The Poisson equation at second order in relativistic cosmology

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We calculate the relativistic constraint equation which relates the curvature perturbation to the matter density contrast at second order in cosmological perturbation theory. This relativistic “second order Poisson equation” is presented in a gauge where the hydrodynamical inhomogeneities coincide with their Newtonian counterparts exactly for a perfect fluid with constant equation of state. We use this constraint to introduce primordial non-Gaussianity in the density contrast in the framework of General Relativity. We then derive expressions that can be used as the initial conditions of N-body codes for structure formation which probe the observable signature of primordial non-Gaussianity in the statistics of the evolved matter density field.

I. INTRODUCTION

Our knowledge of the statistics of the galaxy distribution relies upon the vast amount of data obtained by increasingly large galaxy surveys. Among other goals, analysis of the galaxy field allows us to indirectly probe the distribution of the underlying dark matter on non-linear scales (e.g., Refs. [1–4]). On the theoretical side, in order to understand the physics that governs the observed galaxy field, large numerical codes are developed to simulate the evolution of matter inhomogeneities that have formed large scale structure (LSS). This huge task is usually split in two stages. In a first stage, semi-analytical methods are employed to account for the early evolution of fluctuations in the weakly non-linear regime. At the same time, the inhomogeneous in the continuum matter field are related to a discrete distribution of point masses, thus implementing initial conditions for numerical codes. In a second stage, typically at redshifts \( z \sim 50 \), N-body codes evolve inhomogeneities in the strongly non-linear regime up to the present day. As Newtonian N-body codes continue to improve in resolution and volume (e.g., Refs. [7–9]), the implementation of realistic and accurate initial conditions is increasingly important.

Historically, the initial conditions for N-body simulations have been generated by using the Zel’dovich approximation [10], which establishes the correspondence between the matter density fluctuation of standard perturbation theory, and the displacement of mass particles in a grid. Despite its linear nature, this represents an improvement over standard perturbation theory, since it takes advantage of working in Lagrangian coordinates [6, 11]. The caveat to this approximation is that it accounts only for the early non-linear evolution of density fluctuations, and in particular, it employs a linear Poisson constraint, which is used to express the density contrast, \( \delta_N \), in terms of the gravitational potential, \( \phi_N \), that is

\[
\nabla^2 \phi_N = 4\pi G \rho_0 a^2 \delta_N. \tag{1.1}
\]

An improvement to this approximation is second-order Lagrangian perturbation theory (2LPT), which generates initial conditions taking into account non-linearities in Lagrangian coordinates. This has been shown to be more precise and avoids transients present in the Zel’dovich approximation [12, 13]. Since 2LPT takes into account non-linearities, the fact that the gravitational instability is non-local is manifest in corrections to Eq. (1.1) given by tidal effects at non-linear order [14]. With the matter density fluctuations at non-linear order under control, recent studies have used 2LPT to include primordial non-Gaussianity in the matter fluctuations [15, 16].

These and other semi-analytical approximations to the early evolution of inhomogeneities, however, rely on Newtonian physics, thereby ignoring the effects of General Relativity (GR). Cosmological inhomogeneities are well described by Newtonian dynamics only when the modes of the perturbations lie well inside the horizon, i.e. when their
wavenumber is \( k \gg H \), with \( H \) denoting the Hubble parameter in conformal time. Yet, the initial conditions for these approximations come from much earlier times – typically the epoch of decoupling – when some of the scales of interest are comparable to, or even larger than, the cosmological horizon. Therefore, relativistic effects are important and should be taken into account when setting the initial conditions to simulations of structure formation.

Recent studies demonstrate the importance of GR in the analysis of large scale structure. Some have contrasted relativistic and Newtonian fluctuations by the identification of dynamical equations \([18, 19]\). This provides correspondences between Newtonian fluctuations and relativistic perturbations in a specific gauge at linear order in perturbation theory. Additionally, Ref. \([21]\) extends this correspondences to second-order perturbations. In this way, the equivalence of the dynamical equations is established for the restricted case of pressureless matter and neglecting the decaying mode of perturbations. A major motivation to study this correspondence is to discriminate primordial non-Gaussian fluctuations from non-Gaussianities induced by the non-linear dynamics of GR. In search of observational signatures, Ref. \([21]\) studied the effects of relativistic non-linear fluctuations in the halo bias and subsequently its signature in the spectrum of the galaxy distribution (see also \([22]\)).

In this paper we present the Poisson equation at second order in the framework of relativistic cosmological perturbation theory \([23, 24]\). Previous studies have explored this constraint for the limit of a dust universe at small scales \([20]\) (in this case the linear equation \([1.1]\) is recovered), and for a ΛCDM universe at large scales \([28]\). Instead, our analysis yields the Poisson constraint equation in terms of relativistic perturbations that find a direct correspondence with Newtonian inhomogeneities, and without approximations. Furthermore, we extend the constraint to the case of a general perfect fluid. As an example, we subsequently use our result to express the primordial non-Gaussianity in terms of the dark matter density field in equations that include all the relativistic effects. We present results in the form of kernels for the non-linear variables, a form customarily used in the formulation of initial conditions of numerical simulations.

The paper is organised as follows. In the next section we explicitly show how to construct the Poisson equation from Einstein’s field equations combining variables in two gauges for linear perturbations. In Section III we repeat the procedure for the second order variables and arrive at a GR version of the Poisson constraint valid for any perfect fluid including entropy (or non-adiabatic pressure) perturbations. In Section IV we apply the constraint to the case of matter perturbations in a flat universe dominated by pressureless matter and show how to include the primordial non-Gaussian corrections in the Poisson equation. We conclude in Section V discussing the relevance of our result to the initial conditions of numerical simulations.

II. THE POISSON EQUATION AT FIRST ORDER

A. Background and first-order equations

In cosmological perturbation theory, considering scalar perturbations of the metric yields the following line element,

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

where \( \phi \) is the lapse function, \( \psi \) is the curvature perturbation, and \( B \) and \( E \) make up the scalar shear. All these quantities are function of Cartesian coordinates, \( x_j \), and conformal time, \( \eta \). Perturbations are then expanded order-by-order in a series as, e.g., \( \phi = \phi_1 + \frac{1}{2} \phi_2 + \cdots \). In order to define the expansion uniquely, and as an excellent approximation to observations, the first order quantities are chosen to have Gaussian statistics.

