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Hamiltonian cosmological perturbation theory with loop quantum gravity corrections

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Cosmological perturbation equations are derived systematically in a canonical scheme based on Ashtekar variables. A comparison with the covariant derivation and various subtleties in the calculation and choice of gauges are pointed out. Nevertheless, the treatment is more systematic when correction terms of canonical quantum gravity are to be included. This is done throughout the paper for one example of characteristic modifications expected from loop quantum gravity.

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I. INTRODUCTION

The backbone of most of current cosmology is the theory of perturbation equations for metric modes around an isotropic spacetime [1]. It is used, in particular, for cosmological structure formation and for testing alternative theories beyond general relativity such as quantum gravity candidates. The underlying equations of typical interest are the linearized Einstein's equations, and so it is straightforward to include corrections if they come from a Lagrangian modified by quantum or other effects. This is, in fact, the situation encountered in most studies of so-called trans-Planckian issues for the effect of quantum gravity on structure formation. Modifications derived from a Hamiltonian formulation as it is used in canonical quantizations can, however, not be implemented in this direct way.

Since several effective modifications to Hamiltonians have been derived in recent years, in particular, within the framework of loop quantum gravity [2–5], it is of interest to rederive cosmological perturbation equations in a purely Hamiltonian fashion starting from the gravitational Hamiltonian. This is done in detail in this paper in a derivation based, as loop quantum gravity itself, on real Ashtekar variables [6,7]. We will present a detailed derivation for scalar modes in longitudinal gauge around a spatially flat model, pointing out several subtleties compared to the Lagrangian derivation.

Our analysis treats gravitational and matter terms on the same footing, showing how all of them can be obtained from the total Hamiltonian. This presents a systematic formulation of cosmological perturbations in canonical gravity which can be used for both classical analyses as well as applications of canonical quantum gravity. We thus provide the classical basis for a systematic investigation of effective perturbation equations and cosmological implications resulting from canonical quantum gravity. In our calculations, only one type of corrections (from inverse powers of metric components in the Hamiltonian) is used, and their implications are discussed. The classical perturbation equations and their derivation follow immediately from our expressions after omitting quantum corrections.

II. VARIABLES AND EQUATIONS

To set up linear metric perturbations [1], one perturbs the background metric

$$ds^2 = a^2(\eta)(-d\eta^2 + \delta_{ab}dx^a dx^b), \qquad (1)$$

here chosen as a flat isotropic metric written in conformal time η and with spatial coordinates x^a. There are initially ten perturbation functions for the ten metric components, but some of them can be absorbed simply by redefining coordinates. The remaining functions, in gauge-invariant combinations, comprise scalar, vector and tensor modes. We are here primarily interested in scalar modes which in longitudinal gauge lead to a perturbed metric

$$ds^2 = a^2(\eta)(-(1+2\phi)d\eta^2 + (1-2\psi)\delta_{ab}dx^a dx^b) \qquad (2)$$

which is thus diagonal. Moreover, in the absence of anisotropic stress it is consistent with longitudinal gauge to set $\phi = \psi$, reducing the perturbations to a single function. We will also do so in our final equations, but not immediately since it is a consequence of equations of motion and should not be used in the process of deriving such equations. Expanding Einstein's equations to linear order in ψ then leads to

$$\nabla^2\psi - 3\frac{\dot a}{a}\dot\psi - 3\frac{\dot a^2}{a^2}\psi = -\frac{\kappa}{2}a^2\delta T^0_0 \qquad (3)$$

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$$\ddot{\psi} + 3\frac{\dot{a}}{a}\dot{\psi} + 2\left(\frac{\dot{a}}{a}\right)^{\cdot}\psi + \frac{\dot{a}^2}{a^2}\psi = \frac{\kappa}{2}a^2\delta T^a_a \tag{4}$$

$$\partial_a\left(\dot{\psi} + \frac{\dot{a}}{a}\psi\right) = -\frac{\kappa}{2}a^2\delta T^0_a \tag{5}$$

where $\kappa = 8\pi G$ is the gravitational constant and a dot denotes a derivative by conformal time η. The source terms on the right hand side of these equations are components of the energy-momentum tensor provided by the matter ingredients, also perturbed linearly. These components follow from functional derivatives of the matter Lagrangian by metric components, for a scalar field φ with potential $V(\varphi)$ and Lagrangian

