Quantization of perturbations during inflation in the $1 + 3$ covariant formalism

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This note derives the analogue of the Mukhanov-Sasaki variables both for scalar and tensor perturbations in the 1+3 covariant formalism. The possibility of generalizing them to non-flat Friedmann-Lemaître universes is discussed.

The theory of cosmological perturbations is a cornerstone of the modern cosmological model. It contains two distinct features. First, it describes the growth of density perturbations from an initial state in an expanding universe filled with matter and radiation, taking into account the evolution from the super-Hubble to the sub-Hubble regime. Second, it finds the origin of the initial power spectrum of density perturbations in the amplification of vacuum quantum fluctuations of a scalar field during inflation.

Two formalisms are used to describe the evolution of perturbations. The first relies on the parameterization of the most general spacetime close to a Friedmann-Lemaître (FL) universe and on the construction of gauge invariant variables [1]. The second is based on a general $1 + 3$ decomposition of the Einstein equation [2]. The philosophies and advantages of these two formalisms are different.

The Bardeen formalism is restricted to perturbations around a FL universe (with metric $\bar{g}_{\mu\nu}$) and expands the spacetime metric as $g_{\mu\nu} = \bar{g}_{\mu\nu} + \gamma_{\mu\nu}$. The metric perturbation is then decomposed as

$$\gamma_{\mu\nu}\mathrm{d}x^\mu\mathrm{d}x^\nu = 2a^2(\eta)\left[-A\mathrm{d}\eta^2 + \left(D_i B + \bar{B}_i\right)\mathrm{d}x^i\mathrm{d}\eta \right.$$
$$\left. + \left(C\gamma_{ij} + D_i D_j E + D_{(i}\bar{E}_{j)} + \bar{E}_{ij}\right)\mathrm{d}x^i\mathrm{d}x^j\right] \quad (1)$$

and the 10 degrees of freedom are decomposed in 4 scalars (A, C, B, E), 4 vectors $(\bar{E}_i, \bar{B}_i$ with $D_i\bar{B}^i = 0, \dots)$ and 2 tensors $(\bar{E}_{ij}$ with $\bar{E}^i_i = D_i\bar{E}^{ij} = 0)$. During inflation, it was shown that the Mukhanov-Sasaki (MS) variable v, a gauge invariant variable that mixes matter and metric perturbations, must be quantized [3]. This approach is thus completely predictive (initial conditions and perturbations evolution) for an almost flat FL spacetime. It is not straightforward to extend it to less symmetrical inflationary models [6, 7], for which the quantization procedure has not been investigated (see however Ref. [4] for non flat FL universes and Ref. [5] for non-FL spacetimes).

The $1 + 3$ covariant description assumes the existence of a preferred congruence of worldlines representing the average motion of matter. The central object is the 4-velocity u^a of these worldlines together with the kinematical quantities arising from the decomposition

$$\nabla_a u_b = -u_a\dot{u}_b + \frac{1}{3}\Theta h_{ab} + \sigma_{ab} + \omega_{ab} \quad (2)$$

where $h_{ab} = g_{ab} + u_a u_b$. $\Theta = \nabla_a u^a$ is the expansion rate, σ_{ab} the shear (symmetric trace-free with $\sigma_{ab}u^a = 0$), ω_{ab} the vorticity (antisymmetric with $\omega_{ab}u^a = 0$) and $\dot{u}_a \equiv u^b\nabla_b u_a$). A fully orthogonally projected covariant derivative D_a, referred to as a spatial gradient, is defined and a complete set of evolution equations can be obtained for these quantities (together with the electric and magnetic parts of the Weyl tensor, E_{ab} and H_{ab} and the matter variables) without needing to specify the spacetime geometry (see e.g. Ref. [8] for details). The formalism can then be used to study the evolution of perturbations in various spacetimes (see e.g. Ref. [9] for Bianchi universes) and beyond the linear order in the case of almost FL universes [10, 11]). In this case, the perturbation variables have a clear interpretation and have been related to the Bardeen variables both for fluids [12] and scalar fields [13]. On the other hand, the scalar-vector-tensor decomposition is not straightforward [14] and the analogue of the Mukhanov-Sasaki variable v has not been derived so that it is difficult to argue which quantity must be quantized in this formalism.

