Astron. Astrophys. 323, 295–304 (1997)

ASTRONOMY
AND
ASTROPHYSICS

Cosmic density and velocity fields in Lagrangian perturbation theory

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Received 23 May 1996 / Accepted 16 December 1996

Abstract. A first- and second-order relation between cosmic density and peculiar-velocity fields is presented. The calculation is purely Lagrangian and it is derived using the second-order solutions of the Lagrange-Newton system obtained by Buchert & Ehlers. The procedure is applied to two particular solutions given generic initial conditions. In this approach, the continuity equation yields a relation between the over-density and peculiar-velocity fields that automatically satisfies Euler's equation because the orbits are derived from the Lagrange-Newton system. This scheme generalizes some results obtained by Nusser et al. (1991) in the context of the Zel'dovich approximation. As opposed to several other reconstruction schemes, in this approach it is not necessary to truncate the expansion of the Jacobian given by the continuity equation in order to calculate a first- or second-order expression for the density field. In these previous schemes, the density contrast given by (a) the continuity equation and (b) Euler's equation are mutually incompatible. This inconsistency arises as a consequence of an improper handling of Lagrangian and Eulerian coordinates in the analysis. Here, we take into account the fact that an exact calculation of the density is feasible in the Lagrangian picture and therefore an accurate and consistent description is obtained.

Key words: cosmology: theory – large-scale structure of the universe

1. Introduction

An important aim of cosmology is to determine a relationship between the cosmic density contrast δ and the peculiar-velocity field $\boldsymbol{u}$ under the assumption that these fields have evolved under the action of gravity. In the Eulerian theory of gravitational instability, retaining only the linear growing-mode solution, this relationship is simply given by[1]

$$\delta(t,\boldsymbol{q}) = -\frac{D}{a\dot{D}}\,\nabla_q \cdot \boldsymbol{u}(t,\boldsymbol{q}), \tag{1}$$

where $D(t)$ is the usual linear growth factor, such that $D(t) = a(t) = (t/t_0)^{2/3}$ in an Einstein-de Sitter universe. Beyond linear theory, in the weakly non-linear regime, (1) has been used to good effect as an estimate of the density contrast field from observed peculiar-velocities (e.g. Bertschinger & Dekel 1989; Dekel et al. 1990; Bertschinger et al. 1990). On the other hand, the POTENT method and other quasi-linear reconstruction procedures involve the Zel'dovich approximation (ZA)(Nusser et al. 1991; Nusser & Dekel 1992). The ZA does not however, strictly speaking, provide an exact algebraic relation between the fields $\boldsymbol{u}(t,\boldsymbol{q})$ and $\delta(t,\boldsymbol{q})$. It can however yield (as shown in Nusser et al. 1991) a relation between the fields that is self-consistent within the order of the approximation, i.e. within $O(D^2)$. In the ZA, from the Lagrangian integral of the continuity equation we have

$$\frac{1+\delta(t,\boldsymbol{X})}{1+\delta(t_0,\boldsymbol{X})} = \det\left[\delta_{ij} + \frac{D}{a\dot{D}}\frac{\partial u_i(t,\boldsymbol{X})}{\partial X_j}\right]^{-1}, \tag{2}$$

and the fields are mapped back to Eulerian space via the ZA map for the orbits of the particles. Initial conditions are specified at an arbitrary early time $t_0 \geq 0$. Also, it is customary to make the assumption of smoothness at early times, $\delta(t_0,\boldsymbol{X}) \approx 0$, by virtue of the amplitude of the fluctuations in the microwave background. From (2) we obtain the linear relation (1) by truncating the expansion of the determinant (2) to the lowest order in the perturbation field $\boldsymbol{u}$ and replacing Lagrangian by Eulerian coordinates ($\boldsymbol{X} \approx \boldsymbol{q}$).

These schemes have been generalized further (Gramann 1993a, 1993b; for their Eulerian analogue, see Bernardeau 1992) by starting out with a parametrization of the particle orbits $\boldsymbol{q} = \boldsymbol{F}(t,\boldsymbol{X})$ of the type:

$$\boldsymbol{F}(t,\boldsymbol{X}) = \boldsymbol{X} + D\nabla_X\Phi^{(1)}(\boldsymbol{X}) + D^2\nabla_X\Phi^{(2)}(\boldsymbol{X}), \tag{3}$$

In the case of a flat Universe, the leading second-order term in perturbation theory (Bouchet et al. 1992) is indeed $\propto D^2(t)$. Therefore, the coordinate map (3) is in principle well-motivated (for a numerical comparison of the different models, see e.g. Dekel 1994). However, as shown in Gramann (1993b), orbits of

[1] Throughout this article, $\boldsymbol{q}$ and $\boldsymbol{X}$ denote (comoving) Eulerian and Lagrangian coordinates respectively.

the type (3) do not yield a self-consistent relation for the cosmic density and velocity fields; the density fields obtained via (a) the continuity equation and (b) the Euler equation differ within the order of the approximation. The reason for this is that, as we shall see, (3) is only an approximate second-order solution of the Lagrange-Newton system. Thus, we wish to call the attention of the reader to the fact that the reconstruction models derived from (3) and, more generally, from an ansatz including higher orders in $D(t)$,

$$\boldsymbol{F}(t, \boldsymbol{X}) = \boldsymbol{X} + \sum_{n=1}^{N} D^n \, \nabla_X \Phi^{(n)}(\boldsymbol{X}) \qquad (4)$$

(for arbitrary N), do not follow a rigorous line of analysis (in the case of an arbitrary Ω) for the following reasons:

I In these models, the parametrization of the orbits is given ad hoc and it is not derived as a solution of the Lagrangian evolution equations for the flow field. In particular, the absence of lower-order growing modes, that are present in the general perturbation theory solution, implies that the derivation of δ through the continuity equation neglects couplings of these modes with leading-order terms.

II The density contrast δ_c obtained from the continuity equation in perturbation theory and δ_e satisfying Euler's equation are mutually incompatible.

III There is no reason to justify that $D(t)$ is a good perturbative parameter (in terms of the convergence of the solutions) and that a meaningful generalization of the family of solutions where the ZA belongs can be realized as a polynomial in $D(t)$.

It is easy to see that (II) follows as a consequence of (I). Regarding (I) and (III), it has been shown that the correct coordinate map between Eulerian and Lagrangian coordinates in Lagrangian perturbation theory is obtained by calculating the perturbative solution of the Lagrange-Newton system for the trajectories $\boldsymbol{q} = \boldsymbol{F}(t, \boldsymbol{X})$. These evolution equations are obtained by transforming the Euler-Newton system to Lagrangian coordinates and eliminating all Eulerian fields by using exact Lagrangian integrals for the Eulerian acceleration and density (Buchert & Götz 1987; Buchert 1989). Within this scheme, the ZA is recovered as a subclass of solutions (Buchert 1992), and hence, one can obtain a self-consistent solution for the overdensity field in terms of the velocities as in Nusser et al. (1991). Furthermore, the second- and third-order solutions obtained in the Lagrangian framework (Buchert & Ehlers 1993, Buchert 1994; and in a slightly different approach Bouchet et al. 1992, 1995; Catelan 1995) are unique and well-defined at all times from a fiducial time t_0, where initial data are specified,[2] until shell-crossing, provided we impose periodic boundary conditions and fix some global gauge conditions (Ehlers & Buchert 1997) as opposed to the orbits described by polynomials in $D(t)$, which are expected to have poor convergence (for a discussion in the context of the variational approach to the solutions see Susperregi & Binney 1994). Although the leading terms of the longitudinal parts of the perturbation solutions seem to confirm this polynomial approach (e.g. Bouchet et al. 1992, for the second-order solutions), this is not a mathematically consistent motivation for using $D(t)$ as an expansion parameter by going to higher orders in perturbation theory. On the contrary, the structure of the Lagrangian perturbation scheme is such that, starting at third order, the presence of interaction terms among perturbations of different orders are an obstacle to convergence, and in fact for $n > 3$ all terms are interaction terms (see Buchert 1994). Therefore, for $n \geq 3$ an ansatz of the form (4) cannot reproduce gravitational dynamics, as stated in (III). This is an especially critical point to bear in mind in the context of reconstruction models in which higher-order couplings of flow field gradients show up in the density-velocity relation.

