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Manifestly gauge-invariant general relativistic perturbation theory: I. Foundations

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Abstract

Linear cosmological perturbation theory is pivotal to a theoretical understanding of current cosmological experimental data provided e.g. by cosmic microwave anisotropy probes. A key issue in that theory is to extract the gauge-invariant degrees of freedom which allow unambiguous comparison between theory and experiment. When one goes beyond first (linear) order, the task of writing the Einstein equations expanded to nth order in terms of quantities that are gauge-invariant up to terms of higher orders becomes highly non-trivial and cumbersome. This fact has prevented progress for instance on the issue of the stability of linear perturbation theory and is a subject of current debate in the literature. In this series of papers we circumvent these difficulties by passing to a manifestly gauge-invariant framework. In other words, we only perturb gauge-invariant, i.e. measurable quantities, rather than gauge variant ones. Thus, gauge invariance is preserved non-perturbatively while we construct the perturbation theory for the equations of motion for the gauge-invariant observables to all orders. In this first paper we develop the general framework which is based on a seminal paper due to Brown and Kuchař as well as the relational formalism due to Rovelli. In the second, companion, paper we apply our general theory to FRW cosmologies and derive the deviations from the standard treatment in linear order. As it turns out, these deviations are negligible in the late universe, thus our theory is in agreement with the standard treatment. However, the real strength of our formalism is that it admits a straightforward and unambiguous, gauge-invariant generalization to higher orders. This will also allow us to settle the stability issue in a future publication.

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1. Introduction

General relativity is our best theory for gravitational physics and, so far, has stood the test of time and experiments. Its complicated, highly nonlinear equations of motion, however, mean that the calculation of many gravitational processes of interest has to rely on the use of approximations. One important class of such approximations is given by perturbation theory, where, generally speaking, one perturbs quantities of interest, such as the metric and matter degrees of freedom around an exact, known solution which, typically, displays a high degree of symmetry.

It is well known that perturbation techniques in general relativity pose challenges above and beyond those typically associated with them in other areas of physics, such as stability, convergence issues, etc. The reason is that general relativity is a gauge theory, the gauge group being the diffeomorphism group Diff(M) of the spacetime manifold M. As a result, all metric and matter variables transform non-trivially under gauge transformations. This creates the problem of differentiating between (physical) perturbations of a given variable and the effect of a gauge transformation on the latter. The obvious solution to this situation would be to calculate only with observables and perturb those. It has proved extremely difficult, however, to find observables in the full theory, with the exception of a few special situations, such as for asymptotically flat spacetimes. As a way out of this conundrum, one usually resorts to calculating in a specific gauge, carefully ensuring that all calculated quantities are gauge-independent. Alternatively, one tries to construct quantities that are observables up to a certain order. In the cosmological standard model this has been successfully done in linear order and forms an integral part of the modern lore of cosmology. In fact, there have been attempts to extend this even to second order and beyond, see, e.g., [1–4]. The sheer complexity of those calculations, however, shows that there is a natural limit to how far that approach can be pushed. Furthermore, it is not clear whether it will succeed for other backgrounds, such as a black hole spacetime, etc.

This clearly makes the search for a more general framework for perturbation theory of observable quantities highly desirable. Another motivation comes from the prospects of developing perturbation methods for non-perturbative quantum gravity approaches, such as loop quantum gravity [5]. It is clear that the standard methods mentioned earlier will be extremely difficult, if not impossible to implement.

This paper, the first in a series dedicated to this challenge, lays the foundations at the level of the full theory. Subsequent papers will deal with simplified cases of particular interest, such as perturbations around an FRW background.

After this brief overview of the motivations behind our paper, let us now discuss some of these issues in more detail. The crucial ingredient in our undertaking is the construction of observables for the full theory. To that end let us first recall the counting of the true degrees of freedom of general relativity: the temporal–temporal as well as the temporal–spatial components of the Einstein equations do not contain temporal derivatives of four metric functions (known as lapse and shift). Thus, in the Lagrangian picture, these four sets of equations can be used, in principle, in order to eliminate the temporal–temporal and temporal–spatial components of the metric in terms of the spatial–spatial components[4]. In addition,

[4] In the Hamiltonian picture, these equations relate canonical momenta to canonical configuration coordinates. There are four additional (so-called primary) constraints which impose that the momenta conjugate to lapse and shift vanish which leaves only two independent momenta. These eight constraints are of the first class type in Dirac's terminology [6].

diffeomorphism gauge invariance displays four additional degrees of freedom as pure gauge[5]. This is why general relativity in vacuum (without matter) has only two true (configuration) degrees of freedom (gravitons).

In the canonical picture, the ten equations split into four plus six equations. The four equations are the aforementioned constraints which canonically generate spacetime diffeomorphisms, that is, gauge transformations. The other six equations are canonically generated by a canonical 'Hamiltonian' which is actually a linear combination of these constraints, and thus also generates gauge transformations and even is constrained to vanish. It is customary not to call it a Hamiltonian but rather a Hamiltonian constraint. The interpretation of Einstein's equations as evolution equations is therefore unconvincing. Instead, the correct interpretation seems to be that they actually describe the flow of unphysical degrees of freedom under gauge transformations. Thus we contend that their primary use is to extract the true degrees of freedom in the way described below. These true degrees of freedom are gauge invariant and thus have trivial evolution with respect to the canonical Hamiltonian (constraint). This is the famous problem of time of general relativity [8]: there is no true Hamiltonian, only a Hamiltonian constraint and the observable quantities do not move under its flow. Nothing seems to move, everything is frozen, in obvious contradiction to our experience. This begs, of course, the question of what determines the time evolution of the true physical observables.

In [9] a possible answer was proposed. Namely, it was shown that the problem of time can be resolved without affecting the interpretation of Einstein's equations as evolution equations by adding certain matter to the system. The method for doing this is based on Rovelli's relational formalism [10], which was recently extended considerably by Dittrich [11], as well as on the Brown–Kuchař mechanism [12]. This necessarily uses a canonical approach. Furthermore, it was shown in [9] that this in one stroke provides the true degrees of freedom and provides us with a true (physical) Hamiltonian which generates a non-trivial evolution of the gauge-invariant degrees of freedom. Remarkably, these evolution equations look very similar to Einstein's equations for the type of matter considered. The type of matter originally used in [9] was chosen somewhat ad hoc and guided more by mathematical convenience rather than physical arguments[6]. Furthermore, it seems desirable to find the optimal matter which would minimally affect the standard interpretation of Einstein's equations as evolution equations while increasing the number of true degrees of freedom by four. As it turns out, there is a natural candidate, which we will use for our purposes: pressure free dust as introduced in the seminal paper by Brown and Kuchař [12] cited before. The dust particles fill time and space; they are present everywhere and at every instant of time. They follow geodesics with respect to the dynamical four-metric under consideration. However, they only interact gravitationally, not with the other matter and not with itself. The dust serves as a dynamical reference frame solving Einstein's hole problem [13]. It can be used to build gauge-invariant versions of all the other degrees of freedom. In [14, 15] up to linear order gauge-invariant Hamiltonian perturbation theory is discussed for cosmological and spherically symmetric backgrounds respectively. However, in both cases no additional matter is introduced to construct gauge-invariant quantities but for this purpose certain metric components are used.

The dust supplies the physically meaningless spacetime coordinates with a dynamical field interpretation and thus solves the 'problem of time' of general relativity as outlined above. This is its only purpose. For every non-dust variable in the usual formalism without dust there is unique gauge-invariant substitute in our theory. Once these observables, that is gauge-

[5] In the Hamiltonian picture, the eight constraints canonically generate gauge transformations which displays eight out of ten configuration variables as pure gauge.

[6] Also, apart from cosmological settings, the consequences of the deviations of these evolution equations from Einstein's equations was not analysed.

invariant matter and geometry modes, have been constructed as complicated aggregates made out of the non-gauge-invariant matter, geometry and dust modes, the dust itself completely disappears from the screen. The observable matter and geometry modes are now no longer subject to constraints; rather, the constraints are replaced by conservation laws of a gauge-invariant energy–momentum density. This energy–momentum density is the only trace that the dust leaves on the system; it can be arbitrarily small but must not vanish in order that the dust fulfils its role as a material reference frame of 'clocks and rods'. The evolution equations of the observables is generated by a physical Hamiltonian which is simply the spatial integral of the energy density. These evolution equations, under proper field identifications, can be mapped exactly to the six of the Einstein equations for the unobservable matter and geometry modes without dust, up to modifications proportional to the energy–momentum density. Thus again the influence of the dust can be tuned away arbitrarily and so it plays a perfect role as a 'test observer'. It is interesting that in contrast to [12] the dust must be a 'phantom dust', for the same reason that the phantom scalars appeared in [9]: if we use usual dust as in [12], then the physical Hamiltonian would come out negative definite rather than positive definite. Or equivalently, physical time would run backwards rather than forward. Note that general relativistic energy conditions for the gauge-invariant energy–momentum tensor are *not* violated because it does not contain the dust variables and it is the dust free and gauge-invariant energy–momentum tensor that the positive physical Hamiltonian generates. Hence, while the energy conditions for the phantom dust species are violated at the gauge variant level, at the gauge-invariant level there is no problem because the dust has disappeared. Note also that even at the gauge variant level the energy conditions for the total energy–momentum tensor are still satisfied if there is sufficient additional, observable matter present.

Based on these constructions we will develop a general relativistic perturbation theory in this series of papers. In the current work we treat the case of a general background; in the follow-up papers we discuss special cases of particular interest.

The plan of this paper is as follows.

In section 2 we review the seminal work of Brown and Kuchař [12]. We start from their Lagrangian (with opposite sign in order to get phantom dust) and then perform the Legendre transform. This leads to second class constraints which were not discussed in [12] and which we solve in appendix A. After having solved the second class constraints the further analysis agrees with [12]. The Brown–Kuchař mechanism can now be applied to the dust plus geometry plus other matter system and enables us to rewrite the four initial value constraints of general relativity in an equivalent way such that these constraints are not only mutually Poisson commuting but also that the system deparametrizes. That is, they can be solved for the four dust momentum densities, and the Hamiltonian densities to which they are equal no longer depend on the dust variables.

In section 3 we pass to the gauge-invariant observables and the physical Hamiltonian. In situations such as ours where the system deparametrizes, the general framework of [11] drastically simplifies and one readily obtains the Dirac observables and the physical Hamiltonian. Due to general properties of the relational approach, the Poisson algebra among the observables remains simple. More precisely, for every gauge variant non-dust variable we obtain a gauge-invariant analogue and the gauge variant and gauge-invariant observables satisfy the same Poisson algebra. This is also proved for part of the gauge invariance by independent methods in appendix B. The physical time evolution of these observables is generated by a unique, positive Hamiltonian.

In section 4 we derive the equations of motion generated by the physical Hamiltonian for the physical configuration and momentum observables. We also derive the second order in time equations of motion for the configuration observables. Interestingly, these equations can be seen of almost precisely the usual form that they have in the canonical approach [22] if one identifies lapse and shift with certain functions of the canonical variables. Hence we obtain a *dynamical lapse and shift*. The system of evolution equations is supplemented by four sets of conservation laws which follow from the mutual commutativity of the constraints. They play a role quite similar to the initial value constraints for the system without dust written in gauge variant variables but now the constraint functions do not vanish but rather are constants of the motion.

In section 5 we treat the case of asymptotically flat spacetimes and derive the necessary boundary terms to make the Hamiltonian functionally differentiable in that case. Not surprisingly, the boundary term is just the ADM Hamiltonian. However, while in the usual formalism the bulk term is a linear combination of constraints, in our formalism the bulk term does not vanish on the constraint surface; it represents the total dust energy.

In appendix C we perform the inverse Legendre transform from the physical Hamiltonian to an action. This cannot be done in closed form; however, we can write the transform in the form of a fix point equation which can be treated iteratively. The zeroth iteration precisely becomes the Einstein–Hilbert action for geometry and non-dust matter. Including higher orders generates a more complicated 'effective' action which contains arbitrarily high spatial derivatives of the gauge-invariant variables but only first time derivatives.

In section 6 we perturb the equations of motion about a general exact solution to first order, both in the first time derivative order form and in the second time derivative order form. Note that our perturbations are fully gauge invariant. In appendix D we show that one can get the second time derivative equation of motion for the perturbations in two equivalent ways: perturbing the second time derivative equations of motion to first order or deriving the second time order equation from the perturbations to first order of the first time order equations. This is an important check when one derives the equations of motion for the perturbations on a general background and the second avenue is easier at linear order. However, the first avenue is more economic at higher orders. In appendix E we show that the equations of motion up to nth order are generated by the physical Hamiltonian expanded up to $(n+1)$st order. Moreover, we show that the invariants expanded to nth order remain constants of the motion under the $(n+1)$st-order Hamiltonian up to terms of at least order $n+1$. This is important in order to actually derive the second time derivative equations of motion because we can drop otherwise complicated expressions.

In section 8 we compare our new approach to general-relativistic perturbation theory with some other approaches that can be found in the literature.

Finally, in section 9 we conclude and discuss the implications and open problems raised by the present paper.

In appendix F we ask the question whether the qualitative conclusions of the present paper are generic or whether they are special for the dust we chose. In order to test this question we sketch the repetition of the analysis carried out for the phantom dust for the phantom scalar field of [9]. It seems that qualitatively not much changes, although the dust comes closer than the phantom scalar to reproducing Einstein's equations of motion. This indicates that the Brown–Kuchař mechanism generically leads to equations of motion for gauge-invariant observables which completely resemble the equations of motion of their gauge variant counter parts.

Appendix G contains more details concerning some calculations in section 7.

Appendix H derives the connection between our manifestly gauge-invariant formalism and a corresponding gauge fixed version of it.

Finally, our rather involved notation is listed, for the convenience of the reader, as follows.

Notation

As a rule of thumb, gauge non-invariant quantities are denoted by lowercase letters, and gauge-invariant quantities by capital letters. The only exceptions from this rule are the dust fields T, S^j, ρ, W_j, their conjugate momenta P, P_j, I, I^j and their associated primary constraints Z_j, Z, Z^j which however disappear in the final picture. Partially gauge-invariant quantities (with respect to spatial diffeomorphisms) carry a tilde. Background quantities carry a bar. Our signature convention is that of relativists, that is, mostly plus.

Symbol	Meaning
G_N	Newton constant
$\kappa = 16\pi G_N$	gravitational coupling constant
λ	scalar coupling constant
Λ	cosmological constant
M	spacetime manifold
$\mathcal{X}$	spatial manifold
$\mathcal{T}$	dust time manifold
$\mathcal{S}$	dust space manifold
$\mu, \nu, \rho, \ldots = 0, \ldots, 3$	tensor indices on M
$a, b, c, \ldots = 1, 2, 3$	tensor indices on $\mathcal{X}$
$i, j, k, \ldots = 1, 2, 3$	tensor indices on $\mathcal{S}$
X^μ	coordinates on M
x^a	coordinates on $\mathcal{X}$
σ^j	coordinates on $\mathcal{S}$
t	foliation parameter
τ	dust time coordinate
Y_t^μ	one parameter family of embeddings $\mathcal{X} \to M$
$\mathcal{X}_t = Y_t(\mathcal{X})$	leaves of the foliation
$g_{\mu\nu}$	metric on M
q_{ab}	(pullback) metric on $\mathcal{X}$
$\tilde{q}_{ij}$	(pullback) metric on $\mathcal{S}$
Q_{ij}	Dirac observable associated with q_{ab}
p^{ab}	momentum conjugate to q_{ab}
$\tilde{p}^{ij}$	momentum conjugate to $\tilde{q}_{ij}$
P^{ij}	momentum conjugate to Q_{ij}
ζ	scalar field on M
ξ	scalar field on $\mathcal{X}$
$\tilde{\xi}$	pullback scalar field on $\mathcal{S}$
Ξ	Dirac observable associated with ξ
π	momentum conjugate to ξ
$\tilde{\pi}$	momentum conjugate to $\tilde{\xi}$
Π	momentum conjugate to Ξ
v	potential of $\zeta, \xi, \tilde{\xi}, \Xi$
T	dust time field on $\mathcal{X}$
$\tilde{T}$	dust time field on $\mathcal{S}$
S^j	dust space fields on $\mathcal{X}$
ρ	dust energy density on $M, \mathcal{X}$
W_j	dust Lagrange multiplier field on $M, \mathcal{X}$

Symbol	Meaning
$U = -\mathrm{d}T + W_j\,\mathrm{d}S^j$	dust deformation covector field on M
$J = \det(\partial S/\partial x)$	dust field spatial density on $\mathcal{X}$
P	momentum conjugate to T
$\tilde{P}$	momentum conjugate to $\tilde{T}$
P_j	momentum conjugate to S^j
I	momentum conjugate to ρ
I^j	momentum conjugate to W_j
Z_j, Z, Z^j	dust primary constraints on $\mathcal{X}$
μ^j, μ, μ_j	dust primary constraint Lagrange multipliers on$\mathcal{X}$
φ	diffeomorphism of $\mathcal{X}$
n^μ	unit normal of spacelike hypersurface on M
n	coordinate lapse function on $\mathcal{X}$
n^a	coordinate shift function on $\mathcal{X}$
p	momentum conjugate to n
p_a	momentum conjugate to n^a
z, z_a	primary constraint for lapse, shift
ν, ν^a	lapse and shift primary constraint Lagrange multipliers
ϕ, ψ, B, E	MFB scalars on $\mathcal{X}, \mathcal{S}$
S_a, F_a	MFB transversal vectors on $\mathcal{X}$
S_j, F_j	MFB transversal vectors on $\mathcal{S}$
h_{ab}	MFB transverse tracefree tensor on $\mathcal{X}$
h_{jk}	MFB transverse tracefree tensor on $\mathcal{S}$
Φ, Ψ	linear gauge-invariant completions of ϕ, ψ
V_a	linear gauge-invariant completions of F_a
V_j	linear gauge-invariant completions of F_j
c_a^{tot}	total spatial diffeomorphism constraint on $\mathcal{X}$
$c_j^{\mathrm{tot}} = S_j^a c_a^{\mathrm{tot}}$	total spatial diffeomorphism constraint on $\mathcal{X}$
c^{tot}	total Hamiltonian constraint on $\mathcal{X}$
c_a	non-dust contribution to spatial diffeomorphism constraint on $\mathcal{X}$
$c_j = S_j^a c_a$	non-dust contribution to spatial diffeomorphism constraint on $\mathcal{X}$
$\tilde{c}_j$	non-dust contribution to spatial diffeomorphism constraint on $\mathcal{S}$
$C_j \neq \tilde{c}_j$	momentum density: Dirac observable associated with $\tilde{c}_j$
c	non-dust contribution to Hamiltonian constraint on $\mathcal{X}$
$\tilde{c}$	non-dust contribution to Hamiltonian constraint on $\mathcal{S}$
$C \neq \tilde{c}$	Dirac observable associated with $\tilde{c}$
h	energy density on $\mathcal{X}$
$\tilde{h}$	energy density on $\mathcal{S}$
$H = \tilde{h}$	energy density: Dirac observable associated with $\tilde{h}$
$h_j = c_j^{\mathrm{tot}} - P_j$	auxiliary density on $\mathcal{X}$
ϵ	numerical energy density on $\mathcal{S}$
ϵ_j	numerical momentum density on $\mathcal{S}$
$\mathbf{H} = \int_{\mathcal{S}} \mathrm{d}^3\sigma\, H$	physical Hamiltonian, energy
L	Lagrange density associated with H
$\mathbf{L} = \int_{\mathcal{S}} \mathrm{d}^3\sigma\, L$	physical Lagrangian
V_{jk}	velocity associated with Q_{jk}
Υ	velocity associated with Ξ
$N = C/H$	dynamical lapse function on $\mathcal{S}$

Symbol	Meaning
$N_j = -C_j/H$	dynamical shift function on $\mathcal{S}$
$N^j = Q^{jk}N_k$	dynamical shift function on $\mathcal{S}$
∇_μ	$g_{\mu\nu}$ compatible covariant differential on M
D_a	q_{ab} compatible covariant differential on $\mathcal{X}$
$\tilde{D}_j$	$\tilde{q}_{jk}$ compatible covariant differential on $\mathcal{S}$
D_j	Q_{jk} compatible covariant differential on $\mathcal{S}$
$\bar{Q}_{jk}$	background spatial metric
$\bar{P}^{jk}$	background momentum conjugate to $\bar{Q}_{jk}$
$\bar{\Xi}$	background scalar field
$\bar{\Pi}$	background momentum conjugate to $\bar{\Xi}$
$\bar{\rho} = \frac{1}{2\lambda}[\dot{\bar{\Xi}}^2 + v(\bar{\Xi})]$	background scalar energy density
$\bar{p} = \frac{1}{2\lambda}[\dot{\bar{\Xi}}^2 - v(\bar{\Xi})]$	background scalar pressure
$G_{jkmn} = Q_{j(m}Q_{n)k} - \frac{1}{2}Q_{jk}Q_{mn}$	physical DeWitt bimetric
$[G^{-1}]^{jkmn} = Q^{j(m}Q^{n)k} - Q^{jk}Q^{mn}$	inverse physical DeWitt bimetric
$\bar{G}_{jkmn} = \delta_{j(m}\delta_{n)k} - \frac{1}{2}\delta_{jk}\delta_{mn}$	flat background DeWitt bimetric
$[\bar{G}^{-1}]^{jkmn} = \delta^{j(m}\delta^{n)k} - \delta^{jk}\delta^{mn}]$	inverse flat background DeWitt bimetric

2. The Brown–Kuchař formalism

In this section we review those elements of the Brown–Kuchař formalism [12] that are most relevant to us. Furthermore, we present an explicit constraint analysis for the system where gravity is coupled to a generic scalar field and the Brown–Kuchař dust, based on a canonical analysis using the full arsenal of Dirac's algorithm for constrained Hamiltonian systems.

For concreteness, we employ dust to deparametrize a system consisting of a generic scalar field ζ on a four-dimensional hyperbolic spacetime (M, g). The corresponding action, $S_{\text{geo}} + S_{\text{matter}}$, is given by the Einstein–Hilbert action

$$S_{\text{geo}} = \frac{1}{\kappa}\int_{\text{M}} \mathrm{d}^4X\sqrt{|\det(g)|}[R^{(4)} + 2\Lambda] \tag{2.1}$$

where $\kappa \equiv 16\pi G_N$, with G_N denoting Newton's constant, $R^{(4)}$ is the Ricci scalar of g and Λ denotes the cosmological constant, and the scalar field action

$$S_{\text{matter}} = \frac{1}{2\lambda}\int_{\text{M}} \mathrm{d}^4X\sqrt{\det(g)|}[-g^{\mu\nu}\zeta_{,\mu}\zeta_{,\nu} - v(\zeta)] \tag{2.2}$$

with λ denoting a coupling constant allowing for a dimensionless ζ and v is a potential term.

2.1. Lagrangian analysis

In their seminal paper [12] Brown and Kuchař introduced the following dust action[7]:

$$S_{\text{dust}} = -\frac{1}{2}\int_{\text{M}} \mathrm{d}^4X\sqrt{|\det(g)|}\rho[g^{\mu\nu}U_\mu U_\nu + 1]. \tag{2.3}$$

Here, g denotes the four-metric on the spacetime manifold M. The dust velocity field is defined by $U = -\mathrm{d}T + W_j\,\mathrm{d}S^j$ $(j \in 1, 2, 3)$. The action S_{dust} is a functional of the fields

[7] A classical particle interpretation of this action will be given in section 2.4.

$\rho, g_{\mu\nu}, T, S^j, W_j$.[8] The physical interpretation of the action will now be given in a series of steps.

First of all, the energy momentum of the dust reads

$$T_{\mu\nu}^{\text{dust}} = -\frac{2}{\sqrt{|\det(g)|}}\frac{\delta S_{\text{dust}}}{\delta g^{\mu\nu}} = \rho U_\mu U_\nu - \frac{\rho}{2} g_{\mu\nu}[g^{\lambda\sigma} U_\lambda U_\sigma + 1]. \tag{2.4}$$

By the Euler–Lagrange equation for ρ,

$$\frac{\delta S_{\text{dust}}}{\delta\rho} = g^{\lambda\sigma} U_\lambda U_\sigma + 1 = 0, \tag{2.5}$$

the second term in (2.4) vanishes on shell. Hence, U is unit timelike on shell. Compared with the energy–momentum tensor of a perfect fluid with energy density ρ, pressure p and unit (timelike) velocity field U

$$T_{\mu\nu}^{\text{pf}} = \rho U_\mu U_\nu + p(g_{\mu\nu} + U_\mu U_\nu) \tag{2.6}$$

shows that the action (2.3) gives an energy–momentum tensor for a perfect fluid with vanishing pressure.

For $\rho \neq 0$, variation with respect to W_j yields an equation equivalent to

$$\mathcal{L}_U S^j = 0 \tag{2.7}$$

where $\mathcal{L}$ denotes the Lie derivative. Hence, the fields S^j are constant along the integral curves of U. Equation (2.7) implies

$$\mathcal{L}_U T = U^\mu T_{,\mu} = U^\mu\left[T_{,\mu} - W_j S^j_{,\mu}\right] = -U^\mu U_\mu = +1 \tag{2.8}$$

so that T defines proper time along the dust flow lines.

Variation with respect to T results in

$$\partial_\mu[\rho\sqrt{|\det(g)|}U^\mu] = \sqrt{|\det(g)|}\nabla_\mu[\rho U^\mu] = 0 \tag{2.9}$$

while variation with respect to S^j gives

$$\partial_\mu[\rho\sqrt{|\det(g)|}U^\mu W_j] = \sqrt{|\det(g)|}\nabla_\mu[\rho U^\mu W_j] = 0. \tag{2.10}$$

Using (2.9), (2.10) reduces to (assuming $\rho \neq 0$)

$$\nabla_U W_j = 0. \tag{2.11}$$

Thus, $\nabla_U U_\mu = 0$, and, as a consequence, the integral curves of U are affinely parametrized geodesics. The physical interpretation of the fields T, S^j is complete: the vector field U is geodesic with proper time T, and each integral curve is completely determined by a constant value of S^j. This determines a dynamical foliation of M, with leaves characterized by constant values of T. A given integral curve intersects each leave at the same value of S^j.

2.2. *Hamiltonian analysis*

In this section we derive the constraints that restrict the phase space of the system of a generic scalar field on a spacetime (M, g), extended by the Brown–Kuchař dust. The reader not interested in the details of the derivation, which uses the full arsenal of Dirac's algorithm for constrained systems, may directly refer to the result (2.32)–(2.34).

We assume (M, g) to be globally hyperbolic in order to guarantee a well-posed initial value problem. As a consequence, M is diffeomorphic to $\mathbb{R} \times \mathcal{X}$, where $\mathcal{X}$ is a three-manifold of arbitrary topology. The spacelike leaves $\mathcal{X}_t$ of the corresponding foliation are obtained as images of a one parameter family of embeddings $t \mapsto Y_t$, see e.g. [22] for more details and our notation table for ranges of indices, etc. The timelike unit normals to the leaves may be written[9] as $n^\mu = \left[Y^\mu_{,t} - n^a Y^\mu_{,a}\right]/n$, where n, n^a are called lapse and shift functions,

[8] Here, T, S^j have dimension of length, W_j is dimensionless and, thus, ρ has dimension length^{-4}. The notation used here is suggestive: T stands for *time*, S^j for *space* and ρ for *dust energy density*.

[9] We have written $Y(t, x) \equiv Y_t(x)$.

respectively. Throughout, n^μ is assumed to be future oriented with respect to the parameter t, which requires $n > 0$.

The three-metric on $\mathcal{X}$ is the pullback of the spacetime metric under the embeddings, that is, $q_{ab}(x,t) = Y^\mu_{,a} Y^\nu_{,b} g_{\mu\nu}$. Denoting the inverse of q_{ab} by q^{ab} it is not difficult to see that

$$g^{\mu\nu} = -n^\mu n^\nu + q^{ab}\, Y^\mu_{,a} Y^\nu_{,b}. \tag{2.12}$$

It follows that the dust action can be written as

$$S_{\mathrm{dust}} = -\frac{1}{2}\int_{\mathbb{R}} \mathrm{d}t \int_{\mathcal{X}} \mathrm{d}^3x\, \sqrt{\det(q)} n\rho \left(-U_n^2 + q^{ab} U_a U_b + 1\right) \tag{2.13}$$

with $U_n \equiv n^\mu U_\mu$, $U_a \equiv Y^\mu_{,a} U_\mu$.

The form (2.13) is useful to derive the momentum fields canonically conjugate to T, S^j, respectively, as

$$\begin{aligned} P &:= \frac{\delta S_{\mathrm{dust}}}{\delta T_{,t}} = -\sqrt{\det(q)} \rho U_n \\ P_j &:= \frac{\delta S_{\mathrm{dust}}}{\delta S^j_{,t}} = \sqrt{\det(q)} \rho U_n W_j. \end{aligned} \tag{2.14}$$

The second relation in (2.14) shows that the Legendre transform is singular, and we obtain the *primary constraint* (*Zwangsbedingung*)

$$Z_j := P_j + W_j P = 0. \tag{2.15}$$

Additional primary constraints arise when we compute the momenta conjugate to ρ and W_j:

$$\begin{aligned} I &:= Z := \frac{\delta S_{\mathrm{dust}}}{\delta \rho_{,t}} = 0 \\ I^j &:= Z^j := \frac{\delta S_{\mathrm{dust}}}{\delta W_{j,t}} = 0. \end{aligned} \tag{2.16}$$

Considering the total action $S \equiv S_{\mathrm{geo}} + S_{\mathrm{matter}} + S_{\mathrm{dust}}$, further primary constraints follow from the calculation of the canonical momentum fields conjugate to lapse and shift n, n^a, respectively,

$$\begin{aligned} p &:= z := \frac{\delta S}{\delta n_{,t}} = 0 \\ p_a &:= z_a := \frac{\delta S}{\delta n^a_{,t}} = 0. \end{aligned} \tag{2.17}$$

The primary constraints signify the fact that we cannot solve for the velocities $\left\{S^j_{,t}, \rho_{,t}, W_{j\,,t}, n_{,t}, n^a_{,t}\right\}$, respectively, in terms of the momenta and configuration variables. Therefore, all primary constraints must be included in the canonical action, together with appropriate Lagrange multipliers $\{\mu^j, \mu, \mu_j, \nu, \nu^a\}$, in order to reproduce the Euler–Lagrange equations.

It is straightforward to solve for $T_{,t}$ and $\zeta_{,t}, q_{ab\,,t}$. For instance,

$$T_{,t} = nT_n + n^a T_{,a} = n\left[-U_n + W_j S^j_n\right] + n^a T_{,a} = n\frac{1}{\rho}\frac{P}{\sqrt{\det(q)}} + S^j_{,t} W_j + n^a\left[T_{,a} - W_j S^j_{,a}\right]. \tag{2.18}$$

How to eliminate the velocities of the scalar field and the three-metric is well known, e.g. [22], and will not be repeated here.

The resulting Hamiltonian constraint for the extended system, $c^{\text{tot}} \equiv c^{\text{geo}} + c^{\text{matter}} + c^{\text{dust}}$, is explicitly given by

$$\begin{aligned}
\kappa c^{\text{geo}} &= \frac{1}{\sqrt{\det(q)}}\left[q_{ac}q_{bd} - \frac{1}{2}q_{ab}q_{cd}\right]p^{ab}p^{cd} - \sqrt{\det(q)}R^{(3)} + 2\Lambda\sqrt{\det(q)} \\
\lambda c^{\text{matter}} &= \frac{1}{2}\left[\frac{\pi^2}{\sqrt{\det(q)}} + \sqrt{\det(q)}(q^{ab}\xi_{,a}\xi_{,b} + v(\xi))\right] \\
c^{\text{dust}} &= \frac{1}{2}\left[\frac{P^2/\rho}{\sqrt{\det(q)}} + \sqrt{\det(q)}\rho(q^{ab}U_aU_b + 1)\right]
\end{aligned} \tag{2.19}$$

with $U_a \equiv -T_{,a} + W_jS^j_{,a}$. The spatial diffeomorphism constraints for the extended system, $c_a^{\text{tot}} \equiv c_a^{\text{geo}} + c_a^{\text{matter}} + c_a^{\text{dust}}$, are explicitly given by

$$\begin{aligned}
\kappa c_a^{\text{geo}} &= -2q_{ac}D_bp^{bc} \\
\lambda c_a^{\text{matter}} &= \pi\xi_{,a} \\
c_a^{\text{dust}} &= P\left[T_{,a} - W_jS^j_{,a}\right].
\end{aligned} \tag{2.20}$$

The total action in canonical form reads

$$\begin{aligned}
S = \int_{\mathbb{R}} \mathrm{d}t \int_{\mathcal{X}} \mathrm{d}^3x &\left(PT_{,t} + P_jS^j_{,t} + I\rho_{,t} + I^jW_{j,t} + pn_{,t} + p_an^a_{,t} + \frac{1}{\kappa}p^{ab}q_{ab,t} + \frac{1}{\lambda}\pi\xi_{,t}\right) \\
&- \int_{\mathbb{R}} \mathrm{d}t\, H_{\text{primary}}
\end{aligned} \tag{2.21}$$

with p^{ab} denoting the momentum field conjugate to q_{ab}, ξ denoting the pullback of ζ to $\mathcal{X}$, π denoting its canonical momentum and D the covariant differential compatible with q_{ab}. Furthermore, the Hamiltonian and spatial diffeomorphism constraints, together with the primary constraints, entered the definition of the primary Hamiltonian

$$H_{\text{primary}} \equiv \int_{\mathcal{X}} \mathrm{d}^3x\, h_{\text{primary}} \tag{2.22}$$

via the density

$$h_{\text{primary}} \equiv \mu^jZ_j + \mu Z + \mu_jZ^j + \nu z + \nu^az_a + nc^{\text{tot}} + n^ac_a^{\text{tot}}. \tag{2.23}$$

Consistency requires that the constraint surface, defined by the primary constraints (2.15), (2.16) and (2.17), is stable under the action of H_{primary}. In order to to check this, we summarize the only non-vanishing elementary Poisson brackets[10]:

$$\begin{aligned}
&\{p^{ab}(x), q_{cd}(y)\} = \kappa\ \delta^a_{(c}\delta^b_{d)}\ \delta(x,y) \\
&\{\pi(x), \xi(y)\} = \lambda\delta(x,y) \\
&\{P(x), T(y)\} = \delta(x,y) \\
&\{P_j(x), S^k(y)\} = \delta^k_j\delta(x,y) \\
&\{I(x), \rho(y)\} = \delta(x,y) \\
&\{I^j(x), W_k(y)\} = \delta^j_k\delta(x,y) \\
&\{p(x), n(y)\} = \delta(x,y) \\
&\{p_a(x), n^b(y)\} = \delta^b_a\delta(x,y).
\end{aligned} \tag{2.24}$$

[10] Note that n, n^a, W_j, ρ, S^j are *not* Lagrange multipliers at this point; they are canonical coordinates just like the other fields.

The primary constraints transform under the action of the primary Hamiltonian H_{primary} as follows:

$$
\begin{aligned}
&z_{,t} = \{H_{\text{primary}}, p\} = -c^{\text{tot}}\\
&z_{a,t} = \{H_{\text{primary}}, p_a\} = -c_a^{\text{tot}}\\
&Z_{,t} = \{H_{\text{primary}}, I\} = \frac{n}{2}\left[-\frac{P^2/\rho^2}{\sqrt{\det(q)}} + \sqrt{\det(q)}(q^{ab}U_aU_b + 1)\right] \equiv \tilde{c} \qquad (2.25)\\
&Z^j_{,t} = \{H_{\text{primary}}, I^j\} = -\mu^j P - n\rho\sqrt{\det(q)}q^{ab}U_a S^j_{,b} + PS^j_{,a}n^a\\
&Z_{j,t} = \{H_{\text{primary}}, P_j + W_j P\} = \mu_j P - \left(n^a - \frac{n\rho\sqrt{\det(q)}}{P}q^{ab}U_b\right)PW_{j,a}.
\end{aligned}
$$

Consistency demands that (2.25) must vanish. Indeed, the last two equations in (2.25) involve the Lagrange multipliers μ^j, μ_j, respectively, and can be solved for them, since the system of equations has maximal rank. However, the first three equations in (2.25) do not involve Lagrange multipliers. Hence, they represent secondary constraints. According to Dirac's algorithm, the secondary constraints in equation (2.25) force us to reiterate the stability analysis, i.e. to calculate the action of H_{primary} on the secondary constraints. A lengthy calculation presented in appendix A shows that the secondary constraints are stable under the Hamiltonian flow generated by H_{primary}. In other words, no tertiary constraints arise in the stability analysis for the secondary constraints. However, the action of H_{primary} on $\tilde{c}$ involves the Lagrange multipliers μ^j, μ_j, μ, and can be solved for μ.

The final set of constraints is given by $\{c^{\text{tot}}, c_a^{\text{tot}}, \tilde{c}, Z_j, Z^j, Z, z_a, z\}$ and it remains to classify them into first and second class, respectively. Obviously,

$$
\begin{aligned}
\{Z^j(x), Z_k(y)\} &= P\delta^j_k\delta(x,y)\\
\{Z(x), \tilde{c}(y)\} &= \frac{nP^2}{\rho^3\sqrt{\det(q)}}\delta(x,y)
\end{aligned}
\qquad (2.26)
$$

does not vanish on the constraint surface defined by the final set of constraints; hence they are of second class. Next, since n appears at most linearly in the constraints, while n^a does not appear at all, it follows immediately that z, z_a are of first class. Further, consider the linear combination of constraints

$$
\begin{aligned}
\tilde{c}_a^{\text{tot}} &\equiv I\rho_{,a} + I^j W_{j,a} + PT_{,a} + P_j S^j_{,a} + pn_{,a} + \mathcal{L}_{\vec{n}}p_a + c_a\\
&= c_a^{\text{tot}} + Z\rho_{,a} + Z^j W_{j,a} + Z_j S^j_{,a} + zn_{,a} + \mathcal{L}_{\vec{n}}z_a
\end{aligned}
\qquad (2.27)
$$

where

$$
c_a \equiv c_a^{\text{geo}} + c_a^{\text{matter}} \qquad (2.28)
$$

is the non-dust contribution to the spatial diffeomorphism constraint c_a^{tot}. Since all constraints are scalar or covector densities of weight one and $\tilde{c}_a^{\text{tot}}$ is the generator of spatial diffeomorphisms, it follows that $\tilde{c}_a^{\text{tot}}$ is first class. Finally, we consider the linear combination

$$
\tilde{c}^{\text{tot}} \equiv c^{\text{tot}} + \alpha^j Z_j + \alpha_j Z^j + \alpha Z \qquad (2.29)
$$

and determine the phase space functions $\alpha^j, \alpha_j, \alpha$ such that $\tilde{c}^{\text{tot}}$ has vanishing Poisson brackets with Z_j, Z^j, Z up to terms proportional to Z_j, Z^j, Z. Then, $\tilde{c}^{\text{tot}}$ is first class, as well. See appendix A for details.

In the final step we should calculate the Dirac bracket [6, 18] $\{f, g\}^*$ for phase space functions f, g. It differs from the Poisson bracket $\{f, g\}$ by linear combinations of terms of the form $\{f, Z_j(x)\}\{g, Z^k(y)\}$ and $\{f, Z(x)\}\{g, \tilde{c}(y)\}$ (and terms with f, g interchanged). Fortunately, the Dirac bracket agrees with the Poisson bracket on functions f, g which only involve $\{T, S^j, q_{ab}, n, n^a\}$ and their conjugate momenta $\{P, P_j, P^{ab}, p, p_a\}$ on which we focus our attention in what follows. Using the Dirac bracket, the second class constraints can be solved strongly:

$$\begin{aligned} Z_j = 0 \quad &\Leftrightarrow \quad W_j = -P_j/P \\ Z^j = 0 \quad &\Leftrightarrow \quad I^j = 0 \\ Z = 0 \quad &\Leftrightarrow \quad I = 0 \\ \tilde{c} = 0 \quad &\Leftrightarrow \quad \rho^2 = \frac{P^2}{\det(q)}(q^{ab}U_aU_b + 1)^{-1}. \end{aligned} \tag{2.30}$$

From the last equation in (2.30) we find

$$\rho = \epsilon \frac{P}{\sqrt{\det(q)}}(\sqrt{q^{ab}U_aU_b + 1})^{-1}, \tag{2.31}$$

with $\epsilon = \pm 1$. We may also partially reduce the phase space subject to (2.30) by setting $z = z_a = 0$ and treating n, n^a as Lagrange multipliers, since they are pure gauge. Then, we are left with two constraints

$$\begin{aligned} c^{\text{tot}} &= c + c^{\text{dust}} \\ c_a^{\text{tot}} &= c_a + c_a^{\text{dust}} \end{aligned} \tag{2.32}$$

where

$$c \equiv c^{\text{geo}} + c^{\text{matter}} \tag{2.33}$$

and

$$\begin{aligned} c^{\text{dust}} &= \epsilon P \sqrt{q^{ab}U_aU_b + 1} \\ c_a^{\text{dust}} &= PT_{,a} + P_j S^j_{\ ,a}. \end{aligned} \tag{2.34}$$

Equations (2.32)–(2.34) are the main result of this subsection. They represent the final constraints that restrict the phase space of the system consisting of a generic scalar field on (M, g), extended by dust. The form of the dust Hamiltonian and spatial diffeomorphism constraints $\{c^{\text{dust}}, c_a^{\text{dust}}\}$, respectively, is of paramount importance for utilizing dust as a deparametrizing system, as we will explain in the next section.