$$L_\varphi = -\int d^3x\sqrt{-\det g}\left(\frac{1}{2}g^{ab}\partial_a\varphi\partial_b\varphi + V(\varphi)\right)$$

we have, for instance, [8]

$$\delta T^0_0 = -\frac{1}{a^2}(\dot{\bar{\varphi}}\delta\dot{\varphi} - \dot{\bar{\varphi}}^2\psi + a^2V_{,\varphi}(\varphi)\delta\varphi) \tag{6}$$

$$\delta T^0_a = -\frac{1}{a^2}\dot{\bar{\varphi}}\delta\varphi_{,a} \tag{7}$$

$$\delta T^a_b = \frac{1}{a^2}(-\dot{\bar{\varphi}}\delta\dot{\varphi} + \dot{\bar{\varphi}}^2\psi + a^2V_{,\varphi}(\varphi)\delta\varphi)\delta^a_b. \tag{8}$$

In addition, the matter Lagrangian determines equations of motion for matter fields such as those of a scalar φ:

$$\ddot{\bar{\varphi}} + 2\frac{\dot{a}}{a}\dot{\bar{\varphi}} + a^2V_{,\varphi}(\bar{\varphi}) = 0 \tag{9}$$

is the background Klein-Gordon equation, whereas

$$\delta\ddot{\varphi} + 2\frac{\dot{a}}{a}\delta\dot{\varphi} - \nabla^2\delta\varphi + a^2V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi + 2a^2V_{,\varphi}(\bar{\varphi})\psi - 4\dot{\bar{\varphi}}\dot{\psi} = 0 \tag{10}$$

describes the perturbed part of the scalar field.

A. Canonical formalism

Cosmological perturbation equations are the Einstein's equations expanded in metric perturbations. Once a gauge is chosen and modes of interest are selected, the perturbed metric is specified and ready to be inserted in the expansion. Since the canonical formalism is equivalent to the Lagrangian one which yields Einstein's equations as the Euler-Lagrange equations of the Einstein-Hilbert action, the same perturbation equations must result. However, some of the derivations are more subtle since one has to fix gauges and select modes at the right places. Moreover, one first starts with a different set of variables and first order differential equations, which are combined to the usual second order equations. Keeping in mind that quantum gravity can lead to several modifications it is helpful to go through the canonical derivation in detailed steps, which is what we do in this paper.

In a canonical formulation [9], the Hamiltonian H rather than Lagrangian L is the basic dynamical object, determining equations of motion of any phase space function f by means of Poisson brackets, $\dot{f} = \{f, H\}$. The Poisson structure defines the kinematical arena, which is usually written in terms of a set of basic canonical variables such as position and momentum in mechanics. While dynamics as well as expressions for momenta follow from the same object in a Lagrangian formulation, they are separate in a Hamiltonian one. The Poisson structure is thus prescribed independently of the Hamiltonian, but both of them are needed to determine dynamics. Basic configuration variables in a Lagrangian formulation of gravity are the components of the spacetime metric g_{ab}, and their momenta are determined as usually by derivatives $\pi^{ab} = \delta L/\delta\dot{g}_{ab}$. The dot refers here to a time coordinate in which the action is written. Since general relativity is covariant under arbitrary changes of spacetime coordinates, the choice of time does not play a physical role. Nevertheless, by definition of its kinematical objects a canonical formulation does not appear manifestly covariant. Indeed, not all components of the spacetime metric appear equal: some of them, the time-time component N and the time-space components N^a do not occur as first order derivatives in the action such that their momenta vanish identically, $\pi_N = 0 = \pi_{N^a}$.

This is a consequence of general covariance and implies the existence of constraints. Since momenta of N and N^a vanish, their equations of motion imply

$$0 = \dot{\pi}_N = \{\pi_N, H\} = -\delta H/\delta N \quad \text{and}$$
$$0 = \dot{\pi}_{N^a} = \{\pi_{N^a}, H\} = -\delta H/\delta N^a$$

as constraint equations on the remaining phase space variables. In fact, because there is no absolute meaning to the time coordinate at all, the total Hamiltonian is a sum of constraints $H = H[N] + D[N^a]$ with the Hamiltonian constraint $H[N] = \int d^3xN(x)\delta H/\delta N$ and the diffeomorphism constraint $D[N^a] = \int d^3xN^a(x)\delta H/\delta N^a$. Coordinate time evolution through Hamiltonian equations of motion is completely specified only when N and N^a are known as functions on spacetime. However, there are no equations of motion for N and N^a themselves; they are not dynamical since their momenta vanish. They have to be chosen in order to fix the gauge in which spacetime properties are computed. That the constraints generate coordinate changes can more easily be seen for the diffeomorphism constraint which satisfies $\{f, D[N^a]\} = \mathcal{L}_{N^a}f$ for any phase space function f, where on the right hand side the Lie derivative occurs. Both constraints receive contributions from gravitational fields (the spatial metric and their momenta) and matter fields.

