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(Dated: November 1, 2018)

We derive the governing equations for multiple scalar fields minimally coupled to gravity in a flat Friedmann-Robertson-Walker (FRW) background spacetime on large scales. We include scalar perturbations up to second order and write the equations in terms of physically transparent gauge-invariant variables at first and second order. This allows us to write the perturbed Klein-Gordon equation at second order solely in terms of the field fluctuations on flat slices at first and second order.

PACS numbers: 98.80.Cq

JCAP11 (2005) 005, astro-ph/0506532v3

## I. INTRODUCTION

Cosmological perturbation theory [1, 2] has become the standard tool to study inflation and its observational consequences for the Cosmic Microwave Background (CMB) and the formation of large scale structure [3]. Linear perturbation theory is sufficient to study the power spectrum of the primordial perturbations generated during inflation, in particular to calculate the spectral index and its scale dependence.

One way to glean more information from the CMB is to go beyond first order perturbation theory, which allows the study of higher order statistics, such as the bispectrum, or to calculate the amount of non-gaussianity expected from ones favourite early universe model.

On super-horizon scales, i.e. scales much larger than the particle horizon, there are mainly two approaches to study higher order effects such as non-gaussianity: the first uses second order perturbation theory following Bardeen [1, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22], the second uses nonlinear theory and different manifestations of the separate universe approximation, either employing a gradient expansion, as originally used by Salopek and Bond [23, 24, 25, 26] or using the  $\Delta N$  formalism [27, 28, 29]<sup>1</sup>. In the formalism used by Salopek and Bond [23] the metric and the matter variables are not expanded into a power series, instead an expansion in spatial gradients is used. The  $\Delta N$  formalism was introduced at linear order by Sasaki and Stewart in [31] (see also [32, 33]) and relates the comoving curvature perturbation to the perturbation in the number of e-foldings and has recently been extended to the non-linear case [28, 29]. In the Bardeen approach the metric and the matter fields are expanded in a power series in a small parameter. There has been increased interest in second order perturbation theory due to the prospect of new high precision data and following the papers by Acquaviva et al. [6] and Maldacena [7] focusing on the study of non-gaussianity from inflation.

In this article we concentrate on the scalar field dynamics at second order on large scales in a universe dominated by multiple scalar fields, including metric perturbations. In linear theory the Klein-Gordon equation, including metric perturbations, can be written as a system of coupled evolution equations in terms of the linear field fluctuations in the flat gauge, the Sasaki-Mukhanov variables [34, 35]. We show here that the Klein-Gordon equation at second order on large scales in the multiple field case can also be written solely in terms of the Sasaki-Mukhanov variables, albeit at second and first order. The Klein-Gordon equation is linear in the second order perturbations, with source terms quadratic in the first order perturbations (the same holds for the field equations). We also give an expression for the curvature perturbation on uniform density slices at second order,  $\zeta_2$ , in terms of the field fluctuations on flat slices at first and second order. After calculating the evolution of the field fluctuations at first and second order we therefore immediately get the evolution of the curvature perturbation  $\zeta_2$ . This is similar to the  $\Delta N$  formalism, where the evolution of the comoving curvature perturbation is given by the scalar field dynamics in the background, but which necessitates the slow roll approximation at higher order.

We consider scalar perturbations including and up to second order in the metric and in the scalar fields using the Bardeen approach. We focus on scales larger than the horizon, which allows us to neglect gradient terms. We do not include first order vector and tensor perturbations since they do not couple to the field fluctuations on large scales; also scalar fields do not support vector modes and the tensor contribution from inflation is small and constant or decaying. The large scale focus also makes the equations more transparent and displays the relevant physics more

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<sup>1</sup> Recently there has also been a covariant study [30].

succinctly, a big bonus at second order. We leave the inclusion of small scales, and vector and tensor perturbations to a future publication [36].

The paper is organised as follows: in the next section we give the field equations and the Klein-Gordon equation up to second order in gauge dependent form. In Section III, after reviewing the behaviour of perturbations at first and second order under gauge transformations, we construct physically transparent gauge-invariant combinations. In Section IV we show how the gauge-invariant variables defined in different gauges are related to each other. We also discuss the construction of total variables in the presence of several fields or fluids. We review the derivation of the Klein-Gordon equation at first order in Section V. In Section VIA we give the field equations at second order in the flat gauge and in Section VIB we finally derive the Klein-Gordon equation at second order. We give the second order Klein-Gordon equation in the single field case in Section VII. In Section VIII we apply the formalism to a simple two field inflation model. We conclude in Section IX.

Throughout this paper we assume a flat Friedmann-Robertson-Walker (FRW) background spacetime and work in conformal time,  $\eta$ . Derivatives with respect to conformal time are denoted by a dash. Greek indices,  $\mu, \nu, \lambda$ , run from 0,  $\dots$  3, while lower case Latin indices,  $i, j, k$ , run from 1,  $\dots$  3. Upper case Latin indices,  $I, J, K$ , denote different scalar fields.

## II. GOVERNING EQUATIONS

The covariant Einstein equations are given by

$$G_{\mu\nu} = 8\pi G T_{\mu\nu}, \quad (2.1)$$

where  $G_{\mu\nu}$  is the Einstein tensor,  $T_{\mu\nu}$  the total energy-momentum tensor, and  $G$  Newton's constant. Through the Bianchi identities, the field equations (2.1) give the local conservation of the total energy and momentum,

$$\nabla_\mu T^{\mu\nu} = 0, \quad (2.2)$$

where  $\nabla_\mu$  is the covariant derivative. The energy momentum tensor for  $N$  scalar fields minimally coupled to gravity is

$$T_{\mu\nu} = \sum_{K=1}^N \left[ \varphi_{K,\mu} \varphi_{K,\nu} - \frac{1}{2} g_{\mu\nu} g^{\alpha\beta} \varphi_{K,\alpha} \varphi_{K,\beta} \right] - g_{\mu\nu} U(\varphi_1, \dots, \varphi_N), \quad (2.3)$$

where  $\varphi_K$  is the  $K$ th scalar field and  $U$  the scalar field potential and  $\varphi_{K,\mu} \equiv \frac{\partial \varphi_K}{\partial x^\mu}$ .

We split tensorial quantities into a background value and perturbations according to

$$\mathbf{T} = \mathbf{T}_0 + \delta\mathbf{T}_1 + \frac{1}{2}\delta\mathbf{T}_2 + \dots, \quad (2.4)$$

where the background part is a time dependent quantity only  $\mathbf{T}_0 \equiv \mathbf{T}_0(\eta)$ , whereas the perturbations depend on time and space coordinates  $x^\mu = [\eta, x^i]$ , that is  $\delta\mathbf{T}_n \equiv \delta\mathbf{T}_n(x^\mu)$ . The order of the perturbation is indicated by a subscript, e.g.  $\delta\mathbf{T}_1 = O(\epsilon)$ .

The metric tensor up to second order, including only scalar perturbations, is

$$g_{00} = -a^2 (1 + 2\phi_1 + \phi_2), \quad (2.5)$$

$$g_{0i} = a^2 \left( B_1 + \frac{1}{2} B_2 \right)_{,i}, \quad (2.6)$$

$$g_{ij} = a^2 [(1 - 2\psi_1 - \psi_2) \delta_{ij} + 2E_{1,ij} + E_{2,ij}], \quad (2.7)$$

where  $a = a(\eta)$  is the scale factor,  $\eta$  conformal time,  $\delta_{ij}$  is the flat background metric,  $\phi_1$  and  $\phi_2$  the lapse function, and  $\psi_1$  and  $\psi_2$  the curvature perturbations at first and second order;  $B_1$  and  $B_2$  and  $E_1$  and  $E_2$  are scalar perturbations describing the shear. The contravariant form of the metric tensor is given in Appendix B.

## A. Einstein tensor

We expand the Einstein tensor in a power series according to Eq. (2.4) up to second order

$$G^\mu{}_\nu \equiv G_{(0)\nu}^\mu + \delta G_{(1)\nu}^\mu + \frac{1}{2}\delta G_{(2)\nu}^\mu. \quad (2.8)$$