In this paper, we approach the reconstruction problem from a purely Lagrangian perspective using the solutions of the Lagrange-Newton system obtained by Buchert & Ehlers (1993). The goal of the paper is to obtain a self-consistent solution for the over-density field that is valid to second order, thus extending the results of Nusser et al. 1991 in the context of the ZA. Our results are purely Lagrangian, but in obtaining them we rely on the fact that there is a one-to-one mapping between Lagrangian and Eulerian coordinates and hence, the reconstruction formulae presented are only valid up to orbit-crossing time. The basic formalism is laid out in Sect. 2, and in Sect. 3 we discuss its application to two different classes of initial conditions. In Sect. 4 we discuss the self-consistency of solutions in perturbation theory models. Sect. 5 compares the model presented with previous reconstruction procedures and Sect. 6 sums up.

2. First- and second-order Lagrangian field reconstruction

In what follows, we shall mainly discuss the physically interesting case where the peculiar-velocity field is parallel to the peculiar-acceleration, up to decaying modes, a property which results from the Eulerian linear theory for irrotational fields, and is also valid for the general irrotational Lagrangian linear solution (the growing-mode solution supports the tendency to becoming parallel, see Buchert (1992)). We will further recall that both fields are practically parallel up to orbit-crossing time, also in the second-order schemes we will consider. The results presented however are not restricted to solutions where this property holds but, as we will see below, apply to a wider class of solutions.

In what follows we shall study subclasses of the second-order Lagrangian perturbation solutions given by Buchert & Ehlers (1993) which are only restricted by the requirement that there exists an arbitrary functional relationship among peculiar-velocity and -acceleration at the initial time. The subclasses are singled out by special assumptions for this functional relationship.

The second-order parametrization of the orbits of the particles in terms of their Lagrangian coordinates and time for the

[2] We make use of the term 'initial' to denote conditions given at t_0, an arbitrary but sufficiently early epoch, not necessarily $t = 0$.

subclasses of solutions which we consider later can be written as follows:

$$\boldsymbol{q} = \boldsymbol{F}(t, \boldsymbol{X}) = \boldsymbol{X} + f_1(t)\nabla_X S^{(1)}(\boldsymbol{X}) + f_2(t)\nabla_X S^{(2)}(\boldsymbol{X}), \quad (5)$$

where $f_1(t)$ and $f_2(t)$ are dimensionless functions of time, calculated from solving the Lagrange-Newton system for deviations from the homogeneous solution to second order. Moutarde et al. (1991) investigated the orbits (5) (rather than (4)), for leading orders of $f_1(t)$ and $f_2(t)$ and for a model of a particular initial potential. In the next section, we will examine two particular solutions for $f_1(t)$ and $f_2(t)$ for different, but generic, initial conditions.

The expansion factor $a(t)$ is normalized to unity at t_0, $a(t) = \left(\frac{t}{t_0}\right)^{2/3}$, (and equal to the linear growth factor $D(t)$ in an Einstein-de Sitter universe considered here). The perturbation potentials $S^{(1)}$ and $S^{(2)}$ are determined by the initial data such that, in general, they have to satisfy the (non-local) boundary conditions:

$$\nabla_X^2 S^{(1)} = I(S)\, t_0, \quad (6)$$

$$\nabla_X^2 S^{(2)} = 2\, II(S^{(1)}), \quad (7)$$

where S denotes the initial peculiar-velocity potential $\boldsymbol{u}(t_0, \boldsymbol{X}) \equiv \nabla_X S(\boldsymbol{X})$, and (following the summation convention)

$$I(S) = S_{,i,i}, \quad (8)$$

$$II(S^{(1)}) \equiv \frac{1}{2}\,(S^{(1)}_{,i,i}S^{(1)}_{,j,j} - S^{(1)}_{,i,j}S^{(1)}_{,j,i}), \quad (9)$$

are the first and second principal invariants of the peculiar-velocity tensor gradient. For periodic boundary conditions and suitable gauge conditions, however, which we shall assume hereafter, we can simplify (6)(7) (see Ehlers & Buchert (1997) for a rigourous proof):

$$\nabla_X S^{(1)} = \nabla S\, t_0 \ , \quad (10)$$

$$\nabla_X^2 S^{(2)} = 2\, II(S)\, t_0^2 \ . \quad (11)$$

Therefore, (5) gives us the trajectory of any given particle by solving (10)(11) for an initial potential S. At the time t_0, both f_1 and f_2 vanish, so Lagrangian and Eulerian coordinates coincide,

$$\boldsymbol{q} = \boldsymbol{F}(t_0, \boldsymbol{X}) = \boldsymbol{X}. \quad (12)$$

Thus, the expression for the density contrast at any given time and for any trajectory field reads:

$$[\,1 + \delta(t, \boldsymbol{X})\,] = [\,1 + \delta(t_0, \boldsymbol{X})\,]\; J^{-1} \ , \quad (13)$$

where the determinant $J(t, \boldsymbol{X})$ is

$$J \equiv \det\left(\frac{\partial F_i}{\partial X_j}\right). \quad (14)$$

In order to calculate δ as a function of Eulerian coordinates, we need to invert the coordinate map (5) so that Lagrangian coordinates are expressed in terms of the Eulerian coordinates and thereby derive the following:

$$[\,1 + \delta(t, \boldsymbol{H}(t, \boldsymbol{q}))\,] = [\,1 + \overset{\circ}{\delta}\,]\; J^E, \quad (15)$$

where $\overset{\circ}{\delta}(\boldsymbol{X})$ is the initial density contrast and the determinant $J^E(t, \boldsymbol{q}) = J^{-1}(t, \boldsymbol{X})$ is

$$J^E \equiv \det\left(\frac{\partial H_i}{\partial q_j}\right). \quad (16)$$

Eq. (15) gives the Eulerian values of the field δ at the Eulerian positions corresponding to a given trajectory labelled by $\boldsymbol{X} = \boldsymbol{H}(t, \boldsymbol{q})$. In principle, we can interpret this as a field $\delta(t, \boldsymbol{q})$ satisfying the Eulerian equations of motion. Nonetheless, it is important to bear in mind that the functional dependence of δ on $\boldsymbol{H}$ is only well-defined while the map between both coordinate spaces remains one-to-one. The peculiar-velocity is given by

$$\boldsymbol{u}(t, \boldsymbol{H}) = a\dot{a}\,\frac{\mathrm{d}}{\mathrm{d}a}\boldsymbol{F} \ \ , \quad (17)$$

and, similarly, the peculiar-acceleration,

$$\boldsymbol{w}(t, \boldsymbol{H}) = (a\ddot{a} + 2\dot{a}^2)\frac{\mathrm{d}}{\mathrm{d}a}\boldsymbol{F} + a\dot{a}^2\frac{\mathrm{d}^2}{\mathrm{d}a^2}\boldsymbol{F} \ \ . \quad (18)$$