The Hamiltonian formulation is thus based on phase space coordinates given by the spatial metric components, matter fields and their momenta. In addition, there are the lapse function N and shift vector N^a which need to be chosen for a particular gauge. Their dynamical behavior is given by Hamiltonian equations of motion derived through Poisson brackets with the constraints. Since the Hamiltonian is usually, and, in particular, in gravity, a quadratic polynomial of the momenta conjugate to metric components, Poisson brackets between configuration variables and the Hamiltonian are linear in momenta. Thus, the Hamiltonian equations of motion for configuration variables relate momenta to first order time derivatives. Equations of motion for the momenta can then be reformulated as second order differential equations for configuration variables which agree with the Euler-Lagrange equations. Moreover, one can replace momenta in the constraint equations by first order derivatives of configuration variables, giving additional first order differential equations. The set of Eqs. (3)–(5) thus consists, from the Hamiltonian perspective, of two constraint equations, the Hamiltonian constraint (3) and the diffeomorphism constraint (5) and one equation of motion (4) for the single scalar mode.

However, this set of equations is not the most general one for a linearized metric. Gauge choices and a selection of modes have been made, the latter excluding vector and tensor modes and equating the lapse perturbation with the scalar mode. These put conditions on the variables and on the multipliers N and N^a. In a Hamiltonian formulation one has to be careful about when to make such choices in the process of deriving the equations of motion. Gauge choices have to be made from the start because this determines what the time variable and other coordinates in the resulting differential equations mean. For instance, the homogeneous mode of the lapse function has to be specified, which is usually chosen as $N = 1$ for proper time or $N = a$ for conformal time. But this is to be done only for equations of motion, not for a derivation of the constraint. It is clear that setting $N = 1$ or equal to the scale factor does not result in the right Hamiltonian constraint $\delta H/\delta N$ which requires N to be an independent variable. Similarly, one often sets the shift vector to zero, while the diffeomorphism constraint $\delta H/\delta N^a$ is to be imposed fully.

The correct procedure is as follows: To derive constraint equations, no gauge choices are to be made. In fact, without knowing the constraints it is impossible to know what gauge freedom one has. In the next step, one derives Hamiltonian equations of motion for the phase space variables, q_{ab} and their momenta in the case of gravity. Here, the gauge has to be chosen before computing Poisson brackets to give meaning to coordinate time derivatives. One can also restrict to specific modes, but other conditions are not to be done. For instance, equating the lapse perturbation to the spatial perturbations is only justified as the result of equations of motion. Doing this before computing Poisson brackets would introduce erroneous relations between independent degrees of freedom. Thus, such a simplification must be made only in the final expressions for equations of motion.

B. Perturbed canonical variables

Also the set of canonical variables matters for a quantization: while classically one can change variables by canonical transformations, their quantum representations can appear very different. Loop quantum gravity crucially depends on properties of Ashtekar variables [6,7] due to their transformation properties. First, one introduces a cotriad e_a^i instead of the spatial metric q_{ab}, related to it by $e_a^i e_b^i = q_{ab}$. (Unlike the position of spatial indices $a, b, \ldots$, the upper or lower positions of indices i are not relevant, and summing over i is understood even though it appears twice in the same position.) An oriented cotriad contains the same information as a metric but has more components as it is not a symmetric tensor. This corresponds to freedom one has in rotating the triple of triad covectors which does not change the metric. Not being of geometrical relevance, this freedom is removed in a canonical formalism by implementing the Gauss constraint introduced below. By inverting the matrix (e_a^i), one obtains the triad e_i^a, a set of vector fields related to the inverse metric by $e_i^a e_i^b = q^{ab}$. Just as the metric determines a compatible Christoffel connection Γ_{ab}^c, a triad determines a compatible spin connection

$$\Gamma_a^i = -\epsilon^{ijk} e_j^b \left(\partial_{[a} e_{b]}^k + \frac{1}{2} e_k^c e_a^l \partial_{[c} e_{b]}^l \right). \tag{11}$$