Then the components of the Einstein tensor at zeroth order are

$$G^0_0 = -\frac{3}{a^2} \frac{a'^2}{a^2}, \quad G^i_j = \frac{1}{a^2} \left[ \frac{a'^2}{a^2} - 2\frac{a''}{a} \right], \quad (2.9)$$

at first order

$$\delta G^0_{(1)0} = \frac{6}{a^2} \left[ \frac{a'^2}{a^2} \phi_1 + \frac{a'}{a} \psi'_1 \right] + O(k^2), \quad (2.10)$$

$$\delta G^0_{(1)i} = -\frac{1}{a^2} \left[ 2\psi'_1 + 2\frac{a'}{a} \phi_1 \right]_{,i} \quad (2.11)$$

$$\delta G^i_{(1)j} = \frac{1}{a^2} \left[ 4 \left( \frac{a''}{a} \phi_1 + \frac{a'}{a} \psi'_1 \right) + 2 \left( \psi''_1 + \frac{a'}{a} \phi'_1 - \frac{a'^2}{a^2} \phi_1 \right) \right] \delta^i_j + O(k^2), \quad (2.12)$$

and at second order

$$\delta G^0_{(2)0} = -\frac{6}{a^2} \left[ \psi_1'^2 - \frac{a'^2}{a^2} \phi_2 - \frac{a'}{a} \psi'_2 + 4 \left( \frac{a'}{a} \phi_1 \psi'_1 + \frac{a'^2}{a^2} \phi_1^2 - \frac{a'}{a} \psi_1 \psi'_1 \right) \right] + O(k^2), \quad (2.13)$$

$$\delta G^0_{(2)i} = -\frac{2}{a^2} \left[ \psi'_2 + \frac{a'}{a} \phi_2 + 4\psi_1 \psi'_1 - 4\frac{a'}{a} \phi_1^2 \right]_{,i} - \frac{4}{a^2} [2\phi_1 \psi'_{1,i} - \psi'_1 \phi_{1,i}] + O(k^3), \quad (2.14)$$

$$\begin{aligned} \delta G^i_{(2)j} &= \frac{2}{a^2} \left[ \psi_1'^2 - 2\phi'_1 \psi'_1 + 8 \left( \frac{a'}{a} \psi_1 \psi'_1 - \frac{a'}{a} \phi_1 \phi'_1 - \frac{a'}{a} \phi_1 \psi'_1 - \frac{a''}{a} \phi_1^2 \right) + 4 \left( \psi_1 \psi_1'' - \phi_1 \psi_1'' + \frac{a'^2}{a^2} \phi_1^2 \right) \right. \\ &\quad \left. + 2 \left( \frac{a''}{a} \phi_2 + \frac{a'}{a} \psi'_2 \right) + \psi_2'' + \frac{a'}{a} \phi_2' - \frac{a'^2}{a^2} \phi_2 \right] \delta^i_j + O(k^2), \end{aligned} \quad (2.15)$$

where  $O(k^n)$  denotes terms of order  $n$  or higher in gradients, since we are mainly interested in the large results, i.e. the case  $k \rightarrow 0$ .

## B. Energy-momentum tensor

We split the scalar fields  $\varphi_I$  into a background and perturbations up to and including second order according to Eq. (2.4),

$$\varphi_I(x^\mu) = \varphi_{0I}(\eta) + \delta\varphi_{1I}(x^\mu) + \frac{1}{2}\delta\varphi_{2I}(x^\mu). \quad (2.16)$$

The potential  $U \equiv U(\varphi_I)$  can be split similarly according to

$$U(\varphi_I) = U_0 + \delta U_1 + \frac{1}{2}\delta U_2, \quad (2.17)$$

where

$$\delta U_1 = \sum_K U_{,\varphi_K} \delta\varphi_{K1}, \quad (2.18)$$

$$\delta U_2 = \sum_{K,L} U_{,\varphi_K \varphi_L} \delta\varphi_{1K} \delta\varphi_{1L} + \sum_K U_{,\varphi_K} \delta\varphi_{2K}. \quad (2.19)$$

and we use the shorthand  $U_{,\varphi_K} \equiv \frac{\partial U}{\partial \varphi_K}$ .

The energy-momentum tensor for  $N$  scalar fields with potential  $U(\varphi_I)$  is then split into background, first, and second order perturbations, using Eq. (2.4), as

$$T^\mu_\nu \equiv T^\mu_{(0)\nu} + \delta T^\mu_{(1)\nu} + \frac{1}{2}\delta T^\mu_{(2)\nu}, \quad (2.20)$$

and we get for the components, from Eq. (2.3), at zeroth order

$$T^0_{(0)0} = -\left(\sum_K \frac{1}{2a^2} \varphi'_{0K}{}^2 + U_0\right), \quad T^i_{(0)j} = \left(\frac{1}{2a^2} \sum_K \varphi'_{0K}{}^2 - U_0\right) \delta^i_j, \quad (2.21)$$

at first order

$$\delta T^0_{(1)0} = -\frac{1}{a^2} \sum_K \left(\varphi'_{0K} \delta \varphi_{1K'} - \varphi'_{0K}{}^2 \phi_1\right) - \delta U_1, \quad (2.22)$$

$$\delta T^0_{(1)i} = -\frac{1}{a^2} \sum_K \left(\varphi'_{0K} \delta \varphi_{1K,i}\right), \quad (2.23)$$

$$\delta T^i_{(1)j} = \frac{1}{a^2} \left[ \sum_K \left(\varphi'_{0K} \delta \varphi_{1K'} - \varphi'_{0K}{}^2 \phi_1\right) - a^2 \delta U_1 \right] \delta^i_j, \quad (2.24)$$

and at second order in the perturbations

$$\delta T^0_{(2)0} = -\frac{1}{a^2} \sum_K \left(\varphi'_{0K} \delta \varphi_{2K'} - 4\varphi'_{0K} \phi_1 \delta \varphi_{1K'} - \varphi'_{0K}{}^2 \phi_2 + 4\varphi'_{0K}{}^2 \phi_1^2 + \delta \varphi_{1K}{}'^2 + a^2 \delta U_2\right) + O(k^2), \quad (2.25)$$

$$\delta T^0_{(2)i} = -\frac{1}{a^2} \sum_K \left(\varphi'_{0K} \delta \varphi_{2K,i} - 4\phi_1 \varphi'_{0K} \delta \varphi_{1K,i} + 2\delta \varphi_{1K'} \delta \varphi_{1K,i}\right), \quad (2.26)$$

$$\delta T^i_{(2)j} = \frac{1}{a^2} \left[ \sum_K \left(\varphi'_{0K} \delta \varphi_{2K'} - 4\varphi'_{0K} \phi_1 \delta \varphi_{1K'} - \varphi'_{0K}{}^2 \phi_2 + 4\varphi'_{0K}{}^2 \phi_1^2 + \delta \varphi_{1K}{}'^2\right) - a^2 \delta U_2 \right] \delta^i_j + O(k^2). \quad (2.27)$$

The 0 – 0 component of the energy momentum tensor gives the corresponding energy density at zeroth, first and second order for a universe filled by  $N$  scalar fields [9],

$$T^0_{(0)0} = -\rho_0, \quad \delta T^0_{(1)0} = -\delta \rho_1, \quad \delta T^0_{(2)0} = -\delta \rho_2. \quad (2.28)$$

### C. Evolution of the background

The evolution of the background is governed by the Friedmann equation given from the 0 – 0 component of the Einstein equations

$$\mathcal{H}^2 = \frac{8\pi G}{3} \left(\frac{1}{2} \sum_K \varphi'_{0K}{}^2 + a^2 U(\varphi_{0I})\right), \quad (2.29)$$

where  $\mathcal{H} \equiv \frac{a'}{a}$ . The scalar fields are governed by the Klein-Gordon equation, which is from the energy conservation equation, (2.2), at zeroth order for the  $I$ th field given by

$$\varphi''_{0I} + 2\mathcal{H}\varphi'_{0I} + a^2 U_{,\varphi_I} = 0. \quad (2.30)$$

### D. Perturbed Klein-Gordon equation

Using the energy momentum tensor given above in Section IIB and the energy conservation equation (2.2) we get the Klein-Gordon equation in the multiple filed case for the field  $I$  at first order

$$\delta \varphi_{1I}'' + 2\mathcal{H}\delta \varphi_{1I}' + 2a^2 U_{,\varphi_I} \phi_1 - 3\varphi'_{0I} \psi_1' - \varphi'_{0I} \phi_1' + a^2 \sum_K U_{,\varphi_I \varphi_K} \delta \varphi_{1K} + O(k^2) = 0. \quad (2.31)$$

We get the Klein-Gordon equation at second order from Eq. (2.2) and using Eq. (2.31)

$$\begin{aligned} \delta\varphi_{2I}'' + 2\mathcal{H}\delta\varphi_{2I}' + 2a^2 U_{,\varphi_I}\phi_2 - 6\psi_1'\delta\varphi_{1I}' - 2\phi_1'\delta\varphi_{1I}' + 4\varphi_{0I}'\phi_1\phi_1' + 4\phi_1 a^2 \sum_K U_{,\varphi_I\varphi_K}\delta\varphi_{1K} \\ - 12\varphi_{0I}'\psi_1\psi_1' - 3\varphi_{0I}'\psi_2' - \varphi_{0I}'\phi_2' + a^2 \sum_K U_{,\varphi_I\varphi_K}\delta\varphi_{2K} + a^2 \sum_{K,L} U_{,\varphi_I\varphi_K\varphi_L}\delta\varphi_{1K}\delta\varphi_{1L} + O(k^2) = 0. \end{aligned} \quad (2.32)$$

Note, that Eqs. (2.31) and (2.32) are in an arbitrary gauge.

### III. VARIABLES

In this section we first calculate the changes coordinate transformations induce in the metric and matter perturbations at first and second order. We then construct physically meaningful gauge-invariant combinations from these variables.