The Jacobian J^E of the transformation $\boldsymbol{H}$ is given explicitly in Appendix B. This general expression involves a number of cross-terms of $\boldsymbol{u}$ and $\boldsymbol{w}$ components. However, we can ignore these by assuming the peculiar-velocity field to be parallel to the peculiar-acceleration, such that

$$\boldsymbol{w}(t, \boldsymbol{H}) = \boldsymbol{u}(t, \boldsymbol{H})\, t^{-1}. \quad (19)$$

This assumption can be justified on physical grounds: after some time, the peculiar-velocity field tends to be parallel to the peculiar-acceleration, for the second-order irrotational solution (5), due to the existence of decaying and growing solutions in the weakly non-linear regime. We will address this issue in detail in Sect. 5, and show that a weaker condition on the gradients of the fields leads to the same result. As in the first-order model (where (19) holds exactly) the growing part supports parallelism, as it is shown in Buchert & Ehlers (1993) for a wide class of irrotational second-order solutions. Indeed, the difference between $\boldsymbol{u}\, t^{-1}$ and $\boldsymbol{w}$ for (5) is given by decaying modes only, as we shall see in the next section. Therefore, we are entitled to express $\boldsymbol{w}$ by some function proportional to $\boldsymbol{u}$, so that the inversion of the map (5) satisfies the implicit equation:

$$\boldsymbol{H}(t, \boldsymbol{q}) = \boldsymbol{q} - h(t)\; \boldsymbol{u}(t, \boldsymbol{H}(t, \boldsymbol{q})), \quad (20)$$

where $h(t)$ is given explicitly in Appendix A for two different models.

In the first-order model, by virtue of (19), the same relation (20) holds with the appropriate $h(t)$ (Appendix A.1). With condition (19) implicit in (20), the determinant J^E reduces to:

$$J^E = 1 - h\; I^E(u_i) + h^2\; II^E(u_i) - h^3\; III^E(u_i). \quad (21)$$

Here, I^E (divergence), II^E (dispersion of diagonal components) and III^E (determinant) denote the three principal scalar invariants of the peculiar-velocity gradient with respect to comoving Eulerian coordinates as given in Appendix B. Therefore, substituting (21) into (15), we derive the relation for the density and velocity fields:

$$\frac{1+\delta(t,\boldsymbol{H}(t,\boldsymbol{q}))}{1+\overset{\circ}{\delta}} = 1 - h\, I^E(u_i) + h^2\, II^E(u_i) - h^3\, III^E(u_i)\ , \tag{22}$$

where $u_i = u_i(t,\boldsymbol{H}(t,\boldsymbol{q}))$. This result is unique and valid up to orbit-crossing time, i.e., while the coordinate inversion $\boldsymbol{X} = \boldsymbol{H}(t,\boldsymbol{q})$ is well-defined. In principle, it enables us to calculate the cosmic density field from observations of the peculiar-velocity field in the weakly non-linear regime at a fixed time, provided we set $\delta(t_0) = 0$. It is interesting to emphasize that, due to the parallelism condition (19), (22) applies at both first- and second-order (the appropriate $h(t)$ for each case is given in Appendix A). The simplicity of (22) is remarkable. It shows that the first- and second-order models contain not only quadratic terms in $u_{i,j}$ (as pointed out in the literature, e.g. Gramann 1993a,b) but also cubic terms, arranged in the form of the principal invariants of the deformation tensor: $I^E(u_i)$, $II^E(u_i)$ and $III^E(u_i)$.

A more general result, albeit a complicated one, can also be derived for the case where we drop the condition (19). The corresponding solution, taking into account all cross-terms, is obtained using the full solution for J^E given in Appendix B. Nonetheless, considering $\boldsymbol{w}$ is not directly measurable from observations, the application of the general solution without the assumption of parallelism would be impractical. In these circumstances (22) provides a useful approximation.

3. Application to specific models

In this section, we will examine two particular solutions of the second-order orbits (5) that are of interest in the reconstruction procedure described in Sect. 2. These are characterized by the nature of the initial conditions at t_0. At this time, only one field, S, is specified. These solutions are derived in Buchert & Ehlers (1993).

3.1. Model I: $\boldsymbol{u}(\boldsymbol{X}) = \boldsymbol{w}(\boldsymbol{X})t_0$

In this case, the velocity and acceleration fields are set to be identically parallel at the initial time. This relation is satisfied in Zel'dovich's ansatz, and it is a natural condition to set in a more general scheme, given the remarkable accuracy of the "Zel'dovich approximation". The initial density perturbation is thus expected to be proportional to the divergence of the peculiar-velocity. The solution (5) then is specified by the functions

$$f_1(t) = \frac{3}{2}[\,a(t) - 1\,], \tag{23}$$

$$f_2(t) = \frac{9}{4}[-\frac{3}{14}a^2(t) + \frac{3}{5}a(t) - \frac{1}{2} + \frac{4}{35}a^{-3/2}(t)\,]. \tag{24}$$

Therefore, the peculiar-velocity reads

$$\boldsymbol{u}(t,\boldsymbol{H}) = a^{1/2}\, t_0^{-1}\, \nabla_X S^{(1)} + \frac{3}{2}(-\frac{3}{7}a^{3/2} + \frac{3}{5}a^{1/2} - \frac{6}{35}a^{-2})\, t_0^{-1}\, \nabla_X S^{(2)}, \tag{25}$$

and the peculiar-acceleration,

$$\boldsymbol{w}(t,\boldsymbol{H}) = a^{-1}\, t_0^{-2}\, \nabla_X S^{(1)} + (-\frac{15}{14} + \frac{9}{10}a^{-1} + \frac{6}{35}a^{-7/2})\, t_0^{-2}\, \nabla_X S^{(2)}. \tag{26}$$

Thus the departure from the parallelism condition (19) is

$$\boldsymbol{u}\, t^{-1} - \boldsymbol{w} = \frac{3}{7}\,(1 - a^{-7/2})\, t_0^{-2}\, \nabla_X S^{(2)}. \tag{27}$$

Hence, this difference is a negligible effect due to the presence of the decaying mode. At $t = t_0$, the RHS of (27) is identically zero and, at later times, the decaying mode vanishes sufficiently fast and the overall coefficient therefore tends to a constant. This constant second-order term could be absorbed in a coordinate transformation. In this case, $h(t)$ in the reconstruction formula (22) is given by (see Appendix A.2 for details)

$$h = \frac{3}{2}\, t_0\, (1 - a^{-7/2})^{-1}(a^{1/2} - a^{-1/2} - a^{-3} + a^{-4}). \tag{28}$$

This is a monotonic function of t, and to the leading order it reads

$$h \approx \frac{3}{2}\, t_0\, a^{1/2}, \tag{29}$$

which is consistent with the results presented in Moutarde et al. (1991).

