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Adam J. Christopherson,[1, *] Juan Carlos Hidalgo,[2, †] Cornelius Rampf,[3, ‡] and Karim A. Malik[4, §]

[1] *Department of Physics, University of Florida, Gainesville, FL 32611, USA*
[2] *Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México,*
Av. Universidad S/N, Cuernavaca, Morelos, 62251, Mexico
[3] *Institute of Cosmology and Gravitation, University of Portsmouth,*
Dennis Sciama Building, Burnaby Road, Portsmouth, PO1 3FX, United Kingdom
[4] *Astronomy Unit, School of Physics and Astronomy,*
Queen Mary University of London, Mile End Road, London, E1 4NS, United Kingdom
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We use gauge-invariant cosmological perturbation theory to calculate the displacement field that sets the initial conditions for N-body simulations. Using first and second-order fully relativistic perturbation theory in the synchronous-comoving gauge, allows us to go beyond the Newtonian predictions and to calculate relativistic corrections to it. We use an Einstein–de Sitter model, including both growing and decaying modes in our solutions. The impact of our results should be assessed through the implementation of the featured displacement in cosmological N-body simulations.

I. INTRODUCTION

Recent years have seen tremendous progress in both observational and theoretical cosmology. The acquisition of new data allows us to test our theories and constrain parameters, enabling us to formulate the standard cosmological model. Observations of the 'late' universe include maps of the large-scale structure, which have been pioneered by the Sloan Digital Sky Survey (SDSS) [1, 2]. Current and future experiments including the Dark Energy Survey [3], the Large Synoptic Survey Telescope (LSST) [4] and the EUCLID satellite [5] will take even more data to build up a three dimensional image of the large-scale structure. By comparing the observed galaxy clustering with simulations, we have fairly conclusive evidence that, at the time of formation, the Universe was dominated by matter and, in turn, that the matter content was dominated by cold dark matter (CDM).

At early times the Universe is close to being homogeneous, and the inhomogeneities that lead to the large scale structure are small in amplitude. Perturbative techniques are therefore extremely powerful tools to model the early seeds of structure formation, such as those imprinted in the cosmic microwave background. To do this, we consider the inhomogeneities as small fluctuations about a homogeneous expanding background.

However, gravity is a nonlinear interaction, and in order to fully understand the process of structure formation, one must consider the (nonlinear) multistream regime. To tackle this, one has to resort in general to Vlasov–Poisson solvers. Commonly used solvers are discretised N-body simulations which aim to approximate the phase-space dynamics to high accuracy. The simulations themselves rely on Newtonian physics. Since the incoming data from surveys is of such high quality, we are now at a stage where relativistic corrections may become important and must be quantified. In particular, the EUCLID collaboration [5] requires its N-body simulations to have percent-level accuracy. Relativistic corrections can be important in simulations even using Newtonian physics and cold dark matter particles, when the size of the simulated box is the same as the horizon size at the time that the initial conditions are set. At that time, effects of general relativity on such large scales could likely become important.

Some recent work has focused on the effects of incorporating relativistic corrections into N-body simulations [6–9], or interpreting Newtonian simulations in terms of General Relativity [10, 11]. Since gravity is nonlinear, the simulations are extremely sensitive to the initial conditions used. So far, the initial conditions have been specified using only linear cosmological perturbation theory [12–14]. In this paper, we compute the second-order corrections to the initial conditions using cosmological perturbation theory and keeping the decaying mode at all orders.

* achristopherson@ufl.edu

† hidalgo@fis.unam.mx

‡ cornelius.rampf@port.ac.uk

§ k.malik@qmul.ac.uk

The paper is structured as follows: in the next section we present the governing equations for the system for background, linear and second-order perturbations. In Section III we solve the governing field equations in the synchronous-comoving gauge, order by order. In Section IV we calculate the Lagrangian displacement field, and in Section V we conclude.

II. GOVERNING EQUATIONS

In this section we present the governing equations needed to derive the relation between the input power spectra and the displacement fields later on. We use gauge-invariant cosmological perturbation theory, following largely the notation of Ref. [15].

Tensorial quantities are split, here using the energy density as an example, as

$$\rho = \rho_0 + \delta\rho_1 + \frac{1}{2}\delta\rho_2 \,, \tag{2.1}$$

up to second order. The background variables depend only on time, whereas the perturbations depend on all four coordinates x^μ. Derivatives with respect to conformal time are denoted by a prime. Greek indices, μ, ν, λ, run from $0, \ldots 3$, while lower case Latin indices, i, j, k, run from $1, \ldots 3$. Einstein summation over repeated indices is implied.

A. Metric tensor

We assume a spatially flat Friedmann–Lemaître–Robertson–Walker (FLRW) background, with metric

$$ds^2 = a^2 \left(-\mathrm{d}\eta^2 + \delta_{ij}\mathrm{d}x^i\mathrm{d}x^j \right) \,, \tag{2.2}$$

where η is conformal time, $a = a(\eta)$ the scale factor, and δ_{ij} is the background 3-metric. Cosmic time, measured by observers at fixed comoving spatial coordinates, x^i, is given by $t = \int a(\eta)\,\mathrm{d}\eta$.

The perturbed part of the metric tensor can be written as

$$\delta g_{00} = -2a^2\phi \,, \qquad \delta g_{0i} = a^2 B_i \,, \qquad \delta g_{ij} = 2a^2 C_{ij} \,. \tag{2.3}$$

The 0-i and the i-j components of the metric tensor can be further decomposed into scalar, vector and tensor parts

$$B_i = B_{,i} - S_i \,, \tag{2.4}$$

$$C_{ij} = -\psi\,\delta_{ij} + E_{,ij} + F_{(i,j)} + \frac{1}{2}h_{ij} \,. \tag{2.5}$$

where ϕ, B, ψ and E are scalar, S_i and F_i are vector, and h_{ij} is a tensor metric perturbation. Note, ϕ is usually referred to as the lapse function, and ψ as the curvature perturbation.

For the results of this paper we will consider only scalar perturbations. We will solely work in the synchronous-comoving gauge, which is specified by the gauge conditions

$$\begin{aligned} \phi_{1\mathrm{scm}} = 0 \,, \qquad B_{1\mathrm{scm}} = 0 \,, \qquad v_{1\mathrm{scm}} = 0 \,, \\ \phi_{2\mathrm{scm}} = 0 \,, \qquad B_{2\mathrm{scm}} = 0 \,, \qquad v_{2\mathrm{scm}} = 0 \,, \end{aligned} \tag{2.6}$$

at first and second order, where $v_{1\mathrm{scm}}$ and $v_{2\mathrm{scm}}$ are the velocity potentials at first and second order, respectively. This renders the remaining first and second-order perturbations gauge-invariant [15, 16].

We work in an Einstein–de Sitter universe, a reasonable restriction considering that we are interested in setting up initial conditions for structure formation at very early times where the impact of the cosmological constant is negligible. We however include also decaying modes, which could have significant impact on the early gravitational dynamics. To avoid cluttering the equations, and since there is no confusion possible, we will drop the subscript "scm" from now on.