The goal of this article is to identify this variable in the $1 + 3$ covariant formalism. In § I, we recall the construction of the Mukhanov-Sasaki variable. We then identify in § II its counterpart in the $1 + 3$ covariant formalism for an almost FL spacetime. § III adresses the question of gravitational waves. Finally we conclude on the use and possible extensions of these variables in § IV.

I. QUANTIZATION OF THE MUKHANOV-SASAKI VARIABLE

Focusing on scalar modes of the decomposition (1), one defines the two gauge invariant potentials, $\Phi = A + \mathcal{H}(B - E') + (B - E')'$ and $\Psi = -C - \mathcal{H}(B - E')$ where $\mathcal{H} = a'/a$. For a universe filled by a single scalar field φ, one can define the gauge invariant field fluctuation $Q = \delta\varphi - \varphi'C/\mathcal{H}$. The curvature perturbation in the comoving gauge is then given by

$$\mathcal{R} = -C + \mathcal{H}\frac{\delta\varphi}{\varphi'} = \frac{\mathcal{H}}{\varphi'}Q, \quad (3)$$

when assuming a background FL universe with flat spatial sections. Introducing the two variables

$$u \equiv \frac{2a\Phi}{\kappa\varphi'}, \qquad \theta \equiv \frac{1}{z} \equiv \frac{\mathcal{H}}{a\varphi'} = \frac{H}{a\dot{\varphi}}, \qquad (4)$$

with $\kappa = 8\pi G$, $\mathcal{R}$ takes the simple form $\mathcal{R} = \theta u' - \theta' u$, where use has been made of the background equation $\theta' = \left(-a\theta\varphi'' + \mathcal{H}' - \mathcal{H}^2\right)/a\varphi' = -\theta\varphi''/\varphi' - \kappa\varphi'/2a$. If we define

$$v \equiv z\mathcal{R} = aQ \qquad (5)$$

it reduces to the simple relation $zv = (uz)'$. Thus, $\mathcal{R}'$ takes the simple form $\mathcal{R}' = \theta u'' - \theta'' u$. Additionnaly, the perturbed Einstein equations imply that $\mathcal{R}' = \theta\Delta u$. Provided $\varphi' \neq 0$, i.e. we are not in a strictly de Sitter phase, this leads to

$$u'' - \left(\Delta + \frac{\theta''}{\theta}\right)u = 0 \qquad (6)$$

which can also be written as

$$z^2\mathcal{R}' = \Delta\left(\int \mathcal{R}z^2\mathrm{d}\eta\right). \qquad (7)$$

This form is strictly equivalent to $\mathcal{R}'' - \Delta\mathcal{R} + 2(z'/z)\mathcal{R}' = 0$, that is to

$$v'' - \left(\Delta + \frac{z''}{z}\right)v = 0. \qquad (8)$$

This is the equation of a harmonic oscillator with time varying mass $m^2 = z''/z$. To show that v is indeed the canonical variable to be quantized (contrary to u which satisfies a similar equation with z replaced by θ), one needs to expand the action of the scalar field coupled to gravity up to second order [3]. The standard procedure is then to promote v to the status of an operator and set the initial conditions by requiring that it is in its vacuum state on sub-Hubble scales (in Fourier space, that is when $k\eta \to -\infty$). At the end of inflation, all cosmologically relevant scales are super-Hubble ($k\eta \ll 1$) and the conservation of $\mathcal{R}$ on these scales is used to propagate the large scale perturbations generated during inflation to the post-inflationary eras.

II. QUANTIZATION IN THE 1+3 FORMALISM

A. Generalities

Let us first stress an important point concerning time derivative. In the coordinate based approach, the dot refers to a derivative with respect to the cosmic time. In the covariant formalism, a natural time derivative is introduced as $u^a\nabla_a$ which is a derivative along the worldline of the observer. For an almost FL spacetime, it is clear that for any order 1 scalar quantity X,

$u^a\nabla_a X = \partial_t X$ since u^a has to be evaluated at the background level. It is indeed not the case anymore for vector or tensor quantities, or at second order in the perturbations. Another time derivative can be constructed from the Lie derivative along u^a, $\mathcal{L}_u$. This derivative exactly matches the derivative with respect to cosmic time for any type of perturbations [15]. For instance, $\mathcal{L}_u X_a = u^b\nabla_b X_a + X_b\nabla_a u^b$, and it is easily checked that the second term exactly compensates the term arising from the divergence of u^a. We recall that the Lie derivative satisfies