3.2. Model II: $\boldsymbol{w}(\boldsymbol{X}) = 0$

Although Model I provides an appropriate initial value setting from the physical point of view, the initial density contrast in this model is strictly non-vanishing. However, for reconstruction models we have to neglect this, since we do not want to specify initial information. Precisely speaking, this implies an error which can be removed by using Model II: Given a vanishing initial peculiar-acceleration field, the initial density contrast $\overset{\circ}{\delta}$ is zero and its growth is induced by the initial velocity perturbations only. In this case, $f_1(t)$ and $f_2(t)$ in the class of solutions for the orbits (5) are given by

$$f_1(t) = \frac{3}{5}\,[\,a(t) - a^{-3/2}(t)\,], \tag{30}$$

$$f_2(t) = \frac{9}{25}\,[\,-\frac{3}{14}a^2(t) + \frac{29}{40}a(t) - \frac{1}{2} - \frac{1}{2}a^{-1/2}(t) + \frac{43}{70}a^{-3/2}(t) - \frac{1}{8}a^{-3}(t)\,]. \tag{31}$$

Therefore, from (17) the peculiar-velocity is

$$\boldsymbol{u}(t,\boldsymbol{H}) = \frac{2}{5}(a^{1/2} + \frac{3}{2}a^{-2})\, t_0^{-1}\, \nabla_X S^{(1)} + \frac{9}{25}\,(-\frac{2}{7}a^{3/2} + \frac{29}{60}a^{1/2} + \frac{1}{6}a^{-1} - \frac{43}{70}a^{-2} + \frac{1}{4}a^{-7/2})\, t_0^{-1}\, \nabla_X S^{(2)}, \tag{32}$$

and the peculiar-acceleration,

$$\boldsymbol{w}(t,\boldsymbol{H}) = \frac{2}{5}\,(a^{-1} - a^{-7/2})\, t_0^{-2}\, \nabla_X S^{(1)} + \frac{3}{25}\,(-\frac{10}{7} + \frac{29}{20}a^{-1} + \frac{43}{35}a^{-7/2} - \frac{5}{4}a^{-5})\, t_0^{-2}\, \nabla_X S^{(2)}. \tag{33}$$

Like in the previous example we can calculate the departure from parallelism which is given in terms of the decaying modes

$$\boldsymbol{u}t^{-1} - \boldsymbol{w} = a^{-7/2}\, t_0^{-2}\, \nabla_X S^{(1)} + \frac{3}{25}(\frac{4}{7} - \frac{1}{2}a^{-5/2} - \frac{43}{14}a^{-7/2} + 2a^{-5})\, t_0^{-2}\, \nabla_X S^{(2)}, \tag{34}$$

such that, it is once more manifest that at late times parallelism is supported by the growing modes. At first sight it might seem that the presence of the first-order potential in (34) is a shortcoming for model II in comparison to model I, where departure from parallelism is a second-order effect, given by (27). However, although the initial fields are non-parallel as indicated by (34), the orders of magnitude involved in the RHS are very small from the outset and these decaying modes soon decrease further to negligible values.

3.3. Parallelism of $\boldsymbol{u}$ and $\boldsymbol{w}$

The assumption of parallelism (19) is justified by the presence of decaying modes in the difference $t\,\boldsymbol{w} - \boldsymbol{u}$ in both models I and II. On the other hand, it is apparent that the exact expression for J^E requires knowledge of the derivatives of the peculiar-acceleration field. Using the parallelism condition to simplify the solution implies neglecting the contribution of the Eulerian derivatives of the vector field $t\,\boldsymbol{w} - \boldsymbol{u}$. In this section we produce an analytical argument to justify this approximation in the weakly nonlinear regime.

A measure of parallelism of $\boldsymbol{u}$ and $\boldsymbol{w}$ is given by the quantity $|\boldsymbol{u} \times \boldsymbol{w}|$ (an alternative measure has been proposed recently by Bagla & Padmanabhan (1996)). We expect this quantity to be small in the regime where $\boldsymbol{u}$ and $\boldsymbol{w}$ are close to being parallel. As is given explicitly in Appendix A, we have

$$\boldsymbol{u}(t,\boldsymbol{H}) = \alpha(t)\nabla_{\boldsymbol{X}} S^{(1)} + \beta(t)\nabla_{\boldsymbol{X}} S^{(2)}, \tag{35}$$

$$\boldsymbol{w}(t,\boldsymbol{H}) = \zeta(t)\nabla_{\boldsymbol{X}} S^{(1)} + \eta(t)\nabla_{\boldsymbol{X}} S^{(2)}, \tag{36}$$

and therefore,

$$\boldsymbol{u} \times \boldsymbol{w} = \left(\alpha\,\zeta - \beta\,\eta\right)\, \nabla_{\boldsymbol{X}} S^{(1)} \times \nabla_{\boldsymbol{X}} S^{(2)}. \tag{37}$$

For the particular case of Model I, for instance, this leads to

$$|\,\boldsymbol{u} \times \boldsymbol{w}\,| = \frac{3}{7} t_0^{-3}\; a^{1/2}\;\; |\, 1 - a^{-7/2}\, |\; |\nabla_{\boldsymbol{X}} S^{(1)} \times \nabla_{\boldsymbol{X}} S^{(2)}|. \tag{38}$$

This quantity vanishes for all models where $\nabla_{\boldsymbol{X}} S^{(1)}$ and $\nabla_{\boldsymbol{X}} S^{(2)}$ are parallel. However this is not so in general, and the integrals of (6)(7) can yield to non-parallel (and non-negligible) gradients $\nabla_{\boldsymbol{X}} S^{(1)}$ and $\nabla_{\boldsymbol{X}} S^{(2)}$. Furthermore, the presence of the coefficient $a^{1/2}(t)$ in (38) indicates that an initial departure from parallelism of the fields $\boldsymbol{u}$ and $\boldsymbol{w}$ will grow in time. At this point it is important to stress that our simplification to derive (22) does not strictly speaking rely on the parallelism of the fields $\boldsymbol{u}$ and $\boldsymbol{w}$ but on that of the spatial gradients $u_{i,j}$ and $w_{i,j}$. The differences of these fields are intimately connected, but the time dependence involved is different as is clear by direct differentiation. Parallelism of the gradients is a weaker condition to impose than that of the fields themselves. It is easy to show that

$$u_{i,j} = \left[\alpha\; \nabla_{ik} S^{(1)} + \beta\; \nabla_{ik} S^{(2)}\right] \left[\delta_{kj} + f_1\; \nabla_{kj} S^{(1)} + f_2\; \nabla_{kj} S^{(2)}\right]^{-1}, \tag{39}$$

and

$$w_{i,j} = \left[\zeta\; \nabla_{ik} S^{(1)} + \eta\; \nabla_{ik} S^{(2)}\right] \left[\delta_{kj} + f_1\; \nabla_{kj} S^{(1)} + f_2\; \nabla_{kj} S^{(2)}\right]^{-1}, \tag{40}$$