#### A. Gauge transformations

We now briefly review how tensorial quantities change under coordinate transformations [4, 5]. We consider two coordinate systems,  $\widetilde{x}^\mu$  and  $x^\mu$ , which are related by the coordinate transformation

$$\widetilde{x}^\mu = e^{\xi^\lambda \frac{\partial}{\partial x^\lambda}} x^\mu, \quad (3.1)$$

where  $\xi^\lambda$  is the vector field generating the transformation and  $\xi^\mu \equiv \xi_1^\mu + \frac{1}{2}\xi_2^\mu + O(\epsilon^3)$ . Equation (3.1) can then be expanded up to second-order as

$$\widetilde{x}^\mu = x^\mu + \xi_1^\mu + \frac{1}{2}(\xi_{1,\nu}^\mu \xi_1^\nu + \xi_2^\mu). \quad (3.2)$$

A tensor  $\mathbf{T}$  transforms under the change of coordinate system defined above as

$$\widetilde{\mathbf{T}} = e^{\mathcal{L}_{\xi^\lambda}} \mathbf{T}, \quad (3.3)$$

where  $\mathcal{L}_{\xi^\lambda}$  denotes the Lie derivative with respect to  $\xi^\lambda$ . Splitting the tensor  $\mathbf{T}$  according to Eq. (2.4) we get [4, 5]

$$\begin{aligned} \widetilde{\delta\mathbf{T}}_1 &= \delta\mathbf{T}_1 + \mathbf{L}_{\xi_1} \mathbf{T}_0 \\ \widetilde{\delta\mathbf{T}}_2 &= \delta\mathbf{T}_2 + \mathbf{L}_{\xi_2} \mathbf{T}_0 + \mathbf{L}_{\xi_1}^2 \mathbf{T}_0 + 2\mathbf{L}_{\xi_1} \delta\mathbf{T}_1. \end{aligned} \quad (3.4)$$

Under a first-order transformation  $\xi_1^\mu = (\alpha_1, \beta_1, {}^i)$ , a four scalar such as the energy density,  $\rho$ , or the scalar field  $\varphi$ , transforms therefore as

$$\widetilde{\delta\rho}_1 = \delta\rho_1 + \rho_0' \alpha_1, \quad (3.5)$$

and or the first order metric perturbations we have

$$\widetilde{\psi}_1 = \psi_1 - \mathcal{H}\alpha_1, \quad (3.6)$$

$$\widetilde{\phi}_1 = \phi_1 + \mathcal{H}\alpha_1 + \alpha_1'. \quad (3.7)$$

At second order, writing  $\xi_2^\mu = (\alpha_2, \beta_2, {}^i)$ , we find from Eq. (3.4) that a four scalar transforms as

$$\begin{aligned} \widetilde{\delta\rho}_2 &= \delta\rho_2 + \rho_0' \alpha_2 + \alpha_1 [\rho_0'' \alpha_1 + \rho_0' \alpha_1' + 2\delta\rho_1'] \\ &\quad + (2\delta\rho_1 + \rho_0' \alpha_1)_{,i} \beta_1, {}^i, \end{aligned} \quad (3.8)$$

and the second order metric perturbations transform as

$$\begin{aligned} \widetilde{\psi}_2 &= \psi_2 - \mathcal{H}\alpha_2 - \alpha_1 [\mathcal{H}\alpha_1' + (\mathcal{H}' + 2\mathcal{H}^2)\alpha_1 - 2\psi_1' - 4\mathcal{H}\psi_1] \\ &\quad - (\mathcal{H}\alpha_1 - 2\psi_1)_{,k} \beta_1, {}^k, \end{aligned} \quad (3.9)$$

$$\begin{aligned} \widetilde{\phi}_2 &= \phi_2 + \mathcal{H}\alpha_2 + \alpha_2' + \alpha_1 [\alpha_1'' + 5\mathcal{H}\alpha_1' + (\mathcal{H}' + 2\mathcal{H}^2)\alpha_1 + 4\mathcal{H}\phi_1 + 2\phi_1'] \\ &\quad + \alpha_1' (2\alpha_1' + 4\phi_1) + \beta_1, {}^k (\alpha_1' + \mathcal{H}\alpha_1 + 2\phi_1), {}^k + \beta_1', {}^k (\alpha_1 - 2B_1 - \beta_1'), {}^k. \end{aligned} \quad (3.10)$$

From Eqs. (3.8), (3.9), and (3.10) we see that on super horizon scales, where gradient terms can be neglected, the definition of the second order perturbations in the “new” coordinate is independent of the spatial coordinate choice (the “threading”) at second order in the gradients. It is therefore sufficient on large scales (at  $O(k^2)$ ) to specify the time slicing by prescribing  $\alpha_1$  and  $\alpha_2$ , in order to define gauge-invariant variables [14, 28]. The procedure to neglect the gradient terms, is explained in detail in Ref. [28]. For the approximation to hold one assumes that each quantity can be treated as smooth on some sufficiently large scale. Formally one multiplies each spatial gradient  $\partial_i$  by a fictitious parameter  $k$ , and expands the exact equations as a power series in  $k$ , keeping only the zero- and first-order terms, finally setting  $k = 1$ .

*Note*, in the following sections we shall omit the symbol  $O(k^n)$  denoting the order of the gradient terms neglected, assuming that if not stated otherwise the equations are valid to  $O(k^2)$ .

## B. Gauge-invariant combinations

Using the transformation behaviour of the perturbations derived in the last section we can now construct combinations of these variables that do not change under gauge transformations, i.e. gauge-invariant variables. The combinations given below have definite physical meaning, such as the curvature perturbation on a hypersurface of uniform density.

We define the various time slicings and then substitute the results into the transformation equations to arrive at the gauge-invariant variables. Whereas the first order results are valid on all scales, we only consider the large scale case at second order.

### 1. First order

Hypersurfaces of uniform  $I$ -field, i.e.  $\widetilde{\delta\varphi_{1I}} = 0$ , are given from Eq. (3.5) by the temporal slicing

$$\alpha_1 = -\frac{\delta\varphi_{1I}}{\varphi'_{0I}}. \quad (3.11)$$

The curvature perturbation on uniform field hypersurfaces [37, 38], or comoving curvature perturbation, can then be defined for each field using Eq. (3.6) as

$$\mathcal{R}_{1I} = \psi_1 + \mathcal{H}\frac{\delta\varphi_{1I}}{\varphi'_{0I}}. \quad (3.12)$$

Flat slices are defined as  $\widetilde{\psi}_1 = 0$  and we therefore get from Eq. (3.6) the first order time shift

$$\alpha_1 = \frac{\psi_1}{\mathcal{H}}. \quad (3.13)$$

The Sasaki-Mukhanov variable [34, 35], or the field fluctuation on uniform curvature hypersurfaces, is then given by

$$\mathcal{Q}_{1I} \equiv \widetilde{\delta\varphi_{1I}} = \delta\varphi_{1I} + \frac{\varphi'_{0I}}{\mathcal{H}}\psi_1. \quad (3.14)$$

The density perturbation on uniform curvature hypersurfaces is defined as

$$\widetilde{\delta\rho_{1\alpha}} = \delta\rho_{1\alpha} + \frac{\rho'_{0\alpha}}{\mathcal{H}}\psi_1, \quad (3.15)$$

where  $\rho_{0\alpha}$  and  $\delta\rho_{1\alpha}$  are the energy density of the  $\alpha$ -fluid in the background and at first order <sup>2</sup>. The curvature perturbation on uniform  $\alpha$ -fluid density hypersurfaces is at first order defined as

$$\zeta_{1\alpha} = -\psi_1 - \mathcal{H}\frac{\delta\rho_{1\alpha}}{\rho'_{0\alpha}}. \quad (3.16)$$

The lapse function on flat slices is from the definition (3.7) and Eq. (3.13) given as

$$\widetilde{\phi}_1 = \phi_1 + \frac{1}{\mathcal{H}}\psi'_1 + \left(1 - \frac{\mathcal{H}'}{\mathcal{H}^2}\right)\psi_1. \quad (3.17)$$

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<sup>2</sup> Greek indices from the beginning of the alphabet,  $\alpha, \beta, \gamma$  will be used to denote different fluids.

At second order uniform field slices are, from Eq. (3.8), defined by the temporal shift

$$\alpha_2 = -\frac{1}{\varphi'_{0I}} \left( \delta\varphi_{2I} - \frac{1}{\varphi'_{0I}} \delta\varphi_{1I}' \delta\varphi_{1I} \right), \quad (3.18)$$

on large scales. The curvature perturbation on uniform  $I$ -field slices is therefore on large scales at second order, from Eq. (3.9) and using (3.11) and (3.18) [14]

$$\mathcal{R}_{2I} = \psi_2 + \frac{\mathcal{H}}{\varphi'_{0I}} \delta\varphi_{2I} - 2\frac{\mathcal{H}}{\varphi'_{0I}{}^2} \delta\varphi_{1I}' \delta\varphi_{1I} - 2\frac{\delta\varphi_{1I}}{\varphi'_{0I}} (\psi_1' + 2\mathcal{H}\psi_1) + \frac{\delta\varphi_{1I}{}^2}{\varphi'_{0I}{}^2} \left( \mathcal{H} \frac{\varphi''_{0I}}{\varphi_{0I}} - \mathcal{H}' - 2\mathcal{H}^2 \right). \quad (3.19)$$

The time shift that defines the flat slicing is at second order, from Eq. (3.9), on large scales given by

$$\alpha_2 = \frac{1}{\mathcal{H}} \left( \psi_2 + 2\psi_1^2 + \frac{1}{\mathcal{H}} \psi_1' \psi_1 \right). \quad (3.20)$$

Then the field fluctuation on uniform curvature hypersurfaces, or Sasaki-Mukhanov variable, at second order for the  $I$ th field, from Eq. (3.8) and definitions of the time shifts (3.13) and (3.20) is [14]

$$\mathcal{Q}_{2I} \equiv \widetilde{\delta\varphi_{2I}} = \delta\varphi_{2I} + \frac{\varphi'_{0I}}{\mathcal{H}} \psi_2 + \left( \frac{\psi_1}{\mathcal{H}} \right)^2 \left[ 2\mathcal{H}\varphi'_{0I} + \varphi''_{0I} - \frac{\mathcal{H}'}{\mathcal{H}} \varphi'_{0I} \right] + 2\frac{\varphi'_{0I}}{\mathcal{H}^2} \psi_1' \psi_1 + \frac{2}{\mathcal{H}} \psi_1 \delta\varphi_{1I}'. \quad (3.21)$$