B. The Einstein and energy-momentum tensors

The Einstein tensor, $G^\mu{}_\nu$, in the background is given by

$$G^0{}_0 = -\frac{3}{a^2}\mathcal{H}^2 \,, \qquad G^0{}_i = 0 \,, \qquad G^i{}_j = \frac{1}{a^2}\left(\mathcal{H}^2 - 2\frac{a''}{a}\right)\delta^i{}_j \,, \tag{2.7}$$

where $\mathcal{H} \equiv a'/a$, and a prime denotes a partial time derivative with respect to conformal time. For later convenience we also give the trace of the spatial part of the Einstein tensor, which in the background is

$$G^k{}_k = \frac{3}{a^2}\left(\mathcal{H}^2 - 2\frac{a''}{a}\right).$$

(2.8)

1. First order Einstein tensor

We now give the Einstein tensor in the synchronous-comoving gauge, for scalar perturbations only. At first order the 0-0 component of the perturbed Einstein tensor is given by

$$G^{0(1)}_0 = \frac{1}{a^2}\left[-2\nabla^2\psi_1 + 2\mathcal{H}\left(3\psi'_1 - \nabla^2 E'_1\right)\right],$$

(2.9)

the 0-i component is

$$G^{0(1)}_i = -\frac{2}{a^2}\psi'_{1,i},$$

(2.10)

and the i-j component is

$$G^{i(1)}_j = \frac{1}{a^2}\left(4\mathcal{H}\psi'_1 - 2\mathcal{H}\nabla^2 E'_1 - \nabla^2\psi_1 + 2\psi''_1 - \nabla^2 E''_1\right)\delta^i{}_j + \frac{1}{a^2}\left(\psi_1 + 2\mathcal{H}E'_1 + E''_1\right)^i{}_{,j}.$$

(2.11)

By contracting Eq. (2.11) with $\delta^j{}_i$ we obtain the first-order spatial trace

$$G^{k(1)}_k = \frac{1}{a^2}\left(12\mathcal{H}\psi'_1 - 4\mathcal{H}\nabla^2 E'_1 - 2\nabla^2\psi_1 + 6\psi''_1 - 2\nabla^2 E''_1\right).$$

(2.12)

2. Second order Einstein tensor

At second order in the perturbations we get for the 0-0 component of the Einstein tensor (e.g. Ref. [17]) in the synchronous-comoving gauge

$$\begin{aligned}
\frac{1}{2}G^{0(2)}_0 = \frac{1}{a^2}\Big[&-\nabla^2\psi_2 + \mathcal{H}\left(3\psi'_2 - \nabla^2 E'_2\right) + 12\mathcal{H}\psi_1\psi'_1 - 4\mathcal{H}\psi_1\nabla^2 E'_1 \\
&- 4\mathcal{H}\psi'_1\nabla^2 E_1 + 4\mathcal{H}E'_{1,ij}E^{ij}_{1,} - 3(\psi'_1)^2 + 2\psi'_1\nabla^2 E'_1 \\
&+ \frac{1}{2}\left(E'_{1,ij}E^{ij'}_{1,} - \nabla^2 E'_1\nabla^2 E'_1\right) - 8\psi_1\nabla^2\psi_1 - 3\psi_{1,k}\psi_1{}^k \\
&+ 2\nabla^2\psi_1\nabla^2 E_1 + 2\psi_{1,k}\nabla^2 E_1{}^k{}_, + 2E_{1,ij}\psi^{ij}_{1,} \\
&+ \frac{1}{2}\left(\nabla^2 E_{1,k}\nabla^2 E_1{}^k - E_{1,ijk}E^{ijk}_1\right)\Big],
\end{aligned}$$

(2.13)

for the 0-i component

$$\begin{aligned}
\frac{1}{2}G^{0(2)}_i = \frac{1}{a^2}\Big(&-\psi'_{2,i} - 4\psi_1\psi'_{1,i} - 4\psi'_1\psi_{1,i} + \nabla^2 E'_1\psi_{1,i} + 2\nabla^2 E_1\psi'_{1,i} - E^{jk'}_{1,}E_{1,jki} \\
&+ \nabla^2 E^k_1 E'_{1,ki} + \psi_1{}^k E'_{1,ki} - 2\psi'_{1,k}E_{1,i}{}^k\Big),
\end{aligned}$$

(2.14)

and for the i-j component

$$\frac{1}{2}G^{i(2)}_{\ j} = \frac{1}{2a^2}\Big(4\mathcal{H}\psi'_2 - 2\mathcal{H}\nabla^2 E'_2 - \nabla^2\psi_2 + 2\psi''_2 - \nabla^2 E''_2\Big)\delta^i_{\ j} + \frac{1}{2a^2}\Big(\psi_2 + 2\mathcal{H}E'_2 + E''_2\Big)_{,\ j}^{\ \ \ i}$$

$$+ \frac{1}{a^2}\Big[8\mathcal{H}\psi'_1\psi_1 - 4\mathcal{H}\left(\psi_1\nabla^2 E'_1 + \psi'_1\nabla^2 E_1\right) + (\psi'_1)^2 + 4\psi_1\psi''_1 - 4\psi_1\nabla^2\psi_1 - \psi'_1\nabla^2 E'_1$$

$$+ 4\mathcal{H}E'_{1,kl}E_1^{\ kl} + \frac{3}{2}E'_{1,kl}E'^{\ kl}_{1,} - \frac{1}{2}E_{1,klm}E_1^{\ klm} + \psi_{1,k}\nabla^2 E_1^{\ k} - 2\psi_1\nabla^2 E''_1 - 2\psi''_1\nabla^2 E_1$$

$$+ 2\nabla^2\psi_1\nabla^2 E_1 + 2E''_{1,kl}E_1^{\ kl} - 2\psi_{1,k}\psi_1^{\ k} + \frac{1}{2}\nabla^2 E_{1,k}\nabla^2 E_1^{\ k} - \frac{1}{2}\nabla^2 E'_1\nabla^2 E'_1\Big]\delta^i_{\ j}$$

$$+ \frac{1}{a^2}\Big[4\psi_1\psi_1^{\ i}_{\ ,j} + E_1^{\ ikl}E_{1,jkl} - 2\psi_1^{\ i}_{\ ,j}\nabla^2 E_1 - \left(\psi_{1,k} + \nabla^2 E_{1,k}\right)E_1^{\ ki}_{,\ j} + 2\psi_1^{\ ik}E_{1,kj}$$

$$+ 2\psi_1 E''_1{}^{\ i}_{,\ j} + 2\left(\psi''_1 + 2\mathcal{H}\psi'_1 - \nabla^2\psi_1\right)E_1^{\ i}_{,\ j} - 2E_1^{\ ik}E''_{1,kj} + \left(\psi'_1 + 4\mathcal{H}\psi_1\right)E'_1{}^{\ i}_{,\ j}$$

$$- 2E'_1{}^{\ ik}E'_{1,kj} - 4\mathcal{H}E_1^{\ ik}E'_{1,kj} + 3\psi_1^{\ i}\psi_{1,j} + \nabla^2 E'_1 E'_1{}^{\ i}_{,\ j}\Big]. \tag{2.15}$$

The trace of the last expression is

$$\frac{1}{2}G^{k(2)}_{\ k} = \frac{1}{2a^2}\Big(12\mathcal{H}\psi'_2 - 4\mathcal{H}\nabla^2 E'_2 - 2\nabla^2\psi_2 + 6\psi''_2 - 2\nabla^2 E''_2\Big)$$

$$+ \frac{1}{a^2}\Big[24\mathcal{H}\psi'_1\psi_1 - 8\mathcal{H}\left(\psi_1\nabla^2 E'_1 + \psi'_1\nabla^2 E_1\right) + 3(\psi'_1)^2 + 12\psi_1\psi''_1 - 8\psi_1\nabla^2\psi_1$$

$$- 2\psi'_1\nabla^2 E'_1 + 8\mathcal{H}E'_{1,kl}E_1^{\ kl} + \frac{5}{2}E'_{1,kl}E'^{\ kl}_{1,} - \frac{1}{2}E_{1,klm}E_1^{\ klm} + 2\psi_{1,k}\nabla^2 E_1^{\ k}$$

$$- 4\psi_1\nabla^2 E''_1 - 4\psi''_1\nabla^2 E_1 + 2\nabla^2\psi_1\nabla^2 E_1 + 4E''_{1,kl}E_1^{\ kl} - 3\psi_{1,k}\psi_1^{\ k}$$

$$+ \frac{1}{2}\nabla^2 E_{1,k}\nabla^2 E_1^{\ k} - \frac{1}{2}\nabla^2 E'_1\nabla^2 E'_1 + 2\psi_{1,jk}E_1^{\ jk}\Big]. \tag{2.16}$$

3. The energy-momentum tensor

As mentioned above, for simplicity we assume a pressureless perfect fluid with vanishing anisotropic stress and work in the synchronous-comoving gauge. For this setup, the time-time component of the energy-momentum tensor, $T^\mu_{\ \nu}$, is, up to second order,

$$^{(0)}T^0_{\ 0} = -\rho_0, \qquad ^{(1)}T^0_{\ 0} = -\delta\rho_1, \qquad ^{(2)}T^i_{\ j} = \delta\rho_2. \tag{2.17}$$

The rest of the components are zero up to second order in perturbations. Note the significant simplifications in the expression for the perturbed energy-momentum tensor compared to the general form (see e.g. Ref. [15]) that stem from the matter content and the choice of gauge.