Therefore, we have that for Model I:

$$u_{i,j}\, t^{-1} - w_{i,j} = \frac{3}{7}\left(1 - a^{-7/2}\right) \nabla_{ik} S^{(2)}\; \Gamma_{kj}, \tag{41}$$

and for Model II:

$$u_{i,j}\, t^{-1} - w_{i,j} = \frac{3}{5} a^{-7/2}\, \nabla_{ik} S^{(1)}\; \Gamma_{kj} + \frac{3}{25}\left(\frac{4}{7} + \frac{1}{2}a^{-5/2} - \frac{43}{14}a^{-7/2} - \frac{1}{2}a^{-5}\right) \nabla_{ik} S^{(2)}\; \Gamma_{kj}, \tag{42}$$

where

$$\Gamma_{ij} \equiv \left[\delta_{ij} + f_1 \nabla_{ij} S^{(1)} + f_2 \nabla_{ij} S^{(2)}\right]^{-1}. \tag{43}$$

In the case of Model I, parallelism is exact in the initial conditions, therefore there is no dependence of the derivatives on the potential $S^{(1)}$. In all other models, the difference $u_{i,j}\, t^{-1} - w_{i,j}$ comes as a linear combination of the double derivatives $\nabla_{ij} S^{(n)}$, $n = 1, 2$, up to the coefficient Γ_{ij} that plays a role when we approach orbit-crossing. For realistic fields, i.e., those that evolve from negligible amplitudes at $t = t_0$, the gradients of the perturbative potentials $S^{(1)}$, $S^{(2)}$ are sufficiently smooth and slowly varying, and therefore they are well under the order of the approximation in the weakly nonlinear regime. We stress, however, as indicated above that in the strongly nonlinear regime (or at the epoch of shell-crossing, respectively), this argument breaks down in the same manner as perturbative solutions at any order do.

4. Self-consistency of perturbative solutions

In our reconstruction procedure we have proposed a simplification of the exact solution (15) under the assumption of parallelism of the fields $\boldsymbol{u}$ and $\boldsymbol{w}$. Thus we are able to obtain an expression for the density in terms of the derivatives of the velocity only. We have seen that this assumption is sufficiently accurate, the difference between both fields is a negligible effect. However, it is not necessary to adopt parallelism, and in this section we will outline a possible scheme to construct iteratively a "self-consistent" solution for $\boldsymbol{w}$ from the velocity field, so that the reconstruction method with the Jacobian (B1) can be employed.

At this point, we would like to call the attention of the reader to the problem of self-consistency of approximations as pointed out by Doroshkevich et al. (1973) (compare the discussion by Buchert (1989)). We enunciate the problem by stating that perturbative solutions of the equations of motion are mutually consistent only within the truncation order. This can be illustrated with the "Zel'dovich approximation". The density contrast as given by the Poisson equation is

$$\delta^{(1)}(t,\boldsymbol{q}) = -\frac{3}{2}\, t_0^2\, a^{-1}\, \nabla_q \cdot \boldsymbol{w}(t,\boldsymbol{q}), \tag{44}$$

and the density contrast as given by mass conservation

$$1+\delta^{(2)}(t,\boldsymbol{H}) = \frac{1+\mathring{\delta}}{J(t,\boldsymbol{H})}. \tag{45}$$

Introducing the dimensionless error

$$\epsilon = \frac{\delta^{(2)}-\delta^{(1)}}{\delta^{(2)}}, \tag{46}$$

this difference for the "Zel'dovich approximation" gives

$$\epsilon = (a-1)^2\, II(S) + (a-1)^3\, III(S), \tag{47}$$

which is within the order of the approximation. In the second-order model we expect an analogous situation. As the orbits we have used are obtained by solving the Lagrange-Newton system perturbatively, Eulerian quantities constructed from these will automatically satisfy all equations to second-order. However, the density contrast constructed from the velocities through (22) is associated to a Newtonian potential causing an acceleration that will in general differ from the acceleration given by the second-order orbits. This difference vanishes only for exact solutions.

Let us denote by a (1) superscript the quantities derived from the particle orbits. Hence,

$$\frac{1+\delta^{(1)}(t,H)}{1+\mathring{\delta}} = - h(t)\, I^E(u_i^{(1)}) + h^2(t)\, II^E(u_i^{(1)}) - h^3\, III^E(u_i^{(1)}), \tag{48}$$

and therefore,

$$\nabla_q\cdot\boldsymbol{w}^{(2)} = -\frac{2}{3t_0^2}\, a\,(1+\mathring{\delta}) \cdot[-h\, I^E(u_i^{(1)}) + h^2\, II^E(u_i^{(1)}) - h^3\, III^E(u_i^{(1)}) - 1]\ , \tag{49}$$

which in general differs from $\boldsymbol{w}^{(1)} = \dot{\boldsymbol{u}}^{(1)} + \frac{\dot a}{a}\boldsymbol{u}^{(1)}$. From $\boldsymbol{w}^{(2)} = \dot{\boldsymbol{u}}^{(2)} + \frac{\dot a}{a}\boldsymbol{u}^{(2)}$ it is possible in principle to solve for $\boldsymbol{u}^{(2)}$, from which $\delta^{(2)}$ is similarly constructed, and we iterate henceforth via the prescription

$$\frac{1+\delta^{(n)}(t,H)}{1+\mathring{\delta}} = -h(t)\, I^E(u_i^{(n)}) + h^2(t)\, II^E(u_i^{(n)}) - h^3\, III^E(u_i^{(n)}), \tag{50}$$

that we use to integrate $\boldsymbol{w}^{(n+1)}$. A consistent solution is then found in the limit

$$\epsilon = \frac{\delta^{(n+1)}-\delta^{(n)}}{\delta^{(n)}} \to 0 \qquad n\to\infty. \tag{51}$$

Note that after each iteration, the condition $\nabla_q \times \boldsymbol{w}^{(n)} = \mathbf{0}$ (arising from the Lagrange equations in the exact case) is preserved at all times. Finding a self-consistent solution to the dynamics by successive iterations is tantamount to minimization of the difference of the particle orbits

$$\Delta\boldsymbol{F}(t,\boldsymbol{X}) = \boldsymbol{F}_{\rm self-consistent}(t,\boldsymbol{X}) - \boldsymbol{F}(t,\boldsymbol{X}), \tag{52}$$

that we estimate at each iteration through the differential equation

$$\boldsymbol{w}^{(n)} - \boldsymbol{w}^{(n-1)} = (a\ddot a + 2\dot a^2)\frac{\rm d}{{\rm d}a}\Delta\boldsymbol{F}^{(n)} + a\dot a^2\frac{{\rm d}^2}{{\rm d}a^2}\Delta\boldsymbol{F}^{(n)}. \tag{53}$$

This is however a non-trivial numerical problem that is beyond the scope of this article and we plan to pursue this possibility in a future work.

5. Comparison with other work

We have calculated a unique and well-defined relation (22) for cosmic density and velocity fields that is a self-consistent solution in the second-order model. Given the second-order ansatz for the particle orbits (5), the Lagrange-Newton system determines the functions of time $f_1(t)$ and $f_2(t)$ for generic initial conditions and it constrains the perturbation potentials $S^{(1)}$, $S^{(2)}$ in terms of the peculiar-velocity potential S at t_0. Consequently, the orbits are determined at all times until shell-crossing, and the density is obtained from the continuity equation by evaluating the Jacobian J^E of the transformation $\boldsymbol{X}\to\boldsymbol{q}$.

For simplicity, we have discussed the formulae on the assumption that the velocity and acceleration fields are parallel. In Sect. 3, it is shown that this assumption is a sufficient condition but by no means necessary, and in general it is sufficient to adopt the condition of parallelism of the gradients of the fields, which is a weaker requirement.