2.3. The Brown–Kuchař mechanism for dust

In the previous section we have shown that the canonical formulation of a classical system, originally described by general relativity and a generic scalar field theory, then extended by a specific dust model, results in a phase space subject to the Hamiltonian and spatial diffeomorphism constraints (2.32)–(2.34). The primary Hamiltonian, after having solved the second class constraints, is a linear combination of those final first class constraints (2.32)–(2.34) and, thus, is constrained to vanish. This holds, in general, independently of the matter content, and is a direct consequence of the underlying spacetime diffeomorphism invariance.

Now, observable quantities are special phase space functions, distinguished by their invariance under gauge transformations. In other words, their Poisson brackets with the constraints must vanish when the constraints hold. In particular, they have vanishing Poisson brackets with the primary Hamiltonian H_{primary} on the constraint surface. This is one of the many facets of the problem of time: observable quantities do not move with respect to the primary Hamiltonian, because the latter generates gauge transformations rather than physical evolution. It follows that physical evolution must be generated by a true Hamiltonian (not constrained to vanish, but still gauge invariant).

In this section we address the questions how to construct a true Hamiltonian from a given Hamiltonian constraint, and, how to construct observable quantities (gauge-invariant phase space functions).

2.3.1. Deparametrization: general theory. The manifest gauge-invariant construction of a true Hamiltonian, generating physical evolution as opposed to mere gauge transformations, becomes particularly simple when the original system under consideration can be extended to a system with constraints in deparametrized form.

Consider first a general system subject to first class constraints c_I. The set of canonical pairs on phase space split into two sets of canonical pairs (q^a, p_a) and (T^I, π_I), respectively, such that the constraints can be solved, at least locally in phase space, for the π_I. In other words,

$$c_I = 0 \quad \Leftrightarrow \quad \tilde{c}_I = \pi_I + h_I(T^J; q^a, p_a) = 0. \tag{2.35}$$

Note that, in general, the functions h_I do depend on the T^J. The first class property guarantees that the $\tilde{c}_I$ are mutually Poisson commuting [32].

A system that deparametrizes allows us to split the set of canonical pairs into two sets of canonical pairs such that (1) equation (2.35) holds globally on phase space[11], and (2) the functions h_I are independent of the T^J.

Property (2) implies that the functions h_I are gauge invariant. Hence, any linear combination of the h_I that is bounded from below is a suitable candidate for a true Hamiltonian in the following sense: let $\tilde{c}_\tau \equiv \tau^I \tilde{c}_I$ be such a linear combination, with real coefficients τ^I in the range of T^I, and consider for any phase space function f the expression

$$O_f(\tau) \equiv \left[\sum_{n=0}^{\infty} \frac{1}{n!}\{\tilde{c}_\tau, f\}_{(n)}\right]_{\tau^I \to (\tau - T)^I}. \tag{2.36}$$

Here[12], the iterated Poisson bracket is inductively defined by $\{\tilde{c}_\tau, f\}_{(0)} = f$, $\{\tilde{c}_\tau, f\}_{(n+1)} = \{\tilde{c}_\tau, \{\tilde{c}_\tau, f\}_{(n)}\}$. Then, $O_f(\tau)$ is an observable quantity. More precisely, it is a gauge-invariant extension of the phase space function f. Furthermore, physical time translations of $O_f(\tau)$ are generated by the functions h_I:

$$\frac{\partial O_f(\tau)}{\partial \tau^I} = \{h_I, O_f(\tau)\} \tag{2.37}$$

provided that f only[13] depends on (q^a, p_a).

The observable quantities $O_f(\tau)$ can also be interpreted from the point of view of choosing a *physical* gauge. Indeed, $O_f(\tau)$ can be interpreted as representing the value of f in the gauge $T^I = \tau^I$.

2.3.2. Deparametrization: scalar fields. The Brown–Kuchař mechanism relies on the observation that free scalar fields lead to deparametrization of general relativity, as we sketch below (see [9] for a detailed discussion).

A free scalar field contributes to the spatial diffeomorphism constraint a term of the form

$$c_a^{\mathrm{scalar}} = \pi \phi_{,a} \tag{2.38}$$

[11] This is not the case for Klein–Gordon fields and many other scalar field theories with a canonical action that is at least quadratic in the π_I.

[12] Note that the substitution of the phase space independent numbers τ^I by the phase space dependent combination $(\tau - T)^I$ is performed only *after* the series has been calculated.

[13] This is no restriction since the π_I can be expressed in terms of the (q^a, p_a) (using (2.35)), and the T^I are pure gauge.

and to the Hamiltonian constraint a function of π^2 and $q^{ab}\phi_{,a}\phi_{,b}$, in the absence of a potential. On the constraint surface, defined by the spatial diffeomorphism constraint, we have the identity

$$q^{ab}\phi_{,a}\phi_{,b} = \frac{q^{ab}c_a^{\text{scalar}}c_b^{\text{scalar}}}{\pi^2} = \frac{q^{ab}c_a c_b}{\pi^2} \tag{2.39}$$

with c_a denoting the contribution to the total spatial diffeomorphism constraint that is independent of the free scalar field. Substitution of (2.39) into the total Hamiltonian and spatial diffeomorphism constraints yields the same constraint surface and gauge flow than before. In other words, the constraints with the substitution (2.39) are equivalent to the original ones. However, the new total Hamiltonian constraint does no longer depend on the free scalar field ϕ. Therefore, at least locally in phase space, we can solve the new total Hamiltonian constraint for the momentum field π and write locally

$$\tilde{c}^{\text{tot}}(x) = \pi(x) + h(x) \tag{2.40}$$

where the scalar density h of weight one is independent of π, ϕ and, typically, positive definite, see [9] for details.

As mentioned above, the constraint (2.40) and $h(x)$ are mutually Poisson commuting, which guarantees that the *physical Hamiltonian*

$$H := \int_{\mathcal{X}} \mathrm{d}^3x\ h(x) \tag{2.41}$$

is observable (it has vanishing Poisson brackets with the spatial diffeomorphism constraint, because h has density weight one).

This is as much as the general theory goes. There are two remaining caveats: first of all, the construction is only local in phase space. Secondly, the construction based on a single free scalar field requires phase space functions that are already invariant under spatial diffeomorphisms. Only those can be completed to fully gauge-invariant quantities[14].

2.3.3. Deparametrization: dust. Dust described by the action (2.3) does not entirely fit into the classification scheme given in [9] and sketched in the last section. It is not simply based on four free scalar fields T, S^j, but in addition leads to second class constraints. However, it has a clear interpretation as a system of test observers in geodesic motion, and circumvents the remaining caveats mentioned at the end of the last subsection as we will see.

Recall the final form of the Hamiltonian constraint (2.32)–(2.32) derived in the previous section:

$$c^{\text{tot}} = c + \epsilon P\sqrt{1 + q^{ab}U_a U_b} \tag{2.42}$$

with $U_a = -T_{,a} + W_j S^j_{,a}$. Solving the second class constraint $Z_j = 0$ for W_j, we find $U_a = -c_a^{\text{dust}}/P$. Inserting the first class spatial diffeomorphism constraint $c_a^{\text{tot}} = c_a + c_a^{\text{dust}}$, we arrive at the equivalent Hamiltonian constraint

$$c^{\text{tot}\,\prime} = c + \epsilon P\sqrt{1 + \frac{q^{ab}c_a c_b}{P^2}}, \tag{2.43}$$

which is already independent of T, S^j and P_j, but still not of the form $\tilde{c}^{\text{tot}} = P + h$, as required for a system that deparametrizes.

[14] This can be circumvented by employing e.g. three more free scalars but this would be somewhat ad hoc.

2.3.4. Deparametrization for dust: sign issues. In order to bring (2.43) into the form $\tilde{c}^{\text{tot}} = P + h$, we have to solve a quadratic equation. Each root describes only one sheet of the constraint surface, unless the sign of P is somehow fixed. As we argue below, this freedom will be fixed by our interpretation of the dust system as a *physical reference system*.

Recall that $P = -\rho\sqrt{\det(q)}U_n$ and $U^\mu\ T_{,\mu} = 1,\ U^\mu\ S^j_{,\mu} = 0$. In accordance with our interpretation, we identify T with proper time along the dust flow lines. Thus, U is timelike and future pointing; hence $U_n < 0$. It follows that $\text{sgn}(P) = \text{sgn}(\rho)$, so $\epsilon = 1$ in (2.31).

In [12] the authors assume $\rho > 0$, as it is appropriate for *observable* dust[15]. In our case, however, the dust serves only as a tool to deparametrize the system and is, by construction, only pure gauge. Therefore, we relax the restriction $\rho > 0$, when solving (2.43) for P:

$$P^2 = c^2 - q^{ab}c_a c_b. \tag{2.44}$$

The right-hand side of (2.44) is *constrained to be* non-negative, albeit it is not manifestly non-negative. But this causes no problem, since it is sufficient to analyse the system in an arbitrarily small neighbourhood of the constraint surface, where $c^2 - q^{ab}c_a c_b \geqslant 0$. Then,

$$\tilde{c}^{\text{tot}} = P - \text{sgn}(P)h, \qquad h = \sqrt{c^2 - q^{ab}c_a c_b} \tag{2.45}$$

is the general solution, globally defined on (the physically interesting portion of) the full phase space. However, $\tilde{c}^{\text{tot}}$ is not yet of the form required by a successful deparametrization, because of the sign function which also renders the constraint non-differentiable.

In order to utilize dust for deparametrization, the choice $P < 0$ is required. Before presenting reasons for this choice, we stress again that the dust itself is not observable. There are three related arguments for the choice of $P < 0$:

(1) *Dynamics*. The deparametrization mechanism supplies us with a physical Hamiltonian of the form

$$\mathsf{H} = \int_{\mathcal{X}} \mathrm{d}^3x\, h. \tag{2.46}$$

In the case where dust is chosen as the clock of the system, the variation of the physical Hamiltonian is given by

$$\delta\mathsf{H} = \int_{\mathcal{X}} \mathrm{d}^3x\ \left(\frac{c}{h}\delta c - q^{ab}\frac{c_b}{h}\delta c_a + \frac{1}{2h}q^{ac}q^{bd}c_c c_d\ \delta q_{ab}\right). \tag{2.47}$$

For $P \neq 0$, then $h \neq 0$ (in a sufficiently small neighbourhood of the constraint surface). Hence, the coefficients of the variations on the right-hand side of (2.47) are non-singular. Moreover, for $P \neq 0$, also $c \neq 0$, as we see from (2.43). In fact, using $\text{sgn}(c) = -\text{sgn}(P)$ (from (2.43)) in a neighbourhood of the constraint surface,

$$\frac{c}{h} = -\text{sgn}(P)\ \sqrt{1 + q^{ab}\frac{c_a}{h}\frac{c_b}{h}} \tag{2.48}$$

has absolute value no less than 1.

Let us now compare (2.47) with the differential of the primary Hamiltonian constraint in the absence of dust:

$$H_{\text{primary}} = \int_{\mathcal{X}} \mathrm{d}^3x(nc + n^a c_a), \tag{2.49}$$

[15] This would be required by the usual energy conditions if the dust is the only observable matter. However, note that only the total energy momentum is subject to the energy conditions, not the individual contributions from various matter species.

which is given by (lapse and shift functions are considered as Lagrange multipliers, i.e. are phase space independent)

$$\mathrm{d}H_{\mathrm{primary}} = \int_{\mathcal{X}} \mathrm{d}^3x(n dc + n^a dc_a). \tag{2.50}$$

Comparison between (2.47) and (2.50) reveals that the differentials coincide, up to the additional term proportional to δq_{ab}, provided we identify $n := c/h$ as dynamical lapse and $n^a := -q^{ab}c_b/h$ as dynamical shift. This is promising in our aim to derive physical equations of motions for observable quantities which nevertheless come close to the usual Einstein equations for gauge-dependent quantities. However, in the standard framework the lapse function is always positive, guaranteeing that the normal vector field is future oriented. This fact is correctly reflected in our framework only if $P < 0$.

(2) *Kinematics*. The identification $n \equiv c/h$ and $n^a \equiv -q^{ab}c_b/h$ can also be motivated as follows. Consider a spacetime diffeomorphism defined by $X^\mu \mapsto (\tau, \sigma^j) := (T(X), S^j(X)) =: Y^\mu(X)$ and let $(\tau, \sigma^j) \to Z^\mu(\tau, \sigma)$ be its inverse. We can define a *dynamical* foliation of M by $T(X) = \tau = \text{const}$ hypersurfaces. The leaves $\mathcal{S}_\tau$ of that foliation are the images of $\mathcal{S}$ (which is the range of the S^j) under the map Z at constant τ. Using the identity

$$\delta^\mu_\nu = Z^\mu_{,\tau}\, T_{,\nu} + Z^\mu_{,j}\, S^j_{,\nu} \tag{2.51}$$

and $U^\mu\, T_{,\mu} = 1, U^\mu\, S^j_{,\mu} = 0$, we find $U^\mu = Z^\mu_{,\tau}$. Thus, as expected, the foliation is generated by the vector field $U = \partial/\partial\tau$, which is unit timelike.

It is useful to decompose the deformation vector field U with respect to the arbitrary coordinate foliation that we used before:

$$U^\mu = g^{\mu\nu}U_\nu = -n^\mu U_n + X^\mu_{,a}q^{ab}U_b. \tag{2.52}$$

From (2.13) and (2.31) with $\epsilon = 1$ we find $U_n = -\sqrt{1 + q^{ab}U_aU_b}$. Next,

$$U_a = -\frac{c_a^{\mathrm{dust}}}{P} = \frac{c_a}{P}. \tag{2.53}$$

On the other hand, $n \equiv c/h = \mathrm{sgn}(P)U_n$ and $n_a \equiv -c_a/h = -\mathrm{sgn}(P)\, U_a$. Therefore, (2.52) can be written as

$$U^\mu = -\mathrm{sgn}(P)\left(nn^\mu + X^\mu_{,a}n^a\right). \tag{2.54}$$

Hence, the sign for which n is positive yields the correct decomposition of the deformation vector field U in terms of lapse and shift. This calculation also reveals the geometrical origin of the identification $n \equiv c/h$ and $n^a \equiv -q^{ab}c_b/h$.

As a side remark, the identity $-n^2 + q^{ab}n_an_b = -1$ is an immediate consequence of the normalization of the deformation vector field, $g_{\mu\nu}U^\mu U^\nu = -1$. That is, the deformation vector field is timelike, future oriented and normalized, but not normal to the leaves of the foliation that it defines.

(3) *Stability and flat spacetime limit*. Of course, we could choose $P > 0$ and use $-h$ instead of h in order to obtain equations of motion. However, in that case the physical Hamiltonian would be unbounded from below, leading to an unstable theory. Alternatively, we could stick to $+h$ for the equations of motion, but then the τ evolution would run backwards.

Moreover, since $c^{\mathrm{tot}} = c + P\sqrt{1 + q^{ab}U_aU_b} = 0$ on the constraint surface, we would have $c < 0$ for $P > 0$. Since $c = c^{\mathrm{geo}} + c^{\mathrm{matter}}$ and $c^{\mathrm{matter}} > 0$, this would enforce $c^{\mathrm{geo}} < 0$. Hence, flat space would not be a solution.

As a side remark, for $c_a/h \ll 1$ and $P < 0$, $h \approx c$, while $h \approx -c$ for $P > 0$. Thus, the physical Hamiltonian density, with respect to dust as a physical reference system, approximates the standard model Hamiltonian density c^{matter} only for $P < 0$.

We emphasize again that the dust used for deparametrization is not observable, and should not be confused with observable matter. It solely provides a dynamical reference frame.

2.4. Dust interpretation

In this section we derive a physical interpretation of the Brown–Kuchař action based on the geodesic motion of otherwise free particles [12].

Consider first the action for a single relativistic particle with mass m on a background g:

$$S_m = -m \int_{\mathbb{R}} \mathrm{d}s \sqrt{-g_{\mu\nu}\dot{X}^\mu \dot{X}^\nu}. \tag{2.55}$$

The momentum conjugate to the configuration variable X^μ is given by

$$P_\mu = \frac{\delta S_m}{\delta \dot{X}^\mu} = m \frac{g_{\mu\nu}\dot{X}^\nu}{\sqrt{-g_{\rho\sigma}\dot{X}^\rho \dot{X}^\sigma}}, \tag{2.56}$$

rendering the Legendre transformation singular. This is a consequence of the reparametrization invariance of the action (2.55). Hence, the system exhibits no physical Hamiltonian, but instead a primary Hamiltonian constraint enforcing the mass shell condition:

$$C = \frac{1}{2m}(m^2 + g^{\mu\nu}P_\mu P_\nu). \tag{2.57}$$

Let us proceed to the canonical formulation. In terms of the embeddings $X \equiv Y_t(x)$, the particle trajectory reads $X(s) = Y_{t(s)}(x(s))$, so that

$$\dot{X}(s) = \dot{t}(s)Y_{,t} + \dot{x}^a(s)Y_{,a} \tag{2.58}$$

where the overdot refers to differentiation with respect to the trajectory parameter s. The momenta are then given by

$$\begin{aligned} p_a &\equiv Y^\mu_{,a}P_\mu = \frac{m}{\sqrt{-g_{\rho\sigma}\dot{X}^\rho\dot{X}^\sigma}} q_{ab}(\dot{t}n^b + \dot{x}^b) \\ p_t &\equiv Y^\mu_{,t}P_\mu = \frac{m}{\sqrt{-g_{\rho\sigma}\dot{X}^\rho\dot{X}^\sigma}} (\dot{t}g_{tt} + q_{ab}\, n^b\dot{x}^a) \end{aligned} \tag{2.59}$$

where $g_{tt} = -n^2 + q_{ab}n^a n^b$. We can only eliminate the spatial velocities $\dot{x}^a$. To do this set $A \equiv g_{ta}\dot{x}^a = q_{ab}n^b\dot{x}^a$ and $B \equiv q_{ab}\dot{x}^a\dot{x}^b$. Then,

$$w \equiv g_{\mu\nu}\dot{X}^\mu\dot{X}^\nu = g_{tt}\dot{t}^2 + 2A\dot{t} + B. \tag{2.60}$$

On the other hand,

$$-\frac{w}{m^2}q^{ab}p_a p_b = B + 2A\dot{t} + q_{ab}n^a n^b \dot{t}^2. \tag{2.61}$$

Substituting w from (2.60) and collecting coefficients of A, B, $\dot{t}^2$ yields

$$\begin{aligned} 0 &= B + 2A\dot{t} + \dot{t}^2 \frac{g_{tt}\frac{q^{ab}p_a p_b}{m^2} + q_{ab}n^a n^b}{1 + \frac{q^{ab}p_a p_b}{m^2}} \\ &= w + \frac{\dot{t}^2 n^2}{1 + \frac{q^{ab}p_a p_b}{m^2}}. \end{aligned} \tag{2.62}$$

Now we can solve the first equation in (2.59) for $\dot{x}^a$:

$$\dot{x}^a = \dot{t}\left(-n^a \pm \sqrt{1 + \frac{q^{ab}p_a p_b}{m^2}}\right). \tag{2.63}$$

Inserting this into the second equation in (2.59) leads to a constraint of the form $C \equiv p_s + h$:

$$C = p_s - n^a p_a \pm n\sqrt{m^2 + q^{ab} p_a p_b} \tag{2.64}$$

while the canonical Hamiltonian is obtained from the Lagrangian in (2.55) as

$$H_{\text{canon}} = P_\mu \dot{X}^\mu - L = \dot{t} C. \tag{2.65}$$

Since the constraint (2.64) is in deparametrized form, the phase space can easily be reduced, leading to the reduced action

$$S_{\text{reduced}} = \int \mathrm{d}s (p_a \dot{x}^a - h). \tag{2.66}$$

We extend this phase space by adding a canonical pair (τ, m) and consider the extended action

$$S_{\text{extended}} = \int \mathrm{d}s (m\dot{\tau} + p_a \dot{x}^a - h) \tag{2.67}$$

where the particle mass m is now considered as a dynamical variable. The equations of motion for m, τ give $\dot{m} = 0$ and $\dot{\tau} = \dot{t}\sqrt{-w}$. Thus, the mass is constant and τ is the proper time (in the gauge $s = t$).

We generalize our results now to the case of many particles. More precisely, let $\mathcal{S}$ be a label set and consider a relativistic particle for each label $\sigma \in \mathcal{S}$. This amounts to providing each variable appearing in the extended action with a corresponding label, i.e. $x_\sigma^a, p_a^\sigma, \tau_\sigma, m^\sigma$, and the total action for those particles is then just the sum over the corresponding actions $S^\sigma_{\text{extended}}$:

$$S_{\text{extended}} = \sum_{\sigma \in \mathcal{S}} S^\sigma_{\text{extended}}. \tag{2.68}$$

Next we consider the limit in which $\mathcal{S}$ becomes a three-manifold, with the labels σ becoming coordinates on this manifold. In this limit, we introduce the following fields:

$$\begin{aligned}
\tilde{T}(\sigma) &\equiv \tau_\sigma \\
\tilde{P}(\sigma)\,\mathrm{d}^3\sigma &\equiv m^\sigma \\
\tilde{S}^a(\sigma) &\equiv x^a_\sigma \\
\tilde{p}_a(\sigma)\,\mathrm{d}^3\sigma &\equiv p_a(x_\sigma) \\
\tilde{n}(\sigma) &\equiv n(x_\sigma) \\
\tilde{n}^a(\sigma) &\equiv n^a(x_\sigma) \\
\tilde{q}_{ab}(\sigma) &\equiv q_{ab}(x_\sigma).
\end{aligned} \tag{2.69}$$

Then, in the specified limit, the extended action (2.68) becomes

$$S_{\text{extended}} = \int \mathrm{d}t \int \mathrm{d}^3\sigma \left(\dot{\tilde{T}}\tilde{P} + \dot{\tilde{S}}^a \tilde{P}_a + \tilde{n}^a \tilde{P}_a \mp \tilde{n}\sqrt{\tilde{P}^2 + \tilde{q}^{ab}\tilde{P}_a \tilde{P}_b}\right). \tag{2.70}$$

Finally, we perform a canonical transformation: instead of the fields $\tilde{S}^a(\sigma)$ with values in $\mathcal{X}$, we would like to consider the inverse fields $S^j(x)$ with values in $\mathcal{S}$, that is $S^j(\tilde{S}(\sigma)) = \sigma^j, \tilde{S}^a(S(x)) = x^a$. This is at the same time a diffeomorphism and we can transform the other fields as well. For instance (T is a scalar and P is a scalar density),

$$\begin{aligned}
T(x) &= \tilde{T}(S(x)) = \int_{\mathcal{S}} \mathrm{d}^3\sigma\; \delta(x, \tilde{S}(\sigma))|\det(\partial\tilde{S}/\partial\sigma)|\tilde{T}(\sigma) \\
P(x) &= \frac{\tilde{P}}{|\det(\partial\tilde{S}/\partial\sigma)|}(S(x)) = \int_{\mathcal{S}} \mathrm{d}^3\sigma\; \delta(x, \tilde{S}(\sigma))\tilde{P}(\sigma) \\
S^j(x) &= \int_{\mathcal{S}} \mathrm{d}^3\sigma\; \sigma^j \delta(x, \tilde{S}(\sigma))|\det(\partial\tilde{S}/\partial\sigma)|.
\end{aligned} \tag{2.71}$$

Calculating the time derivatives and performing integrations by parts, we find

$$\int_{\mathcal{S}} \mathrm{d}^3\sigma\, \dot{\tilde{T}}\tilde{P} = \int_{\mathcal{X}} \mathrm{d}^3x(\dot{T}P - \dot{S}^j S^a_j P T_{,a}) \tag{2.72}$$

with S^a_j denoting the inverse of the matrix $S^j_{,a}$. Using

$$\dot{\tilde{S}}^a(\sigma) = -\left[\dot{S}^j S^a_j\right]_{S(x)=\sigma} \tag{2.73}$$

and defining $P_j(x)$ implicitly through

$$\tilde{P}_a = -\left[\frac{PT_{,a} + P_j S^j_{,a}}{|\det(\partial S/\partial x)|}\right]_{S(x)=\sigma} \tag{2.74}$$

we find that S_{extended} precisely turns into the dust action on $\mathcal{X}$ with the second class constraints eliminated[16].

3. Relational observables and physical Hamiltonian

In this section we present an explicit prescription for constructing gauge-invariant completions of arbitrary phase space functions. The construction is non-perturbative and technically involved, but the physical picture behind it will become crystal clear. Furthermore, the formal expressions are only required to establish certain properties of the construction, but are not required for the calculation of physical properties. This is a great strength of the relational formalism.

Let us summarize the situation. After having solved the second class constraints and having identified lapse and shift fields as Lagrange multipliers, we are left with the following canonical pairs:

$$(q_{ab}, p^{ab}), \quad (\xi, \pi), \quad (T, P), \quad (S^j, P_j), \tag{3.1}$$

subject to the following first class constraints:

$$\begin{aligned} c^{\text{tot}}_a &= c_a + c^{\text{dust}}_a, & c^{\text{dust}}_a &= PT_{,a} + P_j S^j_{,a} \\ c^{\text{tot}} &= c + c^{\text{dust}}, & c^{\text{dust}} &= -\sqrt{P^2 + q^{ab} c^{\text{dust}}_a c^{\text{dust}}_b} \end{aligned} \tag{3.2}$$

where c_a, c are independent of the dust variables $\{T, P, S^j, P_j\}$. We already used $P < 0$.

As explained in section 2.3, we aim at deparametrization of the theory and therefore solve (3.2) for the dust momenta, leading to the equivalent form of the constraints

$$\begin{aligned} \tilde{c}^{\text{tot}} &= P + h, & h &= \sqrt{c^2 - q^{ab} c_a c_b} \\ \tilde{c}^{\text{tot}}_j &= P_j + h_j, & h_j &= S^a_j(-hT_{,a} + c_a) \end{aligned} \tag{3.3}$$

with $S^a_j S^k_{,a} = \delta^k_j$, $S^a_j S^j_{,b} = \delta^a_b$; hence S^a_j is the inverse of $S^j_{,a}$ (assuming, as before, that $S : \mathcal{X} \to \mathcal{S}$ is a diffeomorphism). These constraints are mutually Poisson commuting[17]. However, only $\tilde{c}^{\text{tot}}$ is in deparametrized form (i.e. h is independent of T, S^j), but $\tilde{c}^{\text{tot}}_j$ is not.

[16] The metric field has to be pulled back by the dynamical spatial diffeomorphism, as well. For details, see the next section.

[17] One can either prove this by direct calculation, or one uses the following simple argument: the Poisson bracket between the constraints must be proportional to a linear combination of constraints, because the constraint algebra is first class. Since the constraints are linear in the dust momenta, the result of the Poisson bracket calculation no longer depends on them. Therefore, the coefficients of proportionality must vanish.

In particular, we can only conclude that the $h(x)$ are mutually Poisson commuting. Still, this will be enough for our purposes[18].

Following the works [9–11], we describe the construction of fully gauge-invariant completions of phase space functions. Consider the smeared constraint

$$K_\beta \equiv \int_{\mathcal{X}} \mathrm{d}^3x \big[\beta(x)c^{\mathrm{tot}}(x) + \beta^j(x)c_j^{\mathrm{tot}}(x)\big] \tag{3.4}$$

where $\beta(x), \beta^j(x)$ are phase space independent smearing functions in the range of $T(x), S^j(x)$. Under a gauge transformation generated by this constraint, an arbitrary phase space function f is mapped to

$$\alpha_\beta(f) \equiv \sum_{n=0}^{\infty} \frac{1}{n!}\{K_\beta, f\}_{(n)}. \tag{3.5}$$

The fully gauge-invariant completion of f is given by

$$O_f[\tau,\sigma] \equiv [\alpha_\beta(f)]_{\substack{\beta\to\tau-T\\ \beta^j\to\sigma^j-S^j}}. \tag{3.6}$$

Here, the functions $\tau(x), \sigma^j(x)$ are also in the range of $T(x), S^j(x)$, respectively[19]. It is important to *first* calculate the Poisson brackets appearing in (3.5) with the phase space independent functions β, β^j, and *afterwards* to replace them with the phase space dependent functions $\tau - T, \sigma^j - S^j$, respectively. This connection can be established based on the gauge transformation properties of T, S^j: $\alpha_\beta(T) = T + \beta, \alpha_\beta(S^j) = S^j + \beta^j$. Hence,

$$O_f[\tau,\sigma] \equiv [\alpha_\beta(f)]_{\substack{\alpha_\beta(T)=\tau\\ \alpha_\beta(S^j)=\sigma^j}}. \tag{3.7}$$

Indeed, (3.7) motivates the following interpretation: $O_f[\tau,\sigma]$ is the gauge-invariant completion of f, which in the gauge $T = \tau, S^j = \sigma^j$ takes the value f. This is not the only interpretation we entertain a different one below.

For the purpose of this paper it suffices to consider the infinite series appearing in the gauge-invariant completions as expressions useful for formal manipulations. There is no need to actually calculate these series for any physical problem.

Further important properties [17, 32] of the completion are

$$\{O_f[\tau,\sigma], O_{f'}[\tau,\sigma]\} = \{O_f[\tau,\sigma], O_{f'}[\tau,\sigma]\}^* = O_{\{f,f'\}^*}[\tau,\sigma] \tag{3.8}$$

$$O_{f+f'}[\tau,\sigma] = O_f[\tau,\sigma] + O_{f'}[\tau,\sigma], \qquad O_{f\cdot f'}[\tau,\sigma] = O_f[\tau,\sigma]\cdot O_{f'}[\tau,\sigma]. \tag{3.9}$$

Here, $\{\cdot,\cdot\}^*$ is the Dirac bracket[20] [6] associated with the constraints and the *gauge fixing functions* T, S^j. Relations (3.8) and (3.9) show that the map $f \mapsto O_f[\tau,\sigma]$ is a Poisson homomorphism of the algebra of functions on phase space with pointwise multiplication, equipped with the Dirac bracket[21] as the Poisson structure.

[18] In what follows we will drop the tilde in noting the constraints for notational simplicity.

[19] We denote the *functional dependence* of (3.6) on the functions $\tau(x), \sigma^j(x)$ by square brackets. Below we show that it is sufficient to choose those functions to be constant and replace the square brackets by round ones for notational convenience.

[20] For completeness, we note the definition of the Dirac bracket:

$$\{f,f'\}^* \equiv \{f,f'\} - \int_{\mathcal{X}} \mathrm{d}^3x \sum_{\mu=0}^{3}\big[\{f,c_\mu^{\mathrm{tot}}(x)\}\{f',S^\mu(x)\} - \{f',c_\mu^{\mathrm{tot}}(x)\}\{f,S^\mu(x)\}\big] \tag{3.10}$$

where $c_0^{\mathrm{tot}} \equiv c^{\mathrm{tot}}, S^0 := T$. The Dirac bracket is antisymmetric and $\{f, c_\mu^{\mathrm{tot}}(x)\}^* = \{f, S^\mu(x)\}^* = 0$ everywhere. This follows from the fact that $c_\mu^{\mathrm{tot}}(x)$ and $S^\mu(x)$ are mutually Poisson commuting, and that $\{c_\mu^{\mathrm{tot}}(x), S^\nu(y)\} = \delta(x,y)\delta_\mu^\nu$.

[21] The Dirac bracket coincides with the Poisson bracket on gauge-invariant functions. It is degenerate, since it annihilates constraints and *gauge fixing functions*. Hence, it defines only a Poisson structure, but not a symplectic structure on the full phase space.

In particular, for a general functional $f = f[q_{ab}(x), P^{ab}(x), \xi(x), \pi(x), T(x), P(x), S^j(x), P_j(x)]$ the following useful identity holds:

$$O_f = f\left[O_{q_{ab}(x)}, O_{P^{ab}(x)}, O_{\xi(x)}, O_{\pi(x)}, O_{T(x)}, O_{P(x)}, O_{S^j(x)}, O_{P_j(x)}\right](\tau,\sigma). \tag{3.11}$$

This has important consequences: (3.11) ensures that it suffices to know the completions of the elementary phase space variables. In fact, we are only interested in those functions that are independent of the dust variables $\{T, S^j, P, P_j\}$. The reason for this is that, first of all, P, P_j are expressible in terms of all other variables on the constraint surface. Alternatively, since the constraints are mutually Poisson commuting, we have

$$O_{P(x)} = O_{c^{\mathrm{tot}}(x)} + O_{h(x)} = c^{\mathrm{tot}}(x) + O_{h(x)}, \quad O_{P_j(x)} = O_{c_j^{\mathrm{tot}}(x)} + O_{h_j(x)} = c_j^{\mathrm{tot}}(x) + O_{h_j(x)}. \tag{3.12}$$

Hence, these functions are known once we know the completion of the remaining variables. Secondly,

$$O_{T(x)}[\tau,\sigma] = \tau(x), \qquad O_{S^j(x)}[\tau,\sigma] = \sigma^j(x) \tag{3.13}$$

are phase space independent. Thus, the only interesting variables to consider are $\{q_{ab}, P^{ab}, \xi, \pi\}$.

In what follows we consider only dust-independent functions f. For those (3.8) simplifies to

$$\{O_f[\tau,\sigma], O_{f'}[\tau,\sigma]\} = O_{\{f,f'\}}[\tau,\sigma]. \tag{3.14}$$

Equations (3.9) and (3.8) imply that $f \mapsto O_f[\tau,\sigma]$ is a *Poisson automorphism* of the Poisson subalgebra of functions that do not depend on the dust variables with the ordinary Poisson bracket as the Poisson structure. This will be absolutely crucial for all what follows.

Further useful properties of the completion are

$$O_f[\tau,\sigma] = O^{(2)}_{O_f^{(1)}[\sigma]}[\tau] \tag{3.15}$$

where (recall (3.4), (3.5) and (3.6))

$$\begin{aligned} O_f^{(1)}[\sigma] &= [\alpha_\beta(f)]_{\substack{\beta\to 0 \\ \beta^j\to\sigma^j-S^j}} \\ O_f^{(2)}[\tau] &= [\alpha_\beta(f)]_{\substack{\beta\to\tau-T \\ \beta^j\to 0}}. \end{aligned} \tag{3.16}$$

This follows from the fact that the constraints are mutually Poisson commuting and $\{c^{\mathrm{tot}}(x), S^j(y)\} = 0$. The important consequence of (3.15) is that we can accomplish full gauge invariance in two stages: we establish first invariance under the action of the spatial diffeomorphism constraint, and afterwards achieve invariance with respect to gauge transformations generated by the Hamiltonian constraint. This holds even under more general circumstances [11], i.e. when the constraints cannot be deparametrized.

3.1. Implementing spatial diffeomorphism invariance

Keeping the physical interpretation of the completion in mind, the map $f \mapsto O_f^{(1)}[\sigma]$ can be worked out explicitly. In the first stage of the construction, the corresponding smeared constraint reads

$$K_\beta = \int_{\mathcal{X}} \mathrm{d}^3x\ \beta^j(x)\ c_j^{\mathrm{tot}}(x). \tag{3.17}$$

Given a phase space function f, its completion $O_f^{(1)}$ with respect to gauge transformations generated by K_β becomes

$$\begin{aligned} O_f^{(1)}[\sigma] &= \sum_{n=0}^{\infty} \frac{1}{n!} [\{K_\beta, f\}_{(n)}]_{\beta^j \to \sigma^j - S^j} \\ &= f + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathcal{X}} \mathrm{d}^3 x_1 [\sigma^{j_1}(x_1) - S^{j_1}(x_1)] \ \ldots \int_{\mathcal{X}} \mathrm{d}^3 x_n \ [\sigma^{j_n}(x_n) - S^{j_n}(x_n)] \\ &\quad \times \left\{c_{j_1}^{\mathrm{tot}}(x_1), \left\{c_{j_2}^{\mathrm{tot}}(x_2), \ldots, \left\{c_{j_n}^{\mathrm{tot}}(x_n), f\right\} \ldots\right\}\right\}. \end{aligned} \tag{3.18}$$

Let us begin with $f = \xi(x)$. We claim that

$$\{K_\beta, \xi(x)\}_{(n)} = \left[\beta^{j_1} \ldots \beta^{j_n} \ v_{j_1} \ldots v_{j_n} \cdot \xi\right](x) \tag{3.19}$$

where v_j is the vector field defined by

$$v_j \cdot \xi(x) := S_j^a(x) \ \xi_{,a}(x). \tag{3.20}$$

In fact the vectors v_j are mutually commuting:

$$\begin{aligned} [v_j, v_k] &= S_j^a S_{k,a}^b \partial_b - j \leftrightarrow k \\ &= -S_j^a S_l^b S_{,ca}^l S_k^c \partial_b - j \leftrightarrow k \\ &= -S_j^a S_l^b S_{,ac}^l S_k^c \partial_b - j \leftrightarrow k \\ &= S_j^a S_{l,c}^b S_{,a}^l S_k^c \partial_b - j \leftrightarrow k \\ &= S_{j,c}^b S_k^c \partial_b - j \leftrightarrow k \\ &= S_k^a S_{j,a}^b \partial_b - j \leftrightarrow k \\ &= 0. \end{aligned} \tag{3.21}$$

To prove (3.19) by induction over n we need

$$\left\{K_\beta, S_j^a(x)\right\} = -S_k^a(x) \left\{K_\beta, S_{,b}^k(x)\right\} S_j^b(x) = -S_k^a(x) \beta_{,b}^k(x) S_j^b(x) = -[v_j \cdot \beta^k] S_k^a. \tag{3.22}$$

For $n = 1$ we have

$$\{K_\beta, \xi(x)\}_{(1)} = \left[\beta^j S_j^a \xi_{,a}\right](x) = \beta^j v_j \cdot \xi, \tag{3.23}$$

which coincides with (3.19). Suppose that (3.19) is correct up to n; then

$$\begin{aligned} \{K_\beta, \xi\}_{(n+1)} &= \beta^{j_1} \ldots \beta^{j_n} \ \left\{K_\beta, v_{j_1} \ldots v_{j_n} \cdot \xi\right\} \\ &= \beta^{j_1} \ldots \beta^{j_n} \left[v_{j_1} \ldots v_{j_n} \cdot \{K_\beta, \xi\} + \sum_{l=1}^{n} v_{j_1} \ldots v_{j_{l-1}} \left\{K_\beta, S_{j_l}^a\right\} \partial_a v_{j_{l+1}} \ldots v_{j_n} \cdot \xi \right] \\ &= \beta^{j_1} \ldots \beta^{j_n} \left[v_{j_1} \ldots v_{j_n} \cdot \beta^{j_{n+1}} v_{j_{n+1}} \cdot \xi - \sum_{l=1}^{n} v_{j_1} \ldots v_{j_{l-1}} [v_{j_l} \beta^{j_{n+1}}] v_{j_{n+1}} v_{j_{l+1}} \ldots v_{j_n} \cdot \xi \right] \\ &= \beta^{j_1} \ldots \beta^{j_n} \left[v_{j_1} \ldots v_{j_n} \cdot \beta^{j_{n+1}} v_{j_{n+1}} \cdot \xi - \sum_{l=1}^{n} v_{j_1} \ldots v_{j_{l-1}} [v_{j_l} \beta^{j_{n+1}}] v_{j_{l+1}} \ldots v_{j_{n+1}} \cdot \xi \right] \\ &= \beta^{j_1} \ldots \beta^{j_n} \ \left[v_{j_1} \ldots v_{j_n} \cdot \beta^{j_{n+1}} v_{j_{n+1}} \cdot \xi - \left(v_{j_1} \ldots v_{j_n} \beta^{j_{n+1}} - \beta_{j_{n+1}} v_{j_1} \ldots v_{j_n}\right) v_{j_{n+1}} \cdot \xi\right] \\ &= \beta^{j_1} \ldots \beta^{j_{n+1}} \ v_{j_1} \ldots v_{j_{n+1}} \cdot \xi. \end{aligned} \tag{3.24}$$

where we used commutativity of the v_j and the Leibniz rule.