C. Energy and momentum conservation

The energy-momentum conservation equations are given by

$$\nabla_\mu T^\mu_{\ \nu} = 0, \tag{2.18}$$

where ∇_μ is the covariant derivative. In the background, for the considered fluid, the $\nu = 0$ component from the above gives

$$\rho'_0 + 3\mathcal{H}\rho_0 = 0, \tag{2.19}$$

at first order,

$$\delta\rho'_1 + 3\mathcal{H}\delta\rho_1 - 3\rho_0\psi'_1 + \rho_0\nabla^2 E'_1 = 0, \tag{2.20}$$

and at second order

$$\delta\rho'_2 + 3\mathcal{H}\delta\rho_2 - 3\rho_0\psi'_2 + \rho_0\nabla^2 E'_2 - 6\psi'_1\delta\rho_1 + 2\delta\rho_1\nabla^2 E'_1$$

$$= 2\rho_0\Big(6\psi_1\psi'_1 - 2\psi_1\nabla^2 E'_1 - 2\psi'_1\nabla^2 E_1 + 2E'_{1,ij}E_1^{\ ij}\Big). \tag{2.21}$$

It is also often convenient to work in terms of the density contrast, δ, which is defined as

$$\delta_1 = \frac{\delta\rho_1}{\rho_0}\,, \qquad \delta_2 = \frac{\delta\rho_2}{\rho_0}\,, \tag{2.22}$$

at first and second order, respectively.

D.   Field equations

The Einstein field equations, governing the dynamics of spacetime, are

$$G^\mu{}_\nu = 8\pi G\, T^\mu{}_\nu\,, \tag{2.23}$$

where G is Newton's gravitational constant, and we have set the speed of light to unity. To reiterate, we consider an Einstein–de Sitter universe, i.e., one filled by pressureless dust and vanishing cosmological constant. The dust is modelled as a single and perfect fluid, which amounts to a continuum description for collisionless dark matter, valid before the first instance of shell-crossing.

1.   Background

The 0-0 component of Eq. (2.23) in the background yields the Friedmann equation

$$\mathcal{H}^2 = \frac{8\pi G}{3}\rho_0 a^2\,. \tag{2.24}$$

At zeroth order in perturbation theory, this is the only equation we require in addition to the continuity equation (2.19).

2.   First order

With the assumptions on the matter content given above, namely no pressure and no anisotropic stress, we have the following governing equations in the synchronous-comoving gauge at first order,

$$\psi_1' = 0\,, \tag{2.25}$$
$$\sigma_1' + 2\mathcal{H}\sigma_1 + \psi_1 = 0\,. \tag{2.26}$$

In an arbitrary gauge, the scalar shear is defined as $\sigma_1 \equiv -B_1 + E_1'$. This allows us to write the evolution equation for $\delta\rho_1$ as

$$\delta\rho_1' + 3\mathcal{H}\delta\rho_1 + \rho_0\nabla^2\sigma_1 = 0\,. \tag{2.27}$$

We find, however, more useful to rewrite Eq. (2.26) in terms of the metric function E_1. Using the definition of the shear scalar in the synchronous-comoving gauge,

$$\sigma_1 \equiv E_1'\,, \tag{2.28}$$

we obtain,

$$E_1'' + 2\mathcal{H}E_1' = -\psi_1\,. \tag{2.29}$$

E.   Second order

We now write the governing equations at second order. From integrating in time the divergence of Eq. (2.14), we get

$$\nabla^2\psi_2 = \nabla^2\psi_1\nabla^2 E_1 + 2\psi_{1,i}\nabla^2 E_{1,}{}^i + \psi_{1,ki}E_{1,}{}^{ki} + \frac{1}{2}\nabla^2 E_{1,k}\nabla^2 E_{1,}{}^k - \frac{1}{2}E_{1,ijk}E_{1,}{}^{ijk}\,. \tag{2.30}$$

From the trace of the i-j component of the field equations, Eq. (2.16) above, we find an evolution equation for $\nabla^2 E_2'$, that is

$$\nabla^2 E_2'' + 2\mathcal{H}\nabla^2 E_2' = 3\nabla^{-2}\Bigg[-\nabla^2\psi_1\nabla^2\psi_1 - \nabla^2\psi_{1,k}\left(2\psi_{1,}^{\ k} + \nabla^2 E_{1,}^{\ k}\right)$$

$$-\psi_{1,kl}\psi_{1,}^{\ kl} + \psi_{1,ijk}E_{1,}^{\ ijk} + \nabla^2 E_{1,k}'\nabla^2 E_{1,}^{\prime\ k} - E_{1,ijk}'E_{1,}^{\prime\ ijk}\Bigg]$$

$$-4\psi_1\nabla^2\psi_1 - 3\psi_{1,k}\psi_{1,}^{\ k} - 3E_{1,}^{\ kl}\psi_{1,kl} + \frac{5}{2}E_{1,kl}'E_{1,}^{\prime\ kl} - \frac{1}{2}\nabla^2 E_1'\nabla^2 E_1' + \nabla^2 E_1\nabla^2\psi_1\,, \tag{2.31}$$

where we have used Eq. (2.29), and Eq. (2.30) and its time derivative. Note that Eq. (2.31) is only assuming dust and neither assuming growing mode only nor Einstein–de Sitter.

III. SOLUTIONS TO THE FIELD EQUATIONS

In this section we solve the governing evolution equations as given in the above section, order by order. Here we shall report only the solutions in real space, for results in Fourier space see Appendix A.

A. Background

Equations (2.19) and (2.24) yield the well known dust solutions

$$\rho_0 \propto a^{-3}\,, \qquad a \propto \eta^2\,, \qquad \mathcal{H} = \frac{2}{\eta}\,. \tag{3.1}$$

B. First order

At linear order we find that the solutions to the system of governing equations, Eqs. (2.25)–(2.27), are given by

$$\psi_1 = \psi_{1\text{ini}}(x^i)\,, \tag{3.2}$$

$$\sigma_1(\eta, x^i) = \sigma_{1\text{ini}}\left(\frac{\eta_{\text{ini}}}{\eta}\right)^4 + \frac{1}{5}\psi_{1\text{ini}}(x^i)\eta_{\text{ini}}\left[\left(\frac{\eta_{\text{ini}}}{\eta}\right)^4 - \frac{\eta}{\eta_{\text{ini}}}\right]\,. \tag{3.3}$$

$$\delta\rho_1(\eta, x^i) = \frac{\nabla^2}{4\pi G a^2}\left[\psi_{1\text{ini}}(x^i) + \frac{2}{\eta}\sigma_1(\eta, x^i)\right]\,, \tag{3.4}$$

where the spectrum of the curvature perturbation initially is $\psi_{1\text{ini}}(x^i)$ and we set $\sigma_{1\text{ini}} \equiv \sigma_1(\eta_{\text{ini}}, x^i)$. Hence the dominant contribution to the shear at late times is

$$\sigma_1(\eta, x^i) \simeq -\frac{\eta}{5}\psi_{1\text{ini}}(x^i)\,. \tag{3.5}$$