In the background the metric represents the Friedmann-Lemaître-Robertson-Walker spacetime. The homogeneous equations are the familiar Friedmann and continuity equations:

\[
3H^2 = 8\pi G a^2 \rho_0, \\
\rho_0' = -3H(P_0 + \rho_0),
\]

where the prime denotes a derivative with respect to conformal time and a subscript zero denotes the background, homogeneous quantities.

The fluid equations are derived from the vanishing covariant derivative of the energy momentum tensor\(^1\). At

\[^1\] We consider the usual perfect fluid energy momentum tensor of the form \( T^{\mu}_{\nu} = (\rho + P) u^\mu u_\nu + P \delta^{\mu}_{\nu} \), where \( u^\mu \) is the fluid four velocity and \( P \) and \( \rho \) are the pressure and energy density, respectively.
first-order in perturbation theory, the energy conservation dictates the evolution of the density perturbation $\delta \rho_1$,

$$
\delta \rho_1' + 3\mathcal{H}(\delta \rho_1 + \delta P_1) = (\rho_0 + P_0) \left[3\psi_1' - \nabla^2 (E_1' + v_1)\right],
$$

(2.4)

where $v$ is the scalar velocity potential obtained from the spatial part of the fluid four velocity as $u^i = \frac{1}{a} \partial^i v$, and the energy density and pressure fluctuations are denoted by $\delta \rho$ and $\delta P$, respectively. We define the Laplacian as $\nabla^2 = \partial_i \partial^i$. Note that no gauge has been specified here. In order to obtain the corresponding equation for the evolution of the velocity, we define $V = B + v$, and write the momentum conservation equation, which at first order is

$$
V_{1,i} + \mathcal{H}(1 + c_s^2) V_{1,i} + \left[\frac{\delta P_1}{P_0 + \rho_0} + \phi_1\right]_{,i} = 0,
$$

(2.5)

where we have neglected anisotropic stresses and defined the adiabatic sound speed as $c_s^2 = P_0'/\rho_0'$.

The Einstein field equations yield two constraint equations that are combined to derive the Poisson equation. The $(0,0)$ component of these equations yields the energy constraint equation

$$
3\mathcal{H}(\psi_1' + \mathcal{H}\phi_1) - \nabla^2 \left(\psi_1 + \mathcal{H}(E_1' - B_1)\right) = -4\pi G a^2 \delta \rho_1.
$$

(2.6)

The momentum constraint is derived from the $(0,i)$ component:

$$
\psi_{1,i} + \mathcal{H}\phi_{1,i} = -4\pi G a^2 (\rho_0 + P_0) V_{1,i}.
$$

(2.7)

This is the complete set of equations at first order without the gauge specified. The remaining Einstein equations at this order are related to the ones above through the Bianchi identities.

**B. Constraint in the longitudinal gauge**

In order to overcome the ambiguity in the coordinate freedom, we must specify the gauge in the above equations. We work in the longitudinal or Newtonian gauge [23] to recover the exact Newtonian equations. This is a shear-free gauge, specified by setting $E_\ell = B_\ell = 0$. The absence of anisotropic stresses also guarantees that, in this gauge, $\psi_{1\ell} = \phi_{1\ell}$ and Eq. (2.6) becomes

$$
-3\mathcal{H}(\phi_{1\ell}' + \mathcal{H}\phi_{1\ell}) + \nabla^2 \phi_{1\ell} = 4\pi G a^2 \delta \rho_{1\ell}.
$$

(2.8)

Then, by integrating the overall gradient of the momentum constraint (2.7), we have

$$
\phi_{1\ell}' + \mathcal{H}\phi_{1\ell} = -4\pi G a^2 (\rho_0 + P_0) v_{1\ell},
$$

(2.9)

and combining both equations we find the first-order constraint:

$$
\nabla^2 \phi_{1\ell} = 4\pi G a^2 (\delta \rho_{1\ell} + \rho_0' v_{1\ell}).
$$

(2.10)

**C. The Newtonian expression**

The combination in parentheses in the linear Poisson equation (2.10), $\delta \rho_{1\ell} + \rho_0' v_{1\ell}$, is in fact equivalent to the density contrast in two other gauges, as we will now show. The transformation between two coordinate systems is parametrised through the generating vector $\xi_{1\mu} = (\alpha_1, \beta_{1,i})$, so that, for example, the density perturbation at linear order is transformed as

$$
\tilde{\delta \rho}_1 = \delta \rho_1 + \alpha \rho'_0.
$$

(11.11)

We can define the total matter gauge (denoted with a subscript $\text{tom}$) by a vanishing total momentum at all orders, i.e.

$$
V_{\text{tom}} = v_{\text{tom}} + B_{\text{tom}} = 0.
$$

(2.12)

The transformation rule for $V$ tells us that

$$
\tilde{V}_1 = v_1 + B_1 - \alpha_1,
$$

(2.13)
so that in the case of a transformation from the longitudinal to the total matter gauge we have

$$\alpha_{1\text{tom}|\ell} = v_{1\ell}, \quad (2.14)$$

where the notation $X_{\text{tom}|\ell}$ denotes the value of the gauge generation vector component $X$ for the total matter gauge, evaluated in the longitudinal gauge. In order to fully specify the total matter gauge (i.e. in order to specify $\beta_{1\text{tom}}$) the condition $E_{1\text{tom}} = 0$ is taken. In consequence, the density fluctuation in the total matter gauge is obtained in terms of matter perturbations in the longitudinal gauge as

$$\widetilde{\delta \rho_{\text{1\text{tom}}}} = \delta \rho_{1\ell} + \rho_0 v_{1\ell}. \quad (2.15)$$

It is now straightforward to recover the Newtonian form of the Poisson equation writing

$$\nabla^2 \varphi_{1\ell} = 4\pi G a^2 \rho_0 \delta_{1\text{tom}}, \quad (2.16)$$

where the density contrast is, at first order, $\delta_{1\text{tom}} = \delta \rho_{1\text{tom}}/\rho_0$, and at second order $\delta_{2\text{tom}} = \delta \rho_{2\text{tom}}/\rho_0$.