It follows that

$$O_{\xi(x)}^{(1)}[\sigma] = \xi(x) + \sum_{n=1}^{\infty} \frac{1}{n!} [\sigma^{j_1}(x) - S^{j_1}(x)] \ldots [\sigma^{j_n}(x) - S^{j_n}(x)] \ v_{j_1} \ldots v_{j_n} \cdot \xi(x). \tag{3.25}$$

Using $v_j \cdot S^k = \delta_j^k$ and commutativity of the v_j, we find with $\beta^j := \sigma^j - S^j$ that

$$
\begin{aligned}
v_k \cdot O^{(1)}_{\xi(x)}[\sigma] &= v_k \cdot \xi + \sum_{n=1}^{\infty}\left[\frac{1}{(n-1)!}[v_k\cdot\beta^j]\beta^{j_1}\ldots\beta^{j_{n-1}}\, v_j v_{j_1}\ldots v_{j_{n-1}}\cdot\xi \right.\\
&\quad\left. + \frac{1}{n!}\beta^{j_1}\ldots\beta^{j_n}\, v_k v_{j_1}\ldots v_{j_n}\cdot\xi\right]\\
&= v_k\cdot\xi + \left[v_k\cdot\beta^j\right] v_j\cdot\xi + \sum_{n=1}^{\infty}\frac{1}{n!}\beta^{j_1}\ldots\beta^{j_n}\\
&\quad\times\left[[v_k\cdot\beta^j]v_j v_{j_1}\ldots v_{j_n}\cdot\xi + v_k v_{j_1}\ldots v_{j_n}\cdot\xi\right]\\
&= \sum_{n=0}^{\infty}\frac{1}{(n)!}\beta^{j_1}\ldots\beta^{j_n}[v_k\cdot\sigma^j]v_j v_{j_1}\ldots v_{j_n}\cdot\xi.
\end{aligned}
\tag{3.26}
$$

The interpretation of (3.25) becomes clear for the choice $\sigma^j(x) = \sigma^j = \text{const}$, for which (3.26) vanishes identically. In other words, the completion $O^{(1)}_{\xi(x)}[\sigma]$ does not depend on x at all. Hence, for this choice of σ^j, we are free to choose x in $O^{(1)}_{\xi(x)}[\sigma]$ in order to simplify (3.25). Since (3.25) is a power expansion in $(\sigma^j(x) - S^j)(x)$, and S^j is a diffeomorphism, we choose $x = x_\sigma$, with x_σ being the unique solution of $S^j(x) = \sigma^j$. Then[22],

$$
O^{(1)}_{\xi(x)}(\sigma) = \xi(x_\sigma) = [\xi(x)]_{S^j(x)=\sigma^j}\,. \tag{3.27}
$$

The completion $O^{(1)}_{\xi(x)}(\sigma)$ of $\xi(x)$ has also a simple integral representation:

$$
O^{(1)}_{\xi(x)}(\sigma) = \int_{\mathcal{X}} \mathrm{d}^3x\,|\det(\partial S(x)/\partial x)|\,\delta(S(x),\sigma)\,\xi(x). \tag{3.28}
$$

The significance of choosing $\sigma^j = \text{const}$ is the following: clearly, the choice $\sigma^j(x) = \text{const}$ is not in the range of $S^j(x)$, which is supposed to be a diffeomorphism. Thus, the interpretation of $O^{(1)}_f(\sigma)$ as the value of f in the gauge $S^j = \sigma^j$ is obsolete. However, given a function $\sigma^j(x)$, instead of solving $S^j(x) = \sigma^j(x)$ for the values of the function S^j for all x, we could solve it for x, while keeping the function S^j arbitrary. This is the appropriate interpretation of $O^{(1)}_f(\sigma)$. This is possible because $O^{(1)}_f[\sigma]$ is (at least formally) gauge invariant, whether or not $S^j = \sigma^j$ is a good choice of gauge. It is fully sufficient to do this because, as shown in [12] and as we will show in appendix B, the partially reduced phase space (with respect to the spatial diffeomorphism constraint) is completely determined by the $O^{(1)}_f(\sigma)$; hence, the $O^{(1)}_f[\sigma]$ must be hugely redundant.

We can now compute the spatially diffeomorphism invariant extensions for the remaining phase space variables without any additional effort, by switching first to variables which are spatial scalars on $\mathcal{X}$, using $J := \det(\partial S/\partial x)$, which we assume to be positive (orientation preserving diffeomorphism):

$$
(\xi, \pi/J), \qquad (T, P/J), \qquad \left(q_{jk} \equiv q_{ab}S^a_j S^b_k,\ p^{jk} \equiv S^j_{\ ,a}S^k_{\ ,b}p^{ab}/J\right). \tag{3.29}
$$

The image of these quantities, evaluated at x, under the completion $O^{(1)}_f(\sigma)$ simply consists in replacing x by x_σ, where x_σ solves $S^j(x) = \sigma^j$, just as in (3.27). The scalars (3.29) on $\mathcal{X}$ are the pullbacks of the original tensor (densities) under the diffeomorphism $\sigma \mapsto x_\sigma$ evaluated at σ. Thus, they are tensor (densities) of the same type, but live now on the dust space manifold $\mathcal{S}$.

[22] We switched to the notation $O^{(1)}_f(\sigma)$ to indicate the choice $\sigma^j(x) = \sigma^j = \text{const}$.

This statement sounds contradictory because of the following subtlety: we have e.g. the three quantities $P(x)$, $\tilde{P}(x) = P(x)/J(x)$, $\tilde{P}(\sigma) = \tilde{P}(x_\sigma)$. On $\mathcal{X}$, $P(x)$ is a scalar density while $\tilde{P}(x)$ is a scalar. Pulling back $P(x)$ to $\mathcal{S} = S(\mathcal{X})$ by the diffeomorphism $\sigma \mapsto S^{-1}(\sigma)$ results in $\tilde{P}(\sigma)$. But pulling back $\tilde{P}(x)$ back to $\mathcal{S}$ results in the *same* quantity $\tilde{P}(\sigma)$. Since a diffeomorphism does not change the density weight, we would get the contradiction that $\tilde{P}(\sigma)$ has both density weights zero and one on $\mathcal{S}$. The resolution of the puzzle is that what determines the density weight of $P(x)$ on $\mathcal{X}$ is its transformation behaviour under canonical transformations generated by the total spatial diffeomorphism constraint $c_a^{\text{tot}} = c_a^{\text{dust}} + c_a$ where c_a^{dust}, c_a are the dust and non-dust contributions respectively. After the reduction of c_a^{tot}, what determines the density weight of $\tilde{P}(\sigma)$ on $\mathcal{S}$ is its transformation behaviour under $\big([c_a + PT_{,a}]S_j^a\big/J\big)(x_\sigma) = \tilde{c}_j(\sigma) + \tilde{P}(\sigma)\tilde{T}_{,j}(\sigma)$ and this shows that $\tilde{P}(\sigma)$ has density weight one[23].

We will denote the images under $f \mapsto O_f^{(1)}(\sigma)$ by

$$(\tilde{\xi}(\sigma), \tilde{\pi}(\sigma)), \quad (\tilde{T}(\sigma), \quad \tilde{P}(\sigma)), \quad (\tilde{q}_{ij}(\sigma)\tilde{p}^{ij}(\sigma)). \tag{3.30}$$

In appendix B we show that the quantities (3.30) can also be obtained through symplectic reduction which is an alternative method to show that the pairs in (3.30) are conjugate and as it was done in [12].

3.2. Implementing invariance with respect to the Hamiltonian constraint

Having completed the elementary phase space variables with respect to the spatial diffeomorphism constraint, it remains to render those variables invariant under the action of the Hamiltonian constraint. This amounts to calculating the image of those variables under the map $f \mapsto O_f^{(2)}[\sigma]$, for any f in (3.30). For f independent of T, P, the completion of f with respect to the Hamiltonian constraint is given by

$$O_f^{(2)}[\tau] = \sum_{n=0}^{\infty} \frac{1}{n!}\,\{h[\tau], f\}_{(n)}, \qquad h[\tau] = \int_{\mathcal{X}} \mathrm{d}^3x(\tau(x) - T(x))h(x). \tag{3.31}$$

Only if we choose $\tau(x) = \tau = \text{const}$, (3.31) is invariant under diffeomorphisms. Hence we choose $\tau(x) = \tau = \text{const}$, which allows us to rewrite (3.31) entirely in terms of the variables (3.30). As a reminder of this choice, we denote the completion by $O_f^{(2)}(\tau)$. In this case (3.31) can be written as

$$O_f^{(2)}(\tau) = \sum_{n=0}^{\infty} \frac{1}{n!}\{\tilde{h}(\tau), f\}_{(n)}, \qquad \tilde{h}(\tau) = \int_{\mathcal{S}} \mathrm{d}^3\sigma(\tau - \tilde{T}(\sigma))\tilde{h}(\sigma) \tag{3.32}$$

with $\tilde{h}(\sigma)$ denoting the image of $h(x)$ under the replacement[24] of $\{\xi(x), \pi(x), q_{ab}(x), p^{ab}(x)\}$ by $\{\tilde{\xi}(\sigma), \tilde{\pi}(\sigma), \tilde{q}_{jk}(\sigma), \tilde{p}^{jk}(\sigma)\}$, respectively. Explicitly, denoting

$$\tilde{c}(\sigma) \equiv \left[\frac{c(x)}{J(x)}\right]_{S(x)=\sigma} \tilde{c}_j(\sigma) \equiv \left[\frac{c_j(x)}{J(x)}\right]_{S(x)=\sigma}, \tag{3.33}$$

where, as before, $c_j(x) = S_j^a(x)\, c_a(x)$, we find

$$\tilde{h}(\sigma) = \sqrt{\tilde{c}^2 - \tilde{q}^{jk}\,\tilde{c}_j\tilde{c}_k}(\sigma). \tag{3.34}$$

[23] In order to avoid confusion of the reader we mention that any quantity f on $\mathcal{X}$ which has positive density weight is mapped to zero under $f \mapsto O_f^{(1)}(\sigma)$. Let us again consider the example $f = P$. We have $\tilde{P}(\sigma) = P(x_\sigma)\det(\partial S^{-1}(\sigma)/\partial\sigma)$ which is perfectly finite. However by the Poisson automorphism formula $O_{P(x)}^{(1)} = O_{J(x)\,\tilde{P}(x)}^{(1)} = O_{J(x)}^{(1)}\,\tilde{P}(\sigma) = \det(\partial\sigma/\partial x)\,\tilde{P}(\sigma) = 0$ since $\sigma = \text{const}$.

[24] The proof of this statement is based on the fact that the replacement corresponds to a diffeomorphism and that $h(\tau)$ is the integral of a scalar density of weight on, for $\tau = \text{const}$.

It is easy to see that

$$\frac{\mathrm{d}}{\mathrm{d}\tau} O^{(2)}_f(\tau) = \{\mathbf{H}, O^{(2)}_f(\tau)\} \tag{3.35}$$

with

$$\mathbf{H} := \int_{\mathcal{S}} \mathrm{d}^3\sigma\, \tilde{h}(\sigma) \tag{3.36}$$

is the *physical Hamiltonian* (not Hamiltonian density) of the deparametrized system.

We denote the fully gauge-invariant completions of the Hamiltonian constraint, the spatial diffeomorphism constraints[25] and the physical Hamilton density, respectively, as

$$\begin{aligned} &C(\tau,\sigma) \equiv O^{(2)}_{\tilde{c}(\sigma)}(\tau) C_j(\tau,\sigma) \equiv O^{(2)}_{\tilde{c}_j(\sigma)}(\tau),\\ &H(\tau,\sigma) \equiv O^{(2)}_{\tilde{h}(\sigma)}(\tau). \end{aligned} \tag{3.37}$$

It is worth emphasizing again that $H(\tau,\sigma)$ is the physical energy density associated with the physical Hamiltonian when the dust fields are considered as clocks of the system. The fully gauge-invariant completions of the phase space variables for matter and gravity are denoted by

$$\begin{aligned} &\Xi(\tau,\sigma) \equiv O^{(2)}_{\tilde{\xi}(\sigma)}(\tau) \qquad \Pi(\tau,\sigma) \equiv O^{(2)}_{\tilde{\pi}(\sigma)}(\tau),\\ &Q_{ij}(\tau,\sigma) \equiv O^{(2)}_{\tilde{q}_{ij}(\sigma)}(\tau) \qquad P^{ij}(\tau,\sigma) \equiv O^{(2)}_{\tilde{p}^{ij}(\sigma)}(\tau). \end{aligned} \tag{3.38}$$

The matter scalar field $\Xi(\tau,\sigma)$ and its conjugate momentum $\Pi(\tau,\sigma)$ are observable quantities since gauge invariant. The same applies to the three-metric $Q_{ij}(\tau,\sigma)$ and its canonical momentum field $P^{ij}(\tau,\sigma)$. Moreover, the completion is non-perturbative, i.e. full non-Abelian gauge invariance has been accomplished.

3.3. Constants of the physical motion

In the previous section we successfully constructed fully gauge-invariant quantities for a specific deparametrizing system. In some sense, the construction frees the true degrees of freedom from the constraints, replacing them by conservation laws which govern the physical motion of observable quantities. Indeed, we have the following first integrals of physical motion (*conservation laws*):

$$\frac{\mathrm{d}}{\mathrm{d}\tau} C_j(\tau,\sigma) = 0, \qquad \frac{\mathrm{d}}{\mathrm{d}\tau} H(\tau,\sigma) = 0. \tag{3.39}$$

These equations express invariance under the physical evolution generated by $\mathbf{H}$, as opposed to gauge invariance. The functions C_j, H, representing physical three-momentum and energy, *are* already gauge invariant.

We proceed with the proof of (3.39). Recall that the original constraints $c^{\mathrm{tot}}(x)$, $c^{\mathrm{tot}}_j(x)$ are mutually Poisson commuting. Using (3.3), this means, in particular,

$$\{c^{\mathrm{tot}}(x), c^{\mathrm{tot}}(y)\} = \{P(x) + h(x), P(y) + h(y)\} = \{h(x), h(y)\} = 0 \tag{3.40}$$

where we used that the $P(x)$ are mutually Poisson commuting and that $h(x)$ is independent of the dust variables. Next, consider the smeared spatial diffeomorphism generator

$$c(u) \equiv \int_{\mathcal{X}} \mathrm{d}^3x\, u^a(x) c_a(x). \tag{3.41}$$

[25] Explicit expression for the constraints in terms of the fully gauge-invariant phase space variables are given in the next section, see (3.56).

The smeared constraint acts on $h(y)$ as it should,

$$\{c(u), h(y)\} = [u^a h]_{,a}(y) \tag{3.42}$$

or, after functional differentiation with respect to the smearing functions u^a:

$$\{c_a(x), h(y)\} = \partial_{y^a}(\delta(x, y)h(y)). \tag{3.43}$$

This follows from the properties of c_a, generating spatial diffeomorphisms on the matter and gravity variables, and h, being a scalar density of weight one and only depending on the non-dust variables. Furthermore, the spatial diffeomorphisms form an algebra with $\{c(u), c(u')\} = c([u', u])$. From this follows again by functional differentiation

$$\{c_a(x), c_b(y)\} = [\partial_{y^b}\delta(x, y)]c_a(y) - [\partial_{x^a}\delta(y, x)]c_b(x). \tag{3.44}$$

Let us investigate the implications of (3.40)–(3.44) for

$$\begin{aligned} \tilde{h}(\sigma) &= \left[\frac{h(x)}{J(x)}\right]_{S(x)=\sigma} = \int_{\mathcal{X}} \mathrm{d}^3x\, \delta\,(S(x), \sigma)\, h(x) \\ \tilde{c}_j(\sigma) &= \left[\frac{c_a(x)S^a_j(x)}{J(x)}\right]_{S(x)=\sigma} = \int_{\mathcal{X}} \mathrm{d}^3x\, \delta\,(S(x), \sigma)\, S^a_j(x)c_a(x). \end{aligned} \tag{3.45}$$

First of all,

$$\{\tilde{h}(\sigma), \tilde{h}(\sigma')\} = \int_{\mathcal{X}} \mathrm{d}^3x \int_{\mathcal{X}} \mathrm{d}^3y\, \delta(S(x), \sigma)\delta(S(y), \sigma')\{h(x), h(y)\} = 0 \tag{3.46}$$

where we used that the $S^j(x)$ are mutually commuting, as well as with the $h(y)$. Second, denoting the pullback of the smeared diffeomorphism generator with $\tilde{c}(\tilde{u})$ for some smearing functions $\tilde{u}^j(\sigma)$, we have

$$\begin{aligned} \{\tilde{c}(\tilde{u}), \tilde{h}(\sigma')\} &= \int_{\mathcal{S}} \mathrm{d}^3\sigma\, \tilde{u}^j(\sigma) \int_{\mathcal{X}} \mathrm{d}^3x \int_{\mathcal{X}} \mathrm{d}^3y\, \delta(S(x), \sigma)\delta(S(y), \sigma')S^a_j(x)\{c_a(x), h(y)\} \\ &= \int_{\mathcal{S}} \mathrm{d}^3\sigma\, \tilde{u}^j(\sigma) \int_{\mathcal{X}} \mathrm{d}^3x \int_{\mathcal{X}} \mathrm{d}^3y\, \delta(S(x), \sigma)\delta(S(y), \sigma')S^a_j(x)\partial_{y^a}(\delta(x, y)h(y)) \\ &= -\int_{\mathcal{S}} \mathrm{d}^3\sigma\, \tilde{u}^j(\sigma) \int_{\mathcal{X}} \mathrm{d}^3x\, \delta\,(S(x), \sigma)\,[\partial_{x^a}\delta(S(x), \sigma')]S^a_j(x)h(x) \\ &= -\int_{\mathcal{S}} \mathrm{d}^3\sigma\, \tilde{u}^j(\sigma) \int_{\mathcal{X}} \mathrm{d}^3x\, \delta\,(S(x), \sigma)\,[\partial_{\tilde{\sigma}^k}\delta(\tilde{\sigma}, \sigma')]_{\tilde{\sigma}=S(x)}S^k_{,a}(x)S^a_j(x)h(x) \\ &= -\int_{\mathcal{S}} \mathrm{d}^3\sigma\, \tilde{u}^j(\sigma) \int_{\mathcal{S}} \mathrm{d}^3\sigma_1\, \delta\,(\sigma_1, \sigma)\left[\partial_{\sigma_1^j}\delta\left(\sigma_1, \sigma'\right)\right]\left[\frac{h(x)}{J(x)}\right]_{S(x)=\sigma_1} \\ &= -\int_{\mathcal{S}} \mathrm{d}^3\sigma_1\, \tilde{u}^j(\sigma_1)[\delta(\sigma_1, \sigma')]_{,\sigma_1^j}\tilde{h}(\sigma_1) \\ &= \int_{\mathcal{S}} \mathrm{d}^3\sigma_1[\tilde{u}^j(\sigma_1)\tilde{h}(\sigma_1)]_{,\sigma_1^j}\delta(\sigma_1, \sigma') \\ &= [\tilde{u}^j(\sigma')\tilde{h}(\sigma')]_{,\sigma'^j}. \end{aligned} \tag{3.47}$$

The last implication follows from

$$\tilde{c}(\tilde{u}) = c(u_S), \qquad u^a_S(x) = S^a_j(x)\tilde{u}^j(S(x)) \tag{3.48}$$

where the vector fields u_S are phase space dependent (they depend on S) and using the fact that the $S^j(x)$ and $c_a(y)$ are mutually Poisson commuting. Then,

$$
\begin{aligned}
\{\tilde{c}(\tilde{u}), \tilde{c}(\tilde{u}')\} &= c([u'_S, u_S]) \\
&= \int_{\mathcal{X}} \mathrm{d}^3x \left[u'^b_S(x) u^a_{S,b}(x) - u^b_S(x) u'^a_{S,b}(x) \right] c_a(x) \\
&= \int_{\mathcal{X}} \mathrm{d}^3x \; S^b_j(x) \left[\tilde{u}'^j(S(x)) \big(S^a_k(x) S^l_{,b}(x) \; \tilde{u}^k_{,l}(S(x)) \right. \\
&\quad - S^a_l(x) S^l_{,cb}(x) S^c_k(x) \tilde{u}^k(S(x)) \big) - \tilde{u}^j(S(x)) \big(S^a_k(x) \tilde{u}'^k_{,l}(S(x)) \\
&\quad \left. - S^a_l(x) S^l_{,cb}(x) S^c_k(x) \tilde{u}'^k(S(x)) \big) \right] c_a(x) \\
&= \int_{\mathcal{X}} \mathrm{d}^3x \left[\tilde{u}'^j(S(x)) \tilde{u}^k_{,j}(S(x)) - \tilde{u}^j(S(x)) \tilde{u}'^k_{,j}(S(x)) \right] c_a(x) S^a_k(x) \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma \int_{\mathcal{X}} \mathrm{d}^3x \; \delta(S(x), \sigma) \left[\tilde{u}'^j(\sigma) \tilde{u}^k_{,j}(\sigma) - \tilde{u}^j(\sigma) \tilde{u}'^k_{,j}(\sigma) \right] c_a(x) S^a_k(x) \\
&= \tilde{c}([\tilde{u}', \tilde{u}]).
\end{aligned} \tag{3.49}
$$

Hence, equations (3.40)–(3.44) are exactly reproduced by (3.46), (3.47) and (3.49).

We can now easily finish the proof of (3.39). In (3.32) we introduced $\tilde{h}(\tau)$. From (3.46) it follows that

$$\{\tilde{h}(\tau), \tilde{h}(\sigma)\} = 0. \tag{3.50}$$

This implies in particular that

$$\tilde{h}(\sigma) = H(\sigma) = O^{(2)}_{\tilde{h}(\sigma)}(\tau) \tag{3.51}$$

is already an observable quantity[26]. Hence, from the definition of $\mathbf{H}$ and (3.46) we find $\{\mathbf{H}, \tilde{h}(\sigma)\} = 0$. Furthermore,

$$\{\mathbf{H}, C_j(\tau, \sigma)\} = \left\{ O^{(2)}_{\mathbf{H}}(\tau), O^{(2)}_{\tilde{c}_j(\sigma)}(\tau) \right\} = O^{(2)}_{\{\mathbf{H}, \tilde{c}_j(\sigma)\}}(\tau) = 0. \tag{3.52}$$

Alternatively, a more direct way to understand this result is to make use of the series representation (3.32) and of

$$\tilde{h}(\tau) = \tau \mathbf{H} - \tilde{h}[\tilde{T}] \tilde{h}[\tilde{T}] = \int_{\mathcal{S}} \mathrm{d}^3\sigma \; \tilde{T}(\sigma) \tilde{h}(\sigma). \tag{3.53}$$

Since the Hamiltonian vector fields X_1, X_2 of $\mathbf{H}$ and $\tilde{h}[\tilde{T}]$, respectively, are commuting, we may write for (3.32)

$$
\begin{aligned}
C_j(\sigma, \tau) &= \exp(\tau X_1 - X_2) \cdot \tilde{c}_j(\sigma) = \exp(-X_2) \cdot [\exp(\tau X_1) \cdot \tilde{c}_j(\sigma)] \\
&= \exp(-X_2) \cdot \tilde{c}_j(\sigma) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \{\tilde{h}[\tilde{T}], \tilde{\sigma}_j(\sigma)\}_{(n)},
\end{aligned} \tag{3.54}
$$

which is clearly τ-independent.

We end this section by giving an explicit expressions for the physical Hamiltonian in terms of purely gauge-invariant quantities:

$$H(\sigma) = \sqrt{C(\tau, \sigma)^2 - Q^{jk}(\tau, \sigma) \; C_j(\sigma) \; C_k(\sigma)}. \tag{3.55}$$

Note that C, Q^{jk} are not independent of the physical time τ. Of course, $C(\tau, \sigma), C_j(\sigma)$ are obtained from $\tilde{c}(\sigma), \tilde{c}_j(\sigma)$ simply by replacing everywhere the functional dependence on

[26] Note, however, although $H(\sigma) = \tilde{h}(\sigma)$, this is not true for the corresponding spatial diffeomorphism constraints, $\tilde{c}_j(\sigma) \neq C_j(\sigma)$!

$\{\tilde{\xi}(\sigma), \tilde{\pi}(\sigma), \tilde{q}_{jk}(\sigma), p^{jk}(\sigma)\}$ by that on $\{\Xi(\tau,\sigma), \Pi(\tau,\sigma), Q_{jk}(\tau,\sigma), P^{jk}(\tau,\sigma)\}$. In greater detail,

$$\begin{aligned} C_j(\sigma) &= [-2Q_{jk}(D_k P^{kl}) + \Pi(D_j\Xi)](\tau,\sigma) \\ C(\tau,\sigma) &= \frac{1}{\kappa}\left[\frac{1}{\sqrt{\det(Q)}}\left(Q_{jm}Q_{kn} - \frac{1}{2}Q_{jk}Q_{mn}\right)P^{jk}P^{mn}\right. \\ &\quad \left. - \sqrt{\det(Q)}R^{(3)}[Q] + 2\Lambda\sqrt{\det(Q)}\right](\tau,\sigma) \\ &\quad + \frac{1}{2\lambda}\left[\frac{\Pi^2}{\sqrt{\det(Q)}} + \sqrt{\det(Q)}(Q^{jk}\ (D_j\Xi)\ (D_k\Xi) + v(\Xi))\right](\tau,\sigma) \\ &\equiv C_{\mathrm{geo}}(\tau,\sigma) + C_{\mathrm{matter}}(\tau,\sigma) \end{aligned} \tag{3.56}$$

with D_j denoting the covariant differential compatible with Q_{jk}.

4. Physical equations of motion

In this section[27] we derive the physical evolution of the gauge-invariant functions $\{\Xi, \Pi, Q_{jk}, P^{jk}\}$, generated by the true Hamiltonian $\mathbf{H}$, in the first-order (Hamilton) and second-order (Lagrange) formulation. In other words, we study the true evolution of matter degrees of freedom and gravity with respect to the physical reference system (dust).

4.1. First-order (Hamiltonian) formulation

For a generic observable F, we denote[28] its τ-derivative simply by an overdot, $\dot{F}$. Then,

$$\begin{aligned} \dot{F} &= \{\mathbf{H}, F\} = \int_{\mathcal{S}} \mathrm{d}^3\sigma\{H(\sigma), F\} \\ &= \int_{\mathcal{S}} \mathrm{d}^3\sigma \frac{1}{H(\sigma)}\Big(C(\sigma)\{C(\sigma), F\} - Q^{jk}(\sigma)C_k(\sigma)\{C_j(\sigma), F\} \\ &\quad + \frac{1}{2}Q^{im}(\sigma)C_m(\sigma)Q^{jn}(\sigma)C_n(\sigma)\{Q_{ij}(\sigma), F\}\Big). \end{aligned} \tag{4.1}$$

Let us introduce *dynamical shift* and *dynamical lapse* fields by

$$N_j \equiv -C_j/H \qquad N \equiv C/H = \sqrt{1 + Q^{jk}N_jN_k}. \tag{4.2}$$

Note that N_j is a constant of the physical motion, but neither are N nor $N^j = Q^{jk}N_k$. Then (4.1) can be rewritten in the familiar looking form

$$\dot{F} = \int_{\mathcal{S}} \mathrm{d}^3\sigma\left(N(\sigma)\{C(\sigma), F\} + N^j(\sigma)\{C_j(\sigma), F\} + \frac{1}{2}H(\sigma)N^i(\sigma)N^j(\sigma)\{Q_{ij}(\sigma), F\}\right). \tag{4.3}$$

The first two terms in (4.3) are *exactly the same* as those in the gauge variant derivation of the equation of motion, derived with respect the primary Hamiltonian

$$\mathbf{H}_{\mathrm{primary}}(N, \vec{N}) = \int_{\mathcal{S}} \mathrm{d}^3\sigma(N(\sigma)C(\sigma) + N^j(\sigma)C_j(\sigma)). \tag{4.4}$$

Here, N, N^j are viewed as phase space independent functions. The third term in (4.3), on the other hand, is a genuine correction to the gauge variant formalism. However, it enters only in

[27] For the purposes of this section we assume that $\mathcal{X}$ and, equivalently, $\mathcal{S}$ have no boundary. In order to allow for more general topologies, we consider boundary terms in the next section. The calculations of the present section are not affected by the presence of such a boundary term, because it only cancels the boundary term that would appear in the calculation of this section.

[28] Furthermore, for notational ease we drop the dependence on (τ, σ) when no confusions can arise.

the physical evolution equation of P^{jk}. Hence,

$$
\begin{aligned}
\dot{\Xi} &= \frac{N}{\sqrt{\det(Q)}}\Pi + \mathcal{L}_{\vec{N}}\Xi \\
\dot{\Pi} &= \partial_j\left[N\sqrt{\det(Q)}\; Q^{jk}\,\Xi_{,k}\right] - \frac{N}{2}\sqrt{\det(Q)}v'(\Xi) + \mathcal{L}_{\vec{N}}\Pi \\
\dot{Q}_{jk} &= \frac{2N}{\sqrt{\det(Q)}}\; G_{jkmn}P^{mn} + (\mathcal{L}_{\vec{N}}Q)_{jk} \\
\dot{P}^{jk} &= N\Bigg[-\frac{Q_{mn}}{\sqrt{\det Q}}(2P^{jm}P^{kn} - P^{jk}P^{mn}) + \frac{\kappa}{2}Q^{jk}C \\
&\qquad - \sqrt{\det Q}Q^{jk}\left(2\Lambda + \frac{\kappa}{2\lambda}\left(\Xi^{,m}\Xi_{,m} + v(\Xi)\right)\right)\Bigg] \\
&\qquad + \sqrt{\det Q}[G^{-1}]^{jkmn}\left((D_m D_n N) - N R_{mn}[Q]\right) + \frac{\kappa}{2\lambda}N\sqrt{\det Q}\;\Xi^{,j}\,\Xi^{,k} \\
&\qquad - \frac{\kappa}{2}H Q^{jm}Q^{kn}N_m N_n + (\mathcal{L}_{\vec{N}}P)^{jk}
\end{aligned}
\tag{4.5}
$$

with $\mathcal{L}_{\vec{N}}$ denoting the Lie derivative[29] with respect to the vector field $\vec{N}$ with components $N^j = Q^{jk}N_k$, and we have defined the DeWitt metric on symmetric tensors as

$$G_{jkmn} \equiv \tfrac{1}{2}(Q_{jm}Q_{nk} + Q_{jn}Q_{mk} - Q_{jk}Q_{mn}), \tag{4.6}$$

which has the inverse

$$[G^{-1}]^{jkmn} = \tfrac{1}{2}(Q^{jm}Q^{nk} + Q^{jn}Q^{mk} - 2Q^{jk}Q^{mn}), \tag{4.7}$$

that is $G_{jkmn}[G^{-1}]^{nmpq} = \delta^p_{(j}\delta^q_{k)}$. The Ricci tensor of Q is denoted by $R_{jk}[Q]$ and $C = C_{\text{geo}} + C_{\text{matter}}$ denotes the split of the Hamiltonian constraint (with the dust reference system excluded) into gravitational[30] and matter contribution, as shown explicitly in (3.56).

It is already evident that the dust model we utilized as a physical reference system has the great advantage that, remarkably, equations (4.5) are almost exactly of the same form as the corresponding equations in the gauge variant formalism, the only difference being the last term on the right-hand side of the physical evolution equation for $\dot{P}^{jk}$. In other words, introducing a physical reference system must necessarily lead to corrections compared to gauge fixing, because the physical reference system will communicate via gravitational interaction with the original system under consideration. In the sense described above, the dust reference system creates only a minimal modification—it is the minimal extension of the original gravity–matter system that extracts the true degrees of freedom and allows for their physical evolution.

The other difference is that instead of having constraints imposed on the phase space variables, $C = C_j = 0$, now the dynamics of the true degrees of freedom is subject to conservation laws $\dot{H} = \dot{C}_j = 0$. Thus, in solving (4.5) we may prescribe arbitrary functions $\epsilon(\sigma), \epsilon_j(\sigma)$ which play the role of the (constant in τ-time) energy and momentum density, respectively. The substitution[31] $H = \epsilon, C_j = -\epsilon_j$ will be crucial in what follows. In fact, in order to derive the second order equations of motion, $\dot{\Xi}$, $\dot{Q}_{jk}$ in (4.5) has to be solved for Π, P^{jk}. Without the conservation laws, this would be impossible, since Π, P^{jk} enter the

[29] For the explicit calculation of the Lie derivative it is important to note that Π , P^{jk} are tensor densities of weight one in dust space.

[30] Note that we have included a cosmological constant term $+2\sqrt{\det(q)})\Lambda$ in C_{geo}.

[31] The letter ϵ is chosen to indicate that these values are small, appropriate for *test clocks and rods*. In this way it can be guaranteed that the dust, although gravitationally coupled with the original system, will not alter the dynamics of the original system in an uncontrolled fashion.

expressions for H, C, C_j in a non-trivial way, i.e. solving for them would lead to algebraic equations of higher than fourth order. The substitution will also be crucial for the derivation of the effective Lagrangian, by the inverse Legendre transform, corresponding to **H**, see appendix C.

4.2. Second-order (Lagrangian) formulation

In this section we will use the first-order (Hamiltonian) equations of motion and derive the corresponding second-order (Lagrangian) equations of motion for the configuration variables Ξ and Q_{jk}, respectively. We will sketch the main steps of these calculations in section 4.3. The reader who is just interested in the results should skip this section and go directly to section 4.4 where the final equations are summarized.

4.3. Derivation of the second-order equations of motion

In this section we want to derive the second-order equations of motion for Ξ and Q_{jk}, respectively. These second-order equations will be functions of the configuration variables Ξ, Q_{jk} and their corresponding velocities $\dot{\Xi}, \dot{Q}_{jk}$, respectively. This can be achieved by solving for the conjugate momenta Π and P^{jk} in terms of their corresponding velocities $\dot{\Xi}$ and $\dot{Q}_{jk}$ via the equation of motion. The relation between the conjugate momenta and their velocities is given through the first-order Hamiltonian equations which were displayed in the last section in equation (4.5).

We begin with the matter equation for Ξ. First, we have to take the time derivative of the first-order equation for Ξ given in equation (4.5). This yields

$$\ddot{\Xi} = \left[\frac{\dot{N}}{\sqrt{\det Q}} - N\frac{(\sqrt{\det Q})^{\cdot}}{\det Q}\right]\Pi + \frac{N}{\sqrt{\det Q}}\dot{\Pi} + \mathcal{L}_{\dot{\vec{N}}}\Xi + \mathcal{L}_{\vec{N}}\dot{\Xi}. \tag{4.8}$$

As discussed in section 3.3, the shift vector $N_j := -C_j/H$ is a constant of motion since $\dot{C}_j = \dot{H} = 0$. Therefore for the Lie derivative with respect to $\dot{\vec{N}}$ the only non-vanishing contribution is the one including $\dot{Q}^{ij}$,

$$(\mathcal{L}_{\dot{\vec{N}}}\Xi) = (Q^{ij}N_j)^{\cdot}\Xi_{,i} = \dot{Q}^{ij}N_j\Xi_{,i}. \tag{4.9}$$

We will use this result later on, but for now we will work with the compact form of the Lie derivatives as written in equation (4.8). Solving for Π in terms of $\dot{\Xi}$ we get from equation (4.5)

$$\Pi(\Xi, \dot{\Xi}, Q_{jk}) = \frac{\sqrt{\det Q}}{N}(\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi) \tag{4.10}$$

and thus have expressed Π as a function of the velocity $\dot{\Xi}$. In order to stress that Π has to be understood as a function of $\dot{\Xi}$, we have explicitly written the function's arguments in this section. Note that strictly speaking Π also appears in $N = \sqrt{1 + Q^{jk}C_jC_k/H^2}$ and $N^j = -Q^jkC_k/H$. However, C_j and H are treated as constants of motion as discussed before. The same applies to P^{jk} below. Next we insert this result into equation (4.5), obtaining

$$\begin{aligned}\dot{\Pi}(\Xi, \dot{\Xi}) &= [N\sqrt{\det(Q)}\; Q^{jk}\Xi_{,k}]_{,j} - \frac{N}{2}\sqrt{\det(Q)}\; v'(\Xi) + \mathcal{L}_{\vec{N}}\left(\frac{\sqrt{\det Q}}{N}(\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi)\right)\\ &= [N\sqrt{\det(Q)}\; Q^{jk}\Xi_{,k}]_{,j} - \frac{N}{2}\sqrt{\det(Q)}v'(\Xi) + (\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi)\left(\mathcal{L}_{\vec{N}}\frac{\sqrt{\det Q}}{N}\right)\\ &\quad + \frac{\sqrt{\det Q}}{N}(\mathcal{L}_{\vec{N}}(\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi)).\end{aligned} \tag{4.11}$$

The final second-order equation of motion for Ξ can be derived by inserting equations (4.10) and (4.11) into equation (4.8). The result is

$$\ddot{\Xi} = \left[\frac{\dot{N}}{N} - \frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}} + \frac{N}{\sqrt{\det Q}}\left(\mathcal{L}_{\vec{N}}\frac{\sqrt{\det Q}}{N}\right)\right](\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi)$$
$$+ Q^{jk}\Xi_{,k}\left[\frac{N}{\sqrt{\det Q}}[N\sqrt{\det Q}]_{,j}\right] + N^2\left[\Delta\Xi + [Q^{jk}]_{,j}\Xi_{,k} - \frac{1}{2}\,v'(\Xi)\right]$$
$$+ 2(\mathcal{L}_{\vec{N}}\dot{\Xi}) + (\mathcal{L}_{\dot{\vec{N}}}\Xi) - (\mathcal{L}_{\vec{N}}(\mathcal{L}_{\vec{N}}\Xi)). \tag{4.12}$$

The same procedure has to be repeated for the gravitational equations now. Applying another time derivative to the first-order equation of Q_{jk} in equation (4.5) yields

$$\ddot{Q}_{jk} = \left(2\left[\frac{\dot{N}}{\sqrt{\det Q}} - N\frac{(\sqrt{\det Q})^{\cdot}}{\det Q}\right]G_{jkmn} + \frac{2N}{\sqrt{\det Q}}\dot{G}_{jkmn}\right)P^{mn} + \frac{2N}{\sqrt{\det Q}}G_{jkmn}\dot{P}^{mn}$$
$$+ (\mathcal{L}_{\dot{\vec{N}}}Q)_{jk} + (\mathcal{L}_{\vec{N}}\dot{Q})_{jk}. \tag{4.13}$$

In order to solve for P^{jk} in terms of $\dot{Q}_{jk}$ we use the inverse of the tensor G_{jkmn} denoted by $[G^{-1}]^{jkmn}$ and defined in equation (4.7). This results in

$$P^{jk}(Q_{jk}, \dot{Q}_{jk}) = \frac{\sqrt{\det Q}}{2N}[G^{-1}]^{jkmn}(\dot{Q}_{mn} - (\mathcal{L}_{\vec{N}}Q)_{mn}). \tag{4.14}$$

Since the equation for $\dot{P}^{jk}$ in (4.5) contains C which includes the geometry as well as the matter part of the Hamiltonian constraint (see equation (3.56) for its explicit definition), it is a function of the variables Q_{jk}, P^{jk}, Ξ and Π. This was different for Π where its time derivative involved the matter momentum only. Thus, in order to express $\dot{P}^{jk}$ as a function of configuration variables and velocities, we use equations (4.10) and (4.14) and replace the momenta occurring in $\dot{P}^{jk}$. Rewriting C_{geo} by means of the DeWitt bimetric G_{jkmn} we get

$$C_{\text{geo}} = \frac{1}{\kappa}\left[\frac{1}{\sqrt{\det Q}}G_{jkmn}P^{jk}P^{mn} + \sqrt{\det Q}\,(2\Lambda - R)\right]. \tag{4.15}$$

Using the relation in equation (4.14) and the fact that $G_{jkmn}[G^{-1}]^{jkrs} = \delta^r_{(m}\delta^s_{n)}$, we obtain

$$C_{\text{geo}}(Q_{jk}, \dot{Q}_{jk}) = \frac{1}{\kappa}\left[\frac{\sqrt{\det Q}}{4N^2}[G^{-1}]^{jkmn}(\dot{Q}_{jk} - (\mathcal{L}_{\vec{N}}Q)_{jk})(\dot{Q}_{mn} - (\mathcal{L}_{\vec{N}}Q)_{mn})\right.$$
$$\left. + \sqrt{\det Q}(2\Lambda - R)\right]. \tag{4.16}$$

For the matter part of the Hamiltonian constraint we obtain by means of equation (4.10)

$$C_{\text{matter}}(\Xi, \dot{\Xi}, Q_{jk}) = \frac{1}{2\lambda}\left[\frac{\sqrt{\det Q}}{N^2}(\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi)^2 + \sqrt{\det Q}(Q^{jk}\Xi_{,j}\Xi_{,k} + v(\Xi))\right]. \tag{4.17}$$

There are two other terms in $\dot{P}^{jk}$ which include the conjugate momenta P^{jk}. One is the first term on the right-hand side of equation (4.5) being quadratic in P^{jk} and the second is the Lie derivative of P^{jk}. Reinserting into those terms the relation shown in equation (4.14), we end up with the following expression for $\dot{P}^{jk}$ as a function of configuration and velocity variables:

$$\dot{P}^{jk}(Q_{jk}, \dot{Q}_{jk}, \Xi, \dot{\Xi}) = -\frac{\sqrt{\det Q}}{2N}Q_{mn}\left([G^{-1}]^{jmrs}[G^{-1}]^{kntu} - \frac{1}{2}[G^{-1}]^{mnrs}[G^{-1}]^{jktu}\right)$$
$$\times(\dot{Q}_{rs} - (\mathcal{L}_{\vec{N}}Q)_{rs})(\dot{Q}_{tu} - (\mathcal{L}_{\vec{N}}Q)_{tu})$$
$$+ N\left[\frac{\kappa}{2}Q^{jk}\,C - \sqrt{\det Q}\;Q^{jk}\left(2\Lambda + \frac{\kappa}{2\lambda}(\Xi^m\Xi_m + v(\Xi))\right)\right]$$

$$+\sqrt{\det Q}[G^{-1}]^{jkmn}\,((D_mD_nN)-NR_{mn}[Q])+\frac{\kappa}{2\lambda}N\sqrt{\det Q}\;\Xi^{,j}\,\Xi^{,k}$$
$$+\left((\mathcal{L}_{\vec N}\frac{\sqrt{\det Q}}{2N})[G^{-1}]^{jkmn}+\frac{\sqrt{\det Q}}{2N}(\mathcal{L}_{\vec N}[G^{-1}])^{jkmn}\right)(\dot Q_{mn}-(\mathcal{L}_{\vec N}Q)_{mn})$$
$$+((\mathcal{L}_{\vec N}\dot Q)_{mn}-(\mathcal{L}_{\vec N}(\mathcal{L}_{\vec N}Q))_{mn})\frac{\sqrt{\det Q}}{2N}[G^{-1}]^{jkmn}-\frac{\kappa}{2}HQ^{jm}Q^{kn}N_mN_n. \tag{4.18}$$