We also need the metric function E_1, which is simply the time integrated shear, as defined in Eq. (2.28). The curvature perturbation on uniform density hypersurfaces is defined, see e.g. Ref. [15, 18], as

$$\zeta_1 = -\psi - \frac{\mathcal{H}}{\rho_0'}\delta\rho_1\,, \tag{3.6}$$

where the RHS of Eq. (3.6) is gauge invariant by construction and can therefore also be evaluated in synchronous-comoving gauge. For dust ζ_1 simplifies to $\zeta_1 = -\psi_1 + \delta_1/3$, a constant in time. We will use this variable in the following as a convenient quantity to specify the second initial condition in the solution for E_1, besides $\psi_{1\text{ini}}(x^i)$. We then get the solution to Eq. (2.29) as

$$E_1(\eta, x^i) = -\frac{1}{10}\left(\eta^2 - \eta_{\text{ini}}^2\right)\psi_{1\text{ini}}(x^i) + 3\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3}\nabla^{-2}\left[\zeta_{1\text{ini}}(x^i) + \psi_{1\text{ini}}(x^i)\right]\,, \tag{3.7}$$

where the initial condition for E_1, at the initial time η_{ini}, is simply the pure decaying mode,

$$E_1(\eta_{\text{ini}}, x^i) = 3\nabla^{-2}\left[\zeta_{1\text{ini}}(x^i) + \psi_{1\text{ini}}(x^i)\right] . \tag{3.8}$$

as is also the initial condition for the shear:

$$\sigma_{1\text{ini}} = -\frac{\eta_{\text{ini}}}{5}\left[\psi_{1\text{ini}}(x^i) + 45\eta_{\text{ini}}^{-2}\nabla^{-2}\left(\psi_{1\text{ini}}(x^i) + \zeta_{1\text{ini}}(x^i)\right)\right] . \tag{3.9}$$

With the above results we compute the full first order matter density contrast. We integrate Eq. (2.27) to find

$$\delta_1 = -\nabla^2 E_1 = \frac{1}{10}\eta^2\nabla^2\psi_{1\text{ini}}(x^i) - 3\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3}\left[\zeta_{1\text{ini}}(x^i) + \psi_{1\text{ini}}(x^i)\right] , \tag{3.10}$$

Note that the dominant contributions at late times to E_1 and δ_1, or the growing modes, are thus

$$E_1(\eta, x^i) = -\frac{\eta^2}{10}\psi_{1\text{ini}}(x^i), \qquad \delta_1 = \frac{\eta^2}{10}\nabla^2\psi_{1\text{ini}}(x^i). \tag{3.11}$$

C. Second order

1. Growing mode only

We now give the solutions for the second-order metric functions ψ_2, E_2, and for the density contrast δ_2, taking only the growing mode solutions above into account. Here we present them in real space, for the solutions in Fourier space, see Appendix A. The solutions including the decaying mode are given in the following subsection.

From Eq. (2.30) and using the first-order results for ψ_1 and E_1, we obtain after some simple manipulations the fastest-growing mode solution

$$\psi_2 = -\frac{\eta^2}{10}\left(\psi_{1,m}\psi_1^{;m} + \nabla^{-2}\left[(\nabla^2\psi_1)^2 - \psi_{1,lm}\psi_1^{;lm}\right]\right) + \frac{\eta^4}{200}\nabla^{-2}\left(\psi_{1,lm}^l\psi_{1,k}^{;km} - \psi_{1,klm}\psi_1^{;klm}\right) . \tag{3.12}$$

Hereafter we omit the subscript ini in ψ_1 and ζ_1 for simplicity, but keeping in mind that both perturbations are time-independent. To obtain the fastest-growing mode solution for E_2 we first plug in the first-order solutions in the differential equation (2.31) for E_2. Then, multiplying this differential equation by ∇^{-2} we obtain

$$E_2'' + 2\mathcal{H}E_2' = 6\Theta_0 - 2\psi_1^2 + \frac{\eta^2}{25}\nabla^{-2}\left[\frac{21}{2}\nabla^{-2}\left(\nabla^2\psi_{1,k}\nabla^2\psi_1^{;k} - \psi_{1,klm}\psi_1^{;klm}\right)\right.$$
$$\left. + 10\psi_{1,kl}\psi_1^{;kl} - 3(\nabla^2\psi_1)^2\right], \tag{3.13}$$

where we have defined the kernel

$$\nabla^2\Theta_0 = -\nabla^{-2}\mu_2 - \frac{1}{3}\psi_{1,k}\psi_1^{;k} , \tag{3.14}$$

and

$$\mu_2 = \frac{1}{2}\left[(\nabla^2\psi_1)^2 - \psi_{1,lm}\psi_1^{;lm}\right] . \tag{3.15}$$

The fastest growing solution of (3.13) is then easily obtained, it is

$$E_2 = \frac{3\eta^2}{5}\left(\Theta_0 - \frac{1}{3}\psi_1^2\right) + \frac{\eta^4}{700}\nabla^{-2}\left[\frac{21}{2}\nabla^{-2}\left(\nabla^2\psi_{1,k}\nabla^2\psi_1^{;k} - \psi_{1,klm}\psi_1^{;klm}\right)\right.$$
$$\left. + 10\psi_{1,kl}\psi_1^{;kl} - 3(\nabla^2\psi_1)^2\right]. \tag{3.16}$$

The evolution equation for the second-order density contrast, δ_2, follows from the continuity equation for $\delta\rho_2$, (2.21), and using the definition (2.22). We get

$$\delta_2' = 3\psi_2' - \nabla^2 E_2' - 2\delta_1\nabla^2 E_1' - 4\left[\psi_1\nabla^2 E_1' - E_{1,ij}'E_{1,}^{\ ij}\right] . \tag{3.17}$$

Using the above results, we then obtain for the fastest-growing mode of the second-order density contrast

$$\delta_2 = \frac{\eta^2}{5}\left(\frac{3}{2}\psi_{1,m}\psi_1^{;m} + 4\psi_1\nabla^2\psi_1\right) + \frac{\eta^4}{50}\left(\frac{5}{7}(\nabla^2\psi_1)^2 + \frac{2}{7}\psi_{1,kl}\psi_1^{;kl}\right) . \tag{3.18}$$

This result agrees with Ref. [8] for their $f_{\rm nl} = -5/3$, and agrees with Ref. [19] for their $a_{\rm nl} = 0$.

2. Growing and decaying mode

We now give the solutions for the second-order metric functions ψ_2, E_2, including the growing and decaying modes, that is we use Eq. (3.7). We follow the same steps to calculate the solutions as described in the previous section. To arrive at the expressions below, we have used the identity

$$\left(\nabla^{-2}\partial^k\partial^l - \delta^{kl}\right)\psi_{1,km}\psi_{1,l}^{;m} = \nabla^{-2}\left(\nabla^2\psi_{1,m}\nabla^2\psi_1^{;m} - \psi_{1,klm}\psi_1^{;klm}\right) , \tag{3.19}$$