Alternatively, we can perform a similar transformation and define the comoving gauge (denoted with a subscript $\text{com}$) where the three velocity of the fluid vanishes $v_{\text{com}} = 0$. Then, imposing orthogonality of the constant time hypersurfaces to the four velocity, requires $v_{\text{com}} + B_{\text{com}} = 0$. In this case, one finds that $\alpha_{1\text{com}} = v_{1\ell}$, just as in the total matter gauge. Thus, the matter density in the comoving gauge at linear order, $\delta \rho_{1\text{com}}$ reproduces the expression in (2.14). The corresponding Poisson equation

$$\nabla^2 \varphi_{1\ell} = 4\pi G a^2 \rho_0 \delta_{1\text{com}}, \quad (2.17)$$

has been recovered in previous works [5, 29]. It has further been shown that with the same combination of variables (namely $\delta_{1\text{com}}, \varphi_{1\ell}, v_{1\ell}$) one can reproduce the equations used in Newtonian hydrodynamics at linear order [18, 19], with the exception of fluids with non-vanishing pressure, and which allow for entropy perturbations [30].

However, while at first order the gauge transformation from the longitudinal gauge into both the total matter and comoving gauges requires only knowledge of the temporal component of the gauge generating vector, at second order we require the spatial component scalar $\beta_1$. In particular, the gauge transformation $\delta_{2\ell} \rightarrow \delta_{2\text{com}}$ includes time integrals in $\beta_{1\text{com}}$, which may introduce non-local terms. Therefore, in this work we avoid this additional complication by working with the density fluctuation in the total matter gauge.

Indeed, constructing the scalar $\beta_{1\text{tom}}$, which is determined by the transformation $E_{1\text{tom}} = E_{1\ell} + \beta_{1\text{tom}} = 0$, we note that it does not involve a time integral. Explicitly

$$\beta_{1\text{tom}|\ell} = 0. \quad (2.18)$$

### III. THE CONSTRAINT AT SECOND ORDER

In the previous section we have shown how the linear energy and momentum constraint equations can be combined to obtain a Poisson equation at first order. The same procedure can be followed to write a Poisson-like constraint at second order, although the manipulation of terms is obviously more complicated.

We will only consider scalar perturbations in the following. Whereas at linear order in perturbation theory, scalar, vector, and tensor perturbations decouple, this is no longer the case at second order (see e.g. Ref. [26]). However, since the amplitude of vector and tensor perturbations is in general much smaller than that of the scalars, we will still capture the dominant features of the theory, incurring only a small error. We will revisit this issue in a future publication.
A. Second-order equations

The energy constraint at second order in a non-specific gauge form is
\[ 3H(\psi_2 + H\phi_2) + \nabla^2 \left( H(B_2 - E_2) - \psi_2 \right) + \nabla^2 B_1 \left( \nabla^2 E_1 - \frac{1}{2} B_1 \right) - 2\psi_1 \]
\[ + B_1, 0 \left( H(3HB_1, i - 2\nabla^2 E_1, i - 2(\psi_1 + \phi_1, i)) - 2\psi_1 \right) + 2E_1, ij(\psi_1 - 2HB_1, ij) \]
\[ + 4H(\psi_1 - \phi_1) \left( 3\psi_1 - \nabla^2 (E_1 - B_1) \right) + E_1, ij \left( 4HE_1 + \frac{1}{2} B_1 \right), \]
\[ + \psi_1 \left( 2\nabla^2 (E_1 - 2HE_1) - 3\psi_1 \right) + \psi_1 \left( 2\nabla^2 E_1 - 3\psi_1 \right) + 2\nabla^2 \psi_1 (\nabla^2 E_1 - 4\psi_1) \]
\[ - 12H^2 \phi_1 + \frac{1}{2} \left( B_{1, ij} B_{1, ij} + \nabla^2 E_1, j \nabla^2 E_1, j - E_1, ij E_1, ij - \nabla^2 E_1, ij \right) \]
\[ \times \left( \frac{\phi_1}{3} \right) + 2(\rho_0 + \rho) \left( V_{1, i} - 2(1 + w) v_{1, i} + \delta \rho \right) \]  \hspace{1cm} (3.1)
while the momentum constraint is
\[ \psi_1, ij + H\phi_2, i - E_1, ij (\psi_1 + \phi_1 + \nabla^2 E_1), j + B_{1, ij} (2HB_1 + \phi_1), j \]
\[ - \left[ V_{1, i} (\nabla^2 E_1 - \psi_1) \right] - \phi_1, i \left( 8H\phi_1 + 2\psi_1 + \nabla^2 (E_1 - B_1) \right) \]
\[ - B_{1, j} \psi_1, j + 2\phi_1, ij E_1, i + E_1, ij E_1, ij - \psi_1 (\nabla^2 E_1 + 4\phi_1) - \nabla^2 \psi_1 B_{1, i} \]
\[ = -4\pi Ga^2 \left( \rho_0 + \rho \right) \left( V_{2, i} - 2(1 + w) v_{1, i} + \delta \rho \right) \]  \hspace{1cm} (3.2)
These equations simplify if we specify a particular gauge. We choose the longitudinal gauge, as in the first-order analysis above (this gauge is extended to the Poisson gauge when vectors and tensors are included and also subjected to the shear-free gauge condition). In the longitudinal gauge Eq. (3.1) takes the form
\[ 3H(\psi_2 + H\phi_2) - \nabla^2 \psi_2 - 3\phi_1^2 - 3\phi_1 v_1, k \phi_1, k - 8\phi_1 v_1, k \phi_1, k - 12H^2 \phi_1 \]
\[ = -4\pi Ga^2 \rho_0 \left( \delta \rho_2 + 2(1 + w) v_1, k v_1, k \right) \]  \hspace{1cm} (3.3)
while Eq. (3.2) is reduced to
\[ (\psi_2 + H\phi_2), i + 2(\phi_1, i, \phi_1) - 8H\phi_1, i, \phi_1 - 2\phi_1, i, \phi_1 \]
\[ = -4\pi Ga^2 \rho_0 \left( \left( 1 + w \right) |v_{1, i}| - 6v_{1, i} \phi_1 + 2(1 + 2\phi_1) v_{1, i} \phi_1 + 2 \frac{1}{\rho_0} \delta P_{nadi} v_{1, i} \right) \]  \hspace{1cm} (3.4)
Here \( w = P_0 / \rho_0 \) is the equation of state of the fluid, and the non-adiabatic pressure perturbation, \( \delta P_{nadi} \), is defined as
\[ \delta P_{nadi} = \delta P_1 - c_2^2 \delta \rho \]  \hspace{1cm} (3.5)