Its components define the Ashtekar connection $A_a^i = \Gamma_a^i + \gamma K_a^i$ together with those of extrinsic curvature

$$K_a^i = e_i^b K_{ab} = \frac{1}{2N} e_i^b (\mathcal{L}_t q_{ab} - 2D_{(a}N_{b)}) \tag{12}$$

where the right hand side uses lapse function N and shift vector N^a in addition to the spatial metric q_{ab}. Moreover, $\mathcal{L}_t$ denotes a Lie derivative along a timelike vector field chosen to describe changes in coordinate time, and D_a is the covariant derivative compatible with the spatial metric q_{ab}. In A_a^i, we have the positive real Barbero-Immirzi parameter γ [7,10] which we keep here for generality although it will not play a large role later on.

The Ashtekar connection is thus a measure for curvature, and spatial metric information is described by the densitized triad $E_i^a = |\det e_b^j| e_i^a$ obtained from the triad. By multiplying the triad by the determinant of the cotriad, which is identical to the square root of the determinant of the spatial metric, it becomes canonically conjugate to the Ashtekar connection:

$$\{A_a^i(x), E_j^b(y)\} = \gamma\kappa \delta_a^b \delta_j^i \delta(x, y). \tag{13}$$

This follows from the gravitational action which in a first order formulation contains time derivatives of the connection in the term

$$\frac{1}{\gamma\kappa}\int d^3x \frac{dA_a^i}{dt}E_i^a$$

showing that the connection and the densitized triad are canonically conjugate.

An unperturbed isotropic triad and connection for flat spatial slices [11] can always be chosen of diagonal form $E_i^a = p\delta_i^a$ and $A_a^i = c\delta_a^i$ with canonically conjugate c and p: $\{c, p\} = \frac{1}{3}\gamma\kappa$. In more familiar terms, these variables are related to the scale factor a by $|p| = a^2$ and $c = \gamma da/dt$. With inhomogeneous perturbations, the triad and connection components will become space-dependent, but not in a way that is completely unrelated between E_i^a and A_a^i because of the spin connection. This implies that not both the triad and the connection can remain diagonal even when only scalar perturbations in longitudinal gauge are considered for which the spatial metric is diagonal. (This happens generally in inhomogeneous situations; see also [12].) Another way to see this is by looking at the Gauss constraint

$$\partial_a E_i^a + \epsilon^{ijk}A_a^j E_k^a = 0 \tag{14}$$

which ensures invariance of physical results under rotations of the triad, which do not change the metric. Were both E_i^a and A_a^i diagonal, the second term $\epsilon^{ijk}E_j^a A_a^k$ would vanish, constraining inhomogeneity by $\partial_a E_i^a = 0$.

It is most useful to keep the triad diagonal since this simplifies the classical calculations, and even more so the quantum ones where currently only situations of diagonal triads are sufficiently accessible by explicit calculations. We thus introduce the perturbed triad [13]

$$E_i^a = p(x)\delta_i^a = (\bar{p} + \delta p(x))\delta_i^a \tag{15}$$

which gives rise to a spatial metric of the form $q_{ab} = |\bar{p} + \delta p|\delta_{ab}$. Here and elsewhere, we split off the background part

$$\bar{p} := \frac{1}{V_0}\int p(x)d^3x \tag{16}$$

with the spatial coordinate volume $V_0 = \int d^3x$. The latter is assumed to be finite, using a compact torus topology of space, but will not appear in the final classical equations. Using $\bar{p}$, we then define the perturbation

$$\delta p(x) := p(x) - \bar{p} \text{ such that } \int \delta p(x)d^3x = 0. \tag{17}$$

In the usual notation using the scale factor and the scalar metric mode ψ in longitudinal gauge we have $q_{ab} = a^2(1-2\psi)\delta_{ab}$, leading to the identification $|\bar{p}| = a^2$ and $\delta p = -2\bar{p}\psi$. Remaining spacetime metric components are the lapse function $N = \bar{N} + \delta N$ and the shift vector N^a. Their usual notation $N = a(1+\phi)$ gives $\bar{N} = a$, $\delta N = a\phi$ for the lapse function in conformal time gauge, while N^a is zero for scalar modes in the longitudinal gauge. In the absence of anisotropic stress, i.e. nondiagonal components of the spatial part of the energy-momentum tensor, ϕ is not independent of ψ but has to agree with it. We will make this identification in the final equations, but have to keep N as well as N^a as free Lagrange multipliers in initial steps.