Next we insert the expressions for P^{jk} and $\dot P^{jk}$ in equations (4.14) and (4.18), respectively, into equation (4.13) for $\ddot Q_{jk}$. Keeping in mind that $G_{jkmn}Q^{mn}=-1/2Q_{jk}$, we end up with

$$\ddot Q_{jk}=\left[\frac{\dot N}{N}-\frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}}+\frac{N}{\sqrt{\det Q}}\left(\mathcal{L}_{\vec N}\frac{\sqrt{\det Q}}{N}\right)\right](\dot Q_{jk}-(\mathcal{L}_{\vec N}Q)_{jk})$$
$$-(\dot Q_{rs}-(\mathcal{L}_{\vec N}Q)_{rs})G_{jkmn}$$
$$\Bigg[[\dot G^{-1}]^{mnrs}+(\mathcal{L}[G^{-1}])^{mnrs}+Q_{tu}(\dot Q_{vw}-(\mathcal{L}_{\vec N}Q)_{vw})$$
$$\times\left([G^{-1}]^{mtrs}[G^{-1}]^{nuvw}-\frac{1}{2}[G^{-1}]^{mnvw}[G^{-1}]^{turs}\right)\Bigg]$$
$$-Q_{jk}\left[\frac{N^2\kappa}{2\sqrt{\det Q}}\;C-N^2\left(2\Lambda+\frac{\kappa}{2\lambda}v(\Xi)\right)\right]+N^2\left[\frac{\kappa}{\lambda}\Xi_{,j}\,\Xi_{,k}-2R_{jk}\right]$$
$$+2N(D_jD_kN)-\frac{NH\kappa}{\sqrt{\det Q}}G_{jkmn}N^mN^n$$
$$+2(\mathcal{L}_{\vec N}\dot Q)_{jk}+(\mathcal{L}_{\dot{\vec N}}Q)_{jk}-(\mathcal{L}_{\vec N}(\mathcal{L}_{\vec N}Q))_{jk}. \tag{4.19}$$

Here we used that $\dot G_{jkmn}[G^{1-}]^{mnrs}=-G_{jkmn}[\dot G^{-1}]^{jkrs}$ which follows from $(G_{jkmn}[G^{-1}]^{mnrs})^{\cdot}=0$ and

$$\frac{2N}{\sqrt{\det Q}}G_{jkmn}\left[-N\sqrt{\det Q}\;Q^{mn}\frac{\kappa}{2\lambda}\Xi^{,r}\,\Xi_{,r}+N\sqrt{\det Q}\;\frac{\kappa}{2\lambda}\Xi^{,m}\,\Xi^{,n}\right]$$
$$=\frac{2N}{\sqrt{\det Q}}\left[+\frac{N\sqrt{\det Q}\;\kappa}{4\lambda}\;Q_{jk}\Xi^{,r}\,\Xi_{,r}+\frac{N\sqrt{\det Q}\;\kappa}{2\lambda}\;\Xi_{,j}\,\Xi_{,k}-\frac{N\sqrt{\det Q}\kappa}{4\lambda}\;Q_{jk}\Xi^{,r}\,\Xi_{,r}\right]$$
$$=N^2\frac{\kappa}{\lambda}\Xi_{,j}\,\Xi_{,k}. \tag{4.20}$$

A straightforward, but tedious calculation shows that the second term on the right-hand side of the equation for $\ddot Q_{jk}$ simplifies greatly:

$$-(\dot Q_{rs}-(\mathcal{L}_{\vec N}Q)_{rs})G_{jkmn}\big[[\dot G^{-1}]^{mnrs}+(\mathcal{L}[G^{-1}])^{mnrs}+Q_{tu}(\dot Q_{vw}-(\mathcal{L}_{\vec N}Q)_{vw})$$
$$\times\big([G^{-1}]^{mtrs}[G^{-1}]^{nuvw}-\tfrac{1}{2}[G^{-1}]^{mnvw}[G^{-1}]^{turs}\big)\big]$$
$$=Q^{mn}(\dot Q_{mj}-(\mathcal{L}_{\vec N}Q)_{mj})(\dot Q_{nk}-(\mathcal{L}_{\vec N}Q)_{nk}). \tag{4.21}$$

Consequently, the final form for the second-order equation of motion for Q_{jk} is given by

$$\ddot Q_{jk}=\left[\frac{\dot N}{N}-\frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}}+\frac{N}{\sqrt{\det Q}}\left(\mathcal{L}_{\vec N}\frac{\sqrt{\det Q}}{N}\right)\right](\dot Q_{jk}-(\mathcal{L}_{\vec N}Q)_{jk})$$
$$+Q^{mn}(\dot Q_{mj}-(\mathcal{L}_{\vec N}Q)_{mj})(\dot Q_{nk}-(\mathcal{L}_{\vec N}Q)_{nk})$$
$$+Q_{jk}\left[-\frac{N^2\kappa}{2\sqrt{\det Q}}\;C+N^2\left(2\Lambda+\frac{\kappa}{2\lambda}v(\Xi)\right)\right]$$

$$+ N^2 \left[\frac{\kappa}{\lambda}\Xi_{,j}\Xi_{,k} - 2R_{jk}\right] + 2N(D_k D_k N)$$
$$+ 2(\mathcal{L}_{\vec{N}}\dot{Q})_{jk} + (\mathcal{L}_{\dot{\vec{N}}}Q)_{jk} - (\mathcal{L}_{\vec{N}}(\mathcal{L}_{\vec{N}}Q))_{jk} - \frac{NH\kappa}{\sqrt{\det Q}}G_{jkmn}N^m N^n. \tag{4.22}$$

This finishes our derivation of the (general) second-order equation of motion for Ξ and Q_{jk}, respectively.

4.4. Summary of second-order equations of motion

The second-order equations of motion for the (manifestly) gauge-invariant matter scalar field Ξ and the (manifestly) gauge-invariant three-metric Q_{jk} have the following form:

$$\ddot{\Xi} = \left[\frac{\dot{N}}{N} - \frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}} + \frac{N}{\sqrt{\det Q}}\left(\mathcal{L}_{\vec{N}}\frac{\sqrt{\det Q}}{N}\right)\right](\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi)$$
$$+ Q^{jk}\Xi_{,k}\left[\frac{N}{\sqrt{\det Q}}[N\sqrt{\det Q}]_{,j}\right] + N^2\left[\Delta\Xi + [Q^{jk}]_{,j}\Xi_{,k} - \frac{1}{2}\,v'(\Xi)\right]$$
$$+ 2(\mathcal{L}_{\vec{N}}\dot{\Xi}) + (\mathcal{L}_{\dot{\vec{N}}}\Xi) - (\mathcal{L}_{\vec{N}}(\mathcal{L}_{\vec{N}}\Xi)) \tag{4.23}$$

and

$$\ddot{Q}_{jk} = \left[\frac{\dot{N}}{N} - \frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}} + \frac{N}{\sqrt{\det Q}}\left(\mathcal{L}_{\vec{N}}\frac{\sqrt{\det Q}}{N}\right)\right]\left(\dot{Q}_{jk} - \left(\mathcal{L}_{\vec{N}}Q\right)_{jk}\right)$$
$$+ Q^{mn}(\dot{Q}_{mj} - (\mathcal{L}_{\vec{N}}Q)_{mj})(\dot{Q}_{nk} - (\mathcal{L}_{\vec{N}}Q)_{nk})$$
$$+ Q_{jk}\left[-\frac{N^2\kappa}{2\sqrt{\det Q}}\,C + N^2\left(2\Lambda + \frac{\kappa}{2\lambda}v(\Xi)\right)\right]$$
$$+ N^2\left[\frac{\kappa}{\lambda}\Xi_{,j}\Xi_{,k} - 2R_{jk}\right] + 2N(D_j D_k N)$$
$$+ 2(\mathcal{L}_{\vec{N}}\dot{Q})_{jk} + (\mathcal{L}_{\dot{\vec{N}}}Q)_{jk} - (\mathcal{L}_{\vec{N}}(\mathcal{L}_{\vec{N}}Q))_{jk} - \frac{NH\kappa}{\sqrt{\det Q}}G_{jkmn}N^m N^n. \tag{4.24}$$

The term $C = C_{\text{geo}} + C_{\text{matter}}$ occurring in the equation for $\ddot{Q}_{jk}$ has to be understood as a function of configuration and velocity variables and is explicitly given by

$$C_{\text{geo}} = \frac{1}{\kappa}\left[\frac{\sqrt{\det Q}}{4N^2}[G^{-1}]^{jkmn}(\dot{Q}_{jk} - (\mathcal{L}_{\vec{N}}Q)_{jk})(\dot{Q}_{mn} - (\mathcal{L}_{\vec{N}}Q)_{mn}) + \sqrt{\det Q}(2\Lambda - R)\right]$$
$$C_{\text{matter}} = \frac{1}{2\lambda}\left[\frac{\sqrt{\det Q}}{N^2}(\dot{\Xi} - \mathcal{L}_{\vec{N}}\Xi)^2 + \sqrt{\det Q}(Q^{jk}\Xi_{,j}\Xi_{,k} + v(\Xi))\right]. \tag{4.25}$$

Apart from the fact that we have a dynamical lapse function given by $N = C/H$, as well as a dynamical shift vector defined as $N_j = -C_j/H$, the only deviation from the standard Einstein equations in canonical form is the last term on the right-hand side of equation (4.24). This term, being quadratic in N_j and therefore quadratic in $C_j = C_j^{\text{geo}} + C_j^{\text{matter}}$, vanishes for instance when FRW spacetimes are considered. In our companion paper [16], we specialize these equations precisely to this context and show that the equations above reproduce the correct FRW equations.

5. Physical Hamiltonian, boundary term and ADM Hamiltonian

As long as the dust space $\mathcal{S}$ (and therefore $\mathcal{X}$) has no boundary, **H** is functionally differentiable, which we always assumed so far. However, for more general topologies we are forced to consider boundary conditions. In this section we show how to deal with asymptotically flat boundary conditions for illustrative purposes. More general situations can be considered analogously.

Recall [33] that asymptotically flat initial data are subject to the following boundary conditions:

$$\begin{aligned} q_{ab}(x) &= \delta_{ab} + \frac{f_{ab}(\Omega)}{r} + \mathcal{O}(r^{-2}), \qquad & p^{ab}(x) &= \frac{g^{ab}(\Omega)}{r} + \mathcal{O}(r^{-3}), \\ \xi(x) &= \frac{f(\Omega)}{r^2} + \mathcal{O}(r^{-3}), & \pi(x) &= \frac{g(\Omega)}{r^2} + \mathcal{O}(r^{-3}). \end{aligned} \tag{5.1}$$

Here, x^a is an asymptotic coordinate system, $r^2 \equiv \delta_{ab}x^a x^b$ and Ω denotes the angular dependence of the unit vector x^a/r (on the asymptotic sphere). The functions f_{ab}, f, g^{ab}, g are assumed to be smooth. Moreover, f_{ab} is an even function under reflection at spatial infinity on the sphere, while g^{ab} is odd (f, g do not underly parity restrictions). Note that these boundary conditions directly translate into analogous ones for the substitutions $Q_{jk} \leftrightarrow q_{ab}, P^{jk} \leftrightarrow p^{ab}, \Xi \leftrightarrow \xi, \Pi \leftrightarrow \pi$, because switching from $\mathcal{X}$ to $\mathcal{S}$ is just a diffeomorphism.

The part of the differential of $\mathbf{H}$ that gives rise to a boundary term is

$$\delta_{\text{boundary}}\mathbf{H} = \int_{\mathcal{S}} \mathrm{d}^3\sigma [N\delta_{\text{boundary}}C + N^j\delta_{\text{boundary}}C_j], \tag{5.2}$$

which coincides precisely with the boundary terms produced by the canonical Hamiltonian[32]

$$H_{\text{canonical}} = \int_{\mathcal{X}} \mathrm{d}^3x[nc + n^a c_a] \tag{5.3}$$

without dust. Here, the lapse and shift functions n, n^a are Lagrange multiplier rather than dynamical quantities like N, N^j. Therefore, the usual boundary terms [33] can be adopted once the asymptotic behaviour of the dynamical lapse and shift functions N, N^j have been determined, which, in turn, is completely specified by N_j because $N^j = Q^{jk}N_k, N = \sqrt{1 + Q^{jk}N_jN_k}$. The scalar field contribution to C, C_j decays as $1/r^4$; thus, it is sufficient to consider the geometrical contribution. $C_j^{\text{geo}} = -2D_kP_j^k$ decays as $1/r^3$ and is even asymptotically. The term quadratic in P^{jk} and the term quadratic in the Christoffel symbols in C^{geo} decay as $1/r^4$, while the term linear in the Cristoffel symbols decays as $1/r^3$ and is even. We conclude that $N_j = -\frac{C_j}{H}$ (with $H = \sqrt{C^2 - Q^{jk}C_jC_k}$) is asymptotically constant and even. The same is true for N, which is anyway bounded from below by unity. The usual computation [18, 33] yields

$$\begin{aligned} \delta_{\text{boundary}}\mathbf{H} &= -\delta B'(N) - \delta\vec{B}'(\vec{N}') \\ \kappa\delta B'(N) &= \int_{S^2} \sqrt{\det(Q)}Q^{jk}Q^{mn}[(D_jN)\,\mathrm{d}S_k\delta(Q_{mn} - \delta_{mn}) - (D_mN)\,\mathrm{d}S_n\delta(Q_{jk} - \delta_{jk})] \\ &\quad + \int_{S^2} \sqrt{\det(Q)}Q^{jk}N\left[-\mathrm{d}S_j\delta\Gamma^m_{mk} + S_k\delta\Gamma^k_{jk}\right] \\ \kappa\delta\vec{B}'(\vec{N}) &= 2\int_{S^2} \mathrm{d}S_j\; N^k\delta P^j_k, \end{aligned} \tag{5.4}$$

where $\mathrm{d}S_j = x^j/r\,\mathrm{d}\Omega$, with $\mathrm{d}\Omega$ the volume element of S^2. The prime is to indicate that, contrary to what the notation suggests, the terms shown are, *a priori*, not total differentials. In the usual formalism they are, because lapse and shift functions are Lagrange multipliers and do not depend on phase space. Here, however, they are dynamical and we must worry about the variation δN_j.

[32] With the substitutions $\mathcal{S} \leftrightarrow \mathcal{X}$, $Q_{jk} \leftrightarrow q_{ab}$, $P^{jk} \leftrightarrow p^{ab}$, $\Xi \leftrightarrow \xi$, $\Pi \leftrightarrow \pi$ implied.

It turns out that the boundary conditions need to be refined in order to make $\mathbf{H}$ differentiable. We will not analyse the most general boundary conditions in this paper, but just make a specific choice that will be sufficient for our purposes. Namely, we will impose in addition that $C_j^{\text{geo}} = -2D_k P_j^k$ decays as $1/r^{3+\epsilon}$ $(\epsilon > 0)$ at spatial infinity. Then also C_j falls off as $1/r^{3+\epsilon}$. Since C decays like $1/r^3$, it follows also that $H = \sqrt{C^2 - Q^{jk}C_jC_k}$ decays as $1/r^3$, whence $N_j = -C_j/H$ decays as $1/r^{\epsilon}$. This implies that δN_j decays as[33] $1/r^{\epsilon}$. Thus, $\delta N = [Q^{jk}N_k\delta N_j + N_jN_k\delta Q^{jk}/2]/N$ decays as[34] $1/r^{2\epsilon}$.

It follows that $\delta\vec{B}'(\vec{N}) = 0$ and

$$\kappa\delta B'(N) = \kappa\delta E_{\text{ADM}}, \qquad E_{\text{ADM}} = \int_{S^2} \sqrt{\det(Q)}Q^{jk}\left[-\mathrm{d}S_j\ \Gamma^m_{mk} + S_k\delta\Gamma^k_{jk}\right] \tag{5.5}$$

reduces to the variation of the ADM energy. The correct Hamiltonian is given by

$$\mathbf{H} = E_{\text{ADM}} + \int_{\mathcal{S}} \mathrm{d}^3\sigma\, H(\sigma). \tag{5.6}$$

It is reassuring that in the asymptotically flat context, we have automatically a boundary term in the Hamiltonian, which is just the ADM energy. The additional bulk term comes from the dust energy density and *does not vanish* on the constraint surface.

Before we close this section, let us also mention the physical Hamiltonian system under consideration there exists a Lagrangian from which derives by Legendre transformation on the phase space defined by the physical observables. Curiously, the corresponding effective action turns out to be non-local in dust space but local in dust time. It can be computed via a fixed point equation to any order in the spatial derivatives of the fields. Details can be found in appendix C.

6. Linear, manifestly gauge-invariant perturbation theory

In section 4 we derived the (manifestly) gauge-invariant second-order equation of motion for the scalar field Ξ and the three-metric Q_{jk}. Now we consider small perturbations around a given background whose corresponding quantities will be denoted by a bar, namely $\overline{\Xi}$, $\overline{Q}_{jk}$. The linear perturbations are then defined as $\delta\Xi := \Xi - \overline{\Xi}$ and $\delta Q_{jk} := Q_{jk} - \overline{Q}_{jk}$, respectively. Note that these perturbations are also (manifestly) gauge invariant because they are defined as a difference of two gauge-invariant quantities. Consequently, any power of $\delta\Xi$ and δQ_{jk} will also be a (manifestly) gauge-invariant quantity such that in the framework introduced in this paper gauge-invariant perturbation theory up to arbitrary order is not only possible, but also straightforward. This is a definite strength of our approach compared to the traditional one, see section 7 for a detailed discussion.

However, in this section we will restrict ourselves to linear (manifestly) gauge-invariant perturbation theory. That is any function $F(Q_{jk}, \Xi)$ will be expanded up to linear order in the perturbations $\delta\Xi$ and δQ_{jk}. We denote by δF the linear order term in the Taylor expansion of the expression $F(Q_{jk}, \Xi) - F(\overline{Q}_{jk}, \overline{\Xi})$. A calculation of higher order terms will be the content of a future publication. Usually, in cosmological perturbation theory one chooses an FRW background and considers small perturbations around it. Here we will derive the equations of motion for the linear perturbations assuming an arbitrary background. In our

[33] We could more generally have imposed that δN_j falls off like $1/r^{\epsilon}$ at spatial infinity.

[34] The choice $\epsilon = 1/2$ seems to be appropriate in order to reproduce the asymptotic Schwarzschild decay for dynamical lapse and shift. However, this is not the case here, because we are automatically in a freely falling (dust) frame and τ is proper time. Hence, $g_{\tau\tau} = -N^2 + Q^{jk}N_jN_k - 1$, whatever choice for N_j is made, it is independent of τ.

companion paper, we will specialize the results derived here to the case of an FRW background and show that we can reproduce the standard results as presented, e.g., in [7]. The reader who is only interested in the final form of the perturbed equation of motions should go directly to section 6.3, where a summary of the results is provided.

6.1. Derivation of the equation of motion for $\delta\Xi$

Let us go back to the second-order equation of motion for Ξ shown in equation (4.23). Since its perturbation involves several terms we will, for reasons of book keeping, split this equation into several parts and consider the perturbation of those parts separately. Comparing the equation of Ξ with the one for Q_{ij} in equation (4.24), we realize that in both equations the first term on the right-hand side includes an identical term, namely the expression in the square brackets. Therefore, it is convenient to derive its perturbation in a closed form such that the result can then also be used for the derivation of the equation of motion of δQ_{ij}. Throughout this section we will repeatedly need the perturbation of $\sqrt{\det Q}$ and its inverse, given by

$$\begin{aligned}\delta\sqrt{\det Q} &= \frac{1}{2}\sqrt{\det\overline{Q}}\;\overline{Q}^{ij}\delta Q_{ij}\\ \delta\left(\frac{1}{\sqrt{\det Q}}\right) &= -\frac{1}{2}\frac{1}{\sqrt{\det\overline{Q}}}\;\overline{Q}^{ij}\delta Q_{ij}.\end{aligned}\tag{6.1}$$

Next, considering the definition of the lapse functions given by $N = C/H$ and the definition of $H = \sqrt{C^2 - Q^{ij}C_iC_j}$ we obtain $N = \sqrt{1 + Q^{ij}N_iN_j}$. Thus, as mentioned before, N is not an independent variable, but can be expressed in terms of Q_{ij} and the shift vector, which itself is a function of the elementary variables Ξ, Q_{ij}. However, as shown in our companion paper [16], the perturbation of N_j is again a constant of motion, that is $\delta\dot{N}_j = 0$. For this reason it is convenient to work with δQ_{jk}, $\delta\Xi$ and δN_j, although, strictly speaking, δN_j is not an independent perturbation. Keeping this in mind the perturbation of N yields

$$\delta N = \left[-\frac{\overline{N}}{2}\left(\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right]\delta Q_{jk} + \left[\overline{N}\frac{\overline{N}^j}{\overline{N}^2}\right]\delta N_j.\tag{6.2}$$

From the explicit form of δN and $\delta\sqrt{\det Q}$ we can derive the following expressions which we will need below:

$$\begin{aligned}\delta\left(\frac{\dot{N}}{N}\right) &= \left[-\frac{\partial}{\partial\tau}\frac{1}{2}\left(\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right]\delta Q_{jk} + \left[\left(\frac{\overline{N}^j}{\overline{N}^2}\right)^{\cdot}\;\right]\delta N_j\\ \delta\left(-\frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}}\right) &= \left[-\frac{\partial}{\partial\tau}\frac{1}{2}\overline{Q}^{jk}\right]\delta Q_{jk}.\end{aligned}\tag{6.3}$$

Here the derivative with respect to τ is understood to act on everything to its right, including the perturbations. We also used that δN_j is a constant of motion, so the term proportional to $\delta\dot{N}_j$ does not contribute. In order to calculate the perturbation of the Lie derivative term occurring in the square brackets in equation (4.23), we compute

$$\begin{aligned}\delta\left(\frac{N}{\sqrt{\det Q}}\right) &= \left[-\left(\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\right)\frac{1}{2}\left(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right]\delta Q_{jk} + \left[\frac{\overline{N}^j}{\overline{N}^2}\right]\delta N_j\\ \delta\left(\frac{\sqrt{\det Q}}{N}\right) &= \left[\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\frac{1}{2}\left(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right]\delta Q_{jk} + \left[-\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\frac{\overline{N}^j}{\overline{N}^2}\right]\delta N_j.\end{aligned}\tag{6.4}$$

The Lie derivative term then yields

$$\delta\left(\left(\mathcal{L}_{\vec{N}}\frac{\sqrt{\det Q}}{N}\right)\right)=\left[\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\frac{1}{2}\left(\overline{Q}^{jk}+\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right)\right]\delta Q_{jk}$$
$$+\left[-\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\left(\frac{\overline{N}^j}{\overline{N}^2}\right)\right]\delta N_j+\left(\mathcal{L}_{\delta\vec{N}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right). \tag{6.5}$$

Similar to the τ-derivative, the Lie derivative $\mathcal{L}_{\vec{\overline{N}}}$ acts on all terms to its right, including the linear perturbations. For the moment we keep the Lie derivative with respect to $\delta\vec{N}$ in the compact form above. At a later stage we will write down these terms explicitly and express them in terms of δQ_{jk} and δN_j. Having calculated the variations of all components of the first square bracket in equation (4.23), we can now give the final result:

$$\delta\left[\frac{\dot{N}}{N}-\frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}}+\frac{N}{\sqrt{\det Q}}\left(\mathcal{L}_{\vec{N}}\frac{\sqrt{\det Q}}{N}\right)\right]$$
$$=\left[-\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{1}{2}\left(\overline{Q}^{jk}+\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right)\right]\delta Q_{jk}$$
$$+\left[\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\frac{\overline{N}^j}{\overline{N}^2}\right]\delta N_j+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\delta\vec{N}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right). \tag{6.6}$$

The last term in this equation can be written explicitly in terms of δQ_{mn} and δN_m as

$$\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\delta\vec{N}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)=\left[-\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^m}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{jm}\overline{N}^k\right)\right]\delta Q_{jk}$$
$$+\left[\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^k}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{jk}\right)\right]\delta N_j. \tag{6.7}$$

As the terms in equation (6.6) are multiplied by $(\dot{\Xi}-(\mathcal{L}_{\vec{N}}\Xi))$ in equation (4.23), we also need the perturbation of the latter term. It is given by

$$\delta(\dot{\Xi}-(\mathcal{L}_{\vec{N}}\Xi))=\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\delta\Xi-(\mathcal{L}_{\delta\vec{N}}\overline{\Xi}). \tag{6.8}$$

Next we determine the perturbation of $Q^{jk}\Xi_{,k}$ which enters the second term on the right-hand side of equation (4.23):

$$\delta(Q^{jk}\Xi_{,k})=[-\overline{Q}^{jm}\overline{Q}^{kn}\Xi_{,k}]\delta Q_{mn}+\left[\overline{Q}^{jk}\frac{\partial}{\partial x^k}\right]\delta\Xi. \tag{6.9}$$

The perturbation of the term that is multiplied with $Q^{jk}\Xi_{,k}$ yields

$$\delta\left[\frac{N}{\sqrt{\det Q}}(N\sqrt{\det Q})_{,j}\right]=\left[-\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{1}{2}\left(\overline{Q}^{jk}+\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)[\overline{N}\sqrt{\det\overline{Q}}]_{,j}\right.$$
$$\left.+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^j}\left(\frac{1}{2}\left(\overline{Q}^{jk}-\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\overline{N}\sqrt{\det\overline{Q}}\right)\right]\delta Q_{jk}$$
$$+\left[\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\overline{N}^j}{\overline{N}^2}\left[\overline{N}\sqrt{\det\overline{Q}}\right]_{,j}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^j}\left(\frac{\overline{N}^j}{\overline{N}^2}\overline{N}\sqrt{\det\overline{Q}}\right)\right]\delta N_j. \tag{6.10}$$

We will split the third term occurring on the right-hand side of equation (4.23) into N^2 and the remaining part given by $(\Delta\Xi + [Q^{jk}]_{,j}\Xi_{,k} - \frac{1}{2}v'(\Xi))$. Their respective perturbations are

$$\delta N^2 = 2\overline{N}\delta N = [-\overline{N}^j\overline{N}^k]\delta Q_{jk} + [2\overline{N}^j]\delta N_j$$
$$\delta\left(\Delta\Xi + [Q^{jk}]_{,j}\Xi_{,k} - \frac{1}{2}v'(\Xi)\right) = \left[-\frac{\partial}{\partial x^n}(\overline{Q}^{jm}\overline{Q}^{kn}\Xi_{,m})\right]\delta Q_{jk}$$
$$+\left[\Delta + [\overline{Q}^{mn}]_{,n}\frac{\partial}{\partial x^m} - \frac{1}{2}v''(\overline{\Xi})\right]\delta\Xi. \tag{6.11}$$

Finally, we have to calculate the perturbation of the last three terms in equation (4.23), involving Lie derivatives of Ξ and $\dot{\Xi}$, respectively. We obtain

$$\delta(2(\mathcal{L}_{\vec{N}}\dot{\Xi}) + (\mathcal{L}_{\dot{\vec{N}}}\Xi) - (\mathcal{L}_{\vec{N}}(\mathcal{L}_{\vec{N}}\Xi))) = \left[\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \frac{\partial}{\partial\tau}\mathcal{L}_{\vec{\overline{N}}}\right]\delta\Xi$$
$$+\left(\mathcal{L}_{\delta N}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\mathcal{L}_{\delta N}\right)[\overline{\Xi}]. \tag{6.12}$$

Adding up all the contributions and factoring out the linear perturbations $\delta\Xi$, δQ_{jk} and δN_j, we can rewrite the second-order EOM as

$$\delta\ddot{\Xi} = \left[\left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}} + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\right.$$
$$+\overline{Q}^{jk}\left[\frac{\overline{N}}{\sqrt{\det\overline{Q}}}(\overline{N}\sqrt{\det\overline{Q}})_{,j}\right]\frac{\partial}{\partial x^k}$$
$$\left.+\overline{N}^2\left(\Delta + [\overline{Q}^{mn}]_{,n}\frac{\partial}{\partial x^m} - \frac{1}{2}v''(\overline{\Xi})\right) + \left(\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \frac{\partial}{\partial\tau}\mathcal{L}_{\vec{\overline{N}}}\right)\right]\delta\Xi$$
$$+\left[-(\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\left[\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{1}{2}\left(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right)\right.\right.$$
$$\left.+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^m}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{jm}\overline{N}^k\right)\right] - \overline{Q}^{jm}\overline{Q}^{kn}\overline{\Xi}_{,n}\left[\frac{\overline{N}}{\sqrt{\det\overline{Q}}}(\overline{N}\sqrt{\det\overline{Q}})_{,m}\right]$$
$$+\left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}} + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right](\overline{Q}^{jm}\overline{\Xi}_{,m}\overline{N}^k)$$
$$+(\overline{Q}^{mn}\overline{\Xi}_{,n})\left(-\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{1}{2}(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2})[\overline{N}\sqrt{\det\overline{Q}}]_{,m}\right.$$
$$\left.+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^m}\left(\frac{1}{2}\left(\overline{Q}^{jk} - \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\overline{N}\sqrt{\det\overline{Q}}\right)\right)$$
$$-\overline{N}^2\left(\Delta\overline{\Xi} + [\overline{Q}^{mn}]_{,m}\overline{\Xi}_{,n} - \frac{1}{2}v'(\overline{\Xi})\right)\left(\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right) - \overline{N}^2\frac{\partial}{\partial x^n}(\overline{Q}^{jm}\overline{Q}^{kn}\overline{\Xi}_{,m})$$
$$\left.-\overline{Q}^{jm}\overline{Q}^{kn}\overline{N}_m[\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})]_{,n} - \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)(\overline{Q}^{jm}\overline{Q}^{kn}\overline{N}_m\overline{\Xi}_{,n})\right]\delta Q_{jk}$$
$$+\left[(\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\left[\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\frac{\overline{N}^j}{\overline{N}^2} + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^k}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{jk}\right)\right]\right.$$

$$
\begin{aligned}
&+2\overline{N}^2\left(\Delta\overline{\Xi}+[\overline{Q}^{mn}]_{,m}\overline{\Xi}_{,n}-\frac{1}{2}v'(\overline{\Xi})\right)\frac{\overline{N}^j}{\overline{N}^2}\\
&+(\overline{Q}^{mn}\overline{\Xi}_{,n})\left(\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\overline{N}^j}{\overline{N}^2}[\overline{N}\sqrt{\det\overline{Q}}]_{,m}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^j}\left(\frac{\overline{N}^j}{\overline{N}^2}\overline{N}\sqrt{\det\overline{Q}}\right)\right)\\
&-\left[\frac{\dot{\overline{N}}}{\overline{N}}-\frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right](\overline{Q}^{jk}\overline{\Xi}_{,k})\\
&+\overline{Q}^{jk}[\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})]_{,k}+\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)(\overline{Q}^{jk}\overline{\Xi}_{,k})\Bigg]\delta N_j.
\end{aligned}
\tag{6.13}
$$

Here we used that the last term occurring in equation (4.23), which involves the Lie derivative with respect to $\delta\vec{N}$, can again be expressed in terms of the perturbations δQ_{jk} and δN_j, explicitly given by

$$
\begin{aligned}
&\left(\mathcal{L}_{\delta N}\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)+\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\mathcal{L}_{\delta N}\right)[\overline{\Xi}]\\
&\quad=\left[\overline{Q}^{jk}[\dot{\Xi}-(\mathcal{L}_{\vec{\overline{N}}}\Xi)]_{,k}+\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)(\overline{Q}^{jk}\Xi_{,k})\right]\delta N_j\\
&\quad\times\left[-\overline{Q}^{jm}\overline{Q}^{kn}\overline{N}_m[\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})]_{,n}-\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)(\overline{Q}^{jm}\overline{Q}^{kn}\overline{N}_m\overline{\Xi}_{,n})\right]\delta Q_{jk}.
\end{aligned}
\tag{6.14}
$$

Analogously, the last term on the right-hand side of equation (6.6), which also involves a Lie derivative with respect to $\delta\vec{N}$, can be expressed as

$$
\begin{aligned}
\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\delta\vec{N}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)&=\left[-\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^m}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{jm}\overline{N}^k\right)\right]\delta Q_{jk}\\
&\quad+\left[\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^k}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{jk}\right)\right]\delta N_j.
\end{aligned}
\tag{6.15}
$$

Moreover $(\mathcal{L}_{\delta\vec{N}}\overline{\Xi})$ occurring in equation (6.8) is given by

$$
(\mathcal{L}_{\delta\vec{N}}\overline{\Xi})=[-\overline{Q}^{jm}\overline{\Xi}_{,m}\overline{N}^k]\delta Q_{jk}+[\overline{Q}^{jk}\,\Xi_{,k}]\delta N_j.
\tag{6.16}
$$

We would like to emphasize again that the partial and Lie derivatives act on everything to their right and therefore also on the perturbations. That is the reason why for instance $\delta\dot{\Xi}$ and $\delta\dot{Q}_{jk}$ have not been factored out separately. This finishes our derivation of the second-order equation of motion for the scalar field perturbation $\delta\Xi$. In the next section we will discuss the corresponding equation for the metric perturbation δQ_{jk}.

6.2. Derivation of the equation of motion for δQ_{jk}

Similar to the derivation of the second-order equation of motion for $\delta\Xi$ we will also split the equation for $\ddot{Q}_{jk}$ in equation (4.24) into several terms whose perturbations are then considered separately. More precisely, we will split the equation into seven separate terms, with the three terms involving Lie derivatives in the last line counted as one. Starting with the first term on the right-hand side, we recall that the perturbation of the sum of terms in the square brackets has already been computed during the derivation of the equation for $\delta\ddot{\Xi}$. Thus, we can take over those results, as shown in equation (6.6). The perturbation of the term $(\dot{Q}_{jk} - (\mathcal{L}_{\vec{N}}Q)_{jk})$ is given by

$$\delta(\dot{Q}_{jk} - (\mathcal{L}_{\vec{N}}Q)_{jk}) = \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\delta Q_{jk} - (\mathcal{L}_{\delta N}\overline{Q})_{jk}, \tag{6.17}$$

whereby

$$\begin{aligned}(\mathcal{L}_{\delta N}Q)_{jk} = &\left[-\overline{Q}^{mr}\overline{N}^{n}[Q_{jk}]_{,r} - \overline{Q}_{km}\frac{\partial}{\partial x^{j}}(\overline{Q}^{mr}\overline{N}^{n}) - \overline{Q}_{jm}\frac{\partial}{\partial x^{k}}(\overline{Q}^{mr}\overline{N}^{n})\right]\delta Q_{mn}\\ &+\left[\overline{Q}^{mn}[Q_{jk}]_{,n} + \overline{Q}_{kn}\frac{\partial}{\partial x^{j}}(\overline{Q}^{mn}) + \overline{Q}_{jn}\frac{\partial}{\partial x^{k}}(\overline{Q}^{mn})\right]\delta N_{m}.\end{aligned} \tag{6.18}$$

Consequently, we have all ingredients needed for the perturbation of the first term. However, we will not present the final expression in the main text since it is quite lengthly. Nevertheless, the interested reader can find the explicit form in appendix G in equation (6.17). The perturbation of the second term on the right-hand side yields

$$\begin{aligned}&\delta(Q^{mn}(\dot{Q}_{mj} - (\mathcal{L}_{\vec{N}}Q)_{mj})(\dot{Q}_{nk} - (\mathcal{L}_{\vec{N}}Q)_{nk}))\\ &\quad= [-\overline{Q}^{mr}\overline{Q}^{ns}(\dot{\overline{Q}}_{rj} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{rj})(\dot{\overline{Q}}_{sk} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{sk})]\delta Q_{mn}\\ &\qquad+\left[2\overline{Q}^{mn}(\dot{\overline{Q}}_{n(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{n(k})\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\right]\delta Q_{j)m}\\ &\qquad+\left[-2\overline{Q}^{mn}(\dot{\overline{Q}}_{n(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{n(k})\right](\mathcal{L}_{\delta N}\overline{Q})_{j)m}.\end{aligned} \tag{6.19}$$

The perturbation of the third term occurring on the right-hand side requires a bit more work, because it involves $C = C^{\rm geo} + C^{\rm matter}$. Thus we will perform this calculation in two steps. First we will ignore the explicit form of δC in terms of $\delta Q_{jk}, \delta\Xi$ and δN_j. The resulting expression looks like

$$\begin{aligned}&\delta\left(Q_{jk}\left[-\frac{N^2\kappa}{2\sqrt{\det Q}}C + N^2\left(2\Lambda + \frac{\kappa}{2\lambda}v(\Xi)\right)\right]\right)\\ &\quad=\left[\overline{Q}_{jk}\left[\frac{1}{2}\left(\overline{Q}^{mn} + \frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)\frac{\kappa\overline{N}^2}{2\sqrt{\det\overline{Q}}}\overline{C} + \frac{\overline{N}^m\overline{N}^n}{2\overline{N}^2}\overline{N}^2\right.\right.\\ &\qquad\left.\left.\times\left(\frac{\kappa}{2\sqrt{\det\overline{Q}}}\overline{C} - 2\left(2\Lambda + \frac{\kappa}{2\lambda}v(\Xi)\right)\right)\right]\right]\delta Q_{mn}\\ &\qquad+\left[\overline{N}^2\left(-\frac{\kappa}{2\sqrt{\det\overline{Q}}}\overline{C} + 2\Lambda + \frac{\kappa}{2\lambda}v(\overline{\Xi})\right)\right]\delta Q_{jk}\\ &\qquad+\left[2\overline{Q}_{jk}\overline{N}^2\left(-\frac{\kappa}{2\sqrt{\det\overline{Q}}}\overline{C} + 2\Lambda + \frac{\kappa}{2\lambda}v(\overline{\Xi})\right)\left(\frac{\overline{N}^m}{\overline{N}^2}\right)\right]\delta N_m\\ &\qquad+\left[-\overline{Q}_{jk}\overline{N}^2\frac{\kappa}{2\sqrt{\det\overline{Q}}}\right]\delta C + \left[\overline{Q}_{jk}\overline{N}^2\frac{\kappa}{2\lambda}v'(\overline{\Xi})\right]\delta\Xi.\end{aligned} \tag{6.20}$$

Due to its length, the explicit calculation of δC can be found in appendix G. However, when actually inserting the expression of δC into equation (6.20), some of the terms in the expression for δC cancel with existing terms in equation (6.20). As a result, the final expression for the perturbation of the third term in equation (6.21) is slightly less involved. It is given by

$$\delta\left(Q_{jk}\left[-\frac{N^2\kappa}{2\sqrt{\det Q}}\,C+N^2\left(2\Lambda+\frac{\kappa}{2\lambda}v(\Xi)\right)\right]\right)$$
$$=\Bigg[-\overline{Q}_{jk}\Bigg(\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\overline{N}^2\Big(2\Lambda-\overline{R}\frac{\kappa}{2\lambda}(v(\overline{\Xi})-\overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s})\Big)+\frac{\overline{N}^2}{2}(\overline{R}^{mn}-[\overline{G}^{-1}]^{mnrs}\overline{D}_r\overline{D}_s)$$
$$+\frac{\kappa}{2\lambda}\overline{Q}^{mr}\overline{Q}^{ns}(\dot{\Xi}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{N}_r\overline{\Xi}_{,s}-\frac{\kappa\overline{N}^2}{2\lambda}\overline{Q}^{rm}\overline{Q}^{sn}\overline{\Xi}_{,r}\overline{\Xi}_{,s}+\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{rs})$$
$$\times\left[[\overline{G}^{-1}]^{mnrs}\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)-(\dot{\overline{Q}}_{tu}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{tu})\overline{Q}^{sn}[\overline{G}^{-1}]^{turm}\right]$$
$$+\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsvw}\left[\overline{Q}^{mt}\overline{N}^n[\overline{Q}_{vw}]_{,t}+2\overline{Q}_{tw}\frac{\partial}{\partial x^v}(\overline{Q}^{mt}\overline{N}^n)\right]\Bigg)\Bigg]\delta Q_{mn}$$
$$\times\Bigg[-\overline{Q}_{jk}\Bigg(-\frac{\overline{N}^m}{\overline{N}^2}\overline{N}^2\left(2\Lambda-\overline{R}-\frac{\kappa}{2\lambda}(v(\overline{\Xi})-\overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s})\right)-\frac{\kappa}{2\lambda}(\dot{\Xi}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{Q}^{mn}\overline{\Xi}_{,n}$$
$$-\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsvw}\left[\overline{Q}^{mt}[\overline{Q}_{vw}]_{,t}+2\overline{Q}_{tw}\frac{\partial}{\partial x^v}(\overline{Q}^{mt})\right]\Bigg)\delta N_m$$
$$+\left[-\overline{Q}_{jk}\left(\frac{\overline{N}^2\kappa}{2\lambda}\left(\frac{1}{\overline{N}^2}(\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)+\overline{Q}^{mn}\overline{\Xi}_{,n}\frac{\partial}{\partial x^m}-\frac{1}{2}v'(\overline{\Xi})\right)\right)\right]\delta\Xi$$
$$+\left[\overline{N}^2\left(-\frac{\kappa}{2\sqrt{\det\overline{Q}}}\overline{C}+2\Lambda+\frac{\kappa}{2\lambda}v(\overline{\Xi})\right)\right]\delta Q_{jk}. \tag{6.21}$$

Proceeding with the next term on the right-hand side of equation (4.24), we obtain for its perturbation the following result:

$$\delta\left(N^2\left(\frac{\kappa}{\lambda}\Xi_{,j}\Xi_{,k}-2R_{jk}\right)\right)=\left[\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\left(-2\overline{N}^2\left(\frac{\kappa}{\lambda}\overline{\Xi}_{,j}\overline{\Xi}_{,k}-2\overline{R}_{jk}\right)\right)+\overline{N}^2\overline{D}_j\overline{D}_k\overline{Q}^{mn}\right]\delta Q_{mn}$$
$$+[\overline{N}^2\overline{D}_m\overline{D}_n\overline{Q}^{mn}]\delta Q_{jk}+[-2\overline{N}^2\overline{D}_n\overline{D}_{(k}\overline{Q}^{mn}]\delta Q_{j)m}$$
$$+\left[\frac{\overline{N}^m}{\overline{N}^2}\left(2\overline{N}^2\left(\frac{\kappa}{\lambda}\overline{\Xi}_{,j}\overline{\Xi}_{,k}-2\overline{R}_{jk}\right)\right)\right]\delta N_m+\left[4\overline{N}^2\frac{\kappa}{\lambda}\overline{\Xi}_{(,k}\frac{\partial}{\partial x^{j)}}\right]\delta\Xi. \tag{6.22}$$

For this calculation we used the fact that the perturbation of the Ricci tensor can be expressed in terms of the perturbations δQ_{jk}. The explicit relation reads

$$\delta R_{jk}=\left[-\frac{1}{2}\overline{D}_m\overline{D}_n\overline{Q}^{mn}\right]\delta Q_{jk}+\left[-\frac{1}{2}\overline{D}_j\overline{D}_k\overline{Q}^{mn}\right]\delta Q_{mn}+[\overline{D}_n\overline{D}_{(k}\overline{Q}^{mn}]\delta Q_{j)m}. \tag{6.23}$$

The next term in equation (4.24) includes covariant derivatives. Therefore we will have to consider the perturbation of the Christoffel symbols Γ^m_{jk}. These can again be written in terms of metric perturbations as shown below:

$$\delta\Gamma^m_{jk}=\frac{\overline{Q}^{mn}}{2}((\overline{D}_j\delta Q_{nk})+(\overline{D}_k\delta Q_{jn})-(\overline{D}_n\delta Q_{jk})). \tag{6.24}$$

Using this we end up with

$$\begin{aligned}\delta(2ND_jD_kN) &= \left[\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}(-4\overline{N}(\overline{D}_j\overline{D}_k\overline{N})) - 2\overline{N}^2\overline{D}_j\overline{D}_k\left(\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)\right]\delta Q_{mn} \\ &\quad + \left[\frac{\overline{N}^m}{\overline{N}^2}(4\overline{N}(\overline{D}_j\overline{D}_k\overline{N})) + 2\overline{N}^2\overline{D}_j\overline{D}_k\left(\frac{\overline{N}^m}{\overline{N}^2}\right)\right]\delta N_m \\ &\quad + [2\overline{N}(\overline{D}_n\overline{N})\overline{D}_{(k}\overline{Q}^{mn}]\delta Q_{j),m} + [-\overline{N}^2(\overline{D}_n\overline{N})\overline{D}_m\overline{Q}^{mn}]\delta Q_{jk}. \end{aligned} \tag{6.25}$$

Note that covariant derivatives surrounded by round bracket such as $(D_jD_k\ldots)$ act on the elements inside the round brackets only. By contrast, covariant derivatives not surrounded by round brackets act on everything to their right, including also the perturbations.