Following the steps of the procedure at first order, we take the spatial divergence of Eq. (3.3) and integrate with the inverse Laplacian operator \( \nabla^{-2} \). We obtain
\[ \psi_2 + H\phi_2 + \left( \phi_1 \right) = -4H\phi_1 - 2\nabla^2 \left( \phi_1, i, \phi_1 \right) \]
\[ = -4\pi Ga^2 \rho_0 \left( \left( 1 + w \right) |v_{2, i} - 6v_{1, i} \phi_1| + 2(1 + 2\phi_1) v_{1, i} \phi_1 + 2 \frac{1}{\rho_0} \delta P_{nadi} v_{1, i} \right) \]  \hspace{1cm} (3.6)
We can now substitute this into Eq. (3.3) to arrive at
\[ \nabla^2 \psi_2 + \frac{3}{2} \nabla^2 \left( \phi_1 \right) + 3 \phi_1 v_1, k \phi_1 + 3H \phi_1 + 6H \nabla^2 \left[ \phi_1, i, \phi_1 \right] \]
\[ = -4\pi Ga^2 \rho_0 \left( \delta 2\rho - 3H(1 + w)v_{2, i} + 2(1 + w)v_{1, i, i} + 6H \nabla^2 \left( \left( 1 + w \right) \phi_1 \right) \right) \]  \hspace{1cm} (3.7)
B. The Poisson equation at second order

To write the second-order equivalent of the Poisson equation in \[2.10\], we must transform the density contrast to the total matter gauge. The transformation rule at second order is given in \[2.26\], Eq. (6.20)]

\[
\begin{align*}
\tilde{\delta}_{2\text{tom}} &= \delta_{2\ell} + \rho_0 \alpha_{2\text{tom}} + \alpha_{1\text{tom}}(\rho_0 \alpha_{1\text{tom}} + \rho_0 \alpha_{1\text{tom}} + 2 \delta'_{1\ell}).
\end{align*}
\] (3.8)

The second-order \(\alpha_{2\text{tom}}\) evaluated in the longitudinal gauge is found with the aid of expression (2.100) in Ref. 31 and using Eqs. (2.14) and (2.15). We obtain

\[
\alpha_{2\text{tom}} = v_{2\ell} - \mathcal{H} v_{2\ell}^2 + \frac{1}{2} (v_{2\ell}')^2 - 4 \nabla^2 \left[ v_{1\ell,j} (\phi_{1\ell} - v_{1\ell}') \right]^j.
\] (3.9)

With the aid of the background equations and the expressions for \(\alpha_{1\text{tom}}\) in Eq. \[2.14\] and \(\delta_{1\text{tom}}\) in Eq. \[2.15\] we obtain the gauge transformation,

\[
\begin{align*}
\tilde{\delta}_{2\text{tom}} &= \delta_{2\ell} - 3 \mathcal{H} (1 + w) v_{2\ell} - 3 \mathcal{H} (1 + w) v_{1\ell} \delta_{1\text{tom}} + 2 v_{1\ell} \delta_{1\text{tom}}^j + 12 \mathcal{H} (1 + w) \nabla^2 \left[ v_{1\ell,j} (\phi_{1\ell} + v_{1\ell}') \right] + 3 \mathcal{H} w' - \frac{3}{2} \mathcal{H}^2 (1 + w) (5 + 9 w) v_{2\ell}.
\end{align*}
\] (3.10)

We substitute the \(\delta_{\ell}\) factors at both orders into Eq. \[3.7\] for the total matter gauge equivalents. The final expression in terms of \(\delta_{1\text{tom}}, \phi_{1\ell}\) and \(v_{1\ell}\) is then

\[
\begin{align*}
\nabla^2 \psi_{2\ell} + \frac{3}{2} \nabla^2 (\phi_{2\ell}') + 3 (\phi_{2\ell}')^2 + 5 \phi_{1\ell} \nabla^2 \phi_{1\ell} + 3 \mathcal{H} (\phi_{2\ell}') - 6 \mathcal{H} \nabla^2 \left[ \phi_{1\ell} \phi_{1\ell}' \right] & = 4 \pi G a^2 \rho_0 \left\{ \delta_{2\text{tom}} + 6 \mathcal{H} (1 + w) v_{1\ell} \delta_{1\text{tom}} - 2 v_{1\ell} \delta_{1\text{tom}}^j + 2 (1 + w) v_{1\ell,j} (1 + w) (3 w - 1) v_{1\ell}
\end{align*}
\] (3.11)

This rather long equation fulfills our first goal, to provide a Poisson equation at second order using the same variables employed in the structure formation studies at the Newtonian limit. It is already clear that adopting the expression \(\nabla^2 \psi_2 = 4 \pi G a^2 \rho_0 \delta_2\) leaves out most of the terms of the actual second order Poisson constraint.