With a diagonal triad, the connection cannot be diagonal in inhomogeneous situations. In fact, for a perturbed triad (15) one can compute the spin connection to be

$$\Gamma_a^i = \frac{1}{2}\epsilon_a{}^{ij}\frac{\partial_j \delta p}{\bar{p} + \delta p} \tag{18}$$

which is antisymmetric and thus nondiagonal. The diagonal part of A_a^i is then contributed solely by extrinsic curvature, which, again in longitudinal gauge where the shift vector vanishes, [16] is proportional to a time derivative of the triad and thus diagonal,

$$K_a^i = k(x)\delta_a^i = (\bar{k} + \delta k(x))\delta_a^i. \tag{19}$$

A perturbed connection then has the form

$$A_a^i = \gamma(\bar{k} + \delta k(x))\delta_a^i + \Gamma_a^i(x) \tag{20}$$

split into the perturbed but diagonal extrinsic curvature part and the nondiagonal (in fact, antisymmetric) part coming from the perturbed spin connection. The direct calculation (18) can easily be seen to solve the Gauss constraint identically. The gravitational variables $\bar{p}$, $\bar{k}$, δp and δk are thus constrained only by the diffeomorphism and Hamiltonian constraints.

C. Constraints

The gravitational contributions to these constraints in terms of Ashtekar variables are the diffeomorphism constraint

$$D_G[N^a] = \frac{1}{\gamma\kappa}\int d^3x N^a F_{ab}^i E_i^b \tag{21}$$

where $F_{ab}^i = \partial_a A_b^i - \partial_b A_a^i + \epsilon^{ijk}A_a^j A_b^k$ is the curvature of the Ashtekar connection, and the Hamiltonian constraint

$$H_G[N] = \frac{1}{2\kappa}\int_\Sigma d^3x N|\det E|^{-1/2}(\epsilon_{ijk}F_{ab}^i E_j^a E_k^b - 2(1+\gamma^2)K_a^i K_b^j E_i^{[a}E_j^{b]}). \tag{22}$$

Note that, strictly speaking, (21) is the so-called vector constraint, i.e. a combination of the diffeomorphism constraint which generates spatial diffeomorphisms and the Gauss constraint (14). Since by our choice of variables we are solving the Gauss constraint identically, we can use (21) as the diffeomorphism constraint.

Clearly, the matrix symmetry of (15), (18), and (19) will lead to simplifications of the Hamiltonian and other constraints. Since constraints are also the places where quantum corrections enter, in particular, in (22) which determines dynamics, one should use simplifications only after such corrections have been implemented.

Specifically, in the effective regime, the terms containing inverse powers of the scale factor, e.g. the spin connection (18) or $|\det E|^{-1/2}$, will have quantum corrections. If one uses (15) first, then the inverse determinant in (22) would *cancel* at the classical level already, thus not acquiring any effective corrections upon quantization. Reliable places for correction terms can thus only be found in the full expressions. In this paper, we will accordingly insert a function of triad components α to take into account possible corrections coming from $|\det E|^{-1/2}$ and a function β multiplying spin connection components (18) to take into account the inverse triad component there [17]. These functions depend on triad components and classically $\alpha = \beta = 1$ in which case we will indeed reproduce the classical equations. We will, however, keep α and β in our equations without specifying them to demonstrate how quantum corrections can easily propagate in more complicated terms when equations of motion are derived; such functions can be found in [15]. The typical behavior is similar to the function $|\bar{p}|^{3/2}d(\bar{p})$ [21,22] used in isotropic models and sketched in Fig. 1. For small arguments these functions are increasing, starting from a value smaller than 1 which is zero in homogeneous models and for perturbative inhomogenities but can be nonzero if non-Abelian features of the full theory and coherent state effects are considered [23,24]. At an intermediate scale, whose value depends on details of the quantization, they peak at a height larger than 1 and then approach the classical value one from above. The small-$\bar{p}$ behavior is thus strongly modified by nonperturbative effects while the large-$\bar{p}$ behavior is perturbative of the form

$$\alpha(\bar{p}) = 1 + c\left(\frac{\ell_{\rm P}^2}{\bar{p}}\right)^n \quad \text{with } c > 0 \quad \text{and} \quad n > 0 \tag{23}$$