Next we deal with the three terms on the right-hand side of equation (4.24) that include Lie derivatives with respect to $\delta\vec{N}$. Those Lie derivatives are again functions of $\delta Q_{jk}, \delta N_j$, and partial derivatives thereof, because we have $\delta N^m = -\overline{Q}^{mr}\overline{Q}^{ns}\overline{N}_s\delta Q_{rn} + \overline{Q}^{mn}\delta N_n$. In this section, however, we will work with the following compact form only:

$$\begin{aligned}\delta(2(\mathcal{L}_{\vec{N}}\dot{Q})_{jk} + (\mathcal{L}_{\dot{\vec{N}}}Q)_{jk} - (\mathcal{L}_{\vec{N}}(\mathcal{L}_{\vec{N}}Q))_{jk}) &= \left[\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \frac{\partial}{\partial\tau}\mathcal{L}_{\vec{\overline{N}}}\right]\delta Q_{jk} \\ &\quad + \left(\mathcal{L}_{\delta N}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\mathcal{L}_{\delta N}\right)[\overline{Q}_{jk}]. \end{aligned} \tag{6.26}$$

In the next section, we will rewrite the second-order equation of motion in a more concise form, using coefficient functions. That will allow us to include the Lie derivative term with respect to $\delta\vec{N}$ in the following, more explicit form:

$$\begin{aligned}&\left(\mathcal{L}_{\delta N}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\mathcal{L}_{\delta N}\right)[\overline{Q}_{jk}] = \Bigg[-\overline{Q}^{mr}\overline{N}^n[\dot{\overline{Q}}_{jk} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk}]_{,r} \\ &\quad - (\dot{\overline{Q}}_{km} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{kr})\frac{\partial}{\partial x^j}(\overline{Q}^{mr}\overline{N}^n) - (\dot{\overline{Q}}_{jm} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jr})\frac{\partial}{\partial x^k}(\overline{Q}^{mr}\overline{N}^n) \\ &\quad + \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\left(-\overline{Q}^{mr}\overline{N}^n[Q_{jk}]_{,r} - \overline{Q}_{km}\frac{\partial}{\partial x^j}(\overline{Q}^{mr}\overline{N}^n) - \overline{Q}_{jm}\frac{\partial}{\partial x^k}(\overline{Q}^{mr}\overline{N}^n)\right)\Bigg]\delta Q_{mn} \\ &\quad + \Bigg[\overline{Q}^{mn}[\dot{\overline{Q}}_{jk} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk}]_{,n} + (\dot{\overline{Q}}_{kn} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{kn})\frac{\partial}{\partial x^j}(\overline{Q}^{mn}) + (\dot{\overline{Q}}_{jn} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jn})\frac{\partial}{\partial x^k}(\overline{Q}^{mn}) \\ &\quad + \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\left(\overline{Q}^{mn}[Q_{jk}]_{,n} + \overline{Q}_{kn}\frac{\partial}{\partial x^j}(\overline{Q}^{mn}) + \overline{Q}_{jn}\frac{\partial}{\partial x^k}(\overline{Q}^{mn})\right)\Bigg]\delta N_m. \end{aligned} \tag{6.27}$$

Another term which includes Lie derivatives with respect to $\delta\vec{N}$ appeared previously as part of equation (6.19). Performing the Lie derivative also in this case, we end up with

$$\begin{aligned}&[-2\overline{Q}^{mn}(\dot{Q}_{n(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{n(k})](\mathcal{L}_{\delta N}Q)_{j)m} = \Bigg[(-2\overline{Q}^{tu}(\dot{\overline{Q}}_{t(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{t(k})) \\ &\quad \times \left(-\overline{Q}^{mr}\overline{N}^n[\overline{Q}_{j)u}]_{,r} - \overline{Q}_{um}\frac{\partial}{\partial x^{j)}}(\overline{Q}^{mr}\overline{N}^n) - \overline{Q}_{j)m}\frac{\partial}{\partial x^u}(\overline{Q}^{mr}\overline{N}^n)\right)\Bigg]\delta Q_{mn} \\ &\quad \times \Bigg[(-2\overline{Q}^{tu}(\dot{Q}_{t(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{t(k})) \Bigg(\overline{Q}^{mn}[\overline{Q}_{j)u}]_{,n} + \overline{Q}_{un}\frac{\partial}{\partial x^{j)}} \\ &\quad \times (\overline{Q}^{mn}) + \overline{Q}_{j)n}\frac{\partial}{\partial x^u}(\overline{Q}^{mn})\Bigg)\Bigg]\delta N_m. \end{aligned} \tag{6.28}$$

The other two terms that include Lie derivatives with respect to $\delta\vec{N}$ are parts of the perturbation of the first term. Their explicit expressions are given in equations (6.7) and (6.18), respectively. Note that these terms are written out explicitly in appendix G, where the final form of the perturbation of the first term is calculated.

Finally, we consider the last remaining term from equation (4.24). It involves the Hamiltonian density H, which we found out to be a constant of motion in section 3.4. In our companion paper [16] we show that also δN_j and δH are constants of motion. Therefore, in complete analogy with the case of δN_j, we will factor out δH. We thus obtain

$$\begin{aligned}\delta\left(-\frac{N\kappa}{\sqrt{\det Q}}HG_{jkmn}N^mN^n\right) &= \left[-\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{N}^n\overline{N}^m\overline{G}_{jkmn}\right]\delta H \\ &+\left[-\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HQ}^{rm}\overline{N}^n\overline{N}^s\overline{G}_{snr(k}\right]\delta Q_{j)m} \\ &+\left[\frac{1}{2}\left(\overline{Q}^{mn}+\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HN}^r\overline{N}^s\overline{G}_{jkrs}\right. \\ &\left.+\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HQ}^{sm}\overline{N}^r\overline{N}^n\overline{G}_{jkrs}\right]\delta Q_{mn}+\left[-\frac{\overline{N}^m}{\overline{N}^2}\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HN}^r\overline{N}^s\overline{G}_{jkrs}\right]\delta N_m.\end{aligned} \tag{6.29}$$

Here we used that

$$\delta G_{jkmn}=-G_{jkrs}G_{mntu}\delta[G^{-1}]^{rstu}. \tag{6.30}$$

Now we have finally derived all the individual parts that are needed in order to write down the equation of motion for δQ_{jk}. However, by just looking at the various individual terms, it is clear that they are already considerably more complicated than for the corresponding case of the matter equation of motion for $\delta\Xi$. Nevertheless, we decided to present the final equation in detailed form on the next page, in particular to convey a sense of how much more involved the geometrical part of the perturbed equations is compared to the matter part. In the next section we will rewrite both equations of motion, the one for $\delta\Xi$ as well as the one for δQ_{jk}, in a more transparent form where all the complicated background coefficients in front of the perturbations are hidden in certain coefficient functions. In our companion paper, we will then specialize those coefficient functions to the case of an FRW spacetime and show that the general equations derived in the last two subsection are (up to small correction caused by our dust clock) in agreement with the well-known perturbation equations as discussed, e.g., in [7]. Note that we still kept the compact form of the Lie derivative with respect to δN in equation (6.31), because we wanted to present this equation on one page only:

$$\begin{aligned}\delta\ddot{Q}_{jk} = \Bigg[&-\overline{Q}_{jk}\left(\frac{\overline{N}^2\kappa}{2\lambda}\left(\frac{1}{\overline{N}^2}(\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\right.\right. \\ &\left.\left.+\overline{Q}^{mn}\overline{\Xi}_{,n}\frac{\partial}{\partial x^m}-\frac{1}{2}v'(\overline{\Xi})\right)\right)+\left(4\overline{N}^2\frac{\kappa}{\lambda}\overline{\Xi}_{(,k}\frac{\partial}{\partial x^{j)}}\right)\Bigg]\delta\Xi \\ &\times\left[\left[\frac{\dot{\overline{N}}}{\overline{N}}-\frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\right. \\ &\times\left(\overline{Q}^{rn}\overline{N}_n[\overline{Q}_{jk}]_{,r}+\overline{Q}_{rk}\frac{\partial}{\partial x^j}(\overline{Q}^{rn}\overline{N}^m)+\overline{Q}_{rj}\frac{\partial}{\partial x^k}(\overline{Q}^{rn}\overline{N}^m)\right)\end{aligned}$$

$$
\begin{aligned}
&-(\dot{\overline{Q}}_{jk}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk})\left(\left(\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{1}{2}\left(\overline{Q}^{mn}+\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)\right)+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^k}\right.\right.\\
&\left.\left.\times\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{N}^m\overline{Q}^{rn}\right)\right)\right)+(-\overline{Q}^{mr}\overline{Q}^{ns}(\dot{\overline{Q}}_{rj}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{rj})(\dot{\overline{Q}}_{sk}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{sk}))\\
&+\left(-\overline{Q}_{jk}\left[\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\overline{N}^2\left(2\Lambda-\overline{R}+\frac{\kappa}{2\lambda}(v(\overline{\Xi})-\overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s})\right)\right.\right.\\
&+\frac{\overline{N}^2}{2}(\overline{R}^{mn}-[\overline{G}^{-1}]^{mnrs}\overline{D}_r\overline{D}_s)+\frac{\kappa}{2\lambda}\overline{Q}^{mr}\overline{Q}^{ns}(\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{N}_r\overline{\Xi}_{,s}\\
&-\frac{\kappa\overline{N}^2}{2\lambda}\overline{Q}^{rm}\overline{Q}^{sn}\overline{\Xi}_{,r}\overline{\Xi}_{,s}+\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{rs})\\
&\times\left[[\overline{G}^{-1}]^{mnrs}\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)-(\dot{\overline{Q}}_{tu}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{tu})\overline{Q}^{sn}[\overline{G}^{-1}]^{turm}\right]\\
&\left.\left.+\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsvw}\left[\overline{Q}^{mt}\overline{N}^n[\overline{Q}_{vw}]_{,t}+2\overline{Q}_{tw}\frac{\partial}{\partial x^v}(\overline{Q}^{mt}\overline{N}^n)\right]\right]\right)\\
&+\left(\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\left(-2\overline{N}^2\left(\frac{\kappa}{\lambda}\overline{\Xi}_{,j}\overline{\Xi}_{,k}-2\overline{R}_{jk}\right)-4\overline{N}(\overline{D}_j\overline{D}_k\overline{N})\right)\right.\\
&\left.+\overline{N}^2\overline{D}_j\overline{D}_k\overline{Q}^{mn}-2\overline{N}^2\overline{D}_j\overline{D}_k\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)+\left(\frac{1}{2}\left(\overline{Q}^{mn}+\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)\right.\\
&\left.\left.\times\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{H}\overline{N}^r\overline{N}^s\overline{G}_{jkrs}+\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{H}\overline{Q}^{sm}\overline{N}^r\overline{N}^n\overline{G}_{jkrs}\right)\right]\delta Q_{mn}\\
&+\left[-\left[\frac{\dot{\overline{N}}}{\overline{N}}-\frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\right.\\
&\times\left(\overline{Q}^{mn}[\overline{Q}_{jk}]_{,n}+\overline{Q}_{nk}\frac{\partial}{\partial x^j}(\overline{Q}^{mn})+\overline{Q}_{nj}\frac{\partial}{\partial x^k}(\overline{Q}^{mn})\right)\\
&+(\dot{\overline{Q}}_{jk}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk})\left(\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{\overline{N}^m}{\overline{N}^2}\right)+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^n}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{mn}\right)\right)\\
&+\left(-\overline{Q}_{jk}\left[-\frac{\overline{N}^m}{\overline{N}^2}\overline{N}^2\left(2\Lambda-\overline{R}-\frac{\kappa}{2\lambda}(v(\overline{\Xi})-\overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s})\right)\right.\right.\\
&-\frac{\kappa}{2\lambda}(\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{Q}^{mn}\overline{\Xi}_{,n}-\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsvw}\\
&\left.\left.\times\left[\overline{Q}^{mt}[\overline{Q}_{vw}]_{,t}+2\overline{Q}_{tw}\frac{\partial}{\partial x^v}(\overline{Q}^{mt})\right]\right]\right)+\left(-\frac{\overline{N}^m}{\overline{N}^2}\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{H}\overline{N}^r\overline{N}^s\overline{G}_{jkrs}\right)\\
&\left.+\left(\frac{\overline{N}^m}{\overline{N}^2}\left(2\overline{N}^2\left(\frac{\kappa}{\lambda}\overline{\Xi}_{,j}\overline{\Xi}_{,k}-2\overline{R}_{jk}\right)+4\overline{N}(\overline{D}_j\overline{D}_k\overline{N})\right)+2\overline{N}^2\overline{D}_j\overline{D}_k\left(\frac{\overline{N}^m}{\overline{N}^2}\right)\right)\right]\delta N_m\\
&+\left[\left[\frac{\dot{\overline{N}}}{\overline{N}}-\frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\right.\\
&+\left(\overline{N}^2\left(-\frac{\kappa}{2\sqrt{\det\overline{Q}}}\overline{C}+2\Lambda+\frac{\kappa}{2\lambda}v(\overline{\Xi})\right)\right)+(\overline{N}^2\overline{D}_m\overline{D}_n\overline{Q}^{mn})
\end{aligned}
$$

$$+(-\overline{N}^2(\overline{D}_n\overline{N})\overline{D}_m\overline{Q}^{mn}) + \left(\left(\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \frac{\partial}{\partial\tau}\mathcal{L}_{\vec{\overline{N}}}\right)\right]\delta Q_{jk}$$
$$+\left[\left(2\overline{Q}^{mn}(\dot{Q}_{n(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{n(k)})\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\right) + (-2\overline{N}^2\overline{D}_n\overline{D}_{(k}\overline{Q}^{mn})\right.$$
$$\left.+(2\overline{N}(\overline{D}_n\overline{N})\overline{D}_{(k}\overline{Q}^{mn}) + \left(-\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HQ}^{rm}\overline{N}^n\overline{N}^s\overline{G}_{snr(k}\right)\right]\delta Q_{j)m}$$
$$+\left[-\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{N}^n\overline{N}^m\overline{G}_{jkmn}\right]\delta H + \left(\mathcal{L}_{\delta N}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\mathcal{L}_{\delta N}\right)[\overline{Q}_{jk}]$$
$$+\left[-2\overline{Q}^{mn}(\dot{Q}_{n(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{n(k)})\right](\mathcal{L}_{\delta N}\overline{Q})_{j)m}. \tag{6.31}$$

6.3. Summary of the equations of motion for $\delta\Xi$ and δQ_{jk}

In the last two sections we derived the second-order equations of motion for $\delta\Xi$ and δQ_{jk}. The results of our calculations can be found in equations (6.13) and (6.31), respectively. However, these equations are quite complex and not very transparent in that form. For this reason, we want to rewrite them in a form where we can still recognize their general form but where they take a much simpler form. We will hide the precise details of the various background quantities that occur as coefficients in front of the linear perturbations in certain coefficient functions that will be introduced below. These coefficients will be operator valued since they also involve objects such as partial or Lie derivatives, as can be seen from equations (6.13) and (6.31). As explained before, apart from the elementary perturbations δQ_{jk} and $\delta\Xi$, the second-order equations of motion contain also the perturbation of the shift vector δN_j and the (physical) Hamiltonian density δH. Both are functions of δQ_{jk} and $\delta\Xi$, and therefore not independent perturbations. However, it turns out that these two quantities are constants of motion, so it is convenient to keep them in the equations.

Starting with the second-order equation for $\delta\Xi$, its general structure is of the kind

$$\boxed{[C_\Xi]\delta\Xi = [C_\Xi]^{jk}\delta Q_{jk} + [C_\Xi]^j\delta N_j} \tag{6.32}$$

where the coefficients are given by

$$[C_\Xi] := \left[\frac{\partial^2}{\partial\tau^2} - \left(\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \frac{\partial}{\partial\tau}\mathcal{L}_{\vec{\overline{N}}}\right) - \left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}} + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\right.$$
$$\times\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) - \overline{Q}^{jk}\left[\frac{\overline{N}}{\sqrt{\det\overline{Q}}}(\overline{N}\sqrt{\det\overline{Q}})_{,j}\right]\frac{\partial}{\partial x^k}$$
$$\left.-\overline{N}^2\left(\Delta + [\overline{Q}^{mn}]_{,n}\frac{\partial}{\partial x^m}\right) + \frac{1}{2}\overline{N}^2 v''(\overline{\Xi})\right] \tag{6.33}$$

and

$$[C_\Xi]^{jk} := \left[-(\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\left[\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{1}{2}\left(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\right)\right.\right.$$
$$\left.+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^m}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{jm}\overline{N}^k\right)\right] - \left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)(\overline{Q}^{jm}\overline{Q}^{kn}\overline{N}_m\overline{\Xi}_{,n})$$
$$-\overline{N}^2\left(\Delta\overline{\Xi} + [\overline{Q}^{mn}]_{,m}\overline{\Xi}_{,n} - \frac{1}{2}v'(\overline{\Xi})\right)\left(\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right) - \overline{N}^2\frac{\partial}{\partial x^n}(\overline{Q}^{jm}\overline{Q}^{kn}\overline{\Xi}_{,m})$$

$$
\begin{aligned}
&- \overline{Q}^{jm}\overline{Q}^{kn}\overline{N}_m[\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})]_{,n} - \overline{Q}^{jm}\overline{Q}^{kn}\overline{\Xi}_{,n}\left[\frac{N}{\sqrt{\det Q}}(N\sqrt{\det Q})_{,m}\right] \\
&+ \left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det \overline{Q}})^{\cdot}}{\sqrt{\det \overline{Q}}} + \frac{\overline{N}}{\sqrt{\det \overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det \overline{Q}}}{\overline{N}}\right)\right](\overline{Q}^{jm}\overline{\Xi}_{,m}\overline{N}^k) \\
&+ (\overline{Q}^{mn}\overline{\Xi}_{,n})\left(-\frac{\overline{N}}{\sqrt{\det \overline{Q}}}\frac{1}{2}\left(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)[\overline{N}\sqrt{\det \overline{Q}}\,]_{,j}\right. \\
&\left.+ \frac{\overline{N}}{\sqrt{\det \overline{Q}}}\frac{\partial}{\partial x^m}\left(\frac{1}{2}\left(\overline{Q}^{jk} - \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\overline{N}\sqrt{\det \overline{Q}}\right)\right)\Bigg].
\end{aligned}
$$

Note that all partial and Lie derivatives act on all terms to their right, including the linear perturbations. This is also the reason why terms such as for instance $\ddot{\Xi}$ or $\dot{Q}_{jk}$ do not occur in the simple form of equation (6.32).

The third coefficient is given by

$$
\begin{aligned}
[C_\Xi]^j :=& \Bigg[\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)(\overline{Q}^{jk}\overline{\Xi}_{,k})(\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})) + (\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})) \\
&\times\left[\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\frac{\overline{N}^j}{\overline{N}^2} + \frac{\overline{N}}{\sqrt{\det \overline{Q}}}\frac{\partial}{\partial x^k}\left(\frac{\sqrt{\det \overline{Q}}}{\overline{N}}\overline{Q}^{jk}\right)\right] \\
&+ 2\overline{N}^2\left(\Delta\overline{\Xi} + [\overline{Q}^{jk}]_{,j}\overline{\Xi}_{,k} - \frac{1}{2}v'(\overline{\Xi})\right)\frac{\overline{N}^j}{\overline{N}^2} \\
&- \left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det \overline{Q}})^{\cdot}}{\sqrt{\det \overline{Q}}} + \frac{\overline{N}}{\sqrt{\det \overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det \overline{Q}}}{\overline{N}}\right)\right](\overline{Q}^{jk}\overline{\Xi}_{,k}) \\
&+ (\overline{Q}^{mn}\overline{\Xi}_{,n})\left(\frac{\overline{N}}{\sqrt{\det \overline{Q}}}\frac{\overline{N}^j}{\overline{N}^2}[\overline{N}\sqrt{\det \overline{Q}}]_{,m}\right. \\
&\left.+ \frac{\overline{N}}{\sqrt{\det \overline{Q}}}\frac{\partial}{\partial x^j}\left(\frac{\overline{N}^j}{\overline{N}^2}\overline{N}\sqrt{\det \overline{Q}}\right)\right) + \overline{Q}^{jk}[\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})]_{,k}\Bigg].
\end{aligned}
\tag{6.35}
$$

As was to be expected, the corresponding equation for the perturbation of the three-metric δQ_{jk} includes more than just three terms. It is of the form

$$
\boxed{[C_Q]\delta Q_{jk} = [A_Q]_{jk}\delta\Xi + [B_Q]_{jk}\delta H + [C_Q]^m_{(k}\delta Q_{j)m} + [C_Q]^{mn}_{jk}\delta Q_{mn} + [C_Q]^m_{jk}\delta N_m}. \tag{6.36}
$$

The various coefficients introduced in the equation above are given as follows:

$$
\begin{aligned}
[C_Q] :=& \Bigg[\frac{\partial^2}{\partial\tau^2} - \left(\left(\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \frac{\partial}{\partial\tau}\mathcal{L}_{\vec{\overline{N}}}\right) - \left(\left(\mathcal{L}_{\vec{\overline{N}}}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) + \frac{\partial}{\partial\tau}\mathcal{L}_{\vec{\overline{N}}}\right)\right.\right. \\
&- (\overline{N}^2\overline{D}_m\overline{D}_n\overline{Q}^{mn}) - \left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det \overline{Q}})^{\cdot}}{\sqrt{\det \overline{Q}}} + \frac{\overline{N}}{\sqrt{\det \overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det \overline{Q}}}{\overline{N}}\right)\right]\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right) \\
&- \left(\overline{N}^2\left(-\frac{\kappa}{2\sqrt{\det \overline{Q}}}\overline{C} + 2\Lambda + \frac{\kappa}{2\lambda}v(\overline{\Xi})\right)\right) - (-\overline{N}^2(\overline{D}_n\overline{N})\overline{D}_m\overline{Q}^{mn})\Bigg].
\end{aligned}
\tag{6.37}
$$

Here we use the notation that covariant derivatives surrounded by round bracket such as $(D_jD_k\ldots)$ act on the elements inside the round brackets only. By contrast, covariant derivatives not surrounded by round brackets act on everything to their right, including also the perturbations. The coefficient for $\delta\Xi$ can be explicitly written as

$$[A_Q]_{jk} := \Bigg[-\overline{Q}_{jk}\Bigg(\frac{\overline{N}^2\kappa}{2\lambda}\Bigg(\frac{1}{\overline{N}^2}(\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\Bigg(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\Bigg) + \overline{Q}^{mn}\overline{\Xi}_{,n}\frac{\partial}{\partial x^m} - \frac{1}{2}v'(\overline{\Xi})\Bigg)\Bigg) + \Bigg(4\overline{N}^2\frac{\kappa}{\lambda}\overline{\Xi}_{(,k}\frac{\partial}{\partial x^{j)}}\Bigg)\Bigg]. \tag{6.38}$$

For the coefficient belonging to the linear perturbation of the Hamiltonian density δH we get

$$[B_Q]_{jk} := \Bigg[-\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{N}^n\overline{N}^m\overline{G}_{jkmn}\Bigg]. \tag{6.39}$$

The coefficient $[C_Q]^m_{(k}$ takes the form

$$[C_Q]^m_{(k} := \Bigg[(2\overline{Q}^{mn}(\dot{\overline{Q}}_{n(k} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{n(k)}\Bigg(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\Bigg)\Bigg) + (-2\overline{N}^2\overline{D}_n\overline{D}_{(k}\overline{Q}^{mn}) + (2\overline{N}(\overline{D}_n\overline{N})\overline{D}_{(k}\overline{Q}^{mn}) + \Bigg(-\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HQ}^{rm}\overline{N}^n\overline{N}^s\overline{G}_{snr(k}\Bigg)\Bigg]. \tag{6.40}$$

The last two coefficients are the ones for δQ_{mn} and δN_m. These are the most complicated ones for the second-order equation of motion of δQ_{jk}. We will list them below:

$$\begin{aligned}
[C_Q]^{mn}_{jk} := \Bigg[\Bigg[&\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}} + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\Bigg(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\Bigg)\Bigg]\\
&\times\Bigg(\overline{Q}^{rn}\overline{N}_n[\overline{Q}_{jk}]_{,r} + \overline{Q}_{rk}\frac{\partial}{\partial x^j}(\overline{Q}^{rn}\overline{N}^m) + \overline{Q}_{rj}\frac{\partial}{\partial x^k}(\overline{Q}^{rn}\overline{N}^m) - (\dot{\overline{Q}}_{jk} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk})\\
&\times\Bigg(\Bigg(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\Bigg)\Bigg(\frac{1}{2}\Bigg(\overline{Q}^{mn} + \frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\Bigg)\Bigg) + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^k}\Bigg(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{N}^m\overline{Q}^{rn}\Bigg)\Bigg)\\
&+(-\overline{Q}^{mr}\overline{Q}^{ns}(\dot{\overline{Q}}_{rj} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{rj})(\dot{\overline{Q}}_{sk} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{sk}))\\
&+\Bigg(-\overline{Q}_{jk}\Bigg[\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\overline{N}^2\Bigg(2\Lambda - \overline{R} + \frac{\kappa}{2\lambda}(v(\overline{\Xi}) - \overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s})\Bigg)\\
&+\frac{\overline{N}^2}{2}(\overline{R}^{mn} - [\overline{G}^{-1}]^{mnrs}\overline{D}_r\overline{D}_s) + \frac{\kappa}{2\lambda}\overline{Q}^{mr}\overline{Q}^{ns}(\dot{\overline{\Xi}} - (\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{N}_r\overline{\Xi}_{,s}\\
&-\frac{\kappa\overline{N}^2}{2\lambda}\overline{Q}^{rm}\overline{Q}^{sn}\overline{\Xi}_{,r}\overline{\Xi}_{,s} + \frac{1}{4}(\dot{\overline{Q}}_{rs} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{rs})\\
&\times\Bigg[[\overline{G}^{-1}]^{mnrs}\Bigg(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\Bigg) - (\dot{\overline{Q}}_{tu} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{tu})\overline{Q}^{sn}[\overline{G}^{-1}]^{turm}\Bigg]\\
&+\frac{1}{4}(\dot{\overline{Q}}_{rs} - (\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsvw}\Bigg[\overline{Q}^{mt}\overline{N}^n[\overline{Q}_{vw}]_{,t} + 2\overline{Q}_{tw}\frac{\partial}{\partial x^v}(\overline{Q}^{mt}\overline{N}^n)\Bigg]\Bigg]\Bigg)\\
&+\Bigg(\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\Bigg(-2\overline{N}^2\Bigg(\frac{\kappa}{\lambda}\overline{\Xi}_{,j}\overline{\Xi}_{,k} - 2\overline{R}_{jk}\Bigg) - 4\overline{N}(\overline{D}_j\overline{D}_k\overline{N})\Bigg)\\
&+\overline{N}^2\overline{D}_j\overline{D}_k\overline{Q}^{mn} - 2\overline{N}^2\overline{D}_j\overline{D}_k\Bigg(\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\Bigg)\Bigg)\\
&+\Bigg(\frac{1}{2}\Bigg(\overline{Q}^{mn} + \frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\Bigg)\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HN}^r\overline{N}^s\overline{G}_{jkrs} + \frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{HQ}^{sm}\overline{N}^r\overline{N}^n\overline{G}_{jkrs}\Bigg)
\end{aligned}$$

$$
\begin{aligned}
&+\Bigg(-\overline{Q}^{mr}\overline{N}^{n}[\dot{\overline{Q}}_{jk}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk}]_{,r}-(\dot{\overline{Q}}_{km}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{kr})\frac{\partial}{\partial x^{j}}(\overline{Q}^{mr}\overline{N}^{n})\\
&-(\dot{\overline{Q}}_{jm}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jr})\frac{\partial}{\partial x^{k}}(\overline{Q}^{mr}\overline{N}^{n})+(-2\overline{Q}^{tu}(\dot{\overline{Q}}_{t(k}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{t(k)})\\
&\times\left(-\overline{Q}^{mr}\overline{N}^{n}[Q_{j)u}]_{,r}-\overline{Q}_{um}\frac{\partial}{\partial x^{j)}}(\overline{Q}^{mr}\overline{N}^{n})-\overline{Q}_{j)m}\frac{\partial}{\partial x^{u}}(\overline{Q}^{mr}\overline{N}^{n})\right)\\
&+\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)(-\overline{Q}^{mr}\overline{N}^{n}[\overline{Q}_{jk}]_{,r}-\overline{Q}_{km}\frac{\partial}{\partial x^{j}}(\overline{Q}^{mr}\overline{N}^{n})-\overline{Q}_{jm}\frac{\partial}{\partial x^{k}}(\overline{Q}^{mr}\overline{N}^{n}))\Bigg)\Bigg].
\end{aligned}
\tag{6.41}
$$

Note that the coefficient for δQ_{mn} in equation (6.31) and the one above are different due to the presence of the last two lines in the equation above. The reason for this is that now we used the explicit expression for the Lie derivatives with respect to $\delta\vec{N}$, which were derived in equations (6.28) and (6.27) and lead to additional terms in δQ_{mn} and δN_m.

Finally, we present the coefficient for δN_m. Similar to the case of δQ_{nm}, we also get additional terms coming from the Lie derivatives in the last line of equation (6.31):

$$
\begin{aligned}
[C_Q]^{m}_{jk} := \Bigg[&-\left[\frac{\dot{\overline{N}}}{\overline{N}}-\frac{(\sqrt{\det\overline{Q}})^{\dot{}}}{\sqrt{\det\overline{Q}}}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\\
&\times\left(\overline{Q}^{mn}[\overline{Q}_{jk}]_{,n}+\overline{Q}_{nk}\frac{\partial}{\partial x^{j}}(\overline{Q}^{mn})+\overline{Q}_{nj}\frac{\partial}{\partial x^{k}}(\overline{Q}^{mn})\right)\\
&+(\dot{\overline{Q}}_{jk}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk})\left(\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{\overline{N}^{m}}{\overline{N}^{2}}\right)+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^{n}}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{mn}\right)\right)\\
&+\Bigg(-\overline{Q}_{jk}\Bigg[-\frac{\overline{N}^{m}}{\overline{N}^{2}}\overline{N}^{2}\left(2\Lambda-\overline{R}-\frac{\kappa}{2\lambda}(v(\Xi)-\overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s})\right)\\
&-\frac{\kappa}{2\lambda}(\dot{\Xi}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{Q}^{mn}\overline{\Xi}_{,n}-\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsvw}\\
&\times\left[\overline{Q}^{mt}[\overline{Q}_{vw}]_{,t}+2\overline{Q}_{tw}\frac{\partial}{\partial x^{v}}(\overline{Q}^{mt})\right]\Bigg]\Bigg)+\left(-\frac{\overline{N}^{m}}{\overline{N}^{2}}\frac{\overline{N}\kappa}{\sqrt{\det\overline{Q}}}\overline{H}\overline{N}^{r}\overline{N}^{s}\overline{G}_{jkrs}\right)\\
&+\left(\frac{\overline{N}^{m}}{\overline{N}^{2}}\left(2\overline{N}^{2}\left(\frac{\kappa}{\lambda}\overline{\Xi}_{,j}\overline{\Xi}_{,k}-2\overline{R}_{jk}\right)+4\overline{N}(\overline{D}_{j}\overline{D}_{k}\overline{N})\right)+2\overline{N}^{2}\overline{D}_{j}\overline{D}_{k}\left(\frac{\overline{N}^{m}}{\overline{N}^{2}}\right)\right)\\
&+\Bigg(\overline{Q}^{mn}[\dot{\overline{Q}}_{jk}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk}]_{,n}+(\dot{\overline{Q}}_{kn}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{kn})\frac{\partial}{\partial x^{j}}(\overline{Q}^{mn})\\
&+(\dot{\overline{Q}}_{jn}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jn})\frac{\partial}{\partial x^{k}}(\overline{Q}^{mn})\Bigg)+\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)\\
&\times(\overline{Q}^{mn}[\overline{Q}_{jk}]_{,n}+\overline{Q}_{kn}\frac{\partial}{\partial x^{j}}(\overline{Q}^{mn})+\overline{Q}_{jn}\frac{\partial}{\partial x^{k}}(\overline{Q}^{mn})\Big)\\
&+(-2\overline{Q}^{tu}(\dot{\overline{Q}}_{t(k}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{t(k)})(\overline{Q}^{mn}[\overline{Q}_{j)u}]_{,n}+\overline{Q}_{un}\frac{\partial}{\partial x^{j)}}\\
&\times(\overline{Q}^{mn})+\overline{Q}_{j)n}\frac{\partial}{\partial x^{u}}(\overline{Q}^{mn}))\Bigg].
\end{aligned}
\tag{6.42}
$$

Although the form of the perturbed equations is quite complicated, they simplify drastically for special backgrounds of interest. For the case of FRW, for instance, all terms proportional to $\overline{N}_j$ vanish, since $\overline{N}_j = -\overline{C}_j/\overline{H} = 0$ for FRW. This is due to the geometry and matter parts of the diffeomorphism constraint vanishing both separately in that case. Furthermore, all terms in the coefficients that contain spatial derivatives applied to background quantities vanish also. Other backgrounds where considerable simplification will occur include Schwarzschild spacetime.

7. Comparison with other frameworks

We now proceed to compare our work with other approaches to general relativistic perturbation theory found in the literature. In the following we will restrict ourselves to discussing works that treat perturbation theory around general backgrounds. Approaches which deal exclusively with cosmological perturbation theory will be looked at in our second paper, specifically dedicated to that topic.

The central point of comparison is how gauge invariance is handled in the various approaches. As that notion often acquires different meanings, especially in the context of general-relativistic perturbation theory, it seems prudent to recall the precise mathematical setting underlying most works. It was developed by Sachs [23] and Stewart and Walker [24], and recently given a very general and elegant formulation by Bruni, Sonego and collaborators [25–27]. The starting point consists of two spacetime manifolds M_0 and M, which represent the background spacetime around which one perturbs and the actual physical spacetime, respectively. It is important to keep in mind that M_0 is only an artificial construct. Perturbations of geometric quantities are then defined by comparing their values in M_0 and M, respectively. This procedure is highly ambiguous, however, in that there is a great freedom inherent in the choice of points where one compares background and 'real' quantities to define the perturbations. Note that this freedom is in addition to the usual coordinate gauge freedom in general relativity. For that reason, Sachs termed it gauge invariance of the second type [23]. Making such a choice, which mathematically amounts to choosing a so-called point identification map between M_0 and M, is therefore nothing but a choice of gauge. Correspondingly, gauge-invariant perturbations are those quantities whose values do not depend on the choice of point identification map. The actual condition for a perturbed quantity to be gauge invariant to first order in this sense was already derived in [23], fully proved in [24] and finally generalized to arbitrary order n in [25]. The result can be succinctly summarized as follows: a geometric quantity T—such as a tensor—is invariant to order n iff all its perturbations to order $n-1$ are either vanishing (spacetime) constant scalars or a combination of Kronecker deltas. This result is often known as the Stewart and Walker lemma. Clearly, the only case of actual interest is the first. An example is given by curvature tensors in linear perturbation theory around Minkowski space. As they vanish in the background, they are gauge invariant to first order. These insights have been the backbone of most attempts to construct gauge-invariant quantities to various orders in perturbation theory or even non-perturbatively. We will now discuss two of them.

In a series of papers [2–4] Nakamura has used these principles to develop formulae for gauge-invariant quantities to second and third order around an arbitrary background. They encompass the invariant parts of various metric and curvature, as well as matter perturbations. These general formulae are, however, implicit only to the extent that Nakamura derives them from the assumption that the corresponding linear order perturbations can be decomposed into gauge-invariant and gauge-variant parts. Consequently, while the construction is, in principle, valid for arbitrary backgrounds, in practice only backgrounds with sufficient symmetries to perform that split at linear order explicitly can be used. Luckily, that applies, of course, to several cases of great interest, such as cosmological and spherically symmetric backgrounds. The latter case is explicitly treated in [4].

A distinctly different approach—let us call it the EB approach—is based on seminal work by Ellis and Bruni [28], which has since inspired a multitude of other works [29–31]. Although the discussions in these papers are geared towards applications in cosmology, the framework itself can be applied to arbitrary spacetimes, in principle, which is why we decided to discuss it here. The basic idea is to use a 1 + 3-approach by employing covariant quantities connected to a family of flow lines or 'fundamental observers'. The prime reason is that these quantities are much more closely related to what one actually measures in astrophysics. Furthermore, by a simple application of the Stewart–Walker lemma, they are automatically gauge invariant if the corresponding quantities in the background spacetime vanish. Unlike in the more common metric-based formalism, these quantities are defined in the physical, perturbed spacetime. As a result, they are fully non-perturbative and in that sense their gauge invariance extends to all orders. The connection to the standard perturbative approach based on perturbations in the background spacetime can be made by suitably expanding the physical quantities to the desired order, see [29]. This approach enjoys a clear geometric and physical interpretation of the quantities used, as well as the advantage of basing perturbation theory on non-perturbative variables.