$$D_a(\dot{X}) = \mathcal{L}_u(D_a X) - \dot{u}_a\dot{X}. \qquad (9)$$

In the $1 + 3$ covariant formalism, the main equations for a spacetime with vanishing vorticity ($\omega_{ab} = 0$ in the decomposition (2)) are the Raychaudhuri equation

$$\dot{\Theta} + \frac{1}{3}\Theta^2 = D_a\dot{u}^a - \frac{\kappa}{2}(\rho + 3P) - 2\sigma^2, \qquad (10)$$

the Gauss-Codacci equation

$$\mathcal{K} = 2\left(-\frac{\Theta^2}{3} + \kappa\rho + \sigma^2\right), \qquad (11)$$

together with the conservation equations

$$\dot{\rho} + \Theta(\rho + P) = 0, \quad D_a P = -(\rho + P)\dot{u}_a \qquad (12)$$

where $2\sigma^2 = \sigma_{ab}\sigma^{ab}$. For a scalar field $\rho = \psi^2/2 + V$ and $P = \psi^2/2 - V$ with $\psi = \dot{\phi}$. We define the scale factor S by the relation $\dot{S}/S = H \equiv \Theta/3$. The previous equations imply that

$$\dot{H} = -\frac{\kappa}{2}\psi^2 - \sigma^2 + \frac{1}{6}\mathcal{K} + D_a\dot{u}^a \qquad (13)$$

and the Gauss equation leads to

$$\dot{\mathcal{K}} = -\frac{2}{3}\Theta(\mathcal{K} + 2D_a\dot{u}^a) + 2(\sigma^2)^{\cdot} + 2\Theta\sigma^2 \qquad (14)$$

and

$$D_a\mathcal{K} = -\frac{4}{3}\Theta D_a\Theta + 2\kappa\psi D_a\psi + 2D_a(\sigma^2). \qquad (15)$$

Let us now introduce the central quantity in our discussion

$$\mathcal{R}_a \equiv \frac{1}{3}\left[\int_{\mathcal{L}}(D_a\Theta)\,\mathrm{d}\tau - D_a\left(\int_{\mathcal{L}}\Theta\mathrm{d}\tau\right)\right] \equiv \frac{v_a}{z} \qquad (16)$$

where τ is the proper time along the fluid flow lines. It follows from the identity (9) that

$$\mathcal{L}_u\mathcal{R}_a = -H\dot{u}_a = H(D_a\psi)/\psi, \qquad (17)$$

which is a useful relation in order to close the equations in $\mathcal{R}_a$. The conservation equation implies that

$\mathcal{L}_u(\psi D_a \psi) = -\psi D_a(\Theta\psi)$ which, combined with Eq. (15), gives

$$\frac{1}{4}S^2 D_a(\mathcal{K} - 2\sigma^2) = U_a + \frac{2\Theta}{3\kappa\psi^2}\left[\mathcal{L}_u U_a + \frac{1}{3}\Theta U_a\right] \quad (18)$$

with $U_a = \kappa S^2 \psi D_a \psi/2$. Now, introducing

$$V_a \equiv zS^2\left[\frac{1}{4}D_a(\mathcal{K} - 2\sigma^2) + (\sigma^2 - \frac{1}{6}\mathcal{K} - D_b\dot{u}^b)\frac{D_a\psi}{\psi}\right] \quad (19)$$

and developing $\mathcal{L}_u(zU_a)$ with the help of Eqs. (18) and (13), it can be shown that

$$\mathcal{L}_u\mathcal{R}_a = \frac{1}{Sz^2}\int \frac{zV_a}{S}\mathrm{d}\tau. \quad (20)$$

This intermediate result holds whatever the shear and the spatial curvature and is exact, that is valid at any order in perturbations. Note its similarity with Eq. (7).

B. Flat FL spacetimes

Let us now focus on homogeneous spacetimes with flat spatial sections; this includes the FL spacetimes for which the shear vanishes and Bianchi I spacetimes. Homegeneity implies that the spatial gradient of any scalar function vanishes ($D_a f = 0$, $\forall f$) and in particular $D_a P = 0$ so that $\dot{u}_a = 0$. Flatness implies that $\mathcal{K} = 0$ and that the 3D-Ricci tensor vanishes, $^{(3)}R_{ab} = 0$, which leads to the simplified equation for the shear

$$\dot{\sigma}_{ab} + \Theta\sigma_{ab} = 0 \Rightarrow (\sigma^2)^{\cdot} + \Theta\sigma^2 = 0. \quad (21)$$

This means that the only non-vanishing quantity are Θ, ϕ, ψ and σ. At first order in the perturbations, we have to consider the gradients of these quantities but also terms like $\dot{u}_a$ and $\mathcal{K}$.