The second order lapse function in the flat gauge is given from Eqs. (3.10), (3.13), and (3.20) as

$$\begin{aligned} \widetilde{\phi}_2 &= \phi_2 + \left( 1 - \frac{\mathcal{H}'}{\mathcal{H}^2} \right) \psi_2 + \frac{1}{\mathcal{H}} \psi_2' + \frac{2}{\mathcal{H}} \left( 5 - 4\frac{\mathcal{H}'}{\mathcal{H}^2} \right) \psi_1' \psi_1 + \left( 4 - 6\frac{\mathcal{H}'}{\mathcal{H}^2} - \frac{\mathcal{H}''}{\mathcal{H}^3} + 4\frac{\mathcal{H}'^2}{\mathcal{H}^4} \right) \psi_1^2 \\ &+ \frac{3}{\mathcal{H}^2} \psi_1'^2 + \frac{2}{\mathcal{H}} \psi_1'' \psi_1 + 4\phi_1 \left[ \frac{1}{\mathcal{H}} \psi_1' + \left( 1 - \frac{\mathcal{H}'}{\mathcal{H}^2} \right) \psi_1 \right] + \frac{2}{\mathcal{H}} \phi_1' \psi_1. \end{aligned} \quad (3.22)$$

The curvature perturbation on uniform  $\alpha$ -density hypersurfaces is at second order on large scales from Eq. (3.9) and using (3.11) and (3.18) given by [14]

$$-\zeta_{2\alpha} = \psi_2 + \frac{\mathcal{H}}{\rho'_{0\alpha}} \delta\rho_{2\alpha} - 2\frac{\mathcal{H}}{\rho'_{0\alpha}{}^2} \delta\rho'_{1\alpha} \delta\rho_{1\alpha} - 2\frac{\delta\rho_{1\alpha}}{\rho'_{0\alpha}} (\psi_1' + 2\mathcal{H}\psi_1) + \frac{\delta\rho_{1\alpha}{}^2}{\rho'_{0\alpha}{}^2} \left( \mathcal{H} \frac{\rho''_{0\alpha}}{\rho'_{0\alpha}} - \mathcal{H}' - 2\mathcal{H}^2 \right), \quad (3.23)$$

and from Eq. (3.8) and the definitions of the time shifts (3.13) and (3.20) we get the second order density perturbation on uniform curvature hypersurfaces [14]

$$\widetilde{\delta\rho_{2\alpha}} \equiv \delta\rho_{2\alpha} + \frac{\rho'_{0\alpha}}{\mathcal{H}} \psi_2 + \frac{1}{\mathcal{H}} \left( 2\rho'_{0\alpha} + \frac{\rho''_{0\alpha}}{\mathcal{H}} - \frac{\rho'_{0\alpha}\mathcal{H}'}{\mathcal{H}^2} \right) \psi_1^2 + 2\frac{\rho'_{0\alpha}}{\mathcal{H}^2} \psi_1' \psi_1 + \frac{2}{\mathcal{H}} \psi_1 \delta\rho'_{1\alpha}. \quad (3.24)$$

#### IV. RELATING VARIABLES

In this section we relate the gauge-invariant variables defined above on different hypersurfaces to each other. Using the field equations we then define total perturbations from the individual field and fluid ones, where possible.

##### A. First order

From Eqs. (4.5) and (3.14) the Sasaki-Mukhanov variable of the field  $I$  is related to the curvature perturbation on uniform field hypersurfaces at linear order simply by

$$\mathcal{Q}_{1I} = \frac{\varphi'_{0I}}{\mathcal{H}} \mathcal{R}_{1I}. \quad (4.1)$$

From Eq. (3.15) and (3.16) we find that the curvature perturbation on uniform density hypersurfaces is related to the density perturbation on uniform curvature hypersurfaces simply as

$$\zeta_{1\alpha} = -\mathcal{H} \frac{\widetilde{\delta\rho_{1\alpha}}}{\rho'_{0\alpha}}. \quad (4.2)$$

The total density perturbation at first order in the flat gauge is given in terms of the density perturbations of individual fluids simply by

$$\widetilde{\delta\rho_1} = \sum_{\alpha} \widetilde{\delta\rho_{1\alpha}}, \quad (4.3)$$

which allows us to relate the total curvature perturbation to the individual fluid curvature perturbations by

$$\zeta_1 = \sum_{\alpha} \frac{\rho'_{0\alpha}}{\rho'_0} \zeta_{1\alpha}. \quad (4.4)$$

We can define the total comoving curvature perturbation (i.e. relative to the average fluid velocity or an “average field”) using the  $0-i$  component of the field equations as

$$\mathcal{R}_{1\varphi} \equiv \frac{1}{\sum_K \varphi'_{0K}{}^2} \sum_I \varphi'_{0I}{}^2 \mathcal{R}_{1I}. \quad (4.5)$$

The total curvature perturbation on uniform density hypersurfaces in terms of the field fluctuations on flat slices is given by

$$\zeta_1 = -\frac{\mathcal{H}}{\sum_L \varphi'_{0L}{}^2} \sum_K \varphi'_{0K} \widetilde{\mathcal{Q}_{K1}}. \quad (4.6)$$

## B. Second order

The Sasaki-Mukhanov variable at second order defined above in Eq. (3.21) can be expressed in terms of the curvature perturbations on uniform field hypersurfaces,  $\mathcal{R}_{1I}$  and  $\mathcal{R}_{2I}$ ,

$$\mathcal{Q}_{2I} = \frac{\varphi'_{0I}}{\mathcal{H}} \mathcal{R}_{2I} + \left( \frac{\mathcal{R}_{1I}}{\mathcal{H}} \right)^2 \left[ 2\mathcal{H}\varphi'_{0I} + \varphi''_{0I} - \frac{\mathcal{H}'}{\mathcal{H}} \varphi'_{0I} \right] + 2 \frac{\varphi'_{0I}}{\mathcal{H}^2} \mathcal{R}'_{1I} \mathcal{R}_{1I}. \quad (4.7)$$

Similarly we can express the curvature perturbations on uniform field hypersurfaces in terms of the Sasaki-Mukhanov variables at first and second order and get,

$$\mathcal{R}_{2I} = \frac{\mathcal{H}}{\varphi'_{0I}} \mathcal{Q}_{2I} - 2 \frac{\mathcal{H}}{\varphi'_{0I}{}^2} \mathcal{Q}'_{1I} \mathcal{Q}_{1I} + \frac{\mathcal{Q}_{1I}^2}{\varphi'_{0I}{}^2} \left( \mathcal{H} \frac{\varphi''_{0I}}{\varphi'_{0I}} - \mathcal{H}' - 2\mathcal{H}^2 \right). \quad (4.8)$$

To define the total comoving curvature perturbation at second order  $\mathcal{R}_{2\varphi}$  in terms of the  $\mathcal{R}_{2I}$  we would need the  $0-i$  Einstein equation at this order in an appropriate form, that is without gradients. Since it is not clear how to arrive at this form of the  $0-i$  Einstein equation (without imposing slow roll, see Section VIA below) we shall leave the definition of  $\mathcal{R}_{2I}$  open for the moment and shall return to this issue in a future publication [36]. We note however, that the definition of the total comoving curvature perturbation at second order  $\mathcal{R}_{2\varphi}$  is not a problem in itself, since it was already shown in Ref. [28] that on large scales  $\mathcal{R}_{2\varphi}$  and  $\zeta_2$  coincide. The definition of the total curvature perturbation  $\zeta_2$  in terms of the field fluctuations is given below in Eq. (4.16), and we can therefore get  $\mathcal{R}_{2\varphi}$  from  $\zeta_2$  if we should need it.

The definition of “total” quantities from quantities defined for a specific field or fluid is not more problematic at second order than at first order, it is a mere question of having the “right” equations. As an example we shall now digress slightly from the main theme of this paper, multiple scalar fields, and analyse the definition of the total curvature perturbation at second order in the case of multiple fluids, which is unlike the definition of the total comoving curvature perturbation, straight forward<sup>3</sup>.

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<sup>3</sup> The relation between scalar fields and fluids at first order, in particular how fields can be treated as fluids, has been studied in detail in Ref. [39].