where $\ell_{\rm P} = \sqrt{\hbar G}$ is the Planck length. The values of c and

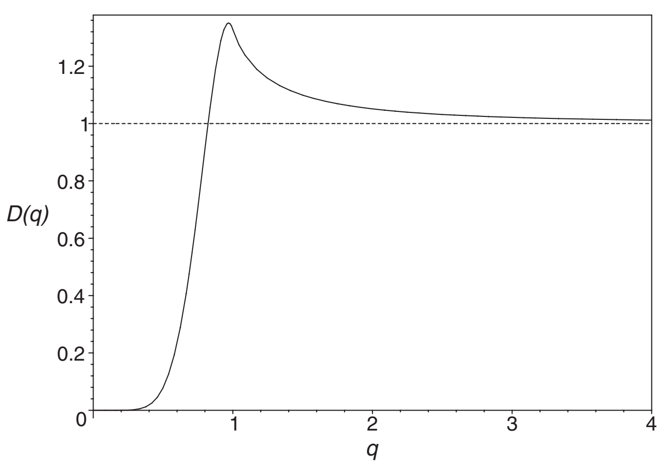

FIG. 1. Typical behavior of correction functions α, β, D and σ which approach one from above for large arguments. For small arguments, the functions are increasing and reach a peak value larger than 1.

n also depend on the quantization but are generally positive. This allows the discussion of characteristic qualitative effects. It is safest to use perturbation theory to the right of the peaks of correction functions.

The constraint (22) can be simplified, if expressed in terms of the spin connection and extrinsic curvature, using $A_a^i = \Gamma_a^i + \gamma K_a^i$. The first term is then written as

$$\begin{aligned} F_{ab}^i &= 2\partial_{[a}\Gamma_{b]}^i + 2\gamma\partial_{[a}K_{b]}^i + \epsilon_{ijk}(\Gamma_a^j + \gamma K_a^j)(\Gamma_b^k + \gamma K_b^k) \\ &= 2\partial_{[a}\Gamma_{b]}^i + 2\gamma\partial_{[a}K_{b]}^i + \gamma\epsilon_{ijk}(\Gamma_a^j K_b^k + \Gamma_b^k K_a^j) \\ &\quad + \epsilon_{ijk}(\Gamma_a^j\Gamma_b^k + \gamma^2 K_a^j K_b^k). \end{aligned} \tag{24}$$

Contracting with the triad, we see that the second term

$$\epsilon_{ijk}\partial_a K_b^i E_j^a E_k^b \propto \epsilon_{ijk}\delta_b^i\delta_j^a\delta_k^b \propto \epsilon_{ijk}\delta_k^i = 0,$$

whereas the cross-term

$$\begin{aligned} \epsilon_{ijk}\epsilon_{ilm}(\Gamma_a^l K_b^m + \Gamma_b^m K_a^l)E_j^a E_k^b &= 2\delta_{[l}^j\delta_{m]}^k E_j^a E_k^b \Gamma_a^l K_b^m \\ &\propto \Gamma_j^j K_k^k - \Gamma_j^k K_k^j \end{aligned}$$

vanishes because K is diagonal and Γ is antisymmetric. Also, the last curvature term in (24) (quadratic in K), can be combined with the last term of (22) yielding

$$\begin{aligned} H_G[N] = \frac{1}{\kappa}\int_\Sigma \mathrm{d}^3x N\alpha|\det E|^{-1/2}(\epsilon_{ijk}\partial_a(\beta\Gamma_b^i) \\ + \beta^2\Gamma_a^j\Gamma_b^k - K_a^j K_b^k)E_j^{[a}E_k^{b]}. \end{aligned} \tag{25}$$

As already announced, here we have included quantum correction functions α and β which depend on the densitized triad and whose classical limit is $\alpha = \beta = 1$. We will present the derivation of perturbation equations from the canonical Hamiltonian in general terms including such unspecified correction functions. The purely classical analysis will be identical and obtained immediately by setting choosing the classical values for all correction functions. To save space, we do not reproduce these classical equations explicitly.