and its equivalent for $(\psi_1 + \zeta_1)$. We find for ψ_2,

$$\begin{aligned}
\psi_2 = &-\frac{(\eta^2 - \eta_{\rm ini}^2)}{10}\left(\psi_{1,m}\psi_1^{;m} + 2\nabla^{-2}\mu_2\right) + \frac{(\eta^2 - \eta_{\rm ini}^2)^2}{200}\nabla^{-2}\left(\psi_{1,lm}^{;l}\psi_{1,k}^{;km} - \psi_{1,klm}\psi_1^{;klm}\right) \\
&+ 3\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}\left[\nabla^{-2}(\psi_{1,j}\psi_{1,}^{\ j}) + \frac{1}{2}\left(\psi_1^2 + \nabla^{-2}\psi_{1,jk}\nabla^{-2}\psi_{1,}^{\ jk}\right)\right] \\
&- \frac{3}{10}(\eta^2 - \eta_{\rm ini}^2)\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}\left[\nabla^{-2}\left(\psi_{1,j}\nabla^2\psi_{1,}^{\ j}\right) - \frac{1}{2}\nabla^{-2}\psi_{1,ijk}\nabla^{-2}\psi_{1,}^{\ ijk}\right] \\
&+ \frac{9}{2}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}\nabla^{-2}\left[\psi_{1,j}\psi_{1,}^{\ j} - \nabla^{-2}\psi_{1,ijk}\nabla^{-2}\psi_{1,}^{\ ijk}\right] \\
&- 3\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}\nabla^{-2}\left[2\psi_{1,i}\zeta_{1,}^{\ i} - \psi_{1,jk}\nabla^{-2}\zeta_{1,}^{\ jk}\right] + \frac{9}{2}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}\nabla^{-2}\left[\zeta_{1,j}\zeta_{1,}^{\ j} - \nabla^{-2}\zeta_{1,ijk}\nabla^{-2}\zeta_{1,}^{\ ijk}\right] \\
&- \frac{3}{10}(\eta^2 - \eta_{\rm ini}^2)\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}\nabla^{-2}\left[\nabla^2\psi_{1,j}\zeta_{1,}^{\ j} - \psi_{1,ijk}\nabla^{-2}\zeta_{1,}^{\ ijk}\right] \\
&+ 9\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}\nabla^{-2}\left[\psi_{1,i}\zeta_{1,}^{\ i} - \nabla^{-2}\psi_{1,ijk}\nabla^{-2}\zeta_{1,}^{\ ijk}\right] .
\end{aligned} \tag{3.20}$$

The growing plus decaying solution for E_2 is derived from expanding Eq. (2.31) in terms of the pure growing mode

ψ_1 and the decaying mode initially given by E_1 in Eq. (3.7):

$$E_2'' + 2\mathcal{H}E_2' = 6\Theta_0 - 2\psi_1^2 + 24\left(\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3} + \frac{3}{4}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-8}\right)\nabla^{-2}\left[\psi_{1,kl}\nabla^{-2}(\zeta_1 + \psi_1),^{kl}\right]$$

$$+ \nabla^{-2}\left\{\frac{\eta^2}{25}\frac{21}{2}\left(1 + \frac{1}{7}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-5} + \frac{9}{14}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\right)\nabla^{-2}\left[\nabla^2\psi_{1,k}\nabla^2\psi_1,^{k} - \psi_{1,klm}\psi_{1,}^{klm}\right]\right.$$

$$+ \frac{243}{\eta^2}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-6}\nabla^{-2}\left[(\zeta_1 + \psi_1),_k(\zeta_1 + \psi_1),^{k} - \nabla^{-2}(\zeta_1 + \psi_1),_{ijk}\nabla^{-2}(\zeta_1 + \psi_1),^{ijk}\right]$$

$$+ \frac{9}{5}\left(\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3} + 4\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-8}\right)\nabla^{-2}\left[(\zeta_1 + \psi_1),_k\nabla^2\psi_1,^{k} + \nabla^{-2}(\zeta_1 + \psi_1),_{ijk}\psi_{1,}^{ijk}\right]$$

$$+ \frac{10}{25}\eta^2\left(1 + \frac{9}{16}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\right)\psi_{1,ij}\psi_{1,}^{ij} + \frac{6}{5}\left(\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3} + \left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-8}\right)(\zeta_1 + \psi_1)\nabla^2\psi_1$$

$$- \frac{3}{25}\eta^2\left(1 - \frac{1}{3}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-5} - \frac{3}{8}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\right)\nabla^2\psi_1\nabla^2\psi_1,$$

$$\left. + \frac{81}{2}\eta^2\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\left[5\nabla^{-2}(\zeta_1 + \psi_1),_{kl}\nabla^{-2}(\zeta_1 + \psi_1),^{kl} - (\zeta_1 + \psi_1)^2\right]\right\}. \tag{3.21}$$

Solving the ODE for E_2 we obtain the following expression

$$E_2 = \frac{3}{5}\eta^2\left(\Theta_0 - \frac{1}{3}\psi_1^2\right) - \frac{3}{5}\eta^2\left(\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3} - \frac{1}{9}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-8}\right)\nabla^{-2}\left[(\zeta_1 + \psi_1)\nabla^2\psi_1\right]$$

$$+ \nabla^{-2}\left\{\frac{\eta^4}{70}\left[1 + \frac{7}{8}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\right]\psi_{1,ij}\psi_{1,}^{ij} - \frac{3\eta^4}{700}\left[1 - \frac{14}{3}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-5} - \frac{7}{12}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\right]\nabla^2\psi_1\nabla^2\psi_1\right.$$

$$+ \frac{3}{2}\frac{\eta^4}{100}\left(1 - 2\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-5} + \left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\right)\nabla^{-2}\left[\nabla^2\psi_{1,k}\nabla^2\psi_1,^{k} - \psi_{1,klm}\psi_{1,}^{klm}\right]$$

$$- \eta^2\left(12\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3} - \left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-8}\right)\psi_{1,kl}\nabla^{-2}(\zeta_1 + \psi_1),^{kl}$$

$$- \frac{9}{10}\eta^2\left(\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3} - \frac{4}{9}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-8}\right)\nabla^{-2}\left[(\zeta_1 + \psi_1),_k\nabla^2\psi_1,^{k} + \nabla^{-2}(\zeta_1 + \psi_1),_{ijk}\psi_{1,}^{ijk}\right]$$

$$+ \frac{27}{2}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-6}\nabla^{-2}\left[(\zeta_1 + \psi_1),_k(\zeta_1 + \psi_1),^{k} - \nabla^{-2}(\zeta_1 + \psi_1),_{ijk}\nabla^{-2}(\zeta_1 + \psi_1),^{ijk}\right]$$

$$\left. + \frac{9}{4}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-10}\left[5\nabla^{-2}(\zeta_1 + \psi_1),_{kl}\nabla^{-2}(\zeta_1 + \psi_1),^{kl} - (\zeta_1 + \psi_1)^2\right]\right\}. \tag{3.22}$$

For completeness we also give the second order density contrast including growing and decaying modes,