FL spacetimes are also isotropic. This implies that $\sigma = 0$ and $S = a$ for the background. Consequently we can discard gradients of σ^2 which are second order. Thus, the only remaining term in the expression (19) of V_a is $\frac{1}{4}zS^2 D_a\mathcal{K}$.

In order to get a closed equation for $\mathcal{R}_a$, we need to express V_a in terms of $\mathcal{R}_a$ in Eq. (20). Taking the spatial gradient of Eq. (14) and using Eq. (9) for handling the time derivative, we obtain the first order relation

$$\mathcal{L}_u\left(\frac{S^2 D_a\mathcal{K}}{4}\right) = \frac{S^2 H}{\psi}D_a(D_b D^b \psi) = S^2 H D_b D^b\left(\frac{D_a\psi}{\psi}\right),$$

where the last equality follows from the flat background assumption. Eq. (17) and the commutation relation $S^2 D_b D^b \mathcal{L}_u X_a = \mathcal{L}_u(S^2 D_b D^b X_a)$, valid at first order, imply $\mathcal{L}_u\left(\frac{S^2 D_a\mathcal{K}}{4}\right) = \mathcal{L}_u(S^2 D_b D^b \mathcal{R}_a)$ which once integrated leads to

$$\frac{S^2 D_a\mathcal{K}}{4} = S^2 D_b D^b \mathcal{R}_a \equiv \Delta\mathcal{R}_a \quad (22)$$

up to a constant F_a satisfying $\mathcal{L}_u F_a = 0$ which can be absorbed in the integration initial boundary surface of Eq. (16). Thus Eq. (20) reads

$$\mathcal{L}_u\mathcal{R}_a = \frac{1}{Sz^2}\int \frac{z^2}{S}\Delta\mathcal{R}_a\mathrm{d}\tau. \quad (23)$$

At this stage, it is useful to introduce a vector field $w_a \equiv Su_a$, and the conformal proper time $\hat{\tau}$ defined by $Sd\hat{\tau} = \mathrm{d}\tau$. It is easily seen that for a spatial vector (i.e. $u^a X_a = 0$) $\mathcal{L}_w X_a = S\mathcal{L}_u X_a$. The Lie derivative along w_a matches at first order the derivative with respect to the conformal time η, as the Lie derivative along u_a was matching the derivative with respect to the cosmic time. For scalars we thus use the notation $X' \equiv \mathcal{L}_w X$. With this definition, Eq. (23) can be recast as

$$z^2\mathcal{L}_w\mathcal{R}_a = \int z^2 \Delta\mathcal{R}_a\mathrm{d}\hat{\tau}, \quad (24)$$

which is similar to Eq. (7). By the same token, we deduce that v_a defined in Eq. (16) satisfies Eq. (8). It can be checked that its spatial components are linked to the MS variable at first order in perturbations by $v_i = \partial_i v$, and consequently the initial conditions obtained from the quantization of v can be used to set the initial conditions for v_a and then $\mathcal{R}_a$. v_a is thus the analogue in the $1 + 3$ formalism of the MS variable v in the Bardeen formalism and it satisfies

$$\mathcal{L}_w^2(v_a) - \left(\Delta + \frac{S''}{S}\right)v_a = 0. \quad (25)$$

III. GRAVITATIONAL WAVES

It can be shown that the magnetic part of the Weyl tensor H_{ab} is a good variable to describe the gravitational waves [14, 16], and it satisfies at first order for flat FL spacetimes

$$\mathcal{L}_w^2 H_{ab} + 2\mathcal{L}_w(\mathcal{H}H_{ab}) - \Delta H_{ab} = 0. \quad (26)$$