In the diffeomorphism constraint we have similar simplifications and some terms do not contribute after writing out the curvature components explicitly. In our variables,

$$\begin{aligned} F_{ab}^i E_i^b &= 2\gamma(\bar{p} + \delta p)\partial_a(\bar{k} + \delta k) \\ &\quad + \epsilon_{bjk}(\Gamma_a^j + \gamma K_a^j)\Gamma_b^k(\bar{p} + \delta p) \\ &= 2\gamma(\bar{p} + \delta p)\partial_a(\bar{k} + \delta k) - (\Gamma_a^j + \gamma K_a^j)\partial_j\delta p \end{aligned}$$

using (18) in the last line. Then, with $\Gamma_a^j\partial_j\delta p = 0$ the constraint

$$D[N^a] = \frac{1}{\kappa}\int \mathrm{d}^3x\delta N^a(2\bar{p}\partial_a\delta k - \tilde{\beta}\,\bar{k}\,\partial_a\delta p)$$

for $\bar{N}^a = 0$ results. Note that we did use the expression for the spin connection in the second term which could thus receive a correction function $\tilde{\beta}$. Since it is coming from the spin connection it should equal β, but we keep it separate because the diffeomorphism constraint is not quantized in infinitesimal form in loop quantum gravity. One rather implements finite diffeomorphisms exactly [25] such that no corrections are expected. As we will see later, effects of $\tilde{\beta}$ are not important such that the precise prescription here does not matter much. Moreover, there is no inverse determinant in the diffeomorphism constraint and no need for a correction function α.

Together with contributions from matter fields, this defines constraints on the basic variables. For a scalar field φ with momentum π and potential $V(\varphi)$, we have a contribution

$$D_\varphi[N^a] = \int d^3x N^a \pi \partial_a \varphi \tag{26}$$

to the diffeomorphism constraint and a contribution by the matter Hamiltonian

$$H_\varphi[N] = \int d^3x N\Big(\frac{1}{2} D \frac{\pi^2}{\sqrt{|\det E|}} + \frac{1}{2}\sigma \frac{E^a_i E^b_i \partial_a\varphi \partial_b \varphi}{\sqrt{|\det E|}} + \sqrt{|\det E|} V(\varphi)\Big) \tag{27}$$

to the Hamiltonian constraint. Again, only the contribution to the Hamiltonian constraint contains inverse powers which occur in two different forms. The kinetic part has a single inverse determinant which we correct by a function D (as it has been used in isotropic models), while the gradient term has additional triad components in the numerator which can lead to a different correction function σ. Note also that, while formally the combination of triad components in the gradient term is the same as that in the gravitational part of the Hamiltonian constraint, it is only the symmetric part in a and b which enters the matter gradient term but the antisymmetric part in the gravitational constraint. We therefore keep the correction functions α and σ independent.

The equations to consider are thus the two constraint equations

$$D[N^a] = D_G[N^a] + D_\varphi[N^a] = 0 \tag{28}$$

$$H[N] = H_G[N] + H_\varphi[N] = 0 \tag{29}$$

together with the Hamiltonian equations of motion

$$\dot{f} = \{f, H[N] + D[N^a]\} \tag{30}$$

for any of the variables $\bar{p}$, $\bar{k}$, $\bar{\varphi}$, $\bar{p}_\varphi$ and the fields δp, δk, $\delta\varphi$ and $\delta\pi$. The components N and N^a, i.e. $\bar{N}$, δN and δN^a play the role of Lagrange multipliers for the constraints. When computing the Poisson brackets in equations of motion (30) one has to keep these multipliers as independent variables at this stage, as discussed before. Only $\bar{N}$ has to be specified to fix the time gauge, with the two most common choices $\bar{N} = 1$ for proper time and $\bar{N} = a$ for conformal time which we will use here. The fields δN and δN^a, on the other hand, must not yet be fixed to ψ or zero, respectively, but be kept independent of the canonical fields.

III. LINEAR PERTURBATION

In order to derive linearized equations of motion, we expand the Hamiltonian to second order in the field perturbations so as to get linear equations after taking Poisson brackets. For the constraint equations themselves, the linear coefficients of δN and δN^a will result as perturbation equations, accompanied by equations of motion for δp, δk, $\delta\varphi$ and $\delta\pi$, which can be combined to 2 s order differential equations of motion for δp and $\delta\varphi$. Spatial integrations of terms linear in perturbations give zero because we have split off the homogeneous background contributions explicitly in definitions such as (17) for δp. The Poisson structure for these variables can then be computed by inserting them in the full action term

$$\frac{1}{\gamma\kappa}\int d^3x \frac{dA^i_a}{dt} E^a_i = \frac{3}{\kappa}\int d^3x \frac{dk(x)}{dt} p(x) = \frac{3V_0}{\kappa}\frac{d\bar{k}}{dt}\bar{p} + \frac{3}{\kappa}\int d^3x \frac{d\delta k}{dt}\delta p \tag{31}$$

such that

$$\{\bar{k}, \bar{p}\} = \frac{\kappa}{3V_0}, \qquad \{\delta k(x), \delta p(y)\} = \frac{\kappa}{3}\delta(x, y). \tag{32}$$