$$
\begin{aligned}
\delta_2 =\ & \frac{3}{10}\left(\eta^2+\eta_{\rm ini}^2\right)\psi_{1,k}\psi_{1,}{}^{k}+\frac{4}{5}\left(\eta^2+\eta_{\rm ini}^2\right)\psi_1\nabla^2\psi_1 \\
& +\frac{\eta^4}{100}\left[\frac{10}{7}-2\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-2}+\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-4}-2\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-5}-\frac{1}{4}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-10}\right]\nabla^2\psi_1\nabla^2\psi_1 \\
& +\frac{\eta^4}{100}\left[\frac{4}{7}-4\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-2}+2\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-4}+3\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-5}-\frac{11}{4}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-10}\right]\psi_{1,ik}\psi_{1,}{}^{ik} \\
& +\frac{3}{100}\eta_{\rm ini}^4\left[\frac{1}{2}-2\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-2}+2\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}+\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-4}-\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-10}\right]\left(\nabla^{-2}(\nabla^2\psi_{1,k}\nabla^2\psi_{1,}{}^{k})-\nabla^{-2}(\psi_{1,ikj}\psi_{1,}{}^{ijk})\right) \\
& -\frac{3}{5}\eta_{\rm ini}^2\nabla^{-2}\left(\psi_{1,ik}\psi_{1,}{}^{ik}\right)-\frac{13}{2}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}(\psi_1+\zeta_1)\psi_1+9\left[\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}+\frac{1}{4}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-10}\right](\psi_1+\zeta_1)^2 \\
& +\frac{3}{5}\eta_{\rm ini}^2\left[\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}-\frac{1}{9}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}\right](\psi_1+\zeta_1)\nabla^2\psi_1+9\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}\nabla^{-2}\left(\psi_{1,k}(\psi_1+\zeta_1),{}^{k}\right) \\
& +\eta_{\rm ini}^2\left[\frac{123}{10}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-1}-\frac{3}{10}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}-\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}\right]\psi_{1,ik}\nabla^{-2}(\psi_1+\zeta_1),{}^{ik} \\
& +9\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}\nabla^{-2}\left(\psi_{1,ik}\nabla^{-2}(\psi_1+\zeta_1),{}^{ik}\right)-\frac{9}{5}\eta_{\rm ini}^2\left[\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-1}-\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-3}\right]\nabla^{-2}\left(\nabla^{-2}(\psi_1+\zeta_1),_{lm}\psi_{1,}{}^{km}\right)^{l}{}_{,k} \\
& +9\left[2\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}-\frac{5}{4}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-10}\right]\nabla^{-2}(\psi_1+\zeta_1),_{kl}\nabla^{-2}(\psi_1+\zeta_1),{}^{kl} \\
& +\frac{9}{10}\eta_{\rm ini}^4\left[\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-1}-\frac{4}{9}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}\right]\nabla^{-2}\left((\psi_1+\zeta_1),_{k}\nabla^2(\psi_1),{}^{k}-\nabla^{-2}(\psi_1+\zeta_1),_{ijk}(\psi_1),{}^{ijk}\right) \\
& +\frac{27}{2}\left(\frac{\eta}{\eta_{\rm ini}}\right)^{-6}\left((\psi_1+\zeta_1),_{k}(\psi_1+\zeta_1),{}^{k}-\nabla^{-2}(\psi_1+\zeta_1),_{ijk}\nabla^{-2}(\psi_1+\zeta_1),{}^{ijk}\right)
\end{aligned}
\tag{3.23}
$$

IV. LAGRANGIAN DISPLACEMENT FIELD

Given the solutions for the metric potentials in the previous sections, we can now determine the metric tensor for scalar perturbations, and use this to calculate the corresponding Lagrangian displacement field.

Let us briefly outline the used method to obtain the displacement field. It requires the knowledge of the metric tensor which, after having established the above results for the metric coefficients, can now be easily constructed. The displacement field can then be extracted from the metric tensor by using a suitable decomposition, which we also motivate briefly in the following (for further details see Ref. [8]).

We begin by writing down the metric tensor γ_{ij} in synchronous-comoving gauge, defined by the line element

$$
\mathrm{d}s^2 = a^2(\tau)\left[-\mathrm{d}\tau^2+\gamma_{ij}\,\mathrm{d}q^i\mathrm{d}q^j\right]\,,
\tag{4.1}
$$

where the q^i are Lagrangian coordinates and thus denote space-like labels of fluid elements on a time-like hypersurface (we assume the vanishing of the spatial vorticity). In this gauge

$$
\gamma_{ij}(\tau,q^m) = \delta_{ij}\left(1-2\psi(\tau,q^m)\right)+2E(\tau,q^m),_{ij}
\tag{4.2}
$$

Let us now turn to a Lagrangian description. Let $\boldsymbol{q}\mapsto\boldsymbol{x}(\eta,\boldsymbol{q})$ be the (spatial) Lagrangian map from the initial position $\boldsymbol{q}$ of the particle to the final position $\boldsymbol{x}$ at time η. The respective Jacobian matrix element is (we neglect vectors)

$$
\mathcal{J}_{ij}(\eta,\boldsymbol{q}) \equiv \delta_{ij}+\mathcal{F}_{,ij}(\eta,\boldsymbol{q})\,,
\tag{4.3}
$$

where $\mathcal{F}$ is the scalar part of the displacement, and ",i" denotes, as before, a partial derivative with respect to Lagrangian coordinates. With these definitions we can utilize the following decomposition for the spatial metric

$$
\gamma_{ij} = \delta_{ab}\left(1-2\mathcal{B}\right)\mathcal{J}^a{}_i\,\mathcal{J}^b{}_j\,,
\tag{4.4}
$$

with $\mathcal{B} = \mathcal{B}_1 + \mathcal{B}_2/2 + \ldots$ and $\mathcal{F} = \mathcal{F}_1 + \mathcal{F}_2/2 + \ldots$ to be determined. We show in the following two subsections how to derive these unknowns, order by order.

A. First order

The spatial metric for scalar perturbations is, substituting the above solutions,

$$
\gamma_{1ij} = \delta_{ij}(1 - 2\psi_1) - 2\frac{\eta_{\text{ini}}}{3}\sigma_{1\text{ini},ij}\left(\frac{\eta_{\text{ini}}}{\eta}\right)^3 - \frac{\eta^2}{5}\psi_{1,ij}\left[1 + \frac{2}{3}\left(\frac{\eta_{\text{ini}}}{\eta}\right)^5\right]. \tag{4.5}
$$

$$
= \delta_{ij}(1 - 2\psi_1) - \frac{1}{5}(\eta - \eta_{\text{ini}})^2\psi_{1,ij} + 6\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3}\nabla^{-2}(\psi_1 + \zeta_1)_{,ij} \tag{4.6}
$$

At late times, or using only the growing mode, this simplifies to

$$
\gamma_{1ij}^+ \simeq \delta_{ij}(1 - 2\psi_1) - \frac{\eta^2}{5}\psi_{1,ij}. \tag{4.7}
$$

To obtain the first-order displacement field, we note that the decomposition (4.4) reduces at first order to

$$
\gamma_{1ij} = \delta_{ij}(1 - 2\mathcal{B}_1) + 2\mathcal{F}_{1,ij}, \tag{4.8}
$$

and thus we can easily read-off the displacement by using our result for γ_{ij}. For the fastest growing mode, i.e., using (4.7), we obtain at first order

$$
\mathcal{B}_1 = \psi_1, \tag{4.9}
$$

$$
\mathcal{F}_1^+ = -\frac{\eta^2}{10}\psi_1, \tag{4.10}
$$

whereas, including the decaying modes (using Eq. (4.5)) we find the same result for $\mathcal{B}_1$ but for the (scalar component of the) first-order displacement we have now

$$
\mathcal{F}_1 = E_1 = -\frac{\eta_{\text{ini}}}{3}\sigma_{1\text{ini}}\left(\frac{\eta_{\text{ini}}}{\eta}\right)^3 - \frac{\eta^2}{10}\psi_1\left[1 + \frac{2}{3}\left(\frac{\eta_{\text{ini}}}{\eta}\right)^5\right],
$$

$$
= -\frac{1}{10}(\eta^2 - \eta_{\text{ini}}^2)\psi_1 + 3\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3}\nabla^{-2}(\psi_1 + \zeta_1). \tag{4.11}
$$

Equation (4.10) is nothing but the Newtonian displacement in the Zel'dovich approximation, whereas Eq. (4.11) is its general relativistic extension including decaying modes. To our knowledge, the laster is a new result. Clearly, at late times the relativistic displacement (4.11) coincides with the Newtonian fastest growing mode as it should.