Comparing the works mentioned so far to ours, a first obvious difference is found to be that we work in a canonical setting versus the covariant setting used by the others. The motivation is first that gauge issues become particularly clear in the canonical picture and second our view towards quantization. The more important difference, however, is our use of dust as a dynamically implemented coordinate system. Our dust clocks serve a twofold purpose: on the one hand they enable us to construct background observables and therefore to solve the standard gauge problem in general relativity. On the other hand they also serve as the point identification map and thus eliminate the gauge freedom of 'second type'. In that sense they represent a logical extension to perturbation theory of the initial conceptual idea by Brown and Kuchar [12] to use dust as a physical and therefore preferred coordinate system.

We should also point out that while our framework employs the metric and its perturbations as fundamental variables, we could equally well use the dust clocks to build a gauge-invariant perturbation theory based on the same variables used in the EB approach. In fact, it seems worthwhile to look a bit more closely at the relationship between the two approaches. Both are non-perturbative in the following sense: they construct quantities which are gauge invariant (with respect to gauge transformations of the second type). Only then perturbation theory is applied, which means that gauge invariance is then automatically guaranteed in each order of perturbation. The difference arises when one looks at the role of gauge transformations of the first kind. The EB approach uses idealized observers that are comoving with the physical matter in the model. Thus the theory is not deparametrized and gauge freedom with respect to the background spacetime remains, as illustrated by the presence of constraints as part of the equations of motion. In our case, the observers are represented by the dust, a component added to the physical matter content of the theory. They are thus dynamically included in the theory via the dust contribution to the Lagrangian, in addition to all the other matter. This allows for a complete deparametrization of the non-dust system with respect to the dust. Time evolution for this subsystem becomes unconstrained and a physical Hamiltonian emerges. The price to pay for this is that the dust contributes to the energy–momentum tensor of the deparametrized system, the size of which is small, however. One might well argue that, for practical purposes at the classical level, the choice between the two approaches is a matter of taste. Our approach, however, offers a clear advantage if one is interested in quantization, eventually. All programs aiming at a quantization of gravity that have been pursued, so far, use the metric as a fundamental building block. It is not obvious to us how to attempt a quantization based on the covariant variables used in the EB approach.

Another argument in favour of our framework is the following: a test observer which by definition does not have any impact is only a mathematical idealization. Physically much more realistic is a dynamically coupled observer fluid like the dust considered here which in particular takes into account the gravitational backreaction.

To summarize, the crucial difference between our approach and the others discussed here is that the latter deal only with gauge freedom of the second type. This can be seen from the fact that they use background variables which are not gauge invariant and is evidenced, e.g., by the presence of constraint equations in addition to evolution equations. Our treatment, by contrast, deals with all variables at all orders in a unified manner. Furthermore, in our opinion the framework developed here allows for a much more straightforward implementation at higher orders. Another advantage is that it allows us to treat arbitrary backgrounds in practice, without the high degree of symmetry necessary for approaches based on the Stewart–Walker lemma to work. Recall that the latter require finding non-trivial quantities that vanish in the background manifold. Only in symmetric backgrounds such as homogeneous spacetimes is that a fairly tractable problem.

Finally, we should briefly discuss the recent work in [21], which is close to ours in terms of motivation and conceptual underpinnings. The authors there also use the general gauge-invariant framework of [11], however, with two differences: first of all, they do not use dust matter to achieve gauge-invariant completions of geometry and matter variables. This prevents them from bringing the constraints into a deparametrized form [9] and thus there is no time-independent physical Hamiltonian. Secondly, while they can develop higher order cosmological perturbation theory, their perturbations of gauge-invariant quantities are still expanded in terms of the perturbations of the the gauge variant quantities which is what we never do. Therefore the basic perturbation variables are different in the two schemes: in our scheme we never care how our gauge-invariant variables are assembled from gauge variant ones, they and their perturbations are fundamental for us and nth-order quantities are nth-order expressions in those. In contrast, in [21] nth order means nth order in the gauge variant quantities. In particular, the nth-order perturbed variables are only invariant with respect to the nth-order constraints up to terms of higher order. In contrast, our perturbed variables are always first order and always fully gauge invariant, it is only in the Hamiltonian that higher orders of gauge-invariant variables appear. It would no doubt be fruitful to translate the schemes into each other and to see which differences and similarities arise.

8. Conclusions and open questions

This is a long and technically involved paper. The reader rightfully will ask why one should dive into its details and what exactly is novel as compared to the existing literature. The following remarks are in order.

(1) *Non-perturbative gauge invariance*. To the best of our knowledge, there exists no generally accepted notion of gauge invariance at nth order of perturbation theory in general relativity. Moreover, at each order of perturbation theory one has to repeat the analysis for how to preserve gauge invariance to the given order. Given those difficulties, it is natural to try to invent a scheme which separates the issue of gauge invariance from the perturbation theory. Hence, one must treat gauge invariance non-perturbatively. This is exactly what we managed to do in this paper.

Thus, one only deals with the exact observables of the theory. All the equations of the theory have to be written in terms of those gauge-invariant quantities. Given such a gauge-invariant function O on the full phase space, we evaluate it on a certain background (data) which is an exact solution to our equations of motion and get a certain value O_0. The perturbation of O is then defined as $\delta O = O - O_0$. We never care to expand δO in terms of the perturbations of the gauge variant degrees of freedom (although we could). However, all the equations are expanded directly in terms of the perturbations of those physical observables.

(2) *Material reference system.* In general relativity it is well known that in order to meaningfully talk about the Einstein equations and to have them describe something observable or measurable, one has to suppose that spacetime is inhabited by (geodesic) test observers. By definition, a test observer has no effect whatsoever on the system. This is of course mathematically convenient but physically worrisome because a test observer is a mathematical idealization. Every real observer interacts at least gravitationally and does leave its fingerprint on the system. One of the achievements of the seminal work [12] of Brown and Kuchař, which in our mind is insufficiently appreciated in the literature, is to have overcome this shortcoming. The authors of [12] have identified a generally covariant Lagrangian which comes as close as possible to describing a non-self-interacting, perfect and geodesically moving fluid that fills out spacetime (congruence). It does leave its fingerprint on the system and thus is physically more realistic than the test observer fluid.

In this paper we have driven the work of [12] to its logical frontier and have asked the question whether the dust when added to the geometry–matter system really accomplishes the goal of keeping the approximate validity of the usual interpretation of the Einstein equations. We have verified that it does which in our mind is an intriguing result.

(3) *Solving the problem of time.* Since general relativity is a generally covariant or reparametrization invariant theory, it is not equipped with a natural Hamiltonian. Rather, the 'dynamics' of the non-observables is described by a linear combination of constraints which really generate gauge transformations rather than physical evolution. Observable quantities are gauge invariant and therefore do not evolve with respect to the 'gauge dynamics'. Therefore it is conceptually unclear what to do with those observables. The achievement of [10, 11] is to have invented a scheme that in principle unfreezes the observables from their non-motion. However, in general that physical motion is far from uniquely selected, there are in general infinitely many such physical notions of time and none of them is preferred. Moreover, the associated Hamiltonians are generically neither preserved nor positive or at least bounded from below.

When combining the frameworks of [12] and [10, 11] we find the remarkable result that there is a preferred Hamiltonian which is manifestly positive, not explicitly dependent on physical time and gauge invariant. It maps a conceptually complicated gauge systems into the safe realm of a conservative Hamiltonian system. The physical Hamiltonian drives the evolution of the physical observables. It reproduces the Einstein equations for the gauge-invariant observables up to corrections which describe the influence of the dust.

(4) *Counting of the physical degrees of freedom.* The price to pay is that one has to assume the existence of the dust as an additional matter species next to those of the standard model[35]. It would maybe be more desirable to have matter species of the standard model

[35] Curiously, what we have done in this paper bears some resemblance to the Stueckelberg formalism. There one also adds additional matter to the Maxwell theory. One can then make the longitudinal mode gauge invariant and thus finds a theory with one more degree of freedom. This is one way to arrive at the Proca theory and more generally at massive vector boson theories via the Higgs mechanism.

or geometry modes playing the role of a dynamical test observer[36]. In principle this is possible; however, the resulting formalism is much more complicated and it does not lead to deparametrization. Thus a conserved physical Hamiltonian would then not be available and the equations of motion would become intractable.

It is true that the dust variables disappear in the final description of the observables which are complicated aggregates built out of all fields. However, the theory has fundamentally four more physical degrees of freedom than without dust and that might eventually rule out our theory if those additional degrees of freedom are not observed.

The truly remarkable feature of the dust is that it replaces the initial value constraints of general relativity which are responsible for having less physical degrees of freedom than one would naively expect, by four conservation laws. That is, in any given solution of our equations of motion, the physical observables must physically evolve with respect to each other in such a way that the conserved quantities do not change. This effectively acts like a constraint and therefore reduces the number of independently evolving observables by four, in agreement with the counting of the degrees of freedom without dust. Thus, at least as long as the value of those conserved quantities is sufficiently small, we will not be able to see those additional degrees of freedom. It is this fact which makes it possible that one effectively does not see more degrees of freedom than in the standard treatment.

As a final objection against our formalism one might raise the fact that the dust contributes with the wrong sign to the matter energy–momentum tensor. However, the formalism not only forces us to do this as we would otherwise have a negative definite Hamiltonian, moreover, as already remarked in the introduction, it is completely acceptable since here we talk about the energy–momentum tensor of non-observables. The energy–momentum tensor of the observables in the final Einstein equations does satisfy the usual energy conditions.

(5) *Complexity of the equations of motion*. Since general relativity is a highly nonlinear, complicated self-interacting theory, experience from much less complicated integrable systems suggests that its invariants, that is, the gauge-invariant observables, satisfy a tremendously complicated Poisson algebra and that the equations of motion are intractable. Surprisingly, this is not at all the case. The observable algebra is almost as simple as the algebra of non-observables and the equations of motion can be solved almost as easily as in the usual gauge variant formalism. Key to that is the presence of the already mentioned conserved current.

In this first paper we have developed the general gauge-invariant formalism and linear perturbation theory about general backgrounds. In the companion paper we apply the general results to flat and FRW backgrounds and find agreement with usual linear perturbation theory for linearly invariant observables. This is a first consistency test that our theory has passed. Thus we hope to have convinced the reader that the present framework has conceptual advantages over previous ones and that it is nonetheless technically not much more complicated. Actually, the pay-off for having a manifestly gauge-invariant approach will really come in at higher order where we believe that our equations of motion will be simpler.

There are many lines of investigations that one can follow from here. An obvious one, the specialization to the all-important case of an FRW background is presented in a companion paper as already mentioned. Investigating perturbations around backgrounds of astrophysical interest, such as Schwarzschild spacetime, is also valuable. Again, for all these cases it should

[36] This would be similar to technicolour theories which declare the Higgs scalar field not as an independent degree of freedom but as a compound object built from the bosons of the electroweak theory. Here one would build four independent scalars e.g. from the geometry field.

also prove very interesting to go beyond the linear to higher orders. Predictions from second-order perturbation theory, e.g. the issue of non-Gaussianity in cosmological perturbations, are the topic of current research and could soon be testable by future experiments such as PLANCK, see [34]. On a more technical and conceptual level, our framework might prove useful to settle the issue of under what conditions general-relativistic perturbation theory is consistent and stable. Finally, with a view towards facilitating the search for physically relevant predictions from approaches to quantum gravity, a quantization of our gauge-invariant formulation of general relativity, together with the development of the corresponding perturbation theory at the quantum level, strikes us as a highly desirable goal. See [20] for first steps.

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Appendix A. Second class constraints of the Brown–Kuchař theory

In this section we provide the calculational details of the constraint analysis of the Brown–Kuchař theory discussed in section 2. In particular, we want to show that no tertiary constraints arise. Our starting point is equation (2.25) which we display once again below for the convenience of the reader:

$$\begin{aligned}
&z_{,t} = \{H_{\text{primary}}, p\} = -c^{\text{tot}} \qquad z_{a,t} = \{H_{\text{primary}}, p_a\} = -c^{\text{tot}}_a \\
&Z_{,t} = \{H_{\text{primary}}, I\} = \frac{n}{2}\left[-\frac{P^2}{\sqrt{\det(q)}\rho^2} + \sqrt{\det(q)}(q^{ab}U_aU_b + 1)\right] =: \tilde{c} \\
&Z^j_{,t} = \{H_{\text{primary}}, I^j\} = -\mu^j P - n\rho\sqrt{\det(q)}q^{ab}U_aS^j_{,b} + PS^j_{,a}n^a \\
&Z_{j,t} = \{H_{\text{primary}}, P_j + W_jP\} = \mu_j P - \left(n^a - \frac{n\rho\sqrt{\det(q)}}{P}q^{ab}U_b\right)PW_{j,a}.
\end{aligned} \tag{A.1}$$

The last two equations involve the Lagrange multipliers μ^j and μ_j and can be solved for them. In contrast we observe that the first three equations are independent of the Lagrange multipliers; they are secondary constraints. We will now proceed with the constraint analysis and show that when the Poisson brackets between the primary Hamiltonian H_{primary} and the secondary constraints are considered no new constraints are generated. Recall that the primary Hamiltonian density was given by

$$h_{\text{primary}} = \mu^j Z_j + \mu Z + \mu_j Z^j + \nu z + \nu^a z_a + n'c^{\text{tot}} + n'^a c^{\text{tot}}_a \tag{A.2}$$

whereby the single constraints are shown below:

$$\begin{aligned}
&c^{\text{tot}} = c^{\text{geo}} + c^{\text{matter}} + c^{\text{D}} \qquad c^{\text{tot}}_a = c^{\text{geo}}_a + c^{\text{matter}}_a + c^{\text{D}}_a \\
&\kappa c^{\text{geo}} = \frac{1}{\sqrt{\det(q)}}\left[P^{ab}P_{ab} - \frac{1}{2}\left(P^a_a\right)^2\right] - \sqrt{\det(q)}R^{(3)} + 2\Lambda\sqrt{\det(q)} \\
&\lambda c^{\text{matter}} = \frac{1}{2}\left[\frac{\pi^2}{\sqrt{\det(q)}} + \sqrt{\det(q)}(q^{ab}\xi_{,a}\xi_{,b} + v(\xi))\right] \\
&c^{\text{D}} = \frac{1}{2}\left[\frac{P^2}{\sqrt{\det(q)}\rho} + \sqrt{\det(q)}\rho(q^{ab}U_aU_b + 1)\right] \\
&\kappa c^{\text{geo}}_a = -2D_bP^b_a \qquad \lambda c^{\text{matter}}_a = \pi\xi_{,a} \qquad c^{\text{D}}_a = P\left[T_{,a} - W_jS^j_{,a}\right].
\end{aligned} \tag{A.3}$$

We begin with the calculation of the Poisson bracket of $H_{\rm primary}$ and the smeared constraint

$$\vec{c}^{\rm tot}(\vec{n}) := \int \mathrm{d}^3x\; n^a(x)c_a^{\rm tot}(x) \tag{A.4}$$

$$\begin{aligned}\{H_{\rm primary}, \vec{c}^{\rm tot}(\vec{n})\} = \int \mathrm{d}^3x \int \mathrm{d}^3y \big(\big\{\mu^j(y)Z_j(y), n^a(x)c_a^{\rm tot}(x)\big\} + \big\{\mu(y)Z(y), n^a(x)c_a^{\rm tot}(x)\big\}\\ + \big\{\mu_j(y)Z^j(y), n^a(x)c_a^{\rm tot}(x)\big\} + \big\{\nu(y)z(y), n^a(x)c_a^{\rm tot}(x)\big\}\\ + \big\{\nu^b(y)z_b(y), n^a(x)c_a^{\rm tot}(x)\big\} + \big\{n'(y)c^{\rm tot}(y), n^a(x)c_a^{\rm tot}(x)\big\}\\ + \big\{n'^b(y)c_b^{\rm tot}(y), n^a(x)c_a^{\rm tot}(x)\big\}\big).\end{aligned} \tag{A.5}$$

For the single Poisson brackets that occur in the equation above we obtain the following result:

$$\begin{aligned}&\int \mathrm{d}^3x \int \mathrm{d}^3y \big\{\mu^j(y)Z_j(y), n^a(x)c_a^{\rm tot}(x)\big\} = \int \mathrm{d}^3x\, n^a P\mu^j W_{j,a}\\ &\int \mathrm{d}^3x \int \mathrm{d}^3y \big\{\mu(y)Z(y), n^a(x)c_a^{\rm tot}(x)\big\} = 0\\ &\int \mathrm{d}^3x \int \mathrm{d}^3y \big\{\mu_j(y)Z^j(y), n^a(x)c_a^{\rm tot}(x)\big\} = -\int \mathrm{d}^3x\, P\mu_j S^j_{,a}n^a\\ &\int \mathrm{d}^3x \int \mathrm{d}^3y \big\{\nu(y)z(y), n^a(x)c_a^{\rm tot}(x)\big\} = 0\\ &\int \mathrm{d}^3x \int \mathrm{d}^3y \big\{\nu^b(y)z_b(y), n^a(x)c_a^{\rm tot}(x)\big\} = \vec{c}^{\rm tot}(\vec{\nu})\\ &\int \mathrm{d}^3x \int \mathrm{d}^3y \big\{n'(y)c^{\rm tot}(y), n^a(x)c_a^{\rm tot}(x)\big\} = c^{\rm tot}(\mathcal{L}_{\vec{n}}n') + \tilde{c}(\mathcal{L}_{\vec{n}'}\rho)\\ &\qquad + \int \mathrm{d}^3x\rho\, n'\, n^a\sqrt{\det(q)}q^{bc}U_b\big(W_{j,a}S^j_c - W_{j,c}S^j_{,a}\big)\\ &\int \mathrm{d}^3x \int \mathrm{d}^3y \big\{n'^b(y)c_b^{\rm tot}(y), n^a(x)c_a^{\rm tot}(x)\big\}\\ &\qquad = \vec{c}(\mathcal{L}_{\vec{n}}\vec{n}') - \int \mathrm{d}^3x (n'^a n^b - n^a n'^b)PS^j_{,a}W_{j,b}.\end{aligned} \tag{A.6}$$

Consequently we can rewrite equation (A.5) as

$$\begin{aligned}\{H_{\rm primary}, \vec{c}^{\rm tot}(\vec{n})\} &= c^{\rm tot}(\mathcal{L}_{\vec{n}}n') + \tilde{c}(\mathcal{L}_{\vec{n}}\rho) + \int \mathrm{d}^3x\; \rho\, n\, n^a\sqrt{\det(q)}q^{bc}U_b\big(W_{j,a}S^j_c - w_{j,c}S^j_a\big)\\ &\quad - \int \mathrm{d}^3x\; \mu_j PS^j_a n^a + \int \mathrm{d}^3x\; \mu^j P w_{j,a}n^a + \vec{c}(\mathcal{L}_{\vec{n}}\vec{n}') + \vec{c}^{\rm tot}(\vec{\nu})\\ &\quad - \int \mathrm{d}^3x (n'^b n^a - n'^a n^b)PW_{j,a}S^j_{,b}\\ &\approx \int \mathrm{d}^3x\; n^a\big(S^j_a(Pn'^bW_{j,b} - \rho\, n\sqrt{\det(q)}q^{bc}U_b w_{j,c} - \mu_j P)\\ &\quad + W_{j,a}\big(-Pn'^bS^j_{,b} + \rho\, n\sqrt{\det(q)}q^{bc}U_bS^j_{,c} + \mu^j P\big)\big).\end{aligned} \tag{A.7}$$

Hence, the result above involves the Lagrange multipliers μ_j and μ^j and can be solved for them such that no new constraints arise from $c_a^{\rm tot}$. Proceeding with $c^{\rm tot}$ whereby the smeared constraint is given by

$$c^{\rm tot}(n) := \int \mathrm{d}^3x\, n(x)c^{\rm tot}(x). \tag{A.8}$$

Thus we get

$$\{H_{\rm primary}, c^{\rm tot}(n)\} = \int \mathrm{d}^3x \int \mathrm{d}^3y \big(\{\mu^j(y)Z_j(y), n(x)c^{\rm tot}(x)\} + \{\mu(y)Z(y), n(x)\tilde{c}(x)\} \\ + \{\mu_j(y)Z^j(y), n(x)c^{\rm tot}(x)\} + \{\nu(y)z(y), n(x)c^{\rm tot}(x)\} \\ + \{\nu^b(y)z_b(y), n(x)c^{\rm tot}(x)\} + \{n'(y)c^{\rm tot}(y), n(x)c^{\rm tot}(x)\} \\ + \big\{n'^b(y)c^{\rm tot}_b(y), n(x)c^{\rm tot}(x)\big\}\big). \tag{A.9}$$

For the single Poisson brackets that occur in the equation above we obtain the following result:

$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{\mu^j(y)Z_j(y), n(x)c^{\rm tot}(x)\} = -\int \mathrm{d}^3x \sqrt{\det(q)}n\rho\mu^j q^{ab}U_b W_{j,a}$$
$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{\mu(y)Z(y), n(x)c^{\rm tot}(x)\} = \int \mathrm{d}^3x\, \mu\frac{n}{n'}\tilde{c}$$
$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{\mu_j(y)Z^j(y), n(x)c^{\rm tot}(x)\} = \int \mathrm{d}^3x\, \mu_j\rho\, n\sqrt{\det(q)}q^{bc}U_b S^j_{,c}$$
$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{\nu(y)z(y), n(x)c^{\rm tot}(x)\} = c^{\rm tot}(\nu)$$
$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{\nu^b(y)z_b(y), n(x)c^{\rm tot}(x)\} = 0$$
$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{n'(y)c^{\rm tot}(y), n(x)c^{\rm tot}(x)\} = \vec{c}^{\,\rm tot}(q^{-1}[n'dn - ndn'])$$
$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{n'^b(y)c^{\rm tot}_b(y), n(x)c^{\rm tot}(x)\} = -c^{\rm tot}(\mathcal{L}_{\vec{n}'}n) - \tilde{c}(\mathcal{L}_{\vec{n}'}\rho) \\ - \int \mathrm{d}^3x\rho n n'^a\sqrt{\det(q)}q^{bc}U_b\big(W_{j,a}S^j_c - W_{j,c}S^j_{,a}\big).$$

Reinserting these results into equation (A.9) yields

$$\{H_{\rm primary}, c^{\rm tot}(n)\} = -\int \mathrm{d}^3x\sqrt{\det(q)}n\rho\mu^j q^{ab}U_bW_{j,a} + \int \mathrm{d}^3x\,\mu\frac{n}{n'}\tilde{c} \\ + \int \mathrm{d}^3x\rho\, n\,\mu_j\sqrt{\det(q)}q^{bc}U_bS^j_{,c} + c^{\rm tot}(\nu) + \vec{c}^{\,\rm tot}[q^{-1}(n'dn - ndn')] \\ - c^{\rm tot}(\mathcal{L}_{\vec{n}'}n) - \tilde{c}(\mathcal{L}_{\vec{n}'}\rho) - \int \mathrm{d}^3x\rho n n'^a\sqrt{\det(q)}q^{bc}U_b\big(W_{j,a}S^j_c - W_{j,c}S^j_{,a}\big) \\ \approx \int \mathrm{d}^3x\sqrt{\det(q)}n\rho q^{bc}U_b\left(W_{j,c}\left(n'^aS^j_{,a} - \mu^j - \frac{\rho\, n'}{P}\sqrt{\det(q)}q^{de}U_dS^j_{,e}\right)\right. \\ \left.\times S^j_{,c}\left(\mu_j - W_{j,a}n'^a + \frac{\rho\, n'}{P}q^{de}U_dW_{j,e}\right)\right) \\ + \int \mathrm{d}^3x\sqrt{\det(q)}n\rho q^{bc}U_b\frac{\rho n'}{P}\sqrt{\det(q)}q^{de}U_d\big(W_{j,c}S^j_{,e} - W_{j,e}S^j_{,c}\big) \\ = \int \mathrm{d}^3x\sqrt{\det(q)}n\rho q^{bc}U_b\left(W_{j,c}\left(n'^aS^j_{,a} - \mu^j - \frac{\rho\, n'}{P}\sqrt{\det(q)}q^{de}U_dS^j_{,e}\right)\right. \\ \left.\times S^j_{,c}\left(\mu_j - W_{j,a}n'^a + \frac{\rho\, n'}{P}q^{de}U_dW_{j,e}\right)\right). \tag{A.11}$$

Here we used in the last step that the last integral in the line before the last line one vanishes, because $W_{j,c}S^j_{,e} - W_{j,e}S^j_{,c}$ is antisymmetric in e, c and multiplied by $q^{bc}q^{de}U_bU_d$ which is symmetric in the indices c, e.

These are again the equation involving the Lagrange multipliers that we have seen before in the calculations for c_a^{tot}.

Finally, let us consider the Poisson bracket of H_{primary} and the secondary constraint $\tilde{c}$ whose smeared version is given by

$$\tilde{c}(u) := \int \mathrm{d}^3x\, u(x)\tilde{c}(x) \tag{A.12}$$

where u is an appropriate smearing function. We obtain

$$\begin{aligned}\{H_{\mathrm{primary}}, \tilde{c}(u)\} = \int \mathrm{d}^3x \int \mathrm{d}^3y \big(&\{\mu^j(y)Z_j(y), u(x)\tilde{c}(x)\} + \{\mu(y)Z(y), u(x)\tilde{c}(x)\} \\ &+ \{\mu_j(y)Z^j(y), u(x)\tilde{c}(x)\} + \{\nu(y)z(y), u(x)\tilde{c}(x)\} + \{\nu^b(y)z_b(y), u(x)\tilde{c}(x)\} \\ &+ \{n'(y)c^{\mathrm{tot}}(y), u(x)\tilde{c}(x)\} + \big\{n'^b(y)c_b^{\mathrm{tot}}(y), u(x)\tilde{c}(x)\big\}\big).\end{aligned} \tag{A.13}$$

In this case we do not need to compute all the individual Poisson bracket in order to convince ourselves that no constraints arise, because the Poisson bracket of $Z(\mu)$ and $\tilde{c}(u)$ yields

$$\int \mathrm{d}^3x \int \mathrm{d}^3y \{\mu(y)Z(y), u(x)\tilde{c}(x)\} = \int \mathrm{d}^3x \mu\, u \frac{nP^2}{\rho^3\sqrt{\det(q)}}, \tag{A.14}$$

which is a new term involving the Lagrange multiplier μ. Thus, we can solve the equation $\{H_{\mathrm{primary}}, \tilde{c}(u)\} = 0$ for μ.

It follows that no new terms are produced not involving μ^j, μ_j, μ in this second iteration step. Consequently, the full set of (primary and secondary) constraints is given by c^{tot}, c_a^{tot}, $\tilde{c}$, Z_j, Z^j, Z, z_a and z and it remains to classify them into first and second class. Obviously,

$$\begin{aligned}\{Z^j(x), Z_k(y)\} &= P\delta_k^j\ \delta(x, y), \\ \{Z(x), \tilde{c}(y)\} &= \frac{\frac{nP^2}{\rho^3}}{\sqrt{\det(q)}}\ \delta(x, y)\end{aligned} \tag{A.15}$$

do not vanish on the constraint surface defined by the final set of constraints; hence they are second class constraints. Since n appears only linearly in $\tilde{c}$ and n^a does not appear at all, it follows that z, z_a are first class.

Let us consider the linear combination

$$\begin{aligned}\tilde{c}_a^{\mathrm{tot}} &\equiv I\rho_{,a} + I^jW_{j,a} + PT_{,a} + P_jS^j_{,a} + pn_{,a} + \mathcal{L}_{\vec{n}}p_a + c_a \\ &= c_a^{\mathrm{tot}} + Z\rho_{,a} + Z^jW_{j,a} + Z_jS^j_{,a} + zn_{,a} + \mathcal{L}_{\vec{n}}z_a\end{aligned} \tag{A.16}$$

where

$$c_a \equiv c_a^{\mathrm{geo}} + c_a^{\mathrm{matter}} \tag{A.17}$$

is the non-dust contribution to the spatial diffeomorphism constraint c_a^{tot}. Since all constraints are scalar or covector densities of weight one and $\tilde{c}_a^{\mathrm{tot}}$ is the generator of spatial diffeomorphisms, it follows that $\tilde{c}_a^{\mathrm{tot}}$ is first class. Finally, we consider as an Ansatz the linear combination

$$\tilde{c}^{\mathrm{tot}} \equiv c^{\mathrm{tot}} + \alpha^jZ_j + \alpha_jZ^j + \alpha Z, \tag{A.18}$$

and determine the phase space functions α^j, α_j, α such that $\tilde{c}^{\mathrm{tot}}$ has vanishing Poisson brackets with Z_j, Z^j, Z up to terms proportional to Z_j, Z^j, Z.

We have

$$\begin{aligned}\{\tilde{c}^{\mathrm{tot}}(x), Z_j(y)\} &= \{c^{\mathrm{tot}}(x), Z_j(y)\} + \alpha_k(x)\{Z^k(x), Z_k(y)\} \\ &= \{c^{\mathrm{tot}}(x), Z_j(y)\} + \alpha_j(x)P(x)\delta^3(x, y).\end{aligned} \tag{A.19}$$

where we used equation (A.15) in the last line. Solving this equation for α_j we end up with

$$\alpha_j(x) = -\int d^3y \frac{1}{P(y)}\{c^{\text{tot}}(x), Z_j(y)\} = \left(\frac{1}{P}\sqrt{\det(q)}\,\rho\, q^{ab}U_b W_{j,a}\right)(x), \tag{A.20}$$

which is a sensible expression since $\{c^{\text{tot}}(x), Z_k(y)\} \sim \delta^3(x, y)$. For the Poisson bracket involving Z^j we get

$$\begin{aligned}\{\tilde{c}^{\text{tot}}(x), Z^j(y)\} &= \{c^{\text{tot}}(x), Z^j(y)\} + \alpha^k(x)\{Z_k(x), Z^j(y)\}\\ &= \{c^{\text{tot}}(x), Z_j(y)\} - \alpha^j(x)P(x)\delta^3(x, y)\end{aligned} \tag{A.21}$$

such that this equation can be solved for α^j explicitly given by

$$\alpha^j(x) = \int d^3y \frac{1}{P(y)}\{c^{\text{tot}}(x), Z^j(y)\} = \left(\frac{1}{P}\rho\sqrt{\det(q)}q^{bc}U_b S^j_{,c}\right)(x). \tag{A.22}$$

Finally, for Z we obtain

$$\{\tilde{c}^{\text{tot}}(x), Z(y)\} = \{c^{\text{tot}}(x), Z(y)\} \sim \tilde{c} \approx 0. \tag{A.23}$$

Hence this Poisson bracket vanishes weakly. Considering now the Poisson bracket between $\tilde{c}$ and $\tilde{c}^{\text{tot}}$ we get

$$\begin{aligned}\{\tilde{c}^{\text{tot}}(x), \tilde{c}(y)\} = \{c^{\text{tot}}(x), \tilde{c}(y)\} &+ \alpha^j(x)\{Z_j(x), \tilde{c}(y)\}\\ &+ \alpha_j(x)\{Z^j(x), \tilde{c}(y)\} + \alpha(x)\{Z(x), \tilde{c}(y)\}.\end{aligned} \tag{A.24}$$

The results of the last three individual Poisson brackets occurring above are listed below:

$$\begin{aligned}\{Z_j(x), \tilde{c}(y)\} &= \left(n\sqrt{\det(q)}q^{ab}U_a W_j P\right)(y)\frac{\partial}{\partial y^b}\delta^3(x, y)\\ \{Z^j(x), \tilde{c}(y)\} &= -\left(n\sqrt{\det(q)}q^{ab}U_a P S^j_{,b}\right)(y)\delta^3(x, y)\\ \{Z(x), \tilde{c}(y)\} &= \left(\frac{nP^2}{\rho^3\sqrt{\det(q)}}\right)(y)\delta^3(x, y).\end{aligned} \tag{A.25}$$

Now, we can solve equation (A.23) for α which yields

$$\alpha(x) = -\int d^3y \frac{\rho^3\sqrt{\det(q)}}{nP^2}(y)\{c^{\text{tot}}(x), \tilde{c}(y)\} \tag{A.26}$$

$$\begin{aligned}&-\left(\frac{\rho^3\sqrt{\det(q)}}{nP^2}\left[n\sqrt{\det(q)}q^{ab}U_a W_j P\right]_{,b}\frac{1}{P}\rho\sqrt{\det(q)}q^{bc}U_b S^j_{,c}\right)(x)\\ &-\left(\frac{\rho^3\sqrt{\det(q)}}{nP^2}\left(n\sqrt{\det(q)}q^{ab}U_a P S^j_{,b}\right)\frac{1}{P}\sqrt{\det(q)}\,\rho\, q^{ab}U_b W_{j,a}\right)(x).\end{aligned} \tag{A.27}$$

Here we reinserted the expressions for α_j and α^j derived before. The final step which includes the construction of the Dirac bracket can again be found in the main text.

Appendix B. Comparison with symplectic reduction

The spatial diffeomorphism invariant quantities

$$(\tilde{\xi}(\sigma), \tilde{\pi}(\sigma)), \qquad (\tilde{T}(\sigma), \tilde{P}(\sigma)), \qquad (\tilde{q}_{ij}(\sigma), \tilde{p}^{ij}(\sigma)) \tag{B.1}$$

shown in equation (3.30) are also obtained in [12] through symplectic reduction which is an alternative method to show that the pairs in (3.30) are conjugate.

To see how this works, we compute

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{T}(\sigma) &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{X}} \mathrm{d}^3x\, \det(\partial S/\partial x)\delta(S(x),\sigma)T(x) \\
&= \int_{\mathcal{X}} \mathrm{d}^3x\, \det(\partial S/\partial x)\Bigg(\delta(S(x),\sigma)\left[\frac{\mathrm{d}}{\mathrm{d}t}T(x)\right] + S^a_j(x)\left[\frac{\mathrm{d}}{\mathrm{d}t}S^j_{,a}(x)\right]\delta(S(x),\sigma)T(x) \\
&\quad + \left[\frac{\mathrm{d}}{\mathrm{d}t}S^j(x)\right]\left[\frac{\partial\delta(\sigma',\sigma)}{\partial\sigma^{j'}}\right]_{\sigma'=S(x)} T(x)\Bigg) \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}t}T(x)\right]_{S(x)=\sigma} + \int_{\mathcal{X}} \mathrm{d}^3x\, \det(\partial S/\partial x)\left[\frac{\mathrm{d}}{\mathrm{d}t}S^j(x)\right]\Bigg(-S^a_j(x)\partial_a\left[\delta(S(x),\sigma)T(x)\right] \\
&\quad + \left[\frac{\partial}{\delta(\sigma',\sigma)}\partial\sigma^{j'}\right]_{\sigma'=S(x)} T(x)\Bigg) \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}t}T(x)\right]_{S(x)=\sigma} - \int_{\mathcal{X}} \mathrm{d}^3x\, \det(\partial S/\partial x)\delta(S(x),\sigma)\left[\frac{\mathrm{d}}{\mathrm{d}t}S^j(x)\right] S^a_j(x)T_{,a}(x) \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}t}T(x) - \left(\frac{\mathrm{d}}{\mathrm{d}t}S^j(x)\right) S^a_j(x)T_{,a}(x)\right]_{S(x)=\sigma}
\end{aligned}
\tag{B.2}
$$

where we have used $\partial_a[S^a_j \det(\partial S/\partial x)] = 0$. Exactly the same calculation reveals

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\xi}(\sigma) &= \left[\frac{\mathrm{d}}{\mathrm{d}t}\xi(x) - \left(\frac{\mathrm{d}}{\mathrm{d}t}S^j(x)\right) S^a_j(x)\xi_{,a}(x)\right]_{S(x)=\sigma} \\
\frac{\mathrm{d}}{\mathrm{d}t}\tilde{q}_{jk}(\sigma) &= \left[\frac{\mathrm{d}}{\mathrm{d}t}q_{jk}(x) - \left(\frac{\mathrm{d}}{\mathrm{d}t}S^l(x)\right) S^a_l(x)q_{jk,a}(x)\right]_{S(x)=\sigma}.
\end{aligned}
\tag{B.3}
$$

Using (B.2) and (B.3) we can now rewrite the symplectic potential in terms of the spatially diffeomorphism invariant variables as follows: $(\dot{\cdot}) := \frac{\mathrm{d}}{\mathrm{d}t}(\cdot)$ and $J = \det(\partial S/\partial x)$):

$$
\begin{aligned}
\Theta &= \int_{\mathcal{X}} \mathrm{d}^3x\left[\dot{\xi}\pi + \dot{T}P + \dot{S}^jP_j + \dot{q}_{ab}p^{ab}\right] \\
&= \int_{\mathcal{X}} \mathrm{d}^3x\left[\dot{\xi}\pi + \dot{T}P + \dot{S}^jP_j + \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(q_{jk}S^j_{,a}S^k_{,b}\right)\right)p^{ab}\right] \\
&= \int_{\mathcal{X}} \mathrm{d}^3x\left[\dot{\xi}\pi + \dot{T}P + \dot{S}^jP_j + \dot{q}_{jk}\left(S^j_{,a}S^k_{,b}p^{ab}\right) + 2q_{jk}\dot{S}^j_{,a}S^k_{,b}p^{ab}\right] \\
&= \int_{\mathcal{X}} \mathrm{d}^3x\left[\dot{\xi}\pi + \dot{T}P + \dot{S}^jP_j + \dot{q}_{jk}\left(S^j_{,a}S^k_{,b}p^{ab}\right) - 2\dot{S}^j\partial_a\left(q_{jk}S^k_{,b}p^{ab}\right)\right] \\
&= \int_{\mathcal{X}} J\mathrm{d}^3x\left[\dot{\xi}\frac{\pi}{J} + \dot{T}\frac{P}{J} + \dot{q}_{jk}\frac{S^j_{,a}S^k_{,b}p^{ab}}{J}\right] + \int_{\mathcal{X}} \mathrm{d}^3x\,\dot{S}^j\left[P_j - 2\partial_a\left(q_{bc}S^c_jp^{ab}\right)\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma\,\tilde{\pi}[[\dot{\xi}]_{S(x)=\sigma} + \tilde{P}[\dot{T}]_{S(x)=\sigma} + \tilde{p}^{jk}[\dot{q}_{jk}]_{S(x)=\sigma}] + \int_{\mathcal{X}} \mathrm{d}^3x\,\dot{S}^j[P_j - 2\partial_a(q_{bc}S^c_jp^{ab})] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma[\tilde{\dot{\xi}}\tilde{\pi} + \tilde{\dot{T}}\widetilde{P} + \tilde{\dot{q}}_{jk}\tilde{p}^{jk}] \\
&\quad + \int_{\mathcal{X}} \mathrm{d}^3x\;\dot{S}^j\;\left[P_j + S^a_j\left(\pi\;\xi_{,a} + PT_{,a} + p^{bc}S^k_{,b}S^l_{,c}S^a_jq_{kl,a}\right) - 2\partial_a\left(q_{bc}S^c_jp^{ab}\right)\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma[\dot{\tilde{\xi}}\tilde{\pi} + \dot{\widetilde{T}}\widetilde{P} + \dot{\tilde{q}}_{jk}\tilde{p}^{jk}]
\end{aligned}
$$

$$+\int_{\mathcal{X}} \mathrm{d}^3x\, \dot{S}^j \left[P_j + S^a_j\left(\pi\ \xi_{,a} + PT_{,a} + p^{bc}S^k_{,b}S^l_{,c}\partial_a\left(S^e_k S^f_l q_{ef}\right)\right) - 2\partial_a\left(q_{bc}S^c_j\ \ p^{ab}\right)\right]$$
$$= \int_{\mathcal{S}} \mathrm{d}^3\sigma[\dot{\tilde{\xi}}\ \tilde{\pi} + \dot{\tilde{T}}\ \widetilde{P} + \dot{\tilde{q}}_{jk}\tilde{p}^{jk}]$$
$$+\int_{\mathcal{X}} \mathrm{d}^3x\, \dot{S}^j\ \left[P_j + S^a_j\left(\pi\ \xi_{,a} + PT_{,a} + p^{bc}\left(q_{bc,a} + 2q_{ec}S^k_{,b}S^e_{k,a}\right)\right) - 2\partial_a\left(q_{bc}S^c_j\ \ p^{ab}\right)\right]$$
$$= \int_{\mathcal{S}} \mathrm{d}^3\sigma[\dot{\tilde{\xi}}\tilde{\pi} + \dot{\tilde{T}}\ \widetilde{P} + \dot{\tilde{q}}_{jk}\tilde{p}^{jk}]$$
$$+\int_{\mathcal{X}} \mathrm{d}^3x\ \dot{S}^j\left[P_j + S^a_j\left(\pi\ \xi_{,a} + PT_{,a} + -2\left[q_{ab}\partial_c p^{bc} + \frac{1}{2}\left(2q_{a(b,c)} - q_{bc,a}\right)p^{bc}\right]\right)\right]$$
$$= \int_{\mathcal{S}} \mathrm{d}^3\sigma[\dot{\tilde{\xi}}\ \tilde{\pi} + \dot{\tilde{T}}\ \widetilde{P} + \dot{\tilde{q}}_{jk}\tilde{p}^{jk}] + \int_{\mathcal{X}} \mathrm{d}^3x\ \dot{S}^j\left[P_j + S^a_j\left(\pi\ \xi_{,a} + PT_{,a} + -2q_{ab}D_c p^{bc}\right)\right]$$
$$= \int_{\mathcal{S}} \mathrm{d}^3\sigma[\dot{\tilde{\xi}}\ \tilde{\pi} + \dot{\tilde{T}}\ \widetilde{P} + \dot{\tilde{q}}_{jk}\tilde{p}^{jk}] + \int_{\mathcal{X}} \mathrm{d}^3x\ \dot{S}^j\ S^j_a c^{\mathrm{tot}}_a \tag{B.4}$$

where we used

$$S^a_j S^k_{,b} S^e_{k,a} = -S^a_j S^k_{,ba} S^e_k = -S^a_j S^k_{,ab} S^e_k = S^a_{j,b} S^k_{,a} S^e_k = S^e_{j,b} \tag{B.5}$$

as well as the definition of the Christoffel symbol in the second to last step (note that p^{ab} is a tensor density so that $D_b p^{ab} = \partial_b p^{ab} + \Gamma^a_{bc} p^{bc}$).

