0')^2, \\
c_\phi^2 &= 1 + \frac{(6 - (\varphi_0')^2)}{3\varphi_0'} V_{,\varphi} / V,
\end{align}

where $V_{,\varphi}$ is the derivative of $V(\varphi_0)$ with respect to $\varphi_0$. It follows from (A.2b) and (A.3) that

\begin{align}
2 - q &= \frac{V}{H^2}, \quad 1 - c_\phi^2 = -\frac{2}{3} \frac{V_{,\varphi}}{\varphi_0'} H^2.
\end{align}

Further, one can derive the background Klein-Gordon equation (1.2) by differentiating (A.3a), and then use the result to obtain

\begin{align}
w_\varphi - c_\phi^2 &= \frac{2}{3} \left( \frac{\varphi_0''}{\varphi_0'} \right).
\end{align}

We will also need the following result

\begin{align}
q' &= 3(1 + q)(w_\varphi - c_\phi^2),
\end{align}

which is an immediate consequence of (A.2b).

We end this section with a brief digression on the Hubble flow functions $\varepsilon_n$, $n = 1, 2, 3 \ldots$ which define the slow-roll regime, although we do not use this approximation. These functions are defined by $\varepsilon_1 = -H' / H$, $\varepsilon_{n+1} = \varepsilon_n / \varepsilon_n$, $n = 1, 2, 3 \ldots$ (see for example, Martin (2016) [16], equation (5)). It follows from $1 + q = -H' / H$ and equations (A.2b), (A.3b) and (A.5) that the Hubble flow functions are related to the scalar field according to

\begin{align}
\varepsilon_1 &= 1 + q = \frac{1}{2} (\varphi_0')^2, \quad \varepsilon_2 = \frac{q'}{1 + q} = 2 \left( \frac{\varphi_0''}{\varphi_0'} \right).
\end{align}

### A.2 Perturbations of the scalar field

For a scalar field we can express the matter variables $((^{(r)}\delta, ^{(r)}P, ^{(r)}V))$, where $^{(r)}P = ^{(r)}p/(\rho_0 + p_0)$, in terms of the scalar field perturbations $^{(r)}\varphi$ and the metric variables $\phi$ and $B$ using equations (A.1a) and (A.1c). The results at first order are

\begin{align}
^{(1)}\delta + ^{(1)}P &= -2(l\partial_N^{(1)} \varphi + ^{(1)}\phi), \\
^{(1)}\delta - ^{(1)}P &= 2H^{-2} l V_{,\varphi} l^{(1)} \varphi, \\
\mathcal{H}^{(1)}V &= l^{(1)} \varphi,
\end{align}
where \( l = -(\varphi_0')^{-1} \) is given by (2.2). The results at second order are:

\[
\begin{align*}
(2) \delta^{(2)} + P &= -2(l \partial_N \phi + \phi') + 2 \left( 2(1) \phi + l \partial_N (1) \phi \right)^2 + 2 H^{-2} \left( D(l(1) \varphi - H(1) B) \right)^2, \quad (A.9a) \\
(2) \delta^{(2)} - P &= 2 H^{-2} \left( V_\varphi l(2) \varphi + V_\varphi \varphi'(l(1) \varphi)^2 \right), \quad (A.9b) \\
\mathcal{H}^{(2)} V &= l(2) \varphi - 2(1) \mathcal{D}_l \mathcal{H}(1) V. \quad (A.9c)
\end{align*}
\]

Before continuing we note two properties of the perturbations of the scalar field that are obtained immediately by choosing the total matter gauge in (A.8) and (A.9), namely that

\[
^{(r)} \varphi_v = 0, \quad r = 1, 2, \tag{A.10}
\]

and hence that

\[
^{(r)} P_v = (r) \delta_v, \quad r = 1, 2. \tag{A.11}
\]

We now derive expressions for the non-adiabatic pressure perturbations \(^{(r)} T\), \( r = 1, 2 \) for a perturbed scalar field. The general expressions are given in UW2 [21] (see equation (23)), which we repeat here

\[
\begin{align*}
(1) \Gamma &= (1) P - \epsilon^2 (1) \delta, \tag{A.12a} \\
(2) \Gamma &= (2) P - \epsilon^2 (2) \delta + \frac{1}{3} \left( \partial_N c_s^2 \right) (1) \delta^2 + \frac{2}{3} (1) \delta \left[ \partial_N - 3(1 + c_s^2) \right] (1) \Gamma. \tag{A.12b}
\end{align*}
\]

The expressions on the right side are independent of choice of timelike gauge once the spatial gauge has been fixed as in UW2 [21]. In the present situation we evaluate them in the total matter gauge and use (A.11) which leads to

\[
\begin{align*}
(1) \Gamma &= (1 - \epsilon^2) (1) \delta_v, \tag{A.13a} \\
(2) \Gamma &= (1 - \epsilon^2) (2) \delta_v + \frac{1}{3} \left( \partial_N c_s^2 \right) (1) \delta_v^2 + \frac{2}{3} (1) \delta_v \left( \partial_N - 3(1 + c_s^2) \right) (1) \Gamma. \tag{A.13b}
\end{align*}
\]