B. Second order

1. Growing mode only

We can now give the metric up to second order. We begin with the metric including only the growing mode solutions for the metric potentials given in Section III C 1. Putting everything together the metric up to second order is

$$\gamma_{ij} = \delta_{ij}\left[1 - 2\psi_1 - \psi_2\right] + 2E_{1,ij} + E_{2,ij} \tag{4.12}$$

$$= \delta_{ij}\left[1 - 2\psi_1 + \frac{\eta^2}{10}\left(\psi_{1,m}\psi_1^{;m} + 2\nabla^{-2}\mu_2\right) - \frac{\eta^4}{200}\nabla^{-2}\left(\nabla^2\psi_{1,m}\nabla^2\psi_1^{;m} - \psi_{1,klm}\psi_1^{;klm}\right)\right]$$

$$- \frac{\eta^2}{5}\psi_{1,ij} + \frac{3\eta^2}{5}\left(\Theta_0 - \frac{1}{3}\psi_1^2\right)_{,ij}$$

$$+ \frac{\eta^4}{700}\nabla^{-2}\left[\frac{21}{2}\nabla^{-2}\left(\nabla^2\psi_{1,k}\nabla^2\psi_1^{,k} - \psi_{1,klm}\psi_1^{,klm}\right) + 10\psi_{1,kl}\psi_1^{;kl} - 3(\nabla^2\psi_1)^2\right]_{,ij}$$

$$= \delta_{ij}\left[1 - 2\psi_1 + \frac{\eta^2}{10}\left(\psi_{1,m}\psi_1^{;m} + 2\nabla^{-2}\mu_2\right)\right]$$

$$- \frac{\eta^2}{5}\psi_{1,ij} + \frac{3\eta^2}{5}\left(\Theta_0 - \frac{1}{3}\psi_1^2\right)_{,ij} + \frac{3\eta^4}{200}\nabla^{-2}\nabla^{-2}D_{ij}\left(\nabla^2\psi_{1,k}\nabla^2\psi_1^{,k} - \psi_{1,klm}\psi_1^{,klm}\right)$$

$$+ \frac{\eta^4}{700}\nabla^{-2}\left[10\psi_{1,kl}\psi_1^{;kl} - 3(\nabla^2\psi_1)^2\right]_{,ij}, \tag{4.13}$$

where in the last step we have made use of the operator

$$D_{ij} = \partial_i\partial_j - \frac{\delta_{ij}}{3}\nabla^2. \tag{4.14}$$

To get the second-order displacement field, we first note that the spatial metric, here for scalar perturbations only but to arbitrary order, can be decomposed as

$$\gamma_{ij} := \frac{\delta_{ij}}{3}\hat{\gamma} + D_{ij}\hat{\gamma}^{\|}, \tag{4.15}$$

where $\hat{\gamma} = \hat{\gamma}_1 + \hat{\gamma}_2/2 + \ldots$ is just the trace of γ_{ij}, whereas $\hat{\gamma}^{\|} = \hat{\gamma}_1^{\|} + \hat{\gamma}_2^{\|}/2 + \ldots$ is its longitudinal part. Applying on this definition the D^{ij} operator then gives the "longitudinal mode extractor"

$$\hat{\gamma}^{\|} = \frac{3}{2}\nabla^{-2}\nabla^{-2}D^{ij}\gamma_{ij}. \tag{4.16}$$

Now, applying $\frac{3}{2}\nabla^{-2}\nabla^{-2}D^{ij}$ on both sides of (4.4), it is straightforward to obtain an expression for the Lagrangian displacement field (valid only up to second order)

$$\mathcal{F} = \frac{3}{4}\nabla^{-2}\nabla^{-2}D^{ij}\left(\gamma_{ij} + 4\mathcal{F}_{,ij}\mathcal{B} - \mathcal{F}_{,il}\mathcal{F}_{,j}^{,l}\right), \tag{4.17}$$

which can be easily solved with the conventional Ansatz $\mathcal{F} = \mathcal{F}_1 + \mathcal{F}_2/2$, i.e., order by order. Restricting for the moment to the fastest growing mode and using the result for γ_{ij}, Eq. (4.13), we then obtain for the scalar part of the displacement field, up to second order

$$\mathcal{F}^+ = -\frac{\eta^2}{10}\psi_1 - \frac{3\eta^4}{700}\nabla^{-2}\mu_2 - \frac{3\eta^2}{10}\Theta_0 - \frac{\eta^2}{5}\psi_1^2, \tag{4.18}$$

with the spatial kernels Θ_0 and μ_2 given in Eqs. (3.14)–(3.15). This result agrees with Ref. [8] for their $f_{\rm nl} = -5/3$, agrees with Ref. [19] for their $a_{\rm nl} = 0$. Note that in order to arrive at the expression (4.17) and subsequent results we have again used the identity in Eq. (3.19).

The first two terms on the RHS of Eq. (4.18) are the well-known Newtonian parts of the displacement field up to second order, whereas the latter terms are relativistic corrections. Finally, we note that the resulting relativistic coordinate transformation

$$\eta(\eta, \boldsymbol{q}) = \eta$$

$$x^i(\eta, \boldsymbol{q}) = q^i - \frac{\eta^2}{10}\psi_1^{;i} - \frac{3\eta^4}{700}\nabla^{-2}\mu_2^{;i} - \frac{3\eta^2}{10}\Theta_0^{;i} - \frac{2\eta^2}{5}\psi_1\psi_1^{;i} \tag{4.19}$$

is the 4D gauge transformation from the synchronous-comoving gauge to the total matter gauge (which also makes use of the proper time coordinate), as already noted in Refs. [8, 19]. Equation (4.19) denotes the relativistic trajectory of fluid elements on constant time-like hypersurfaces up to second order in cosmological perturbation theory, including, however, only the fastest growing modes. In the following section we will show how to incorporate also the decaying modes.

2. Growing and decaying mode

Substituting into Eq. (4.17) the general solutions including decaying modes, and using the same techniques as described in the previous section, we obtain for the displacement up to second order (i.e., including the first-order results)

$$
\begin{aligned}
\mathcal{F} = &-\frac{\eta_{\text{ini}}}{3}\sigma_{1\text{ini}}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3} - \frac{\eta^2}{10}\psi_1\left[1 + \frac{2}{3}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-5}\right] - \frac{3\eta^4}{700}\nabla^{-2}\mu_2 - \frac{3\eta^2}{10}\Theta_0 - \frac{\eta^2}{5}\psi_1^2 \\
&+ \eta_{\text{ini}}^4\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-1}\nabla^{-2}\left(-\frac{1}{40}\nabla^{-2}D^{kl}\psi_{1,km}\psi_{1,l}^{,m} + \frac{1}{100}\psi_{1,lm}\psi_1^{lm} + \frac{1}{100}[\nabla^2\psi_1]^2\right) \\
&+ \eta_{\text{ini}}^4\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-6}\nabla^{-2}\left(\frac{1}{240}\nabla^{-2}D^{kl}\psi_{1,km}\psi_{1,l}^{,m} + \frac{1}{800}\psi_{1,lm}\psi_1^{lm} + \frac{1}{800}[\nabla^2\psi_1]^2\right. \\
&\qquad\qquad\qquad\left. + \frac{9}{8}\left[5\nabla^{-2}(\zeta_1+\psi_1)_{,kl}\nabla^{-2}(\zeta_1+\psi_1)^{,kl} - (\zeta_1+\psi_1)^2\right]\right) \\
&+ \frac{27}{4}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-6}\nabla^{-2}\left[(\zeta_1+\psi_1)_{,k}(\zeta_1+\psi_1)^{,k} - \nabla^{-2}(\zeta_1+\psi_1)_{,ijk}\nabla^{-2}(\zeta_1+\psi_1)^{,ijk}\right] \\
&+ \eta_{\text{ini}}^2\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-1}\nabla^{-2}\left(-\frac{9}{20}\nabla^{-2}\left[(\zeta_1+\psi_1)_{,k}\nabla^2\psi_1^{,k} + \nabla^{-2}(\zeta_1+\psi_1)_{,ijk}\psi_1^{,ijk}\right]\right. \\
&\qquad\qquad\qquad\left. - 6\psi_{1,kl}\nabla^{-2}(\zeta_1+\psi_1)^{,kl} - \frac{3}{10}(\zeta_1+\psi_1)\nabla^2\psi_1\right) \\
&+ \eta_{\text{ini}}^2\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-6}\nabla^{-2}\left(\frac{1}{5}\nabla^{-2}\left[(\zeta_1+\psi_1)_{,k}\nabla^2\psi_1^{,k} + \nabla^{-2}(\zeta_1+\psi_1)_{,ijk}\psi_1^{,ijk}\right]\right. \\
&\qquad\qquad\qquad\left. + \frac{1}{2}\psi_{1,kl}\nabla^{-2}(\zeta_1+\psi_1)^{,kl} + \frac{1}{30}(\zeta_1+\psi_1)\nabla^2\psi_1\right) \\
&- \frac{\eta_{\text{ini}}^2}{5}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3}\left(\frac{\psi_1^2}{3} + 2\Theta_0\right) - \nabla^{-2}\nabla^{-2}D^{ij}\left(\eta_{\text{ini}}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-3}\sigma_{\text{ini},ij}\psi_1\right. \\
&\qquad\qquad\qquad\left. + \frac{\eta_{\text{ini}}^2}{12}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-6}\sigma_{\text{ini},il}\sigma_{\text{ini},j}^{,l} + \frac{\eta_{\text{ini}}^3}{40}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-1}\left\{\sigma_{\text{ini},il}\psi_{1,j}^{,l} + \sigma_{\text{ini},jl}\psi_{1,i}^{,l}\right\}\left[1 + \frac{2}{3}\left(\frac{\eta}{\eta_{\text{ini}}}\right)^{-5}\right]\right). \quad (4.20)
\end{aligned}
$$