Formula (B.4) means that on the full phase space we can switch to the new canonical pairs (B.1) on $\mathcal{X}$ and the canonical pair $\left(S^j, P'_j = S^a_j c^{\mathrm{tot}}_a = c^{\mathrm{tot}}_j\right)$. The pairs (B.1) are thus c^{tot}_j invariant while S^j is pure gauge. The symplectic reduction of the full phase space with respect to c^{tot}_j is therefore precisely coordinatized by (B.1) which is identical to equation (3.30) in the main text.

Appendix C. Effective action and fixed point equation

The aim of the present section is to derive, at least in implicit form, the Lagrangian that corresponds canonically to the physical Hamiltonian. This can be done by calculating the inverse Legendre transform[37] and leads to a fixed point equation, which can be solved order by order, in principle. Interestingly, the Lagrangian turns out to be local in dust time, but will be non-local in dust space. However, the Hamiltonian description is completely local.

The inverse Legendre transform requires to solve for the momenta $P^{jk}(\sigma)$, $\Pi(\sigma)$ in terms of the corresponding velocities $V_{jk}(\sigma)$, $\Upsilon(\sigma)$, respectively, defined by[38]

$$\begin{aligned} V_{jk}(\sigma) &\equiv \dot{Q}_{jk}(\sigma) = \{\mathbf{H}, Q_{jk}(\sigma)\} \\ \Upsilon(\sigma) &\equiv \dot{\Xi}(\sigma) = \{\mathbf{H}, \Xi(\sigma)\}. \end{aligned} \tag{C.1}$$

This can be done by using the first-order equations of motion for $Q_{jk}(\sigma)$, $\Xi(\sigma)$, derived from the physical Hamiltonian $\mathbf{H}$. From the physical Hamiltonian $\mathbf{H}$ we obtain the Lagrangian

$$\mathbf{L}[Q, V; \Xi, \Upsilon] = \int_{\mathcal{S}} \mathrm{d}^3\sigma L(\sigma) = \int_{\mathcal{S}} \mathrm{d}^3\sigma\ \left[\left(\frac{1}{\kappa}P^{jk}V_{jk} + \frac{1}{\lambda}\Pi\Upsilon\right) - \mathbf{H}[Q, P; \Xi, \Pi]\right]_{(\mathrm{C.1})} \tag{C.2}$$

where it it is understood that the solution of (C.1) for P^{jk}, Π has to be inserted.

[37] This is possible because the Legendre transform is regular.

[38] Note that $\dot{Q}_{jk}$ and $\dot{\Xi}$ must be treated as independent variables in addition to Q_{jk} and Ξ.

With the dynamical lapse and shift given by $N = C/H$, $N_j = -C_j/H$, respectively, we obtain for P^{jk}

$$P^{jk} = \frac{\sqrt{\det(Q)}}{2N}[G^{-1}]^{jkmn}(\dot{Q}_{mn} - (\mathcal{L}_{\vec{N}}Q)_{mn}) = \sqrt{\det(Q)}[G^{-1}]^{jkmn}K_{mn}, \tag{C.3}$$

with K_{mn} denoting the extrinsic curvature. This leads to the following expression for the velocities V_{jk} and Υ:

$$V_{jk} = 2[NK_{jk} + D_{(j}N_{k)}] \qquad \text{and} \qquad \Upsilon = \frac{N}{\sqrt{\det(Q)}}\Pi + Q^{jk}N_j\, D_k\Xi. \tag{C.4}$$

We conclude

$$\begin{aligned}
\mathsf{L} &= \int_{\mathcal{S}} \mathrm{d}^3\sigma \left[\frac{1}{\kappa}V_{jk}P^{jk} + \frac{1}{\lambda}\Upsilon\Pi - H\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma \left[\frac{2}{\kappa}(NK_{jk} + D_{(j}N_{k)})P^{jk} + \left(N\frac{\Pi}{\lambda\sqrt{\det(Q)}} + N^jD_j\frac{\Xi}{\lambda}\right)\Pi - H\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma \left[N\left(\frac{2}{\kappa}K_{jk}P^{jk} + \frac{\Pi^2}{\lambda\sqrt{\det(Q)}}\right) + N^jC_j - H\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma \frac{1}{H}\left[C\left(\frac{2}{\kappa}K_{jk}P^{jk} + \frac{\Pi^2}{\lambda\sqrt{\det(Q)}}\right) - Q^{jk}C_jC_k - H^2\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma \frac{C}{H}\left[\frac{2}{\kappa}K_{jk}P^{jk} + \frac{\Pi^2}{\lambda\sqrt{\det(Q)}} - C\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma N\left[\frac{2}{\kappa}\sqrt{\det(Q)}\left(K_{jk}K^{jk} - \left(K_j^j\right)^2\right) + \frac{\Pi^2}{\lambda\sqrt{\det(Q)}} - C\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma N\sqrt{\det(Q)}\left[\frac{1}{\kappa}\left(K_{jk}K^{jk} - \left(K_j^j\right)^2 + R^{(3)}[Q] - 2\Lambda\right)\right. \\
&\quad \left. + \frac{1}{2\lambda}\left(\frac{\Pi^2}{\det(Q)} - [Q^{jk}\Xi_{,j}\Xi_{,k} + v(\Xi)]\right)\right] \\
&= \int_{\mathcal{S}} \mathrm{d}^3\sigma N\sqrt{\det(Q)}\left[\frac{1}{\kappa}\left(K_{jk}K^{jk} - \left(K_j^j\right)^2 + R^{(3)}[Q] - 2\Lambda\right)\right. \\
&\quad \left. + \frac{1}{2\lambda}((\nabla_u\Xi)^2 - (Q^{jk}\Xi_{,j}\Xi_{,k} + v(\Xi)))\right].
\end{aligned} \tag{C.5}$$

In the third step we performed an integration by parts and in the fourth step we substituted the expressions for dynamical lapse and shift, in the sixth we rewrote P^{jk} in terms of K_{jk}, in the seventh we substituted for C and in the last we introduced the vector field $u = \frac{1}{N}(\partial_\tau - N^j\partial_{\sigma^j})$.

If lapse and shift are independent variables, the final expression in (C.6) would coincide with the 3+1-decomposition of the Einstein–Hilbert term minimally coupled to a Klein–Gordon field with potential v! Since N_j is a constant of the physical motion and $N = \sqrt{1 + Q^{jk}N_jN_k}$, we could, in particular, consider the case $N_j = 0$, whence $N = 1$. In that case (C.5) would agree with the usual Lagrangian description on dust spacetime for a static foliation. However, fundamentally lapse and shift are not independent variables, and we must use this fact in (C.1) in order to solve for P^{jk}, Π. We now turn to this task.

By definition

$$N_j = -\frac{C_j}{H} = -\frac{C_j}{C}\frac{C}{H} = -\frac{C_j/\sqrt{\det(Q)}}{C/\sqrt{\det(Q)}}\sqrt{1 + Q^{jk}N_jN_k},$$

$$\frac{C_j}{\sqrt{\det(Q)}} = -\frac{2}{\kappa}\left(D_kK_j^k - D_jK_k^k\right) + \frac{1}{\lambda}(\nabla_u\Xi)\, D_j\Xi,$$

$$\frac{C}{\sqrt{\det(Q)}} = \frac{1}{\kappa}\left(K_{jk}K^{jk} - \left[K^j_j\right]^2 - R^{(3)}[Q]\right) + \frac{1}{2\lambda}\left((\nabla_u \Xi)^2 + Q^{jk}\Xi_{,j}\Xi_{,k} + v(\Xi)\right),$$
$$K_{jk} = \frac{1}{2\sqrt{1+Q^{jk}N_jN_k}}[V_{jk} - 2D_{(j}N_{k)}],$$
$$\nabla_u \Xi = \frac{1}{\sqrt{1+Q^{jk}N_jN_k}}[\Upsilon - Q^{jk}N_jD_k\Xi]. \tag{C.6}$$

The set of equations (C.6), when inserted into each other, yields an equation of the form

$$N_j = G_j[N_k; Q_{kl}, V_{kl}, \Xi, \Upsilon], \tag{C.7}$$

where G_j is a local function of its arguments and their spatial derivatives up to second order (in particular, second spatial derivatives of N_j). Since P^{jk}, Π are known in terms of $Q_{jk}, V_{jk}, \Xi, \Upsilon$, once N_j (and thus N) is known as a function of these arguments, we have reduced the task of performing the inverse Legendre transform to solving the *fixed point equation* (C.7).

Unfortunately, (C.7) is not algebraic in N_j, so a solution just by quadratures is impossible. Also, it represents a highly nonlinear system of partial differential equations of degree 2, so linear solution methods fail, as well. We leave the full investigation of this system for future research. However, the fact that it is a system of fixed point equations suggests to look for a solution by perturbative or fixed point methods.

(1) If we make the Ansatz that N_j is small, in an appropriate sense, then we may expand $G_j[N_k]$ around $N_k = 0$ to linear order and solve the resulting linear system of PDEs.

(2) The fixed point method suggests to write the solution in the form

$$N_j = G_j\big(G_{k_1}\big(G_{k_2}\big(\cdots\big(G_{k_n}(\cdots)\big)\cdots\big)\big)\big). \tag{C.8}$$

If convergence is under control, then an nth-order approximation may be given in the form

$$N_j^{(n)} = G_j\big(G_{k_1}\big(G_{k_2}\big(\cdots\big(G_{k_n}(0)\big)\cdots\big)\big)\big), \tag{C.9}$$

which consists in setting the starting point of the iteration at $N_j = 0$ (which is a reasonable guess if the exact solution is indeed small in an appropriate sense, having a *test clock* in mind) and to iterate n times. Expression (C.9) contains spatial derivatives of the metric of order up to $2(n+1)$, but is only of first order in τ-derivatives, thus establishing that the final Lagrangian is spatially non-local in dust space but temporally local in dust time.

Appendix D. Two routes to second time derivatives of linear perturbations

In this appendix we consider a general Hamiltonian system with canonical coordinates (q, p) and standard Poisson brackets $\{p, q\} = 1$ and a Hamiltonian function $H(q, p)$. We will consider only one degree of freedom but everything generalizes to an arbitrary number of degrees of freedom.

Lemma D.1. *Let* $(q_0(\tau), p_0(\tau))$ *be an exact solution of the Hamiltonian equations of motion*

$$\begin{aligned}\dot q_0(\tau) &= [\{H, q\}(q, p)]_{\substack{q=q_0(\tau)\\ p=p_0(\tau)}}\\ \dot p_0(\tau) &= [\{H, p\}(q, p)]_{\substack{q=q_0(\tau)\\ p=p_0(\tau)}}.\end{aligned} \tag{D.1}$$

Define the perturbations $\delta q := q - q_0(\tau), \delta p := p - p_0(\tau)$. *Let* $H(q, p) = \sum_{n=0}^{\infty} H^{(n)}$ *be the expansion of H(q, p) around* $q_0(\tau), p_0(\tau)$ *in terms of the perturbations where* $H^{(n)}$ *is the nth-order term in terms of the perturbations. Then*

(1) *expanding the full Hamiltonian equations of motion for* $\dot{q}$, $\dot{p}$ *to linear order is equivalent to using the function* $H^{(2)}$ *as a Hamiltonian for the perturbations;*
(2) *expanding the equation for* $\ddot{q}$ *to linear order is equivalent to the equations for* $\dot{\delta q} = \delta\dot{q}$, $\dot{\delta p} = \delta\dot{p}$ *to linear order.*

Proof. Note that $q_0(\tau)$, $p_0(\tau)$ do not carry any phase space dependence in contrast to δq, δp. Therefore $\{\delta q, \delta q\} = \{\delta p, \delta p\} = 0$ and $\{\delta p, \delta q\} = 1$.

(1) Consider the full Hamiltonian equations of motion for a general solution $(q(\tau), p(\tau))$:

$$\dot{q}(\tau) = H_{,p}(q(\tau), p(\tau)) \qquad \text{and} \qquad \dot{p}(\tau) = -H_{,p}(q(\tau), p(\tau)) \tag{D.2}$$

where $H_{,q} = \partial H/\partial q$, $H_{,p} = \partial H/\partial p$. We set $\delta q(\tau) = q(\tau) - q_0(\tau)$ and $\delta p(\tau) = p(\tau) - p_0(\tau)$. Subtracting from (D.2) the equations for $(q_0(\tau), p_0(\tau))$ we obtain

$$\begin{aligned}\dot{\delta q}(\tau) &= H_{,p}(q(\tau), p(\tau)) - H_{,p}(q_0(\tau), p_0(\tau))\\ \delta\dot{p}(\tau) &= -H_{,q}(q(\tau), p(\tau)) + H_{,q}(q_0(\tau), p_0(\tau)),\end{aligned} \tag{D.3}$$

which is still exact. Expanding the right-hand side of (D.3) to first order in $\delta q(\tau)$, $\delta p(\tau)$ we find

$$\begin{aligned}\delta\dot{q}(\tau) &= H_{,pq}(q_0(\tau), p_0(\tau))\delta q(\tau) + H_{,pp}(q_0(\tau), p_0(\tau))\delta p(\tau)\\ \delta\dot{p}(\tau) &= -H_{,qq}(q_0(\tau), p_0(\tau))\delta q(\tau) - H_{,qp}(q_0(\tau), p_0(\tau))\delta p(\tau).\end{aligned} \tag{D.4}$$

On the other hand, we have

$$\begin{aligned}H^{(2)} = \frac{1}{2}H_{,qq}(q_0(\tau), p_0(\tau))[\delta q]^2 &+ \frac{1}{2}H_{,pp}(q_0(\tau), p_0(\tau))[\delta p]^2\\ &+ H_{,qp}(q_0(\tau), p_0(\tau))[\delta q][\delta p].\end{aligned} \tag{D.5}$$

Then it is trivial to check that (D.4) is reproduced by

$$\delta\dot{q}(\tau) = \{H^{(2)}, \delta q\}_{\substack{\delta q=\delta q(\tau)\\ \delta p=\delta p(\tau)}} \qquad \text{and} \qquad \delta\dot{p}(\tau) = \{H^{(2)}, \delta p\}_{\substack{\delta q=\delta q(\tau)\\ \delta p=\delta p(\tau)}}. \tag{D.6}$$

(2) Let $p(\tau) = F(q(\tau), \dot{q}(\tau))$ be the solution of solving $\dot{q}(\tau) = H_{,p}(q(\tau), p(\tau))$ for $p(\tau)$. Then

$$\begin{aligned}\ddot{q}(\tau) &= H_{,pq}(q(\tau), p(\tau))\dot{q}(\tau) + H_{,pp}(q(\tau), p(\tau))\dot{p}(\tau)\\ &= H_{,pq}(q(\tau), p(\tau))\dot{q}(\tau) - H_{,pp}(q(\tau), p(\tau))H_{,q}(q(\tau), p(\tau))\\ &= H_{,pq}(q(\tau), F(q(\tau), \dot{q}(\tau)))\dot{q}(\tau) - H_{,pp}(q(\tau), F(q(\tau), \dot{q}(\tau)))\\ &\quad\times H_{,q}(q(\tau), F(q(\tau), \dot{q}(\tau)))\\ &= G(q(\tau), \dot{q}(\tau)).\end{aligned} \tag{D.7}$$

Equation (D.7) is what we mean by the $\ddot{q}(\tau)$ form of the equations of motion, i.e. an equation only involving $q, \dot{q}, \ddot{q}$ but no longer the momentum. Subtracting from (D.7) the corresponding equation for $\ddot{q}_0(\tau)$ and expanding the right-hand side to first order we obtain with $G = G(q, v)$

$$\ddot{\delta q}(\tau) = G_{,q}(q_0(\tau), \dot{q}_0(\tau))\delta q(\tau) + G_{,v}(q_0(\tau), \dot{q}_0(\tau))\delta\dot{q}(\tau). \tag{D.8}$$

Now

$$\begin{aligned}G_{,q}(q, v) = [H_{,pqq}(q, p)v &- H_{,ppq}(q, p)H_{,q}(q, p) - [H_{,pp}(q, p)H_{,qq}(q, p)]_{p=F(q,v)}\\ &+ [H_{,ppq}(q, p)v - H_{,ppp}(q, p)H_{,q}(q, p)\\ &- H_{,pp}(q, p)H_{,pq}(q, p)]_{p=F(q,v)}F_{,q}(q, v)\\ G_{,v}(q, v) = H_{,pq}(q, p) &+ [H_{,ppq}(q, p)v - H_{,ppp}(q, p)H_{,q}(q, p)\\ &- H_{,pp}(q, p)H_{,pq}(q, p)]_{p=F(q,v)}F_{,v}(q, v).\end{aligned} \tag{D.9}$$

Since $v = H_{,p}(q, F(q, v))$ is an identity we obtain

$$1 = H_{,pp}(q, F(q, v))F_{,v}(q, v) \quad \text{and}$$
$$0 = H_{,pq}(q, F(q, v)) + H_{,pp}(q, F(q, v))F_{,q}(q, v) \tag{D.10}$$

by taking the derivative with respect to the independent variables v, q respectively. This way we can eliminate the derivatives of F:

$$F_{,v}(q, v) = \frac{1}{H_{,pp}(q, F(q, v))} \qquad \text{and} \qquad F_{,q}(q, v) = -\frac{H_{,pq}(q, F(q, v))}{H_{,pp}(q, F(q, v))}. \tag{D.11}$$

Substituting (D.11) into (D.9) we obtain the simplified expressions

$$G_{,v}(q, v) = \left[\left(\frac{H_{,ppq}v - H_{,ppp}H_{,q}}{H_{,pp}}\right)(q, p)\right]_{p=F(q,v)}$$
$$\begin{aligned} G_{,q}(q, v) = {} & [H_{,pqq}(q, p)v - H_{,ppq}(q, p)H_{,q}(q, p) - H_{,pp}(q, p)H_{,qq}(q, p)]_{p=F(q,v)} \\ & -[H_{,ppq}(q, p)v - H_{,ppp}(q, p)H_{,q}(q, p) \\ & - H_{,pp}(q, p)H_{,pq}(q, p)]_{p=F(q,v)}\frac{H_{,pq}}{H_{,pp}}. \end{aligned} \tag{D.12}$$

Now we invert the second equation in (D.4) for δp and obtain

$$\delta p(\tau) = \frac{\delta\dot{q}(\tau) - H_{,pq}(q_0(\tau), p_0(\tau))\delta q(\tau)}{H_{,pp}(q_0(\tau), p_0(\tau)}. \tag{D.13}$$

Taking the time derivative of the first equation in (D.4) and using (D.13) yields after some algebra

$$\begin{aligned} \delta\ddot{q}(\tau) = {} & \left[\dot{H}_{,pq} - H_{,pp}H_{,qq} - \frac{H_{,pq}(\dot{H}_{,pp} - H_{,pp}H_{,pq})}{H_{,pp}}\right](q_0(\tau), p_0(\tau))\delta q(\tau) \\ & + \left[\frac{\dot{H}_{,pp}}{H_{,pp}}\right](q_0(\tau), p_0(\tau))\delta\dot{q}(\tau) \end{aligned} \tag{D.14}$$

where e.g. $\dot{H}_{,pp}(q_0(\tau), p_0(\tau) := \frac{\mathrm{d}}{\mathrm{d}\tau}H_{,pp}(q_0(\tau), p_0(\tau)$. Carrying out the remaining time derivatives in (D.14) and comparing with (D.8) evaluated with the help of (D.12) at $q = q_0(\tau)$, $v = \dot{q}_0(\tau) = H_{,p}(q_0(\tau), p_0(\tau)$ we see that the expressions coincide. □

Appendix E. Constants of the motion of *n*th-order perturbation theory

In this section we will show that for any fully conserved quantity F of a Hamiltonian system with Hamiltonian H, when expanding both the equations of motion and F to order n, then F is still a constant of motion up to terms of order $n + 1$.

Let $m_0(\tau) = (q_0(\tau), p_0(\tau))$ be an exact solution of a Hamiltonian system with canonical coordinates $m = (q, p)$, non-vanishing Poisson brackets $\{p, q\} = 1$ and Hamiltonian $H = H(m) = H(q, p)$. Define $\delta m = m - m_0(\tau)$. Since $m_0(\tau)$ is just a number (for fixed τ) we immediately have the non-vanishing Poisson brackets $\{\delta p, \delta q\} = 1$. For any function F on phase space we consider its Taylor expansion around $m_0(\tau)$ given by

$$F(m) = \sum_{n=0}^{\infty} F^{(n)}(m_0(\tau); \delta m) \tag{E.1}$$

where $F^{(n)}(m_0(\tau); \delta m)$ is a homogeneous polynomial of degree n in δm whose coefficients depend explicitly on the background solution $m_0(\tau)$, that is

$$F^{(n)}(m_0(\tau); \delta m) = \sum_{k=0}^{n} \frac{1}{k!(n-k)!}\left[\frac{\partial^b F}{[\partial q]^k\,[\partial p]^{n-k}}\right](m_0(\tau))\,[\delta q]^k\,[\delta p]^{n-k}. \tag{E.2}$$

Lemma E.1. *The Poisson bracket $\{F, G\}$ can be computed either by first expanding F, G as in (E.1) and then using the Poisson bracket for δm or by using the Poisson bracket for m and then expanding the result as in (E.1).*

Proof. The proof is elementary: since

$$F = \sum_{k,l=0}^{\infty} \frac{1}{k!\,l!} \left[\frac{\partial^{k+l} F}{[\partial q]^k\,[\partial p]^l}\right](m_0(\tau))[\delta q]^k[\delta p]^l, \tag{E.3}$$

we have with the substitution of F by $F_{,q}$

$$F_{,q} = \sum_{k,l=0}^{\infty} \frac{1}{k!\,l!} \left[\frac{\partial^{k+l+1} F}{[\partial q]^{k+1}[\partial p]^l}\right](m_0(\tau))[\delta q]^k[\delta p]^l = F_{,\delta q} \tag{E.4}$$

and similarly $F_{,p} = F_{,\delta p}$. Since one computes Poisson brackets the first way by first expanding and then taking derivatives with respect to $\delta q, \delta p$ while the second way we compute Poisson brackets with respect to q, p and then expand, the assertion follows. □

Lemma E.2. *Suppose we expand the Hamiltonian to nth order in δm with $n \geqslant 1$. Suppose also that F is an exact constant of the motion with respect to the Hamiltonian H. Then:*

(1) The equations of motion up to order n for δm are generated by the Hamiltonian

$$H_n = \sum_{k=2}^{n+1} H^{(k)}. \tag{E.5}$$

(2) The perturbation up to order n of F given by

$$F_n := \sum_{k=1}^{n} F^{(n)} \tag{E.6}$$

is a constant of motion with respect to H_n up to terms of order at least $n + 1$.

Note that the Hamiltonian starts at order 2 and ends at order $n + 1$.

Proof.

(1) Let $m(t)$ be any solution of the exact equation of motion. We have for example

$$\dot{q}(\tau) = [\{H, q\}]_{m=m(\tau)}. \tag{E.7}$$

Subtracting the same equation for $m_0(\tau)$ and setting $\delta q(\tau) = q(\tau) - q_0(\tau)$ we find

$$\delta\dot{q}(\tau) = [\{H, q\}]_{m=m(\tau)} - [\{H, q\}]_{m=m_0(\tau)} = \sum_{k=2}^{\infty} H^{(k)}_{,\delta p} \tag{E.8}$$

from which the assertion follows immediately (the proof for δp is identical).

(2) Using the explicit background dependence of $F^{(k)} = F^{(k)}(m_0(\tau); \delta m(\tau))$ we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau} F^{(k)} &= \frac{\partial F^{(k)}}{\partial q_0}\dot{q}_0(\tau) + \frac{\partial F^{(k)}}{\partial p_0}\dot{p}_0(\tau) + \frac{\partial F^{(k)}}{\partial \delta q}\delta\dot{q}(\tau) + \frac{\partial F^{(k)}}{\partial \delta p}\delta\dot{p}(\tau) \\ &= \frac{\partial F^{(k)}}{\partial q_0}\frac{\partial H^{(1)}}{\partial \delta p} - \frac{\partial F^{(k)}}{\partial p_0}\frac{\partial H^{(1)}}{\partial \delta q} + \frac{\partial F^{(k)}}{\partial \delta q}\frac{\partial H_n}{\partial \delta p} - \frac{\partial F^{(k)}}{\partial \delta p}\frac{\partial H_n}{\partial \delta q}\end{aligned} \tag{E.9}$$

where we used the first part of the lemma as well as the fact that $H_{,q}(m_0) = H^{(1)}_{,\delta q}$, $H_{,p}(m_0) = H^{(1)}_{,\delta p}$. All Poisson brackets are with respect to the coordinates $\delta q, \delta p$.

Now observe the important fact

$$
\begin{aligned}
F^{(k)}_{,q_0} &= \sum_{l=0}^{k} \frac{1}{l!(k-l)!} \frac{\partial^{k+1} F}{[\partial q]^{l+1}\,[\partial p]^{(k+1)-(l+1)}} [\delta q]^l\,[\delta p]^{(k+1)-(l+1)} \\
&= \frac{\partial}{\partial \delta q} \sum_{l=0}^{k} \frac{1}{(l+1)!((k+1)-(l+1))!} \frac{\partial^{k+1} F}{[\partial q]^{l+1}\,[\partial p]^{(k+1)-(l+1)}} [\delta q]^{l+1}\,[\delta p]^{(k+1)-(l+1)} \\
&= \frac{\partial}{\partial \delta q} \sum_{l=1}^{k+1} \frac{1}{l!(k+1-l)!} \frac{\partial^{k+1} F}{[\partial q]^{l}\,[\partial p]^{k+1-l}} [\delta q]^{l}\,[\delta p]^{k+1-l} \\
&= \frac{\partial}{\partial \delta q} \left[F^{(k+1)} - \frac{1}{(k+1)!} \frac{\partial^{k+1} F}{[\partial p]^{k+1}} [\delta p]^{k+1} \right] \\
&= F^{(k+1)}_{,\delta q}
\end{aligned}
\tag{E.10}
$$

and similarly $F^{(k)}_{,p_0} = F^{(k+1)}_{,\delta p}$.

Combining (E.9) and (E.10) we see that

$$
\frac{\mathrm{d}F^{(k)}}{\mathrm{d}\tau} = \{H^{(1)}, F^{(k+1)}\} + \{H_n, F^{(k)}\}
\tag{E.11}
$$

Hence

$$
\frac{\mathrm{d}F_n}{\mathrm{d}\tau} = \sum_{k=1}^{n} \left[\{H^{(1)}, F^{(k+1)}\} + \sum_{l=2}^{n+1} \{H^{(l)}, F^{(k)}\} \right].
\tag{E.12}
$$

We would like to show that the terms up to order n in (E.12) vanish identically. Since $\{H^{(l)}, F^{(k)}\}$ is of order $k+l-2$, for given k we can restrict the sum over l from $l = 2$ until $n+2-k$ up to terms of order $O(\delta^{n+1})$. Note that $n+2-k$ is at least 2 (for $k = n$) and at most $n+1$ (for $k = 1$) for all values of k which is the allowed range of l. It follows

$$
\begin{aligned}
\frac{\mathrm{d}F_n}{\mathrm{d}\tau} + O(\delta^{n+1}) &= \sum_{k=1}^{n} \left[\{H^{(1)}, F^{(k+1)}\} + \sum_{l=2}^{n+2-k} \{H^{(l)}, F^{(k)}\} \right] \\
&= \sum_{k=1}^{n} \left[\{H^{(1)}, F^{(k+1)}\} + \sum_{r=k}^{n} \{H^{(r-k+2)}, F^{(k)}\} \right] \\
&= \sum_{r=1}^{n} \left[\{H^{(1)}, F^{(r+1)}\} + \sum_{k=1}^{r} \{H^{(r-k+2)}, F^{(k)}\} \right] \\
&= \sum_{r=1}^{n} \sum_{k=1}^{r+1} \{H^{(r-k+2)}, F^{(k)}\}
\end{aligned}
\tag{E.13}
$$

where in the second step we have introduced the summation variable $r = k + l - 2$ which for given k takes range in $k, \ldots, n$ (lowest value for $l = 2$ and highest value for $l = n+2-k$) whence $l = r - k + 2$, in the third step we have changed the order of the k and r summation in the second term (keeping in mind the constraint $1 \leqslant k \leqslant r \leqslant n$) while the summation variable k was renamed by r in the first term and in the fourth step we noted that the first and second term can be combined by having the k summation extend to $r+1$.

Now we exploit the fact that F is an exact invariant, that is

$$
0 = \{H, F\} = \sum_{k,l=1}^{\infty} \{H^{(l)}, F^{(k)}\} = \sum_{r=0}^{\infty} \left[\sum_{k=1}^{r+1} \{H^{(r-k+2)}, F^{(k)}\} \right]
\tag{E.14}
$$

where in the second step we collected all terms of order r (note that $l = r - k + 2 \geqslant 1$ as required). Since (E.13) is an identity on the entire phase space, the Taylor coefficients of $[\delta q]^k[\delta p]^l$ have to vanish separately for all $k, l \geqslant 0$. The term corresponding to order r in (E.13) contains *all* terms of the form $[\delta q]^s[\delta p]^{r-s}$, $s = 0, \ldots, r$. Therefore we conclude

$$\sum_{k=1}^{r+1}\{H^{(r-k+2)}, F^{(k)}\} = 0 \tag{E.15}$$

identically for all r. In particular, (E.13) implies

$$\frac{\mathrm{d}F_n}{\mathrm{d}\tau} = O(\delta^{n+1}). \tag{E.16}$$

$\square$

The only n for which the term $O(\delta^{n+1})$ vanishes is for $n = 1$ as one can see from (E.12) since then $k = 1, l = 2$ can only take one value which already contributes to order $r = 1$. Thus for $n = 1$ we even have

$$\frac{\mathrm{d}F_1}{\mathrm{d}\tau} = 0. \tag{E.17}$$

It is instructive to see how the background equations find their way into demonstrating the important result (E.16) which ensures that an exact invariant expanded up to order n remains an invariant up to higher orders for the equations of motion expanded up to order n, thus simplifying the task to integrate those equations of motion.

Appendix F. Generalization to other deparametrizing matter

In this work dust was used as a reference frame in order to define a physical time evolution. We chose dust because then, for the case of no perturbations, the induced physical Hamiltonian yields the exact FRW equations used in standard cosmology. However, when perturbations of the metric and the scalar field are considered, deviations from the standard FRW framework occur, which are, however, still in agreement with observational data. Since general relativity does not tell us which is the right clock to use for cosmology, we chose a clock such that the resulting physical Hamiltonian is as close as possible to the FRW Hamiltonian in standard cosmology, where one uses the Hamiltonian constraint c as a true Hamiltonian. The physical Hamiltonian used here, $H_{\text{dust}} = \sqrt{C^2 - Q^{ij}C_iC_j}$, reduces to $H_{\text{dust}}^{\text{FRW}} = C$ for an FRW universe, namely to the gauge-invariant version of the Hamiltonian constraint. However, the question arises how generic are the results obtained from a dust clock and what changes do we expect when choosing other matter than dust to reparametrize or even deparametrize the constraints of general relativity. To illustrate this issue, let us discuss the phantom clock introduced in [9] which leads to a physical Hamiltonian of the form

$$\mathbf{H}_{\text{phan}} = \int_\chi \mathrm{d}^3\sigma\, H_{\text{phan}}(\sigma), \tag{F.1}$$

with the Hamiltonian density H_{phan} defined as

$$H_{\text{phan}}(\sigma) = \sqrt{\tfrac{1}{2}(F(C, C_i, Q_{ij})) + \sqrt{\tfrac{1}{4}(F(C, C_i, Q_{ij}))^2 - \alpha^2 Q^{ij}(\sigma,\tau)C_iC_j(\sigma)Q(\sigma,\tau)}} \tag{F.2}$$

where

$$F(C, C_i, Q_{ij}) := C^2(\sigma,\tau) - Q^{ij}(\sigma,\tau)C_iC_j(\sigma) - \alpha^2 Q(\sigma,\tau). \tag{F.3}$$

Above we introduced the abbreviation $Q = \det(Q_{ij})$, and $\alpha > 0$ is for the moment an arbitrary constant of dimension cm^{-2} that enters the phantom field action as a free parameter. Recall that the expressions for C and C_j were given by the geometry and matter part of the total Hamiltonian and diffeomorphism constraint, respectively, that is

$$C(\sigma,\tau) = C^{\mathrm{geo}}(\sigma,\tau) + C^{\mathrm{matter}}(\sigma,\tau) \qquad \text{and} \qquad C_j(\sigma) = C_j^{\mathrm{geo}}(\sigma) + C_j^{\mathrm{matter}}(\sigma). \tag{F.4}$$

From now on we will drop the τ dependence of $C(\sigma,\tau)$ and $Q_{ij}(\sigma,\tau)$ in the expression for H_{phan} and write them explicitly only when confusion could arise otherwise.

For the dust Hamiltonian we saw that the first-order equations of motion obtained for Ξ, Π and Q_{ij}, P^{ij} look similar to the standard cosmological equations apart from the fact that in the case of a dust clock we obtain a dynamical, that is phase space dependent, lapse function $N_{\mathrm{dust}} = C/H_{\mathrm{dust}}$ and shift vector $N^i_{\mathrm{dust}} = N^i/H_{\mathrm{dust}}$. Moreover, in the general equations there occurs a term proportional to $N^i_{\mathrm{dust}}N^j_{\mathrm{dust}}$.

With respect to $\mathbf{H}_{\mathrm{phan}}$, we want to analyse now whether it produces a similar effect and leads to possibly more serious deviations from the standard equations. Starting with the first-order equation for Ξ we obtain

$$\begin{aligned}
\dot{\Xi}(\sigma,\tau) &= \{\mathbf{H}_{\mathrm{phan}}, \Xi(\sigma,\tau)\}\\
&= \int_\chi \mathrm{d}^3\sigma' \Bigg[\frac{C}{H_{\mathrm{phan}}}(\sigma') \left(\frac{1}{2} + \frac{(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)(\sigma')}{4\sqrt{\big(\frac{1}{4}(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)^2 - \alpha^2 Q^{ij}C_iC_jQ\big)(\sigma')}} \right)\\
&\quad \times \{C^{\mathrm{matter}}(\sigma'), \Xi(\sigma,\tau)\}\\
&\quad - \frac{Q^{ij}C_j}{H_{\mathrm{phan}}}(\sigma') \left(\frac{1}{2} + \frac{(C^2 - Q^{ij}C_iC_j + \alpha^2 Q)(\sigma')}{4\sqrt{\big(\frac{1}{4}(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)^2 - \alpha^2 Q^{ij}C_iC_jQ\big)(\sigma')}} \right)\\
&\quad \times \{C^{\mathrm{matter}}(\sigma'), \Xi(\sigma,\tau)_i\} \Bigg].
\end{aligned} \tag{F.5}$$

Introducing the dynamical lapse function N_{phan} and the dynamical shift covector N^i_{phan} as

$$\begin{aligned}
N_{\mathrm{phan}}(\sigma) &:= \frac{C}{H_{\mathrm{phan}}}(\sigma) \left(\frac{1}{2} + \frac{(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)(\sigma)}{4\sqrt{\big(\frac{1}{4}(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)^2 - \alpha^2 Q^{ij}C_iC_jQ\big)(\sigma)}} \right)\\
N^i_{\mathrm{phan}}(\sigma) &:= -\frac{Q^{ij}C_j}{H_{\mathrm{phan}}}(\sigma) \left(\frac{1}{2} + \frac{(C^2 - Q^{ij}C_iC_j + \alpha^2 Q)(\sigma)}{4\sqrt{\big(\frac{1}{4}(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)^2 - \alpha^2 Q^{ij}C_iC_jQ\big)(\sigma)}} \right),
\end{aligned} \tag{F.6}$$

we can rewrite the first-order equation of motion for Ξ as

$$\begin{aligned}
\dot{\Xi}(\sigma,\tau) &= \{\mathbf{H}_{\mathrm{phan}}, \Xi(\sigma,\tau)\}\\
&= \int_\chi \mathrm{d}^3\sigma' \big(N_{\mathrm{phan}}(\sigma')\{C^{\mathrm{matter}}(\sigma'), \Xi(\sigma,\tau)\} + N^i_{\mathrm{phan}}\big\{C_i^{\mathrm{matter}}(\sigma'), \Xi(\sigma,\tau)\big\}\big).
\end{aligned} \tag{F.7}$$

Hence, we realize that, similar to the case of the dust clock, the effect of the phantom clock results in the appearance of a dynamical lapse function and a dynamical shift vector. However, due to the more complicated structure of $\mathbf{H}_{\mathrm{phan}}$ as compared to $\mathbf{H}_{\mathrm{dust}}$, N_{phan} and N^i_{phan} are not simply given in terms of C/H_{phan} and $-C_j/H_{\mathrm{phan}}$ respectively. Now also terms occur which include higher than linear powers of the constraints in the nominator and denominator. Since the quantities Π and obviously Q_{ij} also Poisson commute with any function that does depend on Q_{ij} only, the calculation works analogously in these cases and we obtain

$$\begin{aligned}\dot{\Pi}(\sigma,\tau) &= \{\mathbf{H}_{\rm phan},\Pi(\sigma,\tau)\}\\ &= \int_\chi \mathrm{d}^3\sigma'\big(N_{\rm phan}(\sigma')\{C^{\rm matter}(\sigma'),\Xi(\sigma)\} + N^i_{\rm phan}\big\{C^{\rm matter}_i(\sigma'),\Pi(\sigma,\tau)\big\}\big)\end{aligned} \tag{F.8}$$

and

$$\begin{aligned}\dot{Q}_{ij}(\sigma,\tau) &= \{H_{\rm phan},Q_{ij}(\sigma)\}\\ &= \int_\chi \mathrm{d}^3\sigma'\big(N_{\rm phan}(\sigma')\{C^{\rm geo}(\sigma'),Q_{ij}(\sigma,\tau)\} + N^i_{\rm phan}\big\{C^{\rm geo}_i(\sigma'),Q_{ij}(\sigma,\tau)\big\}\big).\end{aligned} \tag{F.9}$$

For the dynamical variable P^{ij} things look slightly different, because P^{ij} does not Poisson commute with functions depending on Q_{ij}. Therefore we get, as in the dust case, an additional contribution proportional to the Poisson bracket $\{Q^{kl}(\sigma'),P^{ij}(\sigma,\tau)\}$. Furthermore, since $\mathbf{H}_{\rm phan}$ includes a term of the form $\alpha^2 Q$, we also obtain a term proportional to the Poisson bracket $\{Q(\sigma'),P^{ij}(\sigma,\tau)\}$. The explicit results for these Poisson brackets are

$$\begin{aligned}\{Q^{kl}(\sigma'),P^{ij}(\sigma,\tau)\} &= \frac{\kappa}{2}(Q^{ik}Q^{lj}+Q^{jk}Q^{il})(\sigma',\tau)\delta^3(\sigma',\sigma)\\ \{Q(\sigma'),P^{ij}(\sigma,\tau)\} &= -\kappa(QQ^{ij})(\sigma',\tau)\delta^3(\sigma',\sigma).\end{aligned} \tag{F.10}$$

Inserting this back into the equation for $\dot{P}^{ij}$, we end up with

$$\begin{aligned}&\dot{P}^{ij}(\sigma,\tau) = \{\mathbf{H}_{\rm phan},P^{ij}(\sigma,\tau)\}\\ &= \int_\chi \mathrm{d}^3\sigma'\big(N_{\rm phan}(\sigma')\{C^{\rm geo}(\sigma'),P^{ij}(\sigma,\tau)\} + N^i_{\rm phan}\big\{C^{\rm geo}_i(\sigma'),P^{ij}(\sigma,\tau)\big\}\big)\\ &-\frac{\kappa}{2}\left(H_{\rm phan}N^i_{\rm phan}N^j_{\rm phan}\left[\frac{1}{2}+\frac{(C^2-Q^{ij}C_iC_j+\alpha^2Q)}{4\sqrt{\big(\frac{1}{4}(C^2-Q^{ij}C_iC_j-\alpha^2Q)^2-\alpha^2Q^{ij}C_iC_jQ\big)}}\right]^{-1}\right)(\sigma,\tau)\\ &+\frac{\kappa}{2}\left(\frac{\alpha^2Q^{ij}Q}{H_{\rm phan}}\left[\frac{1}{2}+\frac{C^2+Q^{ij}C_iC_j-\alpha^2Q}{4\sqrt{\frac{1}{4}(C^2-Q^{ij}C_iC_j-\alpha^2Q)^2-\alpha^2QQ^{ij}C_iC_j}}\right]\right)(\sigma,\tau).\end{aligned} \tag{F.11}$$

The remaining Poisson brackets in the first-order equations for the dynamical variables are the same Poisson brackets that occur when $\mathbf{H}_{\rm dust}$ is used as a Hamiltonian. Inserting the results obtained there into the corresponding equations for the case of $\mathbf{H}_{\rm phan}$, we obtain the following final form of the first-order equations:

$$\begin{aligned}\dot{\Xi}(\sigma,\tau) &= \frac{N_{\rm phan}\Pi}{Q}(\sigma,\tau)+(\mathcal{L}_{\vec{N}^{\rm phan}}\Xi)(\sigma,\tau)\\ \dot{\Pi}(\sigma,\tau) &= [N_{\rm phan}QQ^{ij}\Xi,i]_{,j}(\sigma,\tau)-\frac{1}{2}(N_{\rm phan}QV'(\Xi))(\sigma,\tau)+\big(\mathcal{L}_{\vec{N}_{\rm phan}}\Pi\big)(\sigma,\tau)\\ \dot{Q}_{ij}(\sigma,\tau) &= \frac{2N_{\rm phan}}{Q}(\sigma,\tau)\left(G_{ijmn}P^{mn}\right)(\sigma,\tau)+\big(\mathcal{L}_{\vec{N}_{\rm phan}}Q\big)_{ij}(\sigma,\tau),\end{aligned} \tag{F.12}$$

where

$$G_{ijmn} := \tfrac{1}{2}(Q_{im}Q_{jn}+Q_{in}Q_{jm}-Q_{ij}Q_{mn}), \tag{F.13}$$

with its inverse given by

$$[G^{-1}]^{ijmn} := \tfrac{1}{2}(Q^{im}Q^{jn}+Q^{in}Q^{jm}-2Q^{ij}Q^{mn}). \tag{F.14}$$

For the gravitational momentum we have

$$\begin{aligned}\dot{P}^{ij}(\sigma,\tau) = \Bigg(& N_{\text{phan}}\Bigg[-\frac{Q_{mn}}{\sqrt{\det Q}}(2P^{jm}P^{kn} - P^{jk}P^{mn}) \\ & + \frac{\kappa}{2}Q^{jk}C - \sqrt{\det Q}\,Q^{jk}\left(2\Lambda + \frac{\kappa}{2\lambda}(\Xi^{,m}\Xi_{,m} + v(\Xi))\right)\Bigg] \\ & + \sqrt{\det Q}[G^{-1}]^{jkmn}((D_m D_n N_{\text{phan}}) - N_{\text{phan}}R_{mn}[Q]) \\ & + \frac{\kappa}{2\lambda}N_{\text{phan}}\sqrt{\det Q}\;\Xi^{,j}\Xi^{,k} + \left(\mathcal{L}_{\vec{N}_{\text{phan}}}P\right)^{jk}\Bigg)(\sigma,\tau) \\ -\frac{\kappa}{2}\Bigg(& H_{\text{phan}}N^i_{\text{phan}}N^j_{\text{phan}}\left[\frac{1}{2} + \frac{(C^2 - Q^{ij}C_iC_j + \alpha^2 Q)}{4\sqrt{\left(\frac{1}{4}(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)^2 - \alpha^2 Q^{ij}C_iC_jQ\right)}}\right]^{-1}\Bigg)(\sigma,\tau) \\ +\frac{\kappa}{2}\Bigg(& \frac{\alpha^2 Q^{ij}Q}{H_{\text{phan}}}\left[\frac{1}{2} + \frac{C^2 + Q^{ij}C_iC_j - \alpha^2 Q}{4\sqrt{\frac{1}{4}(C^2 - Q^{ij}C_iC_j - \alpha^2 Q)^2 - \alpha^2 QQ^{ij}C_iC_j}}\right]\Bigg)(\sigma,\tau). \qquad \text{(F.15)}\end{aligned}$$

One can see that the first-order equations for Ξ, Π and Q_{ij} in equation (F.12) are identical to those for the dust Hamiltonian $\mathbf{H}_{\text{dust}}$, apart from the different definitions of the dynamical lapse function N_{phan} and shift vector N^i_{phan} in equation (F.6). However, the equation for $\dot{P}^{ij}$ differs from the corresponding dust Hamiltonian equation. The term in the second last line in equation (F.15) corresponds to the term $-\frac{\kappa}{2}\left(H_{\text{dust}}N^i_{\text{dust}}N^j_{\text{dust}}\right)(\sigma)$ in the equation for $\dot{P}^{ij}$ derived from $\mathbf{H}_{\text{dust}}$. In the present case this term looks a bit more complicated, since we have to divide the whole expression by the term in the square brackets which is identical to one in the case of $\mathbf{H}_{\text{dust}}$. The additional term in the last line of equation (F.15) comes from the terms $\alpha^2 Q$ and $\alpha^2 Q^{ij}C_iC_j$ in $\mathbf{H}_{\text{phan}}$, which are absent in $\mathbf{H}_{\text{dust}}$. Since in this term we cannot factor out C or C_i but only α^2, we are also not able to reexpress this term by means of the dynamical lapse function N_{phan} and the dynamical shift vector N^i_{phan}, respectively, as it was possible for the term in the second last line.