To conclude this section, let us rewrite Eq. \[3.11\] in terms of the potential \(\phi_{2\ell}\) instead of \(\psi_{2\ell}\). This will come handy in the next section since primordial non-Gaussianity is conventionally formulated in terms of this variable. We use the traceless \(ij\) component of the field equations, derived from the Eq. (A.1) in \[31\], written in the longitudinal gauge as

\[
\begin{align*}
\nabla^4 (\psi_{2\ell} - \phi_{2\ell}) = -4 \nabla^4 (\phi_{2\ell}') + 2 \phi_{1\ell,j} \phi_{1\ell,i,j} + 6 \nabla^2 \phi_{1\ell} \nabla^2 \phi_{1\ell} + 8 \phi_{1\ell,j} \nabla^2 \phi_{1\ell,j} + 4 \mathcal{H} \nabla^2 \phi_{1\ell} - 6 \mathcal{H} \phi_{1\ell,j} \phi_{1\ell} 
\end{align*}
\] (3.12)

Upon substitution of this in the constraint equation, Eq. \[3.11\], and with some algebra we arrive at

\[
\begin{align*}
\nabla^4 (\phi_{2\ell}' - 2 \nabla^4 (\phi_{2\ell}') + 7 \nabla^2 (\phi_{1\ell} \nabla^2 \phi_{1\ell}) + 3 \nabla^2 \phi_{1\ell}' \nabla^2 \phi_{1\ell} + 3 \phi_{1\ell} \nabla^2 \phi_{1\ell}' \nabla^2 \phi_{1\ell} + 3 \mathcal{H} \nabla^2 \phi_{1\ell}') - 6 \mathcal{H} \phi_{1\ell,j} \phi_{1\ell} 
\end{align*}
\] (3.13)

This constraint is valid for any perfect fluid. In the following section we show how to insert this constraint in the initial conditions of numerical simulations of structure formation.
IV. NON-GAUSSIAN INITIAL CONDITIONS FOR NUMERICAL SIMULATIONS

The Newtonian Poisson equation is used at all orders as a constraint to the initial conditions in numerical simulations. However, the above constraint is the one that provides consistency with General Relativity. Imposed at an initial time, this constraint is met at all times if the perturbations are evolved in the context of GR. It is therefore useful to write the expression we have derived in terms of variables employed in numerical simulations, namely $\delta_{\text{1tom}}$, and $v_{1\ell}$, evaluated at some initial time. Here we derive such an expression with the aid of the first order equations, Eqs. (2.9), (2.16), and the continuity equation from Ref. [30] in terms of the chosen gauge. These help us to replace $\delta$, to write all of first order variables in terms of the first order Poisson equation (2.16) and the momentum constraint at first order. Explicitly, in Fourier space,

$$
\nabla^4 \phi_{2\ell} - 2\nabla^4 (\phi_{1\ell}^2) + 7\nabla^2 (\phi_{1\ell} \nabla^2 \phi_{1\ell}) + 3(\nabla \phi_{1\ell})^2 - 3\phi_{1\ell} \nabla^4 \phi_{1\ell} = 4\pi G \rho_0 \left\{ \nabla^2 \delta_{\text{2tom}} + 6(1 + w) \left[ v_{1\ell} \nabla^4 v_{1\ell} - (\nabla^2 v_{1\ell})^2 - \frac{2}{3} \nabla^2 (v_{1\ell} \nabla^2 v_{1\ell}) + \frac{3}{4}(1 + w)H^2 \nabla^2 (v_{1\ell}^2) \right] \right. 
$$

$$
\left. + 6H \nabla^2 (v_{1\ell} \delta_{1\ell}) + 6(1 + w)H \left[ v_{1\ell,j} \left( 2\phi_{1\ell} - \frac{c_s^2 - 1}{1 + w} \delta_{\text{1tom}} + \frac{1}{1 + w} \frac{\delta P_{\text{nad1}}}{\rho_0} \right) \right] j \right\}. \tag{4.1}
$$

We emphasise that the Newtonian counterpart of this constraint is a linear equation which includes only the first term at each side of the equality. All the other terms bring relativistic contributions to the Poisson equation. This expression can be used in the numerical simulations that set initial conditions for perturbations of any perfect fluid and allowing for entropy perturbations.

To reduce Eq. (4.1) further, we can either eliminate the density contrast $\delta_{\text{1tom}}$ or the potential $\phi_{1\ell}$ via the first-order Poisson equation (2.16). This proves useful when we want to make contact with formulations like the so-called renormalised perturbation theory (RPT) [32], where the initial conditions are set, order by order in Fourier space, via recursive relations in powers of $\delta_{\text{IN}}$ (see, e.g., Ref. [3]). To reduce things further, let us focus on the case of an Einstein-de Sitter universe, a flat space-time filled by dust, i.e., where $w = 0$ as well as $\delta P_1 = 0$ and $\Lambda = 0$. In this case, Eq. (4.1) is reduced to

$$
\nabla^4 \phi_{2\ell} - 2\nabla^4 (\phi_{1\ell}^2) + 7\nabla^2 (\phi_{1\ell} \nabla^2 \phi_{1\ell}) + 3\phi_{1\ell} \nabla^4 \phi_{1\ell} + 3(\nabla^2 \phi_{1\ell})^2 = 4\pi G \rho_0 \left\{ \nabla^2 \delta_{\text{2tom}} + \frac{9}{2} H^2 \nabla^2 v_{1\ell}^2 + 2 \left[ 3v_{1\ell} \nabla^4 v_{1\ell} - 3(\nabla^2 v_{1\ell})^2 - 2\nabla^2 (v_{1\ell} \nabla^2 v_{1\ell}) \right] \right. 
$$

$$
\left. + 6H \nabla^2 (v_{1\ell} \delta_{1\ell}) + 6H \left[ v_{1\ell,j} \left( 2\phi_{1\ell} - \delta_{\text{1tom}} \right) j \right] \right\}. \tag{4.2}
$$

With the aim of incorporating our result as an initial constraint in the formulation of non-linear initial conditions for numerical simulations, we transform Eq. (4.2) to the Fourier space. Additionally, as is customary in structure formation studies, we work exclusively with the growing mode of perturbations, where $\phi_{1\ell} = \text{const}$. It is then possible to write all of first order variables in terms of $\delta_{\text{1tom}}$ (as in the standard perturbation theory, c.f. Ref. [3]) with the aid of the first order Poisson equation (2.16) and the momentum constraint at first order. Explicitly, in Fourier space,

$$
\phi_{1\ell}(k) = -\frac{3}{2} \frac{H^2}{k^2} \delta_{\text{1tom}}(k), \quad v_{1\ell}(k) = \frac{H}{k^2} \delta_{\text{1tom}}(k). \tag{4.3}
$$