This is our main result. Only a few terms in this expression, namely the fastest growing modes, have been reported in the literature. All terms including decaying modes have not been reported before. The relativistic trajectory, including also the decaying modes, can then be easily obtained by observing that $x^i = q^i + \mathcal{F}^{,i}$, where the scalar $\mathcal{F}$ is given in Eq. (4.20), and q^i denote the initial position of the fluid elements.

V. DISCUSSION AND CONCLUSIONS

In this paper we have derived the Lagrangian displacement field using second order relativistic cosmological perturbation theory, working in synchronous-comoving gauge and using gauge-invariant scalar perturbations. For simplicity we restricted our derivation to an Einstein–de Sitter universe, although the calculations can be readily extended to other models of the Universe. Here we have focused on determining all the terms in the solutions, including the decaying modes of the displacement field, which were so far unknown and could become important at early times, where

the influence of the cosmological constant should be negligible. For the fastest growing mode of the displacement field, we recover known results from the literature, that is, the most dominant contribution to the displacement comes from the well-known Newtonian part, whereas the fastest growing mode of the general relativistic corrections to this displacement should become relevant to cosmological structure formation only on very large scales.

For the decaying modes, the impact of the general relativistic corrections is difficult to estimate by analytical means, however it is expected that these corrections could play an important role at early times — on a wealth of scales. This expectation should be tested by using our novel displacement field for generating initial conditions for N-body simulations, and then analysing the impact of these *relativistic transients* on the late-time gravitational dynamics in comparison with standard methods used in the literature (e.g., 2LPT). For a possible practical implementation of our expressions, existing algorithms for generating initial conditions (e.g., Refs. [20, 21]) could be modified to include the relativistic corrections.

Finally, we note that our results allow us write down the synchronous-comoving metric for scalar perturbations up to second order, including decaying modes, which also has not been published before. We did not write down this expression explicitly, but using ψ_2 and E_2 given in Section III C 1, it is straightforward to obtain the corresponding metric for growing and decaying modes.

There are many avenues to extend the results reported in this paper in future work. To set the initial conditions at later times it will be useful to use a ΛCDM background model. This will also require the use of more than one fluid, and allowing for pressure (as done, for example, in [22] at first order), to get a realistic model. In this work we only used scalar perturbations at first and second order. Another extension will be to include contributions from vector and tensor perturbations (in the case of vectors at first *and* second order, since in multi-fluid systems second order vector perturbations will be generated inevitably, [23] This will result in smaller corrections since the contribution are supposed to be sub-dominant compared to scalars, at least on large scales, but might nevertheless have observable effects. Gravity is after all nonlinear.

Appendix A: Solutions in Fourier space

In Fourier space the solution to Eq. (2.30) for ψ_2 can be rewritten in terms of the growing mode solutions

$$\widetilde{\psi_2(\mathbf{k})} = \int \int \frac{d^3 k_1 d^3 k_2}{(2\pi)^3} \delta_D(\mathbf{k}_q) \psi_1(\mathbf{k}_1) \psi_1(\mathbf{k}_2) \left\{ \frac{\eta^2}{10} \left[\frac{k_1^2 k_2^2}{k^2} + \frac{(k_1^2 + k_2^2)\mathbf{k}_1 \cdot \mathbf{k}_2}{k^2} + \frac{(\mathbf{k}_1 \cdot \mathbf{k}_2)^2}{k^2} \right] \right.$$
$$\left. + \frac{\eta^4}{200} \left[\frac{(k_1^2 k_2^2)\mathbf{k}_1 \cdot \mathbf{k}_2}{k^2} - \frac{(\mathbf{k}_1 \cdot \mathbf{k}_2)^3}{k^2} \right] \right\}, \qquad (A1)$$

where $\mathbf{k}$, $\mathbf{k}_1$ and $\mathbf{k}_2$ are independent vectors in Fourier space. $\mathbf{k}_q \equiv \mathbf{k} - \mathbf{k}_1 - \mathbf{k}_2$, and the Dirac delta $\delta_D(\mathbf{k}_q)$ guarantees momentum conservation. Also we have symmetrised over $\mathbf{k}_1$ and $\mathbf{k}_2$. Similarly, the real-space solution for E_2 (Eq. (3.16)) is easily transformed to Fourier space:

$$E_2 = \int \int \frac{d^3 k_1 d^3 k_2}{(2\pi)^3} \delta_D(\mathbf{k}_q) \frac{1}{k^2} \left[\frac{1}{10} \mathfrak{K}_1 \eta^2 + \frac{1}{28} \mathfrak{K}_2 \eta^4 \right] \psi_1(\mathbf{k}_1) \psi_1(\mathbf{k}_2). \qquad (A2)$$

where

$$\mathfrak{K}_1 = - \left[2\left(k_1^2 + k_2^2\right) + 3\mathbf{k}_1 \cdot \mathbf{k}_2 \right] - \frac{3}{k^2} \left[k_1^2 k_2^2 + \left(k_1^2 + k_2^2\right) \mathbf{k}_1 \cdot \mathbf{k}_2 + \left(\mathbf{k}_1 \cdot \mathbf{k}_2\right)^2 \right], \qquad (A3)$$

$$\mathfrak{K}_2 = -\left[\frac{20}{50}\left(\mathbf{k}_1 \cdot \mathbf{k}_2\right)^2 - \frac{6}{50}k_1^2 k_2^2\right] + \frac{3}{k^2}\mathbf{k}_1 \cdot \mathbf{k}_2\left[-\frac{7}{50}\,k_1^2 k_2^2 + \frac{7}{50}\left(\mathbf{k}_1 \cdot \mathbf{k}_2\right)^2\right],\tag{A4}$$

and we again symmetrised over $\mathbf{k}_1$ and $\mathbf{k}_2$.

For the second-order solution of the density contrast in Fourier space we get, using Eq. (3.18),

$$\delta_2 = \int \int \frac{d^3 k_1 d^3 k_2}{(2\pi)^3}\,\delta_D(\mathbf{k}_q)\left\{-4(k_1^2 + k_2^2) - 3\mathbf{k}_1 \cdot \mathbf{k}_2 + \frac{\eta^2}{10}\left[\frac{10}{7}k_1^2 k_2^2 + \frac{4}{7}(\mathbf{k}_1 \cdot \mathbf{k}_2)^2\right]\right\}\frac{\eta^2}{10}\psi_1(\mathbf{k}_1)\psi_1(\mathbf{k}_2)\,.\tag{A5}$$

This result is in agreement with Eqs. (94) and (A10) of Ref. [24].

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