$\mathcal{E}_{ab}$ defined by $\mathcal{L}_w\mathcal{E}_{ab} = H_{ab}$ satisfies

$$\mathcal{L}_w^2\mathcal{E}_{ab} + 2\mathcal{H}\mathcal{L}_w(\mathcal{E}_{ab}) - \Delta\mathcal{E}_{ab} = 0 \quad (27)$$

where the integration constant is set to 0 as for the scalar case. This is exactly the equation satisfied by the gravitational waves $\bar{E}_{ij}$. Indeed, these variables are linked at first order by $\mathcal{E}_{ab} = \epsilon^{cd}{}_{<a}\partial_c\bar{E}_{b>d}$ [16], where $\epsilon^{ab}{}_c$ is a completely antisymmetric tensor normalized such that $\epsilon^{12}{}_3 = 1$. With $\mu_{ab} \equiv \frac{S}{\sqrt{8\pi G}}\mathcal{E}_{ab}$, Eq. (27) leads at first order to

$$\mathcal{L}_w^2(\mu_{ab}) - \left(\Delta + \frac{S''}{S}\right)\mu_{ab} = 0 \quad (28)$$

which is the equation for an harmonic oscillator with a time varying mass S''/S. Just as for scalar perturbations case, the quantization of the gravitational waves in perturbation theory, can be used to set the initial conditions for μ_{ab} and thus for $\mathcal{E}_{ab}$ and H_{ab}.

IV. CONCLUSIONS

We have identified the scalar and tensor variables that map to the Mukhanov-Sasaki variables when considering an almost-FL universe with Euclidean spatial sections in the $1 + 3$ covariant formalism. Let us stress that in Ref. [10], $\mathcal{R}_a \equiv -D_a\alpha$ (where $\alpha = \frac{1}{3}\int_{\mathcal{L}}\Theta d\eta$ is the integrated volume expansion along u_a) was proposed. But clearly, this maps at linear order to $\partial_a\left(\mathcal{R} - \frac{1}{3}\int\Delta(V + E')d\eta\right)$, where V is the scalar part of the perturbation of the velocity. The additional term in our definition (16) cancels this discrepancy as it can be seen from the constraint $\frac{2}{3}D_a\Theta = D_b\sigma^b{}_a$ which implies that at first order $D_a\Theta = \frac{1}{a}\partial_a\Delta V$. Alternatively, this can be seen directly on the expression of Θ in terms of perturbation variables by use of the $(0 - i)$ Einstein equation. The two variables agree at leading order on super-Hubble scales.

Two generalizations with less restrictive backgrounds can be considered: flat but anisotropic spatial sections ($K \equiv \frac{S^2\mathcal{K}}{6} = 0$, $\sigma \neq 0$), and isotropic but non-flat FL spacetimes ($K \neq 0$, $\sigma = 0$). The cornerstone of the derivation of § II is the possibility of expressing V_a only in terms of $\mathcal{R}_a$ to get a closed equation from Eq. (20).

In the first case, two other terms in Eq. (19) contribute at first order. $zS^2\sigma^2\frac{D_a\psi}{\psi}$ changes the definition of the effective varying mass, but the term $\frac{zS^2}{2}D_a(\sigma^2)$ acts as a source in the R.H.S of Eq. (8). This term represents a coupling of the gravitational waves (σ_{ab} at first order)

with the shear of the background spacetime. As for $\mathcal{E}_{ab}$, Eq. (27) will be supplemented with an integral non trivial source term which couples the background shear to the electric part of the Weyl tensor [16]. Thus both equations are mixed with these new source terms, which are of the same order of magnitude as the quantized variables. Note that this not surprising since at second order in the perturbations around a FL spacetime the scalar and tensor degrees of freedom are coupled [16, 18].

In the second case ($K \neq 0$, $\sigma = 0$),

$$V_a = z\left[\frac{S^2}{4}D_a\mathcal{K} - K\frac{D_a\psi}{\psi}\right] \equiv \frac{z}{4}\tilde{C}_a. \qquad (29)$$

The spatial gradient of Eq. (14) leads at first order to

$$\mathcal{L}_u\tilde{C}_a = \frac{S^2H}{\psi}D_a\left(D_bD^b\psi\right) - 3K\mathcal{L}_u\zeta_a \qquad (30)$$

where $\zeta_a \equiv D_a\alpha + \frac{D_a\psi}{3\psi}$ is a possible nonlinear generalization of the curvature perturbation on uniform density hypersurfaces. From the conservation equation (12) it can be shown [11, 15] that ζ_a is conserved (in the sense of the Lie derivative) on large scales for adiabatic perturbations, and thus $\tilde{C}_a$ is also conserved in the same sense on super-Hubble scales for adiabatic perturbations [17]. Because of this term, $\tilde{C}_a$ cannot be expressed solely in terms of $\mathcal{R}_a$ as it has been done with Eq. (22). Indeed, it contains an additional term involving ζ_a [10].

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