The second relation above follows directly from Eq. (2.10) and the first equivalence above, keeping in mind that we are working with the growing mode exclusively. The reduced Poisson equation at second order is

$$
k^4 \phi_{2\ell}(k) + \frac{3}{2} k^2 H^2 \delta_{\text{2tom}}(k) = \frac{3}{2} \int d^3p d^3q \delta_D(p + q - k) \left\{ \frac{H^4}{p^2 q^2} \times \left\{ 3|p| + q^4 + \frac{15}{4} (p^4 + q^4) - \frac{35}{4} |p + q|^2 (p^2 + q^2) - \frac{15}{2} q^2 - \frac{9}{2} H^2 |p + q|^2 \right\} \delta_{\text{1tom}}(p) \delta_{\text{1tom}}(q) \right\}, \tag{4.4}
$$

where $\delta_D(k)$ is the Dirac delta function and where $k$-modes in the integral are represented by $k = |p + q|$. This equation represents a concrete constraint for initial conditions of numerical simulations, consistent with GR, and written in terms of relativistic equivalents to the gravitational potential and the matter density perturbation. Note that, while the linear equation of Ref. [20] is valid for these second order variables at small scales, the relativistic corrections obtained here become increasingly important as the perturbation modes approach the horizon scale.

Since this constraint already carries couplings between different perturbation modes, there will be some intrinsic non-Gaussianity induced by this second-order correspondence. This is a known effect of GR which has recently been
explored in the CMB through the use of second order Boltzmann codes \cite{33,35}, and in the matter density field \cite{28}. Here we disentangle the effect of the initial constraint from the influence of the non-linear evolution of perturbations. To observe the type of non-Gaussianity induced by the GR constraint, we introduce three templates that constitute a basis for the non-Gaussian $\phi_2$. These templates are also a basis to represent the initial conditions of the density contrast with primordial non-Gaussianity, and consistent with GR, for a given model of structure formation.

Following the convention of \cite{34}, for the non-Gaussianity in the lapse function, the local template is,

$$\phi_2^{loc} = \phi_{2G} + f_{NL}^{loc} [\phi_{2G} - \langle \phi_{2G} \rangle].$$

(4.5)

This is preserved in super-horizon scales since $\phi_2$ is constant when the universe is filled with dust. Therefore, we can directly substitute the primordial $\phi_2$ in the Poisson constraint (4.4).

In Fourier space, the local configuration in Eq. (4.5) yields

$$\frac{1}{2}f_2^{loc}(k) = \frac{9}{4}f_{NL}^{loc} \int d^3p d^3q \frac{1}{p^2 q^2} \delta^3_D(p + q - k) \left( \frac{H^4}{p^2 q^2} \right) \delta_{1tom}(p) \delta_{1tom}(q),$$

(4.6)

and we can generate a kernel for $\delta_{2tom}^{loc}$,

$$\frac{k^2}{H^2} \delta_{2tom}^{loc}(k) = \int d^3p d^3q \frac{1}{p^2 q^2} \delta^3_D(p + q - k) \times \left\{ 3 \left[ 1 - f_{NL}^{loc} \right] |p + q|^4 + \frac{15}{4} (p^4 + q^4) - \frac{35}{4} (p^2 + q^2)^2 - \frac{15}{2} p^2 q^2 + \frac{9}{2} H^2 |p + q|^2 \right\} \delta_{1tom}(p) \delta_{1tom}(q).$$

(4.7)

Note that the primordial non-Gaussianity of the local configuration has the same momentum dependence as one of the terms if the relativistic constraint in Eq. (4.4). This is shown explicitly in the last equation and we can interpret this as an intrinsic relativistic contribution to the non-Gaussianity observable in the Large scale structure. We denote this GR contribution as $f_{NL}^{GR}$ with a numerical value $f_{NL}^{GR} = -1$. Repeating the procedure for the equilateral and orthogonal configurations, we can provide initial conditions for $\delta_{2tom}$ in a complete basis for primordial non-Gaussian perturbations. We borrow the templates implemented in Ref. \cite{17}. For the equilateral configuration, this template is

$$\frac{1}{2}f_2^{eq}(k) = \frac{9}{4}f_{NL}^{eq} \int d^3p d^3q \frac{1}{p^2 q^2} \delta^3_D(p + q - k) \times \left\{ -3 |p + q|^4 + (p^2 - q^2)^2 |p + q|^2 + 2(p + q) |p + q|^3 \right\},$$

(4.8)

while in the orthogonal case

$$\frac{1}{2}f_2^{ort}(k) = \frac{9}{4}f_{NL}^{ort} \int d^3p d^3q \frac{1}{p^2 q^2} \delta^3_D(p + q - k) \times \left\{ -9 |p + q|^4 + (p^2 - q^2)^2 |p + q|^2 + 5(p + q) |p + q|^3 \right\}.$$  

(4.9)

Finally the complementary equilateral and orthogonal kernels for $\delta_{2tom}$ are

$$\frac{k^2}{H^2} \delta_{2tom}^{eq}(k) = \int d^3p d^3q \frac{1}{p^2 q^2} \delta^3_D(p + q - k) \times \left\{ 3 \left[ 1 + 3 f_{NL}^{eq} \right] |p + q|^4 - \frac{1}{4} (12 f_{NL}^{eq} + 35) |p + q|^2 (p^2 + q^2) + 6 f_{NL}^{eq} (p^2 + q^2 |p + q|^2 - |p + q|^3 (p + q)) 

+ \frac{15}{4} (p^4 + q^4) - \frac{15}{2} p^2 q^2 + \frac{9}{2} H^2 |p + q|^2 \right\} \delta_{1tom}(p) \delta_{1tom}(q),$$