We can relate the curvature perturbation on uniform  $\alpha$ -fluid hypersurfaces, Eq. (3.23), to the density perturbation on flat slices, Eq. (3.24),

$$-\zeta_{2\alpha} = \frac{\mathcal{H}}{\rho'_{0\alpha}} \widetilde{\delta\rho_{2\alpha}} - 2 \frac{\mathcal{H}}{\rho'_{0\alpha}} \widetilde{\delta\rho_{1\alpha}}' \widetilde{\delta\rho_{1\alpha}} + \frac{\widetilde{\delta\rho_{1\alpha}}^2}{\rho'_{0\alpha}} \left( \mathcal{H} \frac{\rho''_{0\alpha}}{\rho'_{0\alpha}} - \mathcal{H}' - 2\mathcal{H}^2 \right), \quad (4.9)$$

and similarly the density perturbation of the  $\alpha$ -fluid at second order on flat slices in terms of  $\zeta_{1\alpha}$  and  $\zeta_{2\alpha}$ ,

$$\widetilde{\delta\rho_{2\alpha}} = -\frac{\rho'_{0\alpha}}{\mathcal{H}} \zeta_{2\alpha} + 2 \frac{\rho'_{0\alpha}}{\mathcal{H}^2} \zeta'_{1\alpha} \zeta_{1\alpha} + \zeta_{1\alpha}^2 \left( 2 \frac{\rho'_{0\alpha}}{\mathcal{H}} + \frac{\rho''_{0\alpha}}{\mathcal{H}^2} - \frac{\rho'_{0\alpha} \mathcal{H}'}{\mathcal{H}^3} \right). \quad (4.10)$$

The total density perturbation at second order on flat slices is given in terms of the density perturbations of individual fluids on large scales simply by

$$\widetilde{\delta\rho_2} = \sum_{\alpha} \widetilde{\delta\rho_{2\alpha}}, \quad (4.11)$$

which allows us to write the total curvature perturbation at second order to the individual fluid curvature perturbations, using Eq. (4.10), as

$$\zeta_2 = \sum_{\alpha} \frac{\rho'_{0\alpha}}{\rho'_0} \zeta_{2\alpha} - (1 + 3c_s^2) \zeta_1^2 + \sum_{\alpha} \left[ (1 + 3c_s^2) \frac{\rho'_{0\alpha}}{\rho'_0} + \frac{1}{\rho'_0 \mathcal{H}} \left( Q_{\alpha} \frac{\mathcal{H}'}{\mathcal{H}} - Q'_{\alpha} \right) \right] \zeta_{1\alpha}^2 - \frac{2}{\mathcal{H}} \sum_{\alpha} \zeta_{1\alpha} (\zeta'_{1\alpha} - \zeta'_1), \quad (4.12)$$

where we used the background energy conservation equation for the  $\alpha$ -fluid, Eq. (A7), given in Appendix A,  $c_s^2$  is the adiabatic sound speed of the  $\alpha$ -fluid, and the total adiabatic sound speed is denoted  $c_s^2$ .<sup>4</sup>

The relative entropy (or isocurvature) perturbation at first order is defined as [41, 42]

$$\mathcal{S}_{1\alpha\beta} \equiv 3(\zeta_{1\alpha} - \zeta_{1\beta}), \quad (4.13)$$

which can be used to rewrite Eq. (4.12) in terms of adiabatic and non-adiabatic quadratic first order terms as

$$\begin{aligned} \zeta_2 &= \sum_{\alpha} \frac{\rho'_{0\alpha}}{\rho'_0} \zeta_{2\alpha} - \frac{2}{3\mathcal{H}} \sum_{\alpha} \frac{\rho'_{0\alpha}}{\rho'_0} \left( \zeta_1 + \frac{1}{3} \sum_{\gamma} \frac{\rho'_{0\gamma}}{\rho'_0} \mathcal{S}_{1\alpha\gamma} \right) \sum_{\gamma} \left( \frac{\rho'_{0\gamma}}{\rho'_0} \mathcal{S}_{1\alpha\gamma} \right)' \\ &\quad + \frac{1}{3} \sum_{\alpha} \left[ (1 + 3c_s^2) \frac{\rho'_{0\alpha}}{\rho'_0} + \frac{1}{\rho'_0 \mathcal{H}} \left( Q_{\alpha} \frac{\mathcal{H}'}{\mathcal{H}} - Q'_{\alpha} \right) \right] \sum_{\gamma} \frac{\rho'_{0\gamma}}{\rho'_0} \mathcal{S}_{1\alpha\gamma} \left( 2\zeta_1 + \frac{1}{3} \sum_{\gamma} \frac{\rho'_{0\gamma}}{\rho'_0} \mathcal{S}_{1\alpha\gamma} \right). \end{aligned} \quad (4.14)$$

The evolution equation for the relative entropy perturbation at first order,  $\mathcal{S}_{1\alpha\gamma}$ , was given in [39]. We see that there is a purely non-adiabatic contribution to  $\zeta_2$ , quadratic in  $\mathcal{S}_{1\alpha\gamma}$ . Note that for purely adiabatic first order perturbations Eq. (4.14) simplifies to

$$\zeta_2 = \sum_{\alpha} \frac{\rho'_{0\alpha}}{\rho'_0} \zeta_{2\alpha}. \quad (4.15)$$

Turning back to scalar fields, the curvature perturbation  $\zeta_2$  in terms of field fluctuations on flat slices at first and second order is, using Eq. (3.23) evaluated for a single fluid, the energy densities in terms of scalar fields Eq. (2.28), and the definitions for the Sasaki-Mukhanov variables Eqs. (3.14) and (3.21), given by

$$\begin{aligned} \zeta_2 &= \frac{\rho_0}{3U_0 \sum_L \varphi'_{0L}{}^2} \sum_K \left( \varphi'_{0K} \mathcal{Q}'_{2K} + \mathcal{Q}'_{1K}{}^2 + a^2 \widetilde{\delta U_2} \right) - \frac{2\mathcal{H}}{\sum_L \varphi'_{0L}{}^2} \left( \frac{2a^2 U_0 - \sum_L \varphi'_{0L}{}^2}{U_0 \sum_K \varphi'_{0K}{}^2} \right) \sum_{K,L} U_{,\varphi_K} \varphi'_{0L} \mathcal{Q}_{1K} \mathcal{Q}_{1L} \\ &\quad - \mathcal{H}^2 \left( \frac{\sum_K \varphi'_{0K} \mathcal{Q}_{1K}}{\sum_L \varphi'_{0L}{}^2} \right)^2 \left[ 7 - 3c_s^2 - \frac{6 \sum_L \varphi'_{0L}{}^2}{a^2 \rho_0} \right], \end{aligned} \quad (4.16)$$

<sup>4</sup> The relation between the total  $\zeta_2$  and the curvature perturbations of the individual fluids,  $\zeta_{2\alpha}$ , has been given in the two field case in Ref. [40].

where  $\widetilde{\delta U}_2$  is given from Eq. (2.19) above evaluated on flat slices,

$$\widetilde{\delta U}_2 = \sum_{K,L} U_{,\varphi_K \varphi_L} \mathcal{Q}_{1K} \mathcal{Q}_{1L} + \sum_K U_{,\varphi_K} \mathcal{Q}_{2K}, \quad (4.17)$$

and the adiabatic sound speed for a universe filled by  $N$  scalar fields is given by

$$c_s^2 = 1 + \frac{2}{3\mathcal{H}} \frac{\sum_K U_{,\varphi_K} \varphi'_{0K}}{\frac{1}{a^2} \sum_K \varphi'_{0K}{}^2}, \quad (4.18)$$

and  $\rho_0$  is the background energy density defined in Eq. (2.28) above.

Equation (4.16) can be readily evaluated either analytically or numerically given the Sasaki-Mukhanov variables at first and second order,  $\mathcal{Q}_{1I}$  and  $\mathcal{Q}_{2I}$ . However, in Section VII below we use  $0-i$  Einstein equation at second order in the single field case and in Section VIII we use the slow roll approximation in a particular model to simplify Eq. (4.16) further, without the time derivatives of the Sasaki-Mukhanov variables.

## V. GOVERNING EQUATIONS IN THE UNIFORM CURVATURE GAUGE AT FIRST ORDER

We begin this section by giving the field equations at first order in the uniform curvature gauge and then review the derivation of the Klein-Gordon equation for multiple scalar fields at first order on large scales.

### A. Field equations

The components of the Einstein tensor and the energy-momentum tensor are given in Sections II A and II B. Substitution into Eq. (2.1) then gives for the  $0-0$  component of the Einstein equations gives at first order

$$2a^2 U_0 \widetilde{\phi}_1 + \sum_K \varphi'_{0K} \mathcal{Q}_{1K}' + a^2 \widetilde{\delta U}_1 = 0, \quad (5.1)$$

and from the  $i-j$  component of the Einstein equation we get

$$\frac{a'}{a} \widetilde{\phi}_1' - 8\pi G \sum_K \varphi'_{0K} \mathcal{Q}_{1K}' = 0. \quad (5.2)$$

At first order the  $0-i$  components of the Einstein tensor, Eq. (2.11), and energy momentum tensor, Eq. (2.23), are linear in the spatial gradients (by definition the background quantities are only time dependent), which allows us to write the  $0-i$  Einstein equation without gradients as

$$\frac{a'}{a} \widetilde{\phi}_1 - 4\pi G \sum_K \varphi'_{0K} \mathcal{Q}_{1K} = 0. \quad (5.3)$$

Combining Eqs. (5.1) and (5.3) we get

$$\sum_K \varphi'_{0K} \mathcal{Q}_{1K}' = -a^2 \sum_K \left( U_{,\varphi_K} + \frac{8\pi G}{\mathcal{H}} U_0 \varphi'_{0K} \right) \mathcal{Q}_{1K}, \quad (5.4)$$

relating the time derivative of the field fluctuations to the field fluctuations themselves.