The constraints (A.8c) and (A.9c) play a central role in that they determine the perturbations of the scalar field in terms of the velocity perturbations in an arbitrary gauge. We can write (A.9c) in terms of the hatted variables, in a form that will be useful later, as follows. We combine (A.8a) and (A.8c) to obtain

\[
(1) \delta + (1) P = -2 \left( \partial_N + 1 + q \right) (H(1) V) + (1) \phi - \frac{3}{2} (1 + c_s^2) H(1) V, \tag{A.14}
\]

using \( t'/l = -(1 + q) + \frac{3}{2} (1 + c_s^2) \). The perturbed conservation of momentum equation (UW2 [21], section 4) when applied to a scalar field using (A.13a) gives

\[
(\partial_N + 1 + q) (H(1) V) + (1) \phi = - (1) \delta_v, \tag{A.15}
\]

which when substituted in (A.14) yields

\[
(1) \delta + (1) P = 3(1 + c_s^2) H(1) V + 2(1) \delta_v. \tag{A.16}
\]

\footnote{Formulas for \(^{(r)} T^a_b\), \( r = 1, 2 \), for the stress-energy tensor (A.1a) have been given for example, by Acquaviva et al. (2003) [1] (see equations (9)–(16)), by Malik (2007) [13] (see equations (C12)–(C14)) and by Nakamura (2009) [19] (see equations (4.45)–(4.52)). The expressions we have given can be obtained using the relation

\[
(2) T^a_b = (\rho_0 + p_0)(T^a_b + T^a_{ch}), \tag{A.17}
\]

see UW2 [21].}
We substitute this expression in (A.9c) and introduce the hatted variables \( \hat{\phi} \) defined in (2.4b) and \( H^{(2)} \hat{V} = H^{(2)}V + (1 + q)(H^{(1)}V)^2 \). Together with (A.8c) we obtain

\[
\begin{align*}
I^{(1)} \phi &= H^{(1)}V, \\
I^{(2)} \hat{\phi} &= H^{(2)} \hat{V} + 2S^i[\delta, D_i H V].
\end{align*}
\]

(A.17a)

(A.17b)

### A.3 Alternative forms for the perturbed Klein-Gordon equation

We first transform the differential equation (3.6) to Fourier space \( D^2 \rightarrow -k^2 \) and introduce conformal time \( \eta \) obtaining

\[
\left( \partial^2_\eta + 2(\partial_\eta z/z) \partial_\eta + k^2 \right)(l^{(1)} \phi_c) = 0, \quad z = h/\sqrt{H} = a/l.
\]

(A.18)

We make the transition from \( N \) to \( \eta \) by using

\[
\partial_\eta = H \partial_N, \quad \partial^2_\eta = H^2 (\partial^2_N - q \partial_N).
\]

(A.19)

Alternatively one can transform the above differential equation to the so-called Mukhanov-Sasaki form by scaling \( l^{(1)} \phi_c \) with \( z \):

\[
\left( \partial^2_\eta - (\partial^2_\eta z/z) - k^2 \right)(a^{(1)} \phi_c) = 0, \quad z = a/l.
\]

(A.20)

On recalling that the comoving curvature perturbation is given by \( \mathcal{R} = \psi_v = -l^{(1)} \phi_c \) these differential equations can be written with \( \mathcal{R} \) and \( z \mathcal{R} \), respectively, as the dependent variable. See, for example, Weinberg (2008) [25], equation (10.3.1) and page 481, and Durrer (2008) [3], equation (3.35) and page 113, respectively. In the case of power-law inflation and when using the slow-roll approximation equations (A.18) and (A.20) reduce to particular forms of Bessel’s equation, and hence can be solved. See for example [3], pages 113–115, and in [25], pages 481–482 and 488–491.

Finally, if we use \( \phi_c \) as the dependent variable, the differential equation (3.6) assumes the following form:

\[
\partial^2_N \phi_c + \frac{V}{H^2} \partial_N \phi_c + \left( \frac{V_{,\phi\phi} + 2\phi_0' V_{,\phi} + (\phi_0')^2 V}{H^2} \right) \phi_c = -H^{-2} D^2 \phi_c = 0,
\]

(see for example, Huston and Malik (2009) [7], equation (3.9), in the Fourier domain, noting that \( \delta \dot{\phi} \) denotes differentiation with respect to \( N \) in this reference.). If we change to conformal time we obtain

\[
\partial^2_\eta \phi_c + 2H \partial_\eta \phi_c + a^2 \left( V_{,\phi\phi} + 2\phi_0' V_{,\phi} + (\phi_0')^2 V \right) \phi_c - D^2 \phi_c = 0,
\]

(A.21)

(A.22)

with \( \phi'_0 = \partial_\eta \phi_0 / H \) (see for example [7], equation (2.13), noting that ‘ denotes differentiation with respect to conformal time in this reference.) One can see by inspection that the coefficients of (A.21) and (A.22) are well-defined when \( \phi'_0 = 0 \).
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