(4.10)

$$\frac{k^2}{H^2} \delta_{2tom}^{ort}(k) = \int d^3p d^3q \frac{1}{p^2 q^2} \delta^3_D(p + q - k) \times \left\{ 3 \left[ 1 + 9 f_{NL}^{ort} \right] |p + q|^4 - \frac{1}{4} (48 f_{NL}^{ort} + 35) |p + q|^2 (p^2 + q^2) + 3 f_{NL}^{ort} (8 |p + q|^2 pq - 5 |p + q|^3 (p + q)) 

+ \frac{15}{4} (p^4 + q^4) - \frac{15}{2} p^2 q^2 + \frac{9}{2} H^2 |p + q|^2 \right\} \delta_{1tom}(p) \delta_{1tom}(q).$$

(4.11)
These three kernels represent a complete basis for the primordial bispectrum. The kernels above show that the Poisson constraint yields different contributions for the local, equilateral and orthogonal configurations. The relativistic initial conditions can mimic non-Gaussian contributions as discussed after Eq. (4.7). This intrinsic relativistic non-Gaussian imprint in the matter fluctuation has a value in the local template of $f_{NL}^{loc(\text{GR})} = -1$ (this is particularly relevant in studies of LSS since it is the dominant configuration contributing to the halo bias \cite{37,38}).

In the equilateral configuration, we can read the intrinsic GR contributions to $f_{NL}$ from the parentheses in Eq. (4.10). The dominant contribution is $f_{NL}^{eq(\text{GR})} = 35/12$, while for the orthogonal configuration, we read from Eq. (4.11) $f_{NL}^{ort(\text{GR})} = 35/48$ as a dominant contribution. Note that, although there is an extra contribution of GR to $f_{NL}^{\text{GR}}$ in each one of these configurations, we quote the largest numerical value for each case.

The result obtained for the intrinsic non-Gaussianity in the local configuration is compared with that of Ref. \cite{28}, for the equivalent case of the Poisson gauge, in the appendix A. A detailed analysis of the modification of $f_{NL}$ separating initial constraints from the non-linear evolution of $\delta^2$ in the synchronous-comoving gauge is the subject of a recent paper \cite{39}. For our purposes, it suffices to emphasise that the results of this section are written in terms of the GR variables that find a direct correspondence with the Newtonian ones, since we intend to present initial conditions for the numerical studies of galaxy formation.

V. DISCUSSION

In this paper we have derived the relationship between the energy density fluctuation and the curvature perturbation at second order in the context of cosmological perturbation theory. This Poisson equation at second order, presented in Eq. (4.1) in full generality for a single fluid including entropy perturbations, is expressed in terms of variables equivalent to an Eulerian set in Newtonian hydrodynamics. We found that the Poisson equation takes a particularly simple form at second order if the matter density fluctuation is expressed in the total matter gauge, and not the comoving orthogonal gauge which has been used before at first order. For the Poisson equation, the difference of the two gauges only becomes apparent at second order in perturbation theory.

As an example, we calculate the second order Poisson equation in the case of an Einstein-de Sitter universe, and present the result in Eq. (4.4) in Fourier space. We show how to incorporate primordial non-Gaussianity into the matter perturbation at second order in an equation consistent with GR. In this way, we can also quantify the non-Gaussianity intrinsic to GR contributions. Our results generalise the non-Gaussian kernels presented in terms of Newtonian physics in Ref. \cite{17} to include relativistic terms. We show that the non-linearity of GR induces a non-Gaussian signature in addition to the primordial value. In particular we find, in the local configuration, a value $f_{NL}^{loc(\text{GR})} = -1$, consistent with that obtained in Ref. \cite{28} in the Poisson gauge.

Achieving consistency with the result of \cite{28} in this limit shows the strength of our results since we can recover the primordial and the GR contribution to non-Gaussianity in $\delta^2(\tau, x)$ in a $\Lambda$-CDM universe without solving the field equations. Our result, the Poisson equation at second order, and the example presented in this paper provide fairly simple equations that can be directly incorporated into generators of initial conditions for numerical simulations which take care of the evolution of fluctuations. The initial conditions generated in this way account for general relativistic effects in N-body codes and other numerical simulations of structure formation.

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Appendix A: Comparison with previous work

In this appendix we show that our result is consistent with that reported in \cite{28} at the level of initial conditions, and that the difference at face is only due to the definitions used in that paper.

Let us first note that the transformations performed to change the matter variable $\delta^2_x$ to $\delta^2_{\text{com}}$ do not modify the curvature sector of the Poisson equation as can be seen from comparing Eqs. (3.7) and (3.11). The only modification
to the curvature dependence is due to the change of variables from \( \psi_{2\ell} \) to \( \phi_{2\ell} \). The relevant terms that determine the local configuration of non-Gaussianity and its GR correction are, from Eq. (5.13),

\[
\nabla^4 \phi_{2\ell} - 2\nabla^4 (\phi_{1\ell}^2) + \ldots
\]

(A.1)

Note that the analysis of Sec. IV does not modify these terms and ultimately, using the definition (A.5), this second term is responsible for the GR induced non-Gaussianity, which yields \( f_{\text{NL}}^{\text{loc} (GR)} = -1 \).

The above argument shows that the same value for induced non-Gaussianity is recovered when we work with all variables in the longitudinal gauge. The corresponding result in [28] is derived from the first term of Eq. (31), that is,

\[
f_{NL}^R \supset \left[ \frac{5}{3} (a_{NL} - 1) + 1 - \frac{g(\tau)}{g_{in}} - \frac{1}{2} \frac{B_1(\tau)}{g(\tau)g_{in}} \right],
\]

(A.2)

where the functions of time have an explicit argument and play no role in the initial conditions. The parameter \( a_{NL} \) is defined in terms of the curvature perturbation in uniform density hypersurfaces by the equivalence \( \zeta = 2 \zeta^2 \).