### B. Klein Gordon equation

At first order the Klein-Gordon equation for the field  $I$ , on flat slices, is from Eq. (2.31) given by

$$\mathcal{Q}_{1I}'' + 2\mathcal{H} \mathcal{Q}_{1I}' + 2a^2 U_{,\varphi_I} \widetilde{\phi}_1 - \varphi'_{0I} \widetilde{\phi}_1' + a^2 \sum_K U_{,\varphi_I \varphi_K} \mathcal{Q}_{1K} = 0, \quad (5.5)$$

which can be simplified using Eqs. (5.1) and (5.2), to give

$$\mathcal{Q}_{1I}'' + 2\mathcal{H}\mathcal{Q}_{1I}' - \left( \frac{U_{,\varphi I}}{U_0} + \varphi'_{0I} \frac{8\pi G}{\mathcal{H}} \right) \sum_K \varphi'_{0K} \mathcal{Q}_{1K}' + a^2 \sum_K \left( U_{,\varphi I \varphi K} - \frac{1}{U_0} U_{,\varphi I} U_{,\varphi K} \right) \mathcal{Q}_{1K} = 0. \quad (5.6)$$

Equation (5.6) can be further rewritten using Eq. (5.4) above, to give [43, 44, 45]

$$\mathcal{Q}_{1I}'' + 2\mathcal{H}\mathcal{Q}_{1I}' + \sum_K \left[ a^2 U_{,\varphi I \varphi K} - \frac{8\pi G}{a^2} \left( a^2 \varphi'_{0I} \left( \frac{\varphi'_{0K}}{\mathcal{H}} \right) \right)' \right] \mathcal{Q}_{1K} = 0, \quad (5.7)$$

which now displays the ‘‘canonical’’ time derivatives (in conformal time)  $\partial^2/\partial\eta^2 + 2\mathcal{H}\partial/\partial\eta$ , but has a rather involved mass term.

## VI. GOVERNING EQUATIONS IN THE UNIFORM CURVATURE GAUGE AT SECOND ORDER

In this section we first give the field equation in the uniform curvature gauge at second order, highlighting problems arising from the  $0 - i$  equation at second order and possible ways to solve them. We then give the Klein-Gordon equation in the multiple field case on large scales in terms of the Sasaki-Mukhanov variables.

### A. Field equations

In this section we present the field equations in the uniform curvature gauge at second order on large scales. The components of the Einstein tensor and the energy-momentum tensor are given in Sections II A and II B. Substitution into Eq. (2.1) then gives for the  $0 - 0$  field equation in the flat gauge at second order is

$$2a^2 U_0 \left( 4\widetilde{\phi}_1'^2 - \widetilde{\phi}_2' \right) = \sum_K \left( \varphi'_{0K} \mathcal{Q}'_{2K} - 4\varphi'_{0K} \widetilde{\phi}_1 \mathcal{Q}'_{1K} + \mathcal{Q}'_{1K}{}^2 \right) + a^2 \delta \widetilde{U}_2. \quad (6.1)$$

and, using Eq. (5.3) and Eq. (6.1) above, the  $i - j$  Einstein equation can be rewritten as

$$\frac{a'}{a} \left( \widetilde{\phi}_2' - 4\widetilde{\phi}_1' \widetilde{\phi}_1 \right) = 8\pi G \left[ \sum_K \left( \varphi'_{0K} \mathcal{Q}'_{2K} + \mathcal{Q}'_{1K}{}^2 \right) \right]. \quad (6.2)$$

The  $0 - i$  Einstein equation at second order is given by

$$\mathcal{H} \left( \widetilde{\phi}_{2,i} - 4\widetilde{\phi}_1 \widetilde{\phi}_{1,i} \right) - 4\pi G \sum_K \left( \varphi'_{0K} \mathcal{Q}_{2K,i} + 2\mathcal{Q}_{1K}' \mathcal{Q}_{1K,i} \right) + O(k^3) = 0, \quad (6.3)$$

where we used Eq. (5.3). The left hand side of Eq. (6.3) can be rewritten as  $\mathcal{H} \left( \widetilde{\phi}_2 - 2\widetilde{\phi}_1^2 \right)_{,i}$ , with the spatial derivative outside the brackets. However the right hand side of Eq. (6.3) can't be written, in the general case, as an overall gradient, as can be seen above: whereas the  $\mathcal{Q}_{2K,i}$  term is multiplied by a background quantity, similar to the first order case, the  $\mathcal{Q}_{1K}' \mathcal{Q}_{1K,i}$  term can't be written as an overall gradient and the  $0 - i$  Einstein equation at second order cannot be brought into scalar form immediately.

In order to recast Eq. (6.3) in a more useful form, without the gradients, we have several possibilities:

- The easiest solution is to require  $\mathcal{Q}_{1K} = \text{const}$  or  $\mathcal{Q}_{1K} = 0$ . Unfortunately this case is not particularly interesting, since one of the most interesting applications of second order theory is the study of non-gaussianity, which necessitates the inclusion and evolution of the first order and in particular the first order squared terms. We shall therefore not pursue this option further.
- The next case is to assume we only have one field to consider and we shall study this case in detail in Section VII. Actually, we need only one field at first order, but to assume a single field at first order and multiple field perturbations at second order seems to be rather contrived.

- Another possibility is to use the slow roll approximation such that Eq. (5.7) can be rewritten as  $\mathcal{Q}'_{1I} \propto f(\varphi_{0J})\mathcal{Q}_{1I}$ , where  $f(\varphi_{0J})$  is a function of the background fields, which allows as in the single field case to replace  $\mathcal{Q}'_{1I}\mathcal{Q}_{1I}$  by  $\mathcal{Q}_{1I}^2$  in Eq. (6.3) (for a recent detailed exposition of the slow roll approximation in the multi-field case see e.g. [22]). We shall illustrate this particular case, i.e. using the slow roll approximation, by studying a simple two-field inflation model in Section VIII.
- Finally, we can take the divergence of Eq. (6.3), which we shall do next.

Following Ref. [6] we take the divergence of Eq. (6.3) and get

$$\begin{aligned} \mathcal{H}\nabla^2\widetilde{\phi}_2 - 4\mathcal{H}\left(\widetilde{\phi}_1\nabla^2\widetilde{\phi}_1 + \widetilde{\phi}_{1,k}\widetilde{\phi}_1^k\right) \\ - 4\pi G\sum_K\left[\varphi'_{0K}\nabla^2\mathcal{Q}_{2K} + 2\mathcal{Q}'_{1K}\nabla^2\mathcal{Q}_{1K} + 2\mathcal{Q}'_{1K,j}\mathcal{Q}_{1K}^j\right] + O(k^3) = 0. \end{aligned} \quad (6.4)$$

Using now the inverse Laplacian, defined as  $\nabla^{-2}\nabla^2 X = X$ , Eq. (6.4) can be rewritten as

$$\mathcal{H}\left(\widetilde{\phi}_2 - 4\widetilde{\phi}_1^2\right) - 4\pi G\sum_K\left[\varphi'_{0K}\mathcal{Q}_{2K} + 2\mathcal{Q}'_{1K}\mathcal{Q}_{1K}\right] - R(\widetilde{\phi}_1, \mathcal{Q}_{1I}) + O(k^3) = 0, \quad (6.5)$$

where we define  $R(\widetilde{\phi}_1, \mathcal{Q}_{1I})$  as

$$R(\widetilde{\phi}_1, \mathcal{Q}_{1I}) \equiv 4\mathcal{H}\left[\nabla^{-2}\widetilde{\phi}_1\nabla^2\widetilde{\phi}_1 + \nabla^{-2}\left(\widetilde{\phi}_{1,k}\widetilde{\phi}_1^k\right)\right] + 8\pi G\sum_K\left[\nabla^{-2}\mathcal{Q}'_{1K}\nabla^2\mathcal{Q}_{1K} + \nabla^{-2}\left(\mathcal{Q}'_{1K,j}\mathcal{Q}_{1K}^j\right)\right]. \quad (6.6)$$

But since neither the effect of  $R(\widetilde{\phi}_1, \mathcal{Q}_{1I})$  on the evolution of the field fluctuations nor its large scale limit is clear, we shall not use this form of the  $0-i$  Einstein equation below.

Not being able to make use of the  $0-i$  Einstein equation is inconvenient, but since it is only a constraint equation and therefore redundant, we are able to get a closed system of equations without using it, as shown in Section VI B below, which is sufficient to get the evolution of  $\zeta_2$  from Eq. (4.16). However, the  $0-i$  Einstein equation does allow us to rewrite the Klein Gordon equation in a more compact form with canonical time derivatives (see above the first order case, Section V, and below the single field second order case, Section VII).

## B. Klein Gordon equation

In this section we derive the Klein-Gordon equation in the flat gauge for  $N$  scalar fields on large scales.