The self-consistency of the solution for the density field follows from the fact that the orbits employed are second-order solutions in perturbation theory and not any given ansatz. Our result (22) generalizes previous results in the literature in the following respect. Nusser et al. (1991) obtained two relations for the density constrast in the ZA,

$$\delta_c(t, \boldsymbol{q}) = -D\ I^E(v_i) + D^2\ II^E(v_i) - D^3\ III^E(v_i), \tag{54}$$

and

$$\delta_e(t, \boldsymbol{q}) = -D\ I^E(v_i), \tag{55}$$

where a scaled peculiar velocity is used,

$$v_i \equiv (a\dot{a})^{-1} u_i, \tag{56}$$

and δ_c is derived from the continuity equation and δ_e from Euler's equation. The difference between (54) and (55) is second order and is therefore within the order of the approximation:

$$\delta_c(t, \boldsymbol{q}) - \delta_e(t, \boldsymbol{q}) = D^2\ II^E(v_i) - D^3\ III^E(v_i). \tag{57}$$

Thus, in the ZA, only the first term on the RHS of (54) is significant and consistent with conservation of momentum. In the second-order result (22), we are able to retain two more terms and this relation has a similar form as (54), where D is replaced by h. This form of the over-density field satisfies automatically Euler's equation to second-order, since the orbits are obtained solving the Lagrange-Newton system to this order, and therefore the $II(v_i)$ and $III(v_i)$ terms are a legitimate part of the solution and not higher-order 'error' terms as in (54).

One does not obtain self-consistent solutions in models where an arbitrary perturbative parameter, such as $D(t)$, is singled out, which results in a hybrid Eulerian-Lagrangian scheme. The chief problem inherent to such approaches is that the time dependence is set ab initio on the orbits and it is not determined by the equations of motion as is done in the solutions we have used. This type of ansatz can be employed to good effect in a least-square fit for the dynamics of the particles as a two-boundary condition problem (see for example Susperregi & Binney 1994), but in perturbation theory they are inconsistent and of little predictive power due to their lack of convergence as discussed in the Introduction. In such approaches, both the continuity equation and the equation of motion must be truncated to the given perturbation order and, consequently, the corresponding solutions δ_c and δ_e in general differ. Therefore, from the analysis of the previous section, we can also conclude that δ_c and δ_e do not only differ by a higher order in the approximation, but failure to solve for the orbits perturbatively is conducive to discrepancies in the solutions *at the same order*. Given a parametrization of the orbits such as (3), the second-order solution for the continuity density is given by (Gramann 1993b)

$$\delta_c = -D\ I^E(v_i) + D^2\ II^E(v_i), \tag{58}$$

As shown by Gramann (1993b) the second order term for δ_e differs by a factor of $4/7$ from that of (58). This inconsistency at second order arises as a consequence of using second-order orbits that do not correspond to the actual second-order perturbation theory solutions. In contrast to the solution (22), (58) only accounts for quadratic couplings in u_i. Considering that at first order we already have the relation (22), it is apparent that (58) is not an accurate generalization of the Lagrangian linear theory.

In the scheme discussed here, initial conditions are set at $t = t_0$, and hence we can try to establish a connection with the reconstruction model (58) by specifying these at $t = 0$. However, the normalization chosen for $a(t)$ impedes to set t_0 identically equal to zero. A choice of an arbitrarily small t_0 requires keeping only the growing solutions in the expression for $h(t)$, entirely neglecting the presence of decaying modes. We have to further restrict ourselves to the leading term (which is a particular solution of the second-order differential equation) and neglect the homogeneous second-order solution (which is growing). The leading order in $h(t)$ is, at both first and second order (for model I),

$$h \approx \frac{3}{2}\, t_0\, a^{1/2}, \tag{59}$$

and thus, using definition (56) in (22), we get

$$\begin{aligned}\delta &= -(ha\dot{a})\, I^E(v_i) + (ha\dot{a})^2\, II^E(v_i) - (ha\dot{a})^3\, III^E(v_i) \\ &\approx -(a-1)\, I^E(v_i) + (a-1)^2\, II^E(v_i) - (a-1)^3\, III^E(v_i).\end{aligned} \tag{60}$$

With the normalization chosen for $a(t)$, (60) is in reasonable agreement with (58) at early times. At late times however, the presence of the $III^E(v_i)$ term in (60) diminishes the departures from linearity brought about by the quadratic term whereas this effect is not accounted for in (58).

It must be emphasized that (22) is strictly only valid so long as the inversion $\boldsymbol{H}(t, \boldsymbol{q})$ is well-defined. Indeed, the expression given for $\delta(t, \boldsymbol{H}(t, \boldsymbol{q}))$ provides the Eulerian values of the density contrast and is given as a function of Eulerian positions up to orbit-crossing time. At later times the inversion map becomes singular and this result does not hold.

By integrating the Poisson equation in Eulerian coordinates using $\delta(t, \boldsymbol{H}(t, \boldsymbol{q})$ it is concluded (e.g. Gramann 1993a, eq. (2.20)) that the presence of the quadratic term $II^E(v_i)$ in the density-velocity relation induces a departure from parallelism between peculiar-velocity and -acceleration vectors. The derivation of this relation under the assumption of parallelism proves this conclusion is not correct. Certainly, one would be able to obtain agreement with solutions of Poisson's equation if a self-consistent density contrast were known. It is manifest however that this is far from being the case in these models. Differences in the solutions within the order of the approximation, as it is the case with δ_c and δ_e in Gramann's analysis, imply that any conclusion drawn from Poisson's equation applied to the reconstructed density is not justified as long as approximations are involved.

We finally note that an expansion of the Jacobian to a given order (*after* the solutions are obtained) mirrors formally the mathematical fact that, in principle, we cannot believe terms of higher order than the perturbative order of the trajectories. However, the powerful properties of a Lagrangian approach mainly rely on the existence of an exact integral for the density for *any* given trajectory field, which allows using these approximations until shell-crossing. At this epoch the contributions from second and third invariants is of the same order as that from the first invariant, a fact which underlies the success of the ZA. Whether this extrapolation until shell-crossing is justified at all is another issue. The successes of Lagrangian perturbation methods as summarized by Bouchet et al. (1995) and the success of following trajectories until shell-crossing and even beyond (Melott et al. 1995) strongly argue in favour of this extrapolation.

6. Conclusions

In this paper we have presented a relation between cosmic density and velocity fields following a purely Lagrangian derivation (Eq.(22)) that is self-consistent in the second-order model. The advantage of working in the Lagrangian picture is that the over-density field obtained from the continuity equation is self-consistent and automatically satisfies conservation of momentum. For simplicity, one can adopt the condition (19) of parallelism of the fields $\boldsymbol{u}$ and $\boldsymbol{w}$, satisfied at first order and by a large class of irrotational solutions in second-order Lagrangian perturbation theory, and the result (22) holds accurately at both orders. However, as pointed out in Sect. 3, we note that (19) is not a sine qua non condition but a weaker condition of parallelism of the gradients of the fields would yield the same result. It is shown that this condition is well satisfied for generic initial conditions. In each case, the function $h(t)$ is given explicitly in Appendix B.1 and Appendix B.2 respectively. Its range of validity is limited by the epoch when the inversion map $\boldsymbol{H}(t,\boldsymbol{q})$ becomes singular, i.e. up to orbit-crossing time, while its principal range of validity should strictly be estimated by $|p_{i,j}(t_c)| << a(t_c)$, where $\boldsymbol{p}(t,\boldsymbol{X}) = a(t)\,[\boldsymbol{F}(t,\boldsymbol{X}) - \boldsymbol{X}]$ is the displacement field with respect to the Hubble-flow. This condition is probably very conservative in view of the success of these approximations if followed up to shell-crossing.