In summary, when using a phantom scalar field as a clock we also obtain deviations from the standard treatment in which the Hamiltonian constraint is used as a true Hamiltonian. These deviations manifest themselves in the appearance of a dynamical lapse function N_{phan} and a dynamical shift vector N^i_{phan}, analogous to the case where dust is used as a clock. However, the explicit dependence of N_{phan} and N^i_{phan} on the dynamical variables is more complicated than for the corresponding quantities N_{dust} and N^i_{dust}. Another modification occurs in the equation for the gravitational momentum P^{ij}. While it contains a term that is second order in N^i_{phan}, in complete analogy with the case of $\mathbf{H}_{\text{dust}}$, it also features an additional term proportional to α^2.

F.1. The special case of an FRW universe

It is interesting to study the special case of FRW also for $\mathbf{H}_{\text{phan}}$. Recall from [16] that by assuming homogeneity and isotropy, $\mathbf{H}_{\text{dust}}$, N_{dust} and N^i_{dust} reduce to the following quantities:

$$N_{\text{dust}}(\sigma) \xrightarrow{\text{FRW}} 1, \qquad N^i_{\text{dust}}(\sigma) \xrightarrow{\text{FRW}} 0, \qquad H_{\text{dust}}(\sigma) \xrightarrow{\text{FRW}} C^{\text{FRW}}(\sigma), \qquad \text{(F.16)}$$

where

$$C^{\text{FRW}}_{\text{dust}}(\tau) = A^3(\tau)\left(\frac{1}{\kappa}\left(-6\left(\frac{\dot{A}}{A}\right)^2 + 2\Lambda\right) + \frac{1}{2\lambda}\left(\dot{\Xi}^2 + V(\Xi)\right)\right)(\tau). \qquad \text{(F.17)}$$

Here $A = A(\tau)$ is a function of the dust time τ and the dot refers to a derivative with respect to the dust time. In particular, $A(\tau)$ can be understood as the gauge-invariant extension of the ordinary scale factor $a(t)$ used in standard cosmology. The difference between the two is that A is gauge invariant and thus a physical observable whereas a is not, since it does not commute with the Hamiltonian constraint of FRW.

The gravitational canonical variables are given by $Q_{ij} = A^2(\tau)\delta_{ij}$ and $P^{ij} = -2\dot{A}(\tau)\delta^{ij}$. We mentioned previously that a consequence of this behaviour is that the unperturbed equations of motion for (Ξ, Π) and (Q_{ij}, P^{ij}) agree with the FRW equations used in standard cosmology. In particular, the deviation from the general standard equation of motion for P^{ij} vanishes in the case of FRW, because it is quadratic in $N^i_{\rm dust}$.

For the phantom Hamiltonian $\mathsf{H}_{\rm phan}$ things look slightly different. Here we have the following behaviour of $H_{\rm phan}$, $N_{\rm phan}$ and $N^i_{\rm phan}$, when a homogenous and isotropic universe is considered:

$$\begin{aligned} N_{\rm phan}(\sigma) &\stackrel{\rm FRW}{\longrightarrow} N^{\rm FRW}_{\rm phan} := \left(\frac{C^{\rm FRW}_{\rm phan}}{H^{\rm FRW}_{\rm phan}}\right)(\sigma), \qquad N^i_{\rm phan}(\sigma) \stackrel{\rm FRW}{\longrightarrow} 0, \\ H_{\rm phan}(\sigma) &\stackrel{\rm FRW}{\longrightarrow} H^{\rm FRW}_{\rm phan} := \sqrt{\left(C^{\rm FRW}_{\rm phan}\right)^2 - \alpha^2 A^6(\sigma)} \end{aligned} \tag{F.18}$$

with

$$C^{\rm FRW}_{\rm phan}(\tau) = \frac{A^3}{\left(N^{\rm FRW}_{\rm phan}\right)^2}(\tau)\left(\frac{1}{\kappa}\left(-6\left(\frac{\dot{A}}{A}\right)^2 + 2\Lambda\left(N^{\rm FRW}_{\rm phan}\right)^2\right) + \frac{1}{2\lambda}\left(\dot{\Xi}^2 + V(\Xi)\left(N^{\rm FRW}_{\rm phan}\right)^2\right)\right)(\tau). \tag{F.19}$$

Hence, the dust clock and the phantom scalar field clock agree only if the parameter α is chosen to be tiny compared to the Hamiltonian constraint $C^{\rm FRW}_{\rm phan}$, e.g. $\alpha A^3 \ll C^{\rm FRW}_{\rm phan}$. Consequently, the equations of motion generated by $\mathsf{H}_{\rm phan}$ also deviate from the standard FRW equations. The significance of this deviation again depends on the specific value of the parameter α, as was discussed in detail in [9]. For completeness we also list the first-order equations of motion here:

$$\begin{aligned} \dot{\Xi}(\tau) &= \left(N^{\rm FRW}_{\rm phan}\frac{\Pi}{\sqrt{Q}}\right)(\tau) \qquad \dot{\Pi}(\tau) = -\left(N^{\rm FRW}_{\rm phan}\frac{\sqrt{Q}}{2}V'(\Xi)\right)(\tau) \\ \dot{Q}_{ij} &= \left(N^{\rm FRW}_{\rm phan}\frac{2}{\sqrt{Q}}G_{ijmn}P^{mn}\right)(\tau) \\ \dot{P}^{ij} &= N^{\rm FRW}_{\rm phan}(\tau)\left(-\frac{Q_{mn}}{\sqrt{Q}}(2P^{im}P^{jn} - P^{ij}P^{mn}) + \frac{\kappa}{2}Q^{ij}C^{\rm FRW}_{\rm phan}\right. \\ &\quad \left. - Q^{ij}\sqrt{Q}\left(2\Lambda + \frac{\kappa}{2\lambda}V(\Xi)\right) + \frac{\alpha^2\kappa}{2}\frac{Q}{C^{\rm FRW}}Q^{ij}\right)(\tau). \end{aligned} \tag{F.20}$$

Taking into account that $Q_{ij} = A^2\delta_{ij}$ and using the first-order equation for Q_{ij}, we solve for the momenta $P^{ij} = -2\dot{A}\big/N^{\rm FRW}_{\rm phan}\delta^{ij}$ in terms of $\dot{Q}_{jk} = 2A\dot{A}$. In order to derive the corresponding FRW equation with respect to the time generated by $\mathsf{H}^{\rm FRW}_{\rm phan}$, we take the time derivative of the equation for $\dot{Q}_{ij}$ and insert into the resulting equation for $\ddot{Q}_{ij}$ the expression for P^{ij} and $\dot{P}^{ij}$ given above. This yields

$$\begin{aligned} \left(\frac{\ddot{A}}{A}\right) &= -\frac{1}{2}\left(\frac{\dot{A}}{A}\right)^2 + \frac{1}{2}\left(N^{\rm FRW}_{\rm phan}\right)^2\Lambda - \frac{\kappa}{4\lambda}\left(\frac{1}{2}\dot{\Xi}^2 - \frac{1}{2}\left(N^{\rm FRW}_{\rm phan}\right)^2 V(\Xi)\right) \\ &\quad + \frac{\dot{N}^{\rm FRW}_{\rm phan}}{N^{\rm FRW}_{\rm phan}}\left(\frac{\dot{A}}{A}\right) - \frac{\kappa}{4}\left(N^{\rm FRW}_{\rm phan}\right)^2\left(\frac{\alpha^2 A^3}{C^{\rm FRW}_{\rm phan}}\right). \end{aligned} \tag{F.21}$$

Apart from the lapse functions in the equation above which are not present in the standard FRW equations, we get an additional term including the time derivative of the lapse function. Using the explicit definition of the lapse function, we can perform this time derivative, leading to

$$\frac{\dot{N}^{\mathrm{FRW}}_{\mathrm{phan}}}{N^{\mathrm{FRW}}_{\mathrm{phan}}}\left(\frac{\dot{A}}{A}\right) = \frac{3\left(\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2 - 1\right)}{\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2}\left(\frac{\dot{A}}{A}\right)^2. \tag{F.22}$$

Consequently, equation (F.21) can be rewritten as

$$\begin{aligned}\left(\frac{\ddot{A}}{A}\right) &= -\left(\frac{\dot{A}}{A}\right)^2\left(\frac{1}{2} - \frac{3\left(\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2 - 1\right)}{\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2}\right) + \frac{1}{2}\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2\Lambda \\ &\quad - \frac{\kappa}{4\lambda}\left(\frac{1}{2}\dot{\Xi}^2 - \frac{1}{2}\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2 V(\Xi)\right) - \frac{\kappa}{4}\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2\left(\frac{\alpha^2 A^3}{C^{\mathrm{FRW}}_{\mathrm{phan}}}\right).\end{aligned} \tag{F.23}$$

The term $(\dot{A}/A)^2$ can be replaced by considering the energy conservation law $\dot{H}^{\mathrm{FRW}}_{\mathrm{phan}} = 0$, that is $H^{\mathrm{FRW}}_{\mathrm{phan}} = \epsilon_0$, from which we get $C^{\mathrm{FRW}}_{\mathrm{phan}} = \sqrt{\epsilon_0^2 + \alpha^2 A^6}$. Solving this equation for $(\dot{A}/A)^2$ yields

$$\begin{aligned}3\left(\frac{\dot{A}}{A}\right)^2 &= \left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2\Lambda + \frac{\kappa}{2\lambda}\left(\frac{1}{2}\dot{\Xi}^2 + \frac{1}{2}V(\Xi)\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2\right) - \frac{\kappa}{2}\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2\alpha\sqrt{1 + \frac{\epsilon_0}{\alpha^2 A^6}} \\ &= \left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2\Lambda + \frac{\kappa}{2\lambda}\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2(\rho_{\mathrm{matter}} + \rho_{\mathrm{phan}}),\end{aligned} \tag{F.24}$$

where we used in the last line

$$\rho_{\mathrm{matter}} = \frac{1}{2}\frac{1}{\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2}\dot{\Xi}^2 + \frac{1}{2}V(\Xi) \qquad \text{and} \qquad \rho_{\mathrm{phan}} = -\alpha\sqrt{1 + \frac{\epsilon_0}{\alpha^2 A^6}}. \tag{F.25}$$

Reinserting equation (F.24) into equation (F.23), we obtain the phantom FRW equation given by

$$\begin{aligned}3\left(\frac{\ddot{A}}{A}\right) &= \Lambda\left(1 + 4\left(\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2 - 1\right)\right) - \frac{\kappa}{4}\left[\left(\frac{1}{\lambda}\rho_{\mathrm{matter}} + \rho_{\mathrm{phan}}\right)\left(1 - 5\left(\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2 - 1\right)\right)\right. \\ &\quad \left. + 3\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2\left(\frac{1}{\lambda}p_{\mathrm{matter}} + p_{\mathrm{phan}}\right)\right],\end{aligned} \tag{F.26}$$

whereby we introduced

$$\begin{aligned}p_{\mathrm{matter}} &= \frac{1}{2}\frac{1}{\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2}\dot{\Xi}^2 - \frac{1}{2}V(\Xi) \\ p_{\mathrm{matter}} &= -\frac{1}{3A^2}\frac{\mathrm{d}}{\mathrm{d}A}(A^3\rho_{\mathrm{phan}}) = \frac{\alpha^2 A^3}{C^{\mathrm{FRW}}_{\mathrm{phan}}}.\end{aligned} \tag{F.27}$$

That this equation agrees with the one derived in [9] can be seen when expressing $\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2$ in terms of the deviation parameter $x := \epsilon_0/\alpha^2 A^6$ used there, resulting in $\left(N^{\mathrm{FRW}}_{\mathrm{phan}}\right)^2 = 1 + 1/x$.

In general, choosing one clock or the other might have significant effects on the equation of motion. General relativity does not tell us which clock is convenient to work with; hence, additional physical input is needed. The results of the application of this framework for FRW in [16] show that choosing dust as clock reproduces the standard FRW equations. Thus we could call the dust clock the FRW clock. Since so far an (approximate) FRW universe is in agreement with observational data, dust seems to be a good choice. However, the α parameter in $\mathbf{H}^{\mathrm{FRW}}_{\mathrm{phan}}$ can be chosen such that the resulting equation of motion also do not contradict present experiments. Therefore, based on experimental constraints, none of the two clocks is excluded, nor is one of them preferred. From a theoretical point of view, the choice of a clock is mainly guided by the requirement that the constraints can be deparametrized, that is, they can be written in the form $C = p^{\mathrm{clock}} + H^{\mathrm{clock}}$. Here the Hamiltonian density H^{clock} must no longer depend on the clock variables, and furthermore it should be positive definite. Additionally the structure of H^{clock} should not be too complicated such that calculations of, for instance, the equation of motions are still possible. However, in principle, we have a large amount of freedom to choose a clock, as long as the induced equations of motion do not contradict experiments.

Appendix G. linear perturbation theory: some calculations in more detail

In section 6.2 we derived the second-order equation of motion for the linear perturbation of the (manifestly) gauge-invariant three-metric δQ_{jk}. For that we needed the perturbation of the geometry and matter part of the gauge-invariant Hamiltonian constraint, denoted by C^{geo} and C^{matter}, respectively, as these terms occur in the third term on the right-hand side of the unperturbed equation of motion for Q_{jk}, equation (4.24). We omitted the details in the main text due to their length, and also because it turns out that several terms cancel when inserted back into the expression of the perturbation of the third term, shown in equation (6.20). For the interested reader, however, the detailed perturbations of the constraints are given below.

The perturbed geometry constraint δC^{geo} is given by

$$\begin{aligned}\delta C^{\mathrm{geo}} = \Bigg[& \frac{1}{2}\left(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\overline{C}^{\mathrm{geo}} + \frac{1}{2}\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\left(\overline{C}^{\mathrm{geo}} - 2\frac{\sqrt{\det\overline{Q}}}{\kappa}(2\Lambda - \overline{R})\right) \\
& + \frac{\sqrt{\det\overline{Q}}}{\kappa}(\overline{R}^{jk} - [\overline{G}^{-1}]^{jkmn}\overline{D}_m\overline{D}_n) + \frac{\sqrt{\det\overline{Q}}}{2\overline{N}^2\kappa}(\dot{\overline{Q}}_{mn} - (\mathcal{L}_{\overline{\vec{N}}}\overline{Q})_{mn}) \\
& \times \left[[\overline{G}^{-1}]^{jkmn}\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\overline{\vec{N}}}\right) - (\dot{\overline{Q}}_{rs} - (\mathcal{L}_{\overline{\vec{N}}}\overline{Q})_{rs})\overline{Q}^{nk}[\overline{G}^{-1}]^{rsmj}\right] + \frac{\sqrt{\det\overline{Q}}}{2\overline{N}^2\kappa} \\
& \times (\dot{\overline{Q}}_{rs} - (\mathcal{L}_{\overline{\vec{N}}}\overline{Q})_{rs})[\overline{G}^{-1}]^{rsmn}\left[\overline{Q}^{jt}\overline{N}^k[\overline{Q}_{mn}]_{,t} + 2\overline{Q}_{tn}\frac{\partial}{\partial x^m}(\overline{Q}^{jt}\overline{N}^k)\right]\Bigg]\delta Q_{jk} \\
& + \Bigg[-2\frac{\overline{N}^j}{\overline{N}^2}\left(\overline{C}^{\mathrm{geo}} - \frac{\sqrt{\det\overline{Q}}}{\kappa}(2\Lambda - \overline{R})\right) - \frac{\sqrt{\det\overline{Q}}}{2\overline{N}^2\kappa}(\dot{\overline{Q}}_{rs} - (\mathcal{L}_{\overline{\vec{N}}}\overline{Q})_{rs})[\overline{G}^{-1}]^{rsmn} \\
& \times \left[\overline{Q}^{jt}[\overline{Q}_{rs}]_{,t} + 2\overline{Q}_{ts}\frac{\partial}{\partial x^k}(\overline{Q}^{jt})\right]\Bigg]\delta N_j. \qquad \text{(G.1)}\end{aligned}$$

Here we used that the perturbation of the Ricci scalar can be written as

$$\delta R = [[\overline{G}^{-1}]^{jkmn}\overline{D}_m\overline{D}_n - \overline{R}^{jk}]\delta Q_{jk}. \qquad \text{(G.2)}$$

For the perturbed matter part of the constraint $\delta C^{\mathrm{matter}}$ we obtain

$$\begin{aligned}\delta C^{\mathrm{matter}} = \Bigg[& \frac{1}{2}\left(\overline{Q}^{jk} + \frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\right)\overline{C}^{\mathrm{matter}} + \frac{1}{2}\frac{\overline{N}^j\overline{N}^k}{\overline{N}^2}\left(\overline{C}^{\mathrm{matter}} - \frac{\sqrt{\det\overline{Q}}}{\lambda}(\overline{Q}^{jk}\overline{\Xi}_{,j}\overline{\Xi}_{,k} + v(\Xi))\right) \\
& + \frac{\sqrt{\det\overline{Q}}}{\overline{N}^2\lambda}\overline{Q}^{jm}\overline{Q}^{kn}(\dot{\Xi} - (\mathcal{L}_{\overline{\vec{N}}}\overline{\Xi}))\overline{N}_m\overline{\Xi}_{,n} - \frac{\sqrt{\det\overline{Q}}}{2\lambda}\overline{Q}^{jm}\overline{Q}^{jk}\overline{\Xi}_{,m}\overline{\Xi}_{,n}\Bigg]\delta Q_{jk}\end{aligned}$$

$$
+\left[-\frac{\sqrt{\det\overline{Q}}}{\overline{N}^2\lambda}(\dot{\Xi}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{Q}^{jk}\overline{\Xi}_{,k}-2\frac{\overline{N}^j}{\overline{N}^2}\right.
$$

$$
\left.\times\left(\overline{C}^{\text{matter}}-\frac{\sqrt{\det\overline{Q}}}{2\lambda}(\overline{Q}^{jk}\overline{\Xi}_{,j}\overline{\Xi}_{,k}+v(\overline{\Xi}))\right)\right]\delta N_j
$$

$$
+\left[\frac{\sqrt{\det\overline{Q}}}{\lambda}\left(\frac{1}{\overline{N}^2}\left(\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi})\right)\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)+\overline{Q}^{jk}\overline{\Xi}_{,k}\frac{\partial}{\partial x^j}+\frac{1}{2}v'(\overline{\Xi})\right)\right]\delta\Xi. \tag{G.3}
$$

Since the perturbation of $\delta C=\delta C^{\text{geo}}+\delta C^{\text{matter}}$ occurs in equation (6.20) multiplied by a factor of $\frac{\kappa\overline{N}^2}{2\sqrt{\det\overline{Q}}}$, we will present it here already with this factor in front:

$$
\frac{\kappa\overline{N}^2}{2\sqrt{\det\overline{Q}}}\delta C=\left[\frac{1}{2}\left(\overline{Q}^{mn}+\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)\frac{\kappa\overline{N}^2}{2\sqrt{\det\overline{Q}}}\overline{C}+\frac{1}{2}\frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\frac{\kappa\overline{N}^2}{2\sqrt{\det\overline{Q}}}\right.
$$

$$
\times\left(\overline{C}-2\frac{\sqrt{\det\overline{Q}}}{\kappa}(2\Lambda-\overline{R})-\frac{\sqrt{\det\overline{Q}}}{\lambda}(\overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s}+v(\overline{\Xi}))\right)
$$

$$
+\frac{\overline{N}^2}{2}(\overline{R}^{mn}-[\overline{G}^{-1}]^{mnrs}\overline{D}_r\overline{D}_s)+\frac{\kappa}{2\lambda}\overline{Q}^{mr}\overline{Q}^{ns}(\dot{\Xi}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{N}_r\overline{\Xi}_{,s}
$$

$$
-\frac{\kappa\overline{N}^2}{2\lambda}\overline{Q}^{jm}\overline{Q}^{kn}\overline{\Xi}_{,j}\overline{\Xi}_{,k}+\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{rs})
$$

$$
\times\left[[\overline{G}^{-1}]^{mnrs}\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)-(\dot{\overline{Q}}_{tu}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{tu})\overline{Q}^{sn}[\overline{G}^{-1}]^{turm}\right]
$$

$$
\left.+\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsjk}\left[\overline{Q}^{mt}\overline{N}^n[\overline{Q}_{jk}]_{,t}+2\overline{Q}_{tk}\frac{\partial}{\partial x^j}(\overline{Q}^{mt}\overline{N}^n)\right]\right]\delta Q_{mn}
$$

$$
+\left[-2\frac{\kappa\overline{N}^2}{2\sqrt{\det\overline{Q}}}\frac{\overline{N}^m}{\overline{N}^2}\left(\overline{C}-\frac{\sqrt{\det\overline{Q}}}{\kappa}(2\Lambda-\overline{R})-\frac{\sqrt{\det\overline{Q}}}{2\lambda}(\overline{Q}^{rs}\overline{\Xi}_{,r}\overline{\Xi}_{,s}+v(\overline{\Xi}))\right)\right.
$$

$$
-\frac{\kappa}{2\lambda}(\dot{\Xi}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\overline{Q}^{mn}\overline{\Xi}_{,n}-\frac{1}{4}(\dot{\overline{Q}}_{rs}-(\mathcal{L}_{\vec{\overline{N}}}Q)_{rs})[\overline{G}^{-1}]^{rsjk}
$$

$$
\left.\times\left[\overline{Q}^{mt}[\overline{Q}_{jk}]_{,t}+2\overline{Q}_{tk}\frac{\partial}{\partial x^j}(\overline{Q}^{mt})\right]\right]\delta N_m
$$

$$
+\left[\frac{\overline{N}^2\kappa}{2\lambda}\left(\frac{1}{\overline{N}^2}(\dot{\overline{\Xi}}-(\mathcal{L}_{\vec{\overline{N}}}\overline{\Xi}))\left(\frac{\partial}{\partial\tau}-\mathcal{L}_{\vec{\overline{N}}}\right)+\overline{Q}^{mn}\overline{\Xi}_{,n}\frac{\partial}{\partial x^m}+\frac{1}{2}v'(\overline{\Xi})\right)\right]\delta\Xi. \tag{G.4}
$$

Going back to the second-order equation of motion for Q_{jk} shown in equation (4.24), we remind the reader that the perturbation of the first term on the right-hand side involves a term that we had already calculated for the equation of motion of $\delta\Xi$. For this reason, we presented in the main text only the perturbation of the remaining term $(\dot{Q}_{jk}-(\mathcal{L}_{\vec{N}}Q)_{jk})$, not the final result for the full first term. For those interested in more detail, we display it here:

$$
\delta\left(\left[\frac{\dot{N}}{N}-\frac{(\sqrt{\det Q})^{\cdot}}{\sqrt{\det Q}}+\frac{N}{\sqrt{\det Q}}\left(\mathcal{L}_{\vec{N}}\frac{\sqrt{\det Q}}{N}\right)\right](\dot{Q}_{jk}-(\mathcal{L}_{\vec{N}}Q)_{jk})\right)
$$

$$
=\left[\left[\frac{\dot{\overline{N}}}{\overline{N}}-\frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}}+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\right.
$$

$$
\times\left(\overline{Q}^{rn}\overline{N}^n[\overline{Q}_{jk}]_{,r}+\overline{Q}_{rk}\frac{\partial}{\partial x^j}(\overline{Q}^{rn}\overline{N}^m)+\overline{Q}_{rj}\frac{\partial}{\partial x^k}(\overline{Q}^{rn}\overline{N}^m)\right.
$$

$$
\begin{aligned}
&-\left(\dot{\overline{Q}}_{jk} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk}\right)\left(\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{1}{2}\left(\overline{Q}^{mn} + \frac{\overline{N}^m\overline{N}^n}{\overline{N}^2}\right)\right)\right.\\
&\left.\left.+\frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^k}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{N}^m\overline{Q}^{rn}\right)\right)\right]\delta Q_{mn}\\
&+\left[-\left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}} + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\right.\\
&\times\left(\overline{Q}^{mn}[\overline{Q}_{jk}]_{,r} + \overline{Q}_{mk}\frac{\partial}{\partial x^j}(\overline{Q}^{mn}) + \overline{Q}_{mj}\frac{\partial}{\partial x^k}(\overline{Q}^{mn}) + (\dot{\overline{Q}}_{jk} - (\mathcal{L}_{\vec{\overline{N}}}\overline{Q})_{jk})\right.\\
&\left.\left.\times\left(\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\left(\frac{\overline{N}^m}{\overline{N}^2}\right) + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\frac{\partial}{\partial x^k}\left(\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\overline{Q}^{mn}\right)\right)\right)\right]\delta N_m\\
&+\left[\left[\frac{\dot{\overline{N}}}{\overline{N}} - \frac{(\sqrt{\det\overline{Q}})^{\cdot}}{\sqrt{\det\overline{Q}}} + \frac{\overline{N}}{\sqrt{\det\overline{Q}}}\left(\mathcal{L}_{\vec{\overline{N}}}\frac{\sqrt{\det\overline{Q}}}{\overline{N}}\right)\right]\left(\frac{\partial}{\partial\tau} - \mathcal{L}_{\vec{\overline{N}}}\right)\right]\delta Q_{jk}.
\end{aligned}
$$

Appendix H. Gauge-invariant versus gauge fixed formalism

In this appendix we investigate the question under which circumstances a manifestly gauge-invariant formulation of a constrained system can be equivalently described by a gauge fixed version.

We begin quite generally and consider a (finite-dimensional) constrained Hamiltonian system with first class constraints $C_I, I = 1, \ldots, m$, on a phase space with canonical pairs $(q^a, p_a), a = 1, \ldots, n; m \leqslant n$. If there is a true, gauge-invariant Hamiltonian H (not constrained to vanish), enlarge the phase space by an additional canonical pair (q^0, p_0) and additional first class constraint $C_0 = p_0 + H$. The reduced phase space and dynamics of the enlarged system is equivalent to the original one; hence, we consider without loss of generality a system with no true Hamiltonian.

The canonical Hamiltonian of the system is a linear combination of constraints

$$H_{\text{can}} = \lambda^I C_I \tag{H.1}$$

for some Lagrange multipliers λ^I whose range specifies the amount of gauge freedom. A gauge fixing is defined by a set of gauge fixing functions G_I with the property that the matrix with entries $M_{IJ} := \{C_I, G_J\}$ has everywhere (on phase space) non-vanishing determinant[39]. Note that we allow for gauge fixing conditions that display an explicit time dependence. The conservation in time of the gauge fixing conditions

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}G_I = \frac{\partial}{\partial t}G_I + \{H_{\text{can}}, G_I\} = \frac{\partial}{\partial t}G_I + \lambda^J M_{JI} \tag{H.2}$$

uniquely fixes the Lagrange multipliers to be the following phase space dependent functions:

$$\lambda^I = -\frac{\partial G_J}{\partial t}\,(M^{-1})^{JI} =: \lambda^I_0. \tag{H.3}$$

By arbitrarily splitting the set of canonical pairs (q^a, p_a) into two sets $(T^I, \pi_I), I = 1, \ldots, m$, and $(Q^A, P_A), A = 1, \ldots, n-m$, we can solve $C_I = G_I = 0$ for

$$C'_I = \pi_I + h'_I(Q, P) = 0, \qquad G'_I = T^I - \tau^I(Q, P) = 0 \tag{H.4}$$

[39] Ideally, the gauge $G_I = 0$ should define a unique point in each gauge orbit.

for certain functions h, τ which generically will be explicitly time dependent. The variables T, π are called the gauge degrees of freedom and Q, P are called the true degrees of freedom (although typically neither of them is gauge invariant).

The reduced Hamiltonian $H_{\text{red}}(Q, P)$, if it exists, is supposed to generate the same equations of motion for Q, P as the canonical Hamiltonian does, when the constraints and the gauge fixing conditions are satisfied and the Lagrange multipliers assume their fixed values (H.3), that is,

$$\{H_{\text{red}}, f\} = \{H_{\text{can}}, f\}_{C=G=\lambda-\lambda_0=0} = \left[\lambda_0^I\{C_I, f\}\right]_{C=G=\lambda-\lambda_0=0} \tag{H.5}$$

for any function $f = f(Q, P)$. For general gauge fixing functions the reduced Hamiltonian will not exist; the system of PDEs to which (H.5) is equivalent will not be integrable.

However, a so-called coordinate gauge fixing condition $G^I = T^I - \tau^I$ with τ^I independent of the phase space always leads to a reduced Hamiltonian as follows: we can always (locally) write the constraints in the form (at least weakly)

$$C_I = M_{IJ}(\pi_I + h_I(T, Q, P)). \tag{H.6}$$

Then, noting that $M_{IJ} = \{C_I, T_J\}$, (H.5) becomes

$$\{H_{\text{red}}, f\} = [\lambda_0^I M_{IJ}\{h_I, f\}]_{C=G=\lambda-\lambda_0=0} = [\dot{\tau}_I\{h_I, f\}]_{G=0} = \{\dot{\tau}_I\tilde{h}_I, f\} \tag{H.7}$$

with $\tilde{h}_I = h_I(T = \tau, Q, P)$ and we used that f only depends on Q, P. This displays the reduced Hamiltonian as

$$H_{\text{red}}(Q, P; t) = \dot{\tau}_I(t)h_I(T = \tau(t), Q, P)). \tag{H.8}$$

It will be explicitly time dependent unless $\dot{\tau}_I$ is time independent and h_I is independent of T, that is, unless those constraints can be deparametrized for which $\dot{\tau}_I \neq 0$. Hence, deparametrization is crucial for having a conserved Hamiltonian system.

On the other hand, let us consider the gauge-invariant point of view. The observables associated with $f(Q, P)$ are given by

$$O_f(\tau) = [\exp(\beta^I X_I) \cdot f]_{\beta=\tau-T} \tag{H.9}$$

where we have denoted the Abelian Hamiltonian vector fields X_I by $X_I := \{\pi_I + h_I, .\}$. Consider a one parameter family of flows $t \mapsto \tau^I(t)$; then with $O_f(t) := O_f(\tau(t))$ we find

$$\frac{\mathrm{d}}{\mathrm{d}t}O_f(t) = \dot{\tau}^I(t)\sum_{n=0}^{\infty}\frac{\beta^{J_1}\cdots\beta^{J_n}}{n!}\; X_I X_{J_1}\cdots X_{J_n}\cdot f. \tag{H.10}$$

On the other hand, consider $H_I(t) := O_{h_I}(\tau(t))$; then

$$\begin{aligned}\{H_I(t), O_f(t)\} &== O_{\{h_I,f\}^*}(\tau(t)) = O_{\{h_I,f\}}(\tau(t)) = O_{X_I\cdot f}(\tau(t))\\ &= \dot{\tau}^I(t)\sum_{n=0}^{\infty}\frac{\beta^{J_1}\ldots\beta^{J_n}}{n!}\; X_I X_{J_1}\cdots X_{J_n}\cdot f\end{aligned} \tag{H.11}$$

where in the second step we used that neither h_I nor f depends on π_J, in the third we used that f does not depend on T^J and in the last we used the commutativity of the X_J. Thus the physical Hamiltonian that drives the time evolution of the observables is simply given by

$$H(t) := \dot{\tau}^I(t)h_I(\tau(t), O_Q(t), O_P(t)) \tag{H.12}$$

This is exactly the same as (H.8) under the identification $f \leftrightarrow O_f(0)$. Hence we have shown that for suitable gauge fixings the reduced and the gauge-invariant frameworks are equivalent. Note that it was crucial in the derivation that (T^I, π_I) and (Q^A, P_A) are two sets of canonical pairs. If that is not the case, then it would be unclear whether the time evolution of the observables has a canonical generator.

The power of a manifestly gauge-invariant framework lies therefore not in the gauge invariance itself. Rather, it relies on whether the gauge fixing can be achieved globally, whether it can be phrased in terms of separate canonical pairs, whether the observer clocks T_I are such that reduced Hamiltonian system is conserved and whether they do display the time evolution of observables as viewed by a realistic observer. In particular, the reduced Hamiltonian by construction only depends on (Q^A, P_A). In application to gravity, if one does not add an additional matter component such as the dust, then the true degrees of freedom would sit in two of the six canonical pairs (q_{ab}, p^{ab}). However, note that it is not obvious how to split these pairs into gauge and true degrees of freedom in an at least spatially covariant way and moreover it is not possible to solve for four of the p^{ab} algebraically because the spatial diffeomorphism constraint involves their derivatives. Hence the physical or reduced Hamiltonian would become non-local. Furthermore, if one uses gravitational degrees of freedom for reduction, then it is clear that one does not get the full set of Einstein's equations as evolution equations which is something that one may want to keep. Finally, the reduced Hamiltonian will not reduce to the standard model Hamiltonian in the flat space limit (i.e. with unit lapse) nor will it be necessarily positive. Of course, when adding matter like our dust, then similar to the Higgs mechanism the four dust degrees of freedom get absorbed by the metric which develops four additional Goldstone modes. These modes should decouple and they do as we showed explicitly in this paper because of the existence of an infinite number of conserved charges; however, it is not granted to happen when adding arbitrary matter.

We close this section by verifying that the reduced Hamiltonian for the Brown–Kuchař dust model with the obvious choice for the gauge degrees of freedom indeed agrees with the physical Hamiltonian. As gauge fixing conditions we choose

$$G(x) = T(x) - \tau(x;t), \qquad G^j(x) = S^j(x) - \sigma^j \tag{H.13}$$

whence $\tau^j(t,x) = \sigma^j(x)$ is not explicitly time dependent. The stability of (H.13) with respect to the canonical Hamiltonian

$$H_{\text{can}} = \int_{\mathcal{X}} \mathrm{d}^3x \left\{ n[c - \sqrt{P^2 + q^{ab}c_a c_b}] + n^a \left[P T_{,a} + P_j S^j_{,a} + c_a \right] \right\} \tag{H.14}$$

fixes lapse and shift to be

$$n_0 = -\frac{\dot{\tau}\sqrt{P^2 + q^{ab}c_a c_b}}{P}, \qquad n_0^a = 0. \tag{H.15}$$

Hence for any function f independent of the dust degrees of freedom

$$\begin{aligned}
&\{H_{\text{can}}, f\}_{c^{\text{tot}}=\vec{c}^{\text{tot}}=n-n_0=\vec{n}-\vec{n}_0=0} \\
&\quad = \int_{\mathcal{X}} \mathrm{d}^3x \left(n_0 \left[\{c, f\} - \frac{1}{2\sqrt{P^2 + q^{ab}c_a c_b}} \{q^{ab}c_a c_b, f\} \right] \right)_{c^{\text{tot}}=0} \\
&\quad = \int_{\mathcal{X}} \mathrm{d}^3x \, \dot{\tau} \, \frac{c}{h} \left[\{c, f\} - \frac{1}{2c} \{q^{ab}c_a c_b, f\} \right] \\
&\quad = \int_{\mathcal{X}} \mathrm{d}^3x \, \dot{\tau} \, \frac{1}{2h} \left[\{c^2, f\} - \{q^{ab}c_a c_b, f\} \right] \\
&\quad = \int_{\mathcal{X}} \mathrm{d}^3x \, \dot{\tau} \, \{h, f\}]
\end{aligned} \tag{H.16}$$

where we used

$$c^{\text{tot}} = 0 \quad \Leftrightarrow \quad -P = h = \sqrt{c^2 - q^{ab}c_a c_b}. \tag{H.17}$$

Thus the reduced Hamiltonian for $\dot{\tau} = 1$ equals the physical Hamiltonian under the identification $q_{ab} \equiv Q_{jk}$, $p^{ab} \equiv P^{jk}$.

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