At second order the Klein Gordon equations on flat slices is for the field  $I$ , from Eq. (2.32), on large scales given by

$$\begin{aligned} \mathcal{Q}_{2I}'' + 2\mathcal{H}\mathcal{Q}_{2I}' + 2a^2U_{,\varphi_I}\widetilde{\phi}_2 - 2\widetilde{\phi}_1'\mathcal{Q}_{1I}' + 4\varphi'_{0I}\widetilde{\phi}_1\widetilde{\phi}_1' + 4\widetilde{\phi}_1a^2\sum_K U_{,\varphi_I\varphi_K}\mathcal{Q}_{1K} \\ - \varphi'_{0I}\widetilde{\phi}_2' + a^2\sum_K U_{,\varphi_I\varphi_K}\mathcal{Q}_{2K} + a^2\sum_{K,L} U_{,\varphi_I\varphi_K\varphi_L}\mathcal{Q}_{1K}\mathcal{Q}_{1L} = 0. \end{aligned} \quad (6.7)$$

We can rewrite Eq. (6.7) above, using the field equations at first and second order given above in Sections V A and VI A, to substitute for the lapse functions at first and second order,  $\widetilde{\phi}_1$  and  $\widetilde{\phi}_2$ , and get

$$\begin{aligned} \mathcal{Q}_{2I}'' + 2\mathcal{H}\mathcal{Q}_{2I}' + a^2\sum_K\left[U_{,\varphi_I\varphi_K} - \frac{1}{U_0}U_{,\varphi_I}U_{,\varphi_K}\right]\mathcal{Q}_{2K} - \left(\frac{U_{,\varphi_I}}{U_0} + \frac{8\pi G}{\mathcal{H}}\varphi'_{0I}\right)\sum_K\left(\varphi'_{0K}\mathcal{Q}_{2K}' + \mathcal{Q}_{1K}'^2\right) \\ + a^2\sum_{K,L}\left\{U_{,\varphi_I\varphi_K\varphi_L} - \frac{1}{U_0}U_{,\varphi_I}U_{,\varphi_K\varphi_L} + \frac{16\pi G}{\mathcal{H}}\sum_{K,L}\left(U_{,\varphi_I\varphi_K} - \frac{1}{U_0}U_{,\varphi_I}U_{,\varphi_K}\right)\varphi'_{0L}\right\}\mathcal{Q}_{1L}\mathcal{Q}_{1K} \\ + a^2\frac{16\pi G}{\mathcal{H}}\sum_K\left(\frac{U_{,\varphi_K}}{U_0} + \frac{8\pi G}{\mathcal{H}}\varphi'_{0K}\right)\mathcal{Q}_{1K}\mathcal{Q}_{1I}' = 0. \end{aligned} \quad (6.8)$$

This is the gauge-invariant Klein-Gordon equation in the uniform curvature gauge for  $N$  minimally coupled scalar fields on large scales in terms of the field fluctuations in the flat gauge at first and second order,  $\mathcal{Q}_{1I}$  and  $\mathcal{Q}_{2I}$ . It is linear in the second order variables, but quadratic in the first order ones.

Having dealt with the multi-field case in the previous section, we now turn to the single field case. The general form of the Klein Gordon equation at second order, Eq. (6.8), reduces in this case to

$$\begin{aligned} \mathcal{Q}_2'' + 2\mathcal{H}\mathcal{Q}_2' + a^2 \left[ U_{,\varphi\varphi} - \frac{1}{U_0} U_{,\varphi} U_{,\varphi} \right] \mathcal{Q}_2 - \left( \frac{U_{,\varphi}}{U_0} + \frac{8\pi G}{\mathcal{H}} \varphi_0' \right) (\varphi_0' \mathcal{Q}_2' + \mathcal{Q}_1'^2) \\ + a^2 \left\{ U_{,\varphi\varphi\varphi} - \frac{1}{U_0} U_{,\varphi} U_{,\varphi\varphi} + \frac{16\pi G}{\mathcal{H}} \left( U_{,\varphi\varphi} - \frac{1}{U_0} U_{,\varphi} U_{,\varphi} \right) \varphi_0' \right\} \mathcal{Q}_1^2 \\ + a^2 \frac{16\pi G}{\mathcal{H}} \left( \frac{U_{,\varphi}}{U_0} + \frac{8\pi G}{\mathcal{H}} \varphi_0' \right) \mathcal{Q}_I' \mathcal{Q}_K = 0. \end{aligned} \quad (7.1)$$

In the single field case we can use Eq. (5.4) to rewrite the  $0-i$  Einstein equation at second order, Eq. (6.3), as

$$\mathcal{H} \left( \widetilde{\phi}_2 - 2\widetilde{\phi}_1'^2 \right)_{,i} = 4\pi G \left[ \varphi_0' \mathcal{Q}_2 - a^2 \left( \frac{U_{,\varphi}}{\varphi_0'} + 8\pi G \frac{U_0}{\mathcal{H}} \right) \mathcal{Q}_1^2 \right]_{,i} + O(k^3) = 0, \quad (7.2)$$

which allows us to immediately get rid of the spatial gradient in a similar fashion as in the first order case. From Eqs. (6.1) and (7.2) we then get the useful relation, similar to Eq. (5.4) at first order,

$$\begin{aligned} \varphi_0' \mathcal{Q}_2' + \mathcal{Q}_1'^2 = -a^2 U_0 \left( \frac{U_{,\varphi}}{U_0} + \frac{8\pi G}{\mathcal{H}} \varphi_0' \right) \mathcal{Q}_2 - a^2 U_{,\varphi\varphi} \mathcal{Q}_1^2 \\ - a^2 U_0 \frac{8\pi G}{\mathcal{H}} \left[ 2\varphi_0' \frac{U_{,\varphi}}{U_0} + \frac{8\pi G}{\mathcal{H}} \varphi_0'^2 - a^2 \left( \frac{U_{,\varphi}}{\varphi_0'} + \frac{8\pi G}{\mathcal{H}} U_0 \right) \right] \mathcal{Q}_1^2. \end{aligned} \quad (7.3)$$

Substituting Eq. (7.3) into Eq. (7.1) we arrive at the single field Klein Gordon equation at second order,

$$\begin{aligned} \mathcal{Q}_2'' + 2\mathcal{H}\mathcal{Q}_2' + a^2 \left[ U_{,\varphi\varphi} + \frac{16\pi G}{\mathcal{H}} U_0 \varphi_0' \left( \frac{U_{,\varphi}}{U_0} + \frac{4\pi G}{\mathcal{H}} \varphi_0' \right) \right] \mathcal{Q}_2 \\ + a^2 \left\{ U_{,\varphi\varphi\varphi} + \frac{24\pi G}{\mathcal{H}} \varphi_0' U_{,\varphi\varphi} + \frac{8\pi G}{\mathcal{H}} \left[ 3U_{,\varphi} \left( \frac{8\pi G}{\mathcal{H}} (\varphi_0'^2 - 2a^2 U_0) - a^2 \frac{U_{,\varphi}}{\varphi_0'} \right) \right. \right. \\ \left. \left. + \left( \frac{8\pi G}{\mathcal{H}} \right)^2 U_0 \varphi_0' (\varphi_0'^2 - 3a^2 U_0) \right] \right\} \mathcal{Q}_1^2 = 0. \end{aligned} \quad (7.4)$$

now with the time derivatives in canonical form, which is nice.

In the single field case the curvature perturbation on uniform density hypersurfaces at first order in terms of the field fluctuation on the flat slice is given, from Eq. (4.6), as

$$\zeta_1 = -\frac{\mathcal{H}}{\varphi_0'} \mathcal{Q}_1, \quad (7.5)$$

and at second order we get from Eq. (4.16), using Eq. (7.3),

$$\zeta_2 = -\frac{\mathcal{H}}{\varphi_0'} \mathcal{Q}_2 - \left[ 7 - 3c_s^2 - 3 \frac{\varphi_0'^2 - a^2 U_0}{a^2 \rho_0} + 3 \frac{a^2 U_{,\varphi}}{\mathcal{H} \varphi_0'} \right] \left( \frac{\mathcal{H}}{\varphi_0'} \right)^2 \mathcal{Q}_1^2. \quad (7.6)$$

Using Eqs. (7.4) and (7.6) should be sufficient to show the conservation of  $\zeta_2$  on large scales in the single field case, which was shown in Refs. [18, 23], and we will return to this issue in a future work [36].

### VIII. A SIMPLE APPLICATION USING SLOW ROLL

We can now apply the formalism derived in the previous sections to the simple two field model of Ref. [17] which has subsequently been studied in Refs. [20, 29] and most recently in Ref. [46] (for earlier work on two-field inflation at linear order see e.g. [47]). Using the slow-roll approximation we calculate the curvature perturbation at second order,  $\zeta_2$ , in terms of the field fluctuations.

The potential is given as

$$U = \bar{U}_0 + \frac{1}{2}m_1^2\varphi_1^2 + \frac{1}{2}m_2^2\varphi_2^2, \quad (8.1)$$

with the first term,  $\bar{U}_0 = \text{const}$ , dominating and where  $m_I$  denotes the mass of the  $I$ th field. Furthermore we assume slow roll and

$$\varphi_{02} = 0, \quad \varphi'_{02} = 0. \quad (8.2)$$

The background Friedmann constraint, Eq. (2.29), then simplifies to

$$\mathcal{H}^2 = \frac{8\pi G}{3}\bar{U}_0, \quad (8.3)$$

and the background Klein-Gordon equation, Eq. (2.30), gives

$$\varphi'_{01} + \frac{a^2 m_1^2}{3\mathcal{H}}\varphi_{01} = 0. \quad (8.4)$$

From Eq. (4.6) we immediately get the curvature perturbation at first order in terms of the field fluctuations on flat slices in this model,

$$\zeta_1 = 8\pi G \frac{\bar{U}_0}{m_1^2 \varphi_{01}} \mathcal{Q}_{11}. \quad (8.5)$$

The calculation of the second order curvature perturbation in terms of the field fluctuations is slightly more involved. As pointed out in Section IV B, in order to get  $\zeta_2$  solely in terms of the field fluctuations without their time derivatives we have to use the  $0-i$  Einstein equation at second order, and, as discussed in Section VI A, to get the latter in a useful form we need the first order Klein-Gordon equations.

The perturbed Klein-Gordon equation at first order on flat slices, Eq. (5.5), reduces in the slow roll limit for the model specified by Eqs. (8.1) and (8.2) to

$$\mathcal{Q}'_{11} + \frac{a^2 m_1^2}{3\mathcal{H}}\mathcal{Q}_{11} = 0, \quad \mathcal{Q}'_{12} + \frac{a^2 m_2^2}{3\mathcal{H}}\mathcal{Q}_{12} = 0, \quad (8.6)$$

where  $\mathcal{Q}_{11}$  and  $\mathcal{Q}_{12}$  are the field fluctuations in the flat gauge, the Sasaki-Mukhanov variables, at first order for the two fields.