By specifying the initial data at $t \approx 0$ and keeping only the leading terms in the solutions, we are able to recover the leading terms of previous reconstruction models as shown in Sect. 5. Furthermore, the time dependence of the orbits in our model is established by solving the Lagrange-Newton system at each order. This leads to a unique and consistent result for the Eulerian density constrast in terms of the peculiar-velocities.

We finally wish to show some skepticism about the usefulness of the reconstruction formulae given. We want them to be applicable to present day observational data. However, we know confidently that shell-crossing has occurred, i.e. the interesting regime is no longer covered. Instead one would have to investigate a relationship between *smoothed* cosmic over-density and peculiar-velocity fields, where the smoothing window scale has to ensure the absence of vorticity and multi-stream systems in the average flow. Given the present work we should ask whether there is a formally proper way to incorporate smoothing into a consistent Lagrangian reconstruction formalism. With regard to this point, we think that solutions of the Lagrange-Newton system may possibly provide reasonable tools for reconstructing average fields, since averages in Eulerian space of any vector function $\boldsymbol{A}(t,\boldsymbol{H}(t,\boldsymbol{q}))$ are straightforward to calculate: $\langle \boldsymbol{A}\rangle_q \propto \int d^3\boldsymbol{q}\ \boldsymbol{A}(t,\boldsymbol{X}) = \int d^3\boldsymbol{X}\ J(t,\boldsymbol{X})\ \boldsymbol{A}(t,\boldsymbol{X})$. However, we still encounter the fundamental problem of averaging over multi-stream flows, which may not be properly handled in the framework of the Lagrange-Newton system. Rather, such a description has to be based on an approximation of the Vlasov-Poisson system. This major improvement of the methods lies well beyond the scope of present reconstruction techniques and requires the construction of Vlasov-Poisson type approximations.

Acknowledgements. We thank James Binney, Avishai Dekel, Jürgen Ehlers, Adi Nusser and David Weinberg for valuable comments and suggestions. TB is supported by the "Sonderforschungsbereich 375-95 für Astro-Teilchenphysik" der Deutschen Forschungsgemeinschaft. MPS is grateful to the Max-Planck-Institut für Astrophysik at Garching for its hospitality.

Appendix A: determination of $h(t)$

A.1. First-order model I

The first-order particle orbits are

$$\boldsymbol{F}(t,\boldsymbol{X}) = \boldsymbol{X} + f_1(t)\,t_0\,\nabla_X S(\boldsymbol{X}), \tag{A1}$$

where the perturbation potential is related to the initial gravitational potential through the relation

$$\nabla_{\boldsymbol{X}} S = -t_0^2\,\nabla_{\boldsymbol{X}}\phi. \tag{A2}$$

The inversion of (A1) is then:

$$\boldsymbol{H}(t,\boldsymbol{q}) = \boldsymbol{q} - h(t)\,\boldsymbol{u}(t,\boldsymbol{H}) = \boldsymbol{q} - a^{-1/2}\,t_0\,f_1(t)\,\boldsymbol{u}(t,\boldsymbol{H}), \tag{A3}$$

and therefore $h(t)$ is given by:

$$h = \frac{3}{2}\,t_0\,(a^{1/2} - a^{-1/2}). \tag{A4}$$

Thus, we obtain:

$$\boldsymbol{u} = a^{1/2}\,t_0^{-1}\,\nabla_{\boldsymbol{X}} S, \tag{A5}$$

$$\boldsymbol{w}\,t_0 = a^{-1}\,t_0^{-1}\,\nabla_{\boldsymbol{X}} S. \tag{A6}$$

From this we derive the well-known result for the Zel'dovich approximation used in the Sachs-Wolfe effect that

$$\nabla_q\phi = \text{const}, \tag{A7}$$

since

$$\boldsymbol{w} = -\frac{1}{a\,t_0^2}\nabla_q\phi. \tag{A8}$$

A.2. Second-order model I

Eqs. (17)(18) in terms of the perturbation potentials read

$$\begin{bmatrix} \boldsymbol{u}(t,\boldsymbol{H}) \\ \boldsymbol{w}(t,\boldsymbol{H}) \end{bmatrix} = \begin{bmatrix} \alpha(t) & \beta(t) \\ \eta(t) & \zeta(t) \end{bmatrix} \begin{bmatrix} \nabla_X S^{(1)}(\boldsymbol{X}) \\ \nabla_X S^{(2)}(\boldsymbol{X}) \end{bmatrix}, \tag{A9}$$

where

$$\alpha = t_0^{-1}\, a^{1/2}, \tag{A10}$$

$$\beta = \frac{3}{2}\, t_0^{-1} \Big(-\frac{3}{7} a^{3/2} + \frac{3}{5} a^{1/2} - \frac{6}{35} a^{-2} \Big), \tag{A11}$$

$$\eta = t_0^{-2}\, a^{-1}, \tag{A12}$$

$$\zeta = t_0^{-2} \Big(-\frac{15}{14} + \frac{9}{10} a^{-1} + \frac{6}{35} a^{-7/2} \Big). \tag{A13}$$

We write the perturbation potentials in terms of $\boldsymbol{u}$ and $\boldsymbol{w}$ by inverting (A9):

$$\begin{bmatrix} \nabla_X S^{(1)}(\boldsymbol{X}) \\ \nabla_X S^{(2)}(\boldsymbol{X}) \end{bmatrix} = \begin{bmatrix} \alpha'(t) & \beta'(t) \\ \eta'(t) & \zeta'(t) \end{bmatrix} \begin{bmatrix} \boldsymbol{u}(t,\boldsymbol{H}) \\ \boldsymbol{w}(t,\boldsymbol{H}) \end{bmatrix}, \tag{A14}$$

where

$$\alpha' = (1 - a^{-7/2})^{-1} t_0 \,(\frac{5}{2} a^{-1/2} - \frac{21}{10} a^{-3/2} - \frac{2}{5} a^{-4}), \tag{A15}$$

$$\beta' = (1 - a^{-7/2})^{-1} t_0^2 \,(-\frac{3}{2} a + \frac{21}{10} - \frac{3}{5} a^{-5/2}), \tag{A16}$$

$$\eta' = \frac{7}{3} (1 - a^{-7/2})^{-1} t_0\, a^{-3/2}, \tag{A17}$$

$$\zeta' = -\frac{7}{3} (1 - a^{-7/2})^{-1} t_0^2. \tag{A18}$$

Using (A14), we invert (5) in the form

$$\boldsymbol{H}(t,\boldsymbol{q}) = \boldsymbol{q} - (1 - a^{-7/2})^{-1} [\, m_1(t)\, \boldsymbol{u} + m_2(t)\, \boldsymbol{w} \,], \tag{A19}$$

where

$$m_1 = \frac{3}{2}\, t_0 \,(\frac{7}{4} a^{1/2} - \frac{5}{2} a^{-1/2} + \frac{7}{20} a^{-3/2} + \frac{2}{5} a^{-4}), \tag{A20}$$

$$m_2 = \frac{3}{2}\, t_0^2 \,(-\frac{3}{4} a^2 + \frac{3}{2} a - \frac{7}{20} - a^{-3/2} + \frac{3}{5} a^{-5/2}). \tag{A21}$$