Subsequently, the definition of the parameter \( f_{NL}^R \) in Ref. [40] indicates that

\[
\zeta_2 = \left( \frac{6}{5} f_{NL}^R + 2 \right) \zeta_1^2 \Rightarrow a_{NL} - 1 = \frac{3}{5} f_{NL}^R.
\]

(A.3)

This definition is not stated explicitly in [28] but it is implied by the limits discussed at the end of Sec. 2 of that paper. The primordial non-Gaussianity in this case is thus given by \( f_{NL}^R \). We can then subtract the primordial non-Gaussianity from Eq. (A.2) and ignore the time-dependent part to find that

\[
f_{NL}^{P(GR)} = 1.
\]

(A.4)

Let us finally note that the parameter \( f_{NL}^R \) is constructed from the definitions in Eqs. (4) and (5) of [28]. For our variables this implies that

\[
\phi_{2\ell} = -2 f_{NL}^R (\phi_{1\ell} - \phi_{1\ell}^G).
\]

(A.5)

In view of Eq. (A.5) we find the equivalence \( f_{NL}^{P(GR)} = -f_{NL}^{\text{loc} (GR)} \) and thus recover the result obtained in the body of the paper.

[1] E. Hawkins, S. Maddox, S. Cole, D. Madgwick, P. Norberg, et al., Mon.Not.Roy.Astron.Soc. 346, 78 (2003), astro-ph/0212375.
[2] D. J. Eisenstein et al. (SDSS Collaboration), Astron.J. 142, 72 (2011), 1101.1529.
[3] D. Schlegel et al. (BigBoss Experiment) (2011), 1106.1506.
[4] R. Laureijs, J. Amiaux, S. Arduini, J.-L. Augueres, J. Brinchmann, et al. (2011), 1110.3193.
[5] P. Peebles, The Large-Scale Structure of the Universe, Princeton Series in Physics Series (Princeton University Press, 1980), ISBN 9780691082400.
[6] F. Bernardeau, S. Colombi, E. Gaztanaga, and R. Scoccimarro, Phys.Rept. 367, 1 (2002), astro-ph/0112551.
[7] A. Evrard et al. (VIRGO Collaboration), Astrophys.J. 573, 7 (2002), astro-ph/0110246.
[8] M. Crocce, P. Fosalba, F. J. Castander, and E. Gaztanaga, Mon.Not.Roy.Astron.Soc. 403, 1353 (2010), 0907.0019.
[9] S. Habib, V. Morozov, H. Finkel, A. Pope, K. Heitmann, et al. (2012), 1211.4864.
[10] Y. Zeldovich, Astron.Astrophys. 5, 84 (1970).
[11] A. Yoshisato, M. Morikawa, N. Gouda, and H. Mouri, Astrophys.J. 637, 555 (2006), astro-ph/0510107.
[12] M. Croce, S. Pueblas, and R. Scoccimarro, Mon.Not.Roy.Astron.Soc. 373, 369 (2006), astro-ph/0606505.
[13] E. Sirko, Astrophys.J. 634, 728 (2005), astro-ph/0505106.
[14] T. Buchert, A. Melott, and A. Weiss, Astron.Astrophys. 288, 349 (1994), astro-ph/9309056.
[15] N. Dalal, O. Dore, D. Huterer, and A. Shirokov, Phys.Rev. D77, 123514 (2008), 0710.4560.
[16] V. Desjacques, U. Seljak, and I. Iliev (2008), 0811.2748.
[17] R. Scoccimarro, L. Hui, M. Manera, and K. C. Chan, Phys.Rev. D85, 083002 (2012), 1108.5512.
[18] N. E. Chisari and M. Zaldarriaga, Phys.Rev. D83, 123505 (2011), 1101.3555.
[19] S. R. Green and R. M. Wald, Phys.Rev. D85, 063512 (2012), 1111.2997.
[20] J.-c. Hwang, H. Noh, and J.-O. Gong, Astrophys.J. 752, 50 (2012), 1204.3345.
[21] M. Bruni, R. Crittenden, K. Koyama, R. Maartens, C. Pitrou, et al., Phys.Rev. D85, 041301 (2012), 1106.3999.
[22] V. Desjacques and U. Seljak, Class.Quant.Grav. 27, 124011 (2010), 1003.5020.
[23] J. M. Bardeen, Phys. Rev. D22, 1882 (1980).
[24] V. F. Mukhanov, H. A. Feldman, and R. H. Brandenberger, Phys. Rept. **215**, 203 (1992).
[25] H. Kodama and M. Sasaki, Prog. Theor. Phys. Suppl. **78**, 1 (1984).
[26] K. A. Malik and D. Wands, Phys. Rept. **475**, 1 (2009), 0809.4944.
[27] K. A. Malik and D. R. Matravers, Class. Quant. Grav. **25**, 193001 (2008), 0804.3276.
[28] N. Bartolo, S. Matarrese, O. Pantano, and A. Riotto, Class. Quant. Grav. **27**, 124009 (2010), 1002.3759.
[29] D. Wands and A. Slosar, Phys. Rev. **D79**, 123507 (2009), 0902.1084.
[30] A. J. Christopherson, J. C. Hidalgo, and K. A. Malik, JCAP **1301**, 002 (2013), 1207.1870.
[31] A. J. Christopherson, Ph.D. thesis, University of London (2011), 1106.0446.
[32] M. Crocce and R. Scoccimarro, Phys. Rev. **D73**, 063519 (2006), astro-ph/0509418.
[33] Z. Huang and F. Vernizzi (2012), 1212.3573.
[34] S.-C. Su, E. A. Lim, and E. Shellard (2012), 1212.6968.
[35] G. W. Pettinari, C. Fidler, R. Crittenden, K. Koyama, and D. Wands (2013), 1302.0832.
[36] E. Komatsu and D. N. Spergel, Phys. Rev. **D63**, 063002 (2001), astro-ph/0005036.
[37] S. Matarrese, L. Verde, and R. Jimenez, Astrophys. J. **541**, 10 (2000), astro-ph/0001366.
[38] M. Dias, R. H. Ribeiro, and D. Seery (2013), 1303.6009.
[39] M. Bruni, J. C. Hidalgo, N. Meures, and D. Wands (2013), 1307.1478.
[40] D. H. Lyth and Y. Rodriguez, Phys. Rev. **D71**, 123508 (2005), astro-ph/0502578.