The  $0-i$  equation at second order on flat slices, Eq. (6.3), simplifies then using Eqs. (8.6) to

$$\mathcal{H} \left( \tilde{\phi}_2 - 2\tilde{\phi}_1^2 \right) = 4\pi G \left[ \varphi'_{01} \mathcal{Q}_{21} - \frac{a^2 m_1^2}{3\mathcal{H}} \mathcal{Q}_{11}^2 - \frac{a^2 m_2^2}{3\mathcal{H}} \mathcal{Q}_{12}^2 \right]. \quad (8.7)$$

Rewriting Eq. (6.1), the  $0-0$  Einstein equation at second order, in a similar fashion we arrive at the useful relation

$$\sum_K \left( \varphi_{0K} \mathcal{Q}'_{2K} + \mathcal{Q}'_{1K}{}^2 \right) + a^2 \delta U_2 = a^2 \left( m_1^2 \varphi_{01} \mathcal{Q}_{21} + m_1^2 \mathcal{Q}_{11}^2 + m_2^2 \mathcal{Q}_{12}^2 \right), \quad (8.8)$$

which upon substitution in Eq. (4.16) yields

$$\zeta_2 = 8\pi G \frac{\bar{U}_0}{m_1^2 \varphi_{01}^2} \left[ \varphi_{01} \mathcal{Q}_{21} + \frac{m_2^2}{m_1^2} \mathcal{Q}_{12}^2 + \left( 1 + 2 \frac{8\pi G \bar{U}_0}{m_1^2} \right) \mathcal{Q}_{11}^2 \right], \quad (8.9)$$

the curvature perturbation on uniform density hypersurfaces at second order in terms of the field fluctuations on flat slices for the model specified above.

This expression for  $\zeta_2$ , Eq. (8.9) above, agrees with the one found by Lyth and Rodriguez in Ref. [29] using the  $\Delta N$  formalism, if we take into account that  $\zeta_2 = \zeta_{2\text{LR}} + 2\zeta_1^2$  [28]. In particular we find that  $\zeta_2$  does not contain any non-local terms.

However, the curvature perturbation  $\zeta_2$  found here disagrees with the expression for the second order curvature perturbation found by Enqvist and Vaihkonen in Ref. [17], although the order of magnitude estimate published subsequently by Vaihkonen [46] seems to agree with the result found here.

In this paper we have presented the Klein-Gordon equation for multiple minimally coupled scalar fields at second order in the perturbations in a perturbed FRW background on large scales. We have shown that using suitable gauge-invariant variables, namely the field fluctuations in the flat gauge or Sasaki-Mukhanov variables, the Klein-Gordon equation at second order, Eq. (6.8), can be written solely in terms of these variables, as in the first order case, and is linear in the second order variables, but has source terms quadratic in the first order field fluctuations.

We have also given the relation between gauge-invariant quantities in different gauges, and hence on different hypersurfaces, which at second order is non-trivial. In particular we give the curvature perturbation on uniform density hypersurfaces,  $\zeta_2$ , in terms of the Sasaki-Mukhanov variables of the individual fields,  $\mathcal{Q}_{1I}$  and  $\mathcal{Q}_{2I}$  in Eq. (4.16). We calculated  $\zeta_2$  for a particular two-field model during slow-roll inflation, Eq. (8.9), and found excellent agreement with the expression derived using the  $\Delta N$  formalism [29]. In particular we find using second order cosmological perturbation theory that there are no non-local terms in the expression for  $\zeta_2$  in this model.

Having an expression for  $\zeta_2$  solely in terms of the field fluctuations allows us to get the evolution of  $\zeta_2$  directly from solving the Klein-Gordon equations at zeroth, first, and second order, Eqs. (2.30), (5.7), and (6.8), respectively, together with the Friedmann constraint, Eq. (2.29). Alternatively we could have calculated the non-adiabatic pressure due to the multiple scalar fields first and then solve an evolution equation for  $\zeta_2$  [14, 39, 41], but using Eq. (4.16) eliminates the integration of the  $\zeta_2$  evolution equation and is therefore simpler, since the Klein-Gordon equations have to be solved in both cases.

Given suitable initial conditions for the Klein-Gordon equations governing the dynamics of the fields at zeroth, first, and second order the equations can be integrated numerically. The equations can be solved order by order, the background and first order fields acting as source terms for the second order equations, since we do not consider back-reaction of the higher order perturbations on the lower order ones. Solving the second order equations numerically will therefore be very similar to solving the first order system.

Alternatively, employing a slow roll approximation at all orders, the equations can be approximated analytically. It will be particularly interesting to compare the evolution of  $\zeta_2$  from a slow roll version of the Klein-Gordon equation, Eq. (6.8), to the  $\Delta N$ -formalism [29], which also uses slow roll and also gives the evolution of the curvature perturbation directly from the solution of the Klein-Gordon equations, without having to integrate an evolution equation for  $\zeta_2$ .

The next step will be the extension of the formalism presented here to small scales, i.e. deriving a formalism valid on all scales. This will also be an advantage compared to other approaches based on the separate universe paradigm, such as the  $\Delta N$ -formalism, which can not be extended to small scales since it is by assumption only valid on scales of order or larger than the horizon. First steps towards extending the formalism are under way at present, based on the work presented here [36].

### Acknowledgments

The author is grateful to David Lyth, David Matravers, and David Wands for useful discussions and comments. KAM is supported by PPARC grant PPA/G/S/2002/00098. Algebraic computations of tensor components were performed using the GRTENSORII package for Maple.

### APPENDIX A: BACKGROUND FIELD EQUATIONS

The Friedmann equation is given from the 0 – 0 component of the Einstein equations

$$\mathcal{H}^2 = \frac{8\pi G}{3} a^2 \rho_0, \quad (\text{A1})$$

where  $\mathcal{H} \equiv \frac{a'}{a}$ . From the  $i - j$  component we find

$$\left(\frac{a'}{a}\right)^2 - 2\frac{a''}{a} = 8\pi G a^2 P_0. \quad (\text{A2})$$

The two previous equations can be rewritten as

$$\mathcal{H}' = -\frac{4\pi G}{3} a^2 (\rho_0 + 3P_0), \quad (\text{A3})$$

or alternatively as

$$\frac{a''}{a} = \frac{4\pi G}{3} a^2 (\rho_0 - 3P_0) . \quad (\text{A4})$$

Also useful are

$$2 \left( \frac{a'}{a} \right)^2 - \frac{a''}{a} = 4\pi G a^2 (P_0 + \rho_0) , \quad (\text{A5})$$

where the right hand side in the case of scalar fields simplifies to  $a^2 (P_0 + \rho_0) = \sum_K \varphi'_{0K}{}^2$ , and

$$\mathcal{H}' + 2\mathcal{H}^2 = 4\pi G a^2 (\rho_0 - P_0) , \quad (\text{A6})$$

where the right hand side in the case of scalar fields simplifies to  $(\rho_0 - P_0) = 2U_0$ .

The background energy conservation for the  $\alpha$ -fluid is given by [2, 39]

$$\rho'_{0\alpha} = -3\mathcal{H} (\rho_{0\alpha} + P_{0\alpha}) + Q_\alpha , \quad (\text{A7})$$

where  $\rho_{0\alpha}$ ,  $P_{0\alpha}$ , and  $Q_\alpha$  are the energy density, the pressure and the energy transfer to the  $\alpha$ -fluid. Note that the energy transfer defined here is related to the one define in [39],  $\hat{Q}_\alpha$ , by  $aQ_\alpha = \hat{Q}_\alpha$ . The adiabatic sound speed of the  $\alpha$ -fluid is

$$c_\alpha^2 \equiv \frac{P'_{0\alpha}}{\rho'_{0\alpha}} , \quad (\text{A8})$$

related to the total adiabatic sound speed by

$$c_s^2 = \sum_\alpha \frac{\rho'_{0\alpha}}{\rho'_0} c_\alpha^2 . \quad (\text{A9})$$

For more details on the multi-fluid formalism see [39].

## APPENDIX B: THE METRIC TENSOR

The metric tensor up to second order, including only scalar perturbations, is

$$g_{00} = -a^2 (1 + 2\phi_1 + \phi_2) , \quad (\text{B1})$$

$$g_{0i} = a^2 \left( B_1 + \frac{1}{2} B_2 \right)_{,i} , \quad (\text{B2})$$

$$g_{ij} = a^2 [(1 - 2\psi_1 - \psi_2) \delta_{ij} + 2E_{1,ij} + E_{2,ij}] . \quad (\text{B3})$$

and its contravariant form is

$$g^{00} = -a^{-2} [1 - 2\phi_1 - \phi_2 + 4\phi_1^2 - B_{1,k} B_1^k] , \quad (\text{B4})$$

$$g^{0i} = a^{-2} \left[ B_1^i + \frac{1}{2} B_2^i - 2B_{1,k} E_1^{ki} + 2(\psi_1 - \phi_1) B_1^i \right] , \quad (\text{B5})$$

$$g^{ij} = a^{-2} \left[ (1 + 2\psi_1 + \psi_2 + 4\psi_1^2) \delta^{ij} - (2E_1^{ij} + E_2^{ij} - 4E_1^{ik} E_{1,k}^j + 8\psi_1 E_1^{ij} + B_1^i B_1^j) \right] , \quad (\text{B6})$$

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