Therefore, given the condition of parallelism(19), we have that (A19) reduces to (20) with

$$h(t) \equiv (1 - a^{-7/2})^{-1} [\, m_1(t) + t^{-1}\, m_2(t) \,] \tag{A22}$$

$$h = \frac{3}{2}\, t_0 \,(1 - a^{-7/2})^{-1} (a^{1/2} - a^{-1/2} - a^{-3} + a^{-4}). \tag{A23}$$

A.3. Second-order model II

Following the same procedure as in Appendix A.2, we write

$$\begin{bmatrix} \boldsymbol{u}(t,\boldsymbol{H}) \\ \boldsymbol{w}(t,\boldsymbol{H}) \end{bmatrix} = \begin{bmatrix} \alpha(t) & \beta(t) \\ \eta(t) & \zeta(t) \end{bmatrix} \begin{bmatrix} \nabla_X S^{(1)}(\boldsymbol{X}) \\ \nabla_X S^{(2)}(\boldsymbol{X}) \end{bmatrix}, \tag{A24}$$

where

$$\alpha = \frac{2}{5}\, t_0^{-1} \,(a^{1/2} + \frac{3}{2} a^{-2}), \tag{A25}$$

$$\beta = \frac{9}{25}\, t_0^{-1} \,(-\frac{2}{7} a^{3/2} + \frac{29}{60} a^{1/2} + \frac{1}{6} a^{-1} - \frac{43}{70} a^{-2} + \frac{1}{4} a^{-7/2}), \tag{A26}$$

$$\eta = \frac{2}{5}\, t_0^{-2} \,(a^{-1} - a^{-7/2}), \tag{A27}$$

$$\zeta = \frac{3}{25}\, t_0^{-2} \,(-\frac{10}{7} + \frac{29}{20} a^{-1} + \frac{43}{35} a^{-7/2} - \frac{5}{4} a^{-5}). \tag{A28}$$

Therefore, inversion of (A24) leads to:

$$\begin{bmatrix} \nabla_X S^{(1)}(\boldsymbol{X}) \\ \nabla_X S^{(2)}(\boldsymbol{X}) \end{bmatrix} = \gamma(t) \begin{bmatrix} \alpha'(t) & \beta'(t) \\ \eta'(t) & \zeta'(t) \end{bmatrix} \begin{bmatrix} \boldsymbol{u}(t,\boldsymbol{H}) \\ \boldsymbol{w}(t,\boldsymbol{H}) \end{bmatrix}, \tag{A29}$$

where

$$\alpha' = 28\, t_0\, a^2, \tag{A30}$$

$$\beta' = -\frac{9}{5}\, t_0^2 \Big(-\frac{2}{7} a^{3/2} + \frac{29}{60} a^{1/2} + \frac{1}{6} a^{-1} - \frac{43}{70} a^{-2} + \frac{1}{4} a^{-7/2} \Big), \tag{A31}$$

$$\eta' = 2\, t_0 \,(-a^{-1} + a^{-7/2}), \tag{A32}$$

$$\zeta' = t_0^2 \,(2a^{1/2} + 3a^{-2}), \tag{A33}$$

$$\gamma = \Big(-\frac{24}{175} a^{1/2} - \frac{21}{25} a^{-2} + \frac{45}{28} a^{-3} - \frac{9}{25} a^{-9/2} - \frac{27}{100} a^{-7} \Big)^{-1}. \tag{A34}$$

Appendix B: Jacobian J^E

The Jacobian $\det(\partial H_i / \partial q_j)$ is given by:

$$\begin{aligned} J^E = {} & 1 - g_1\, I^E(u_i) - g_2\, I^E(w_i) + g_1^2\, II^E(u_i) + g_2^2\, II(w_i) \\ & + g_1\, g_2\, II'^E(u_i \mid w_j) - g_1^3\, III^E(u_i) - g_2^3\, III^E(w_i) \\ & - g_1^2\, g_2\, III'^E(u_i \mid w_j) - g_1\, g_2^2\, III''^E(u_i \mid w_j), \end{aligned} \tag{B1}$$

where

$$I^E(u_i) = u_{i,i}, \tag{B2}$$

$$II^E(u_i) = \frac{1}{2}(u_{i,i}u_{j,j} - u_{i,j}u_{j,i}), \tag{B3}$$

$$II'^E(u_i \mid w_j) = \frac{1}{2}(u_{i,i}w_{j,j} - u_{i,j}w_{j,i}), \tag{B4}$$

$$III^E(u_i) = \det(u_{i,j}) \tag{B5}$$

$$III'^E(u_i \mid w_j) = u_{2,3}u_{3,2}w_{1,1} - u_{2,2}u_{3,3}w_{1,1} - u_{2,3}u_{3,1}w_{1,2} + u_{2,1}u_{3,3}w_{1,2} + u_{2,2}u_{3,1}w_{1,3} - u_{2,1}u_{3,2}w_{1,3} - u_{1,3}u_{3,2}w_{2,1} + u_{1,2}u_{3,3}w_{2,1} + u_{1,3}u_{3,1}w_{2,2} - u_{1,1}u_{3,3}w_{2,2} - u_{1,2}u_{3,1}w_{2,3} + u_{1,1}u_{3,2}w_{2,3}, \tag{B6}$$

$$III''^E(u_i \mid w_j) = u_{3,3}w_{1,2}w_{2,1} - u_{3,2}w_{1,3}w_{2,1} - u_{3,3}w_{1,1}w_{2,2} + u_{3,1}w_{1,3}w_{2,2} + u_{3,2}w_{1,1}w_{2,3} - u_{3,1}w_{1,2}w_{2,3} - u_{2,3}w_{1,2}w_{3,1} + u_{2,2}w_{1,3}w_{3,1} + u_{1,3}w_{2,2}w_{3,1} - u_{1,2}w_{2,3}w_{3,1} + u_{2,3}w_{1,1}w_{3,2} - u_{2,1}w_{1,3}w_{3,2}, \tag{B7}$$

and the functions $g_1(t)$ and $g_2(t)$ are model-dependent. For instance, for the case of model I of Sect. 3,

$$g_1(t) = (1 - a^{-7/2})^{-1}\ m_1(t), \tag{B8}$$

$$g_2(t) = (1 - a^{-7/2})^{-1}\ m_2(t), \tag{B9}$$

where $m_1(t)$ and $m_2(t)$ are defined in Appendix A.2. The assumption of parallelism (19) adopted, J^E is simplified by making the following substitutions in (B1):

$$\begin{aligned} \boldsymbol{w} &\rightarrow 0 \\ g_1(t) &\rightarrow h(t), \end{aligned} \tag{B10}$$

where

$$h(t) = g_1(t) + t^{-1}\, g_2(t). \tag{B11}$$

Hence, all terms containing w_i are set equal to zero, and thus (B1) simply reads

$$J^E = 1 - h\ I^E(u_i) + h^2\ II^E(u_i) - h^3\ III^E(u_i). \tag{B12}$$

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