A. Variations

All necessary equations follow from variations of the total constraint

$$\begin{aligned} H &= H_G[N] + H_\varphi[N] + D_G[N^a] + D_\varphi[N^a] \\ &= \frac{1}{2\kappa}\int d^3x N(x)\alpha(p)\Big(-6(\bar{k}+\delta k)^2|\bar{p}+\delta p|^{1/2} \\ &\quad + \frac{1}{2}\frac{(\beta(p)^2 + 4\beta'(p)p - 4\beta(p))\partial^a\delta p \partial_a \delta p}{|\bar{p}+\delta p|^{3/2}} \\ &\quad + 2\frac{\beta(p)\nabla^2\delta p}{|\bar{p}+\delta p|^{1/2}}\Big) + \frac{1}{\kappa}\int d^3x \delta N^a(2\bar{p}\partial_a\delta k \\ &\quad - \tilde{\beta}(p)\bar{k}\partial_a\delta p) + H_\varphi[N] + D_\varphi[N^a] \end{aligned} \tag{33}$$

by the independent variables $\bar{N}$, δN, δN^a, $\bar{p}$, δp, $\bar{k}$, δk, $\bar{\varphi}$, $\delta\varphi$, $\bar{\pi}$ and $\delta\pi$. The background shift vector $\bar{N}^a$ does not appear because it vanishes for homogeneous models, as does the background diffeomorphism constraint it would be the Lagrange multiplier of. It would have to be considered when perturbing around an inhomogeneous background.

We then have the following equations:

$$0 = \frac{\partial H[N]}{\partial \bar{N}} = -\frac{3V_0}{\kappa}\alpha\sqrt{|\bar{p}|}\bar{k}^2 + \frac{\partial H_\varphi[N]}{\partial \bar{N}} \tag{34}$$

gives the background Friedmann equation which is corrected by higher order terms such as $\int d^3x\alpha\delta k^2\sqrt{|\bar{p}|}$ in the perturbations if higher orders are retained in the expansion. In this variation, $\bar{N}$ is kept independent because it must be varied, but from now on we set $\bar{N}=\sqrt{|\bar{p}|}$ to choose conformal time, derivatives of which will be denoted by a dot (while a prime is used for $\bar{p}$-derivatives). Then,

$$\begin{aligned}0&=\frac{\delta H[N]}{\delta(\delta N)}\\&=\frac{\sqrt{|\bar{p}|}}{\kappa}\Big(-6\alpha\bar{k}\delta k-3\alpha\bar{k}^2\Big(1+2\bar{p}\frac{\alpha'}{\alpha}\Big)\frac{\delta p}{2\bar{p}}\\&\quad+\frac{\alpha\beta}{\bar{p}}\nabla^2\delta p\Big)+\frac{\delta H_\varphi[N]}{\delta(\delta N)}\end{aligned}\tag{35}$$

gives the first perturbation equation equivalent to (3),

$$0=\kappa\frac{\delta D[N^a]}{\delta(\delta N^a)}=2\bar{p}\partial_a\delta k-\tilde{\beta}\,\bar{k}\,\partial_a\delta p+\kappa\frac{\delta D_\varphi[N^a]}{\delta(\delta N^a)}\tag{36}$$

gives the third perturbation equation equivalent to (5) and

$$\dot{\bar{k}}=\frac{\kappa}{3V_0}\frac{\partial H}{\partial\bar{p}}=-\alpha\bar{k}^2+\frac{\kappa}{3V_0}\frac{\partial H_\varphi[N]}{\partial\bar{p}}\tag{37}$$

gives the background Raychaudhuri equation. In

$$\begin{aligned}\delta\dot{k}&=\frac{\kappa}{3}\frac{\delta H}{\delta(\delta p)}\\&=-\frac{1}{\sqrt{|\bar{p}|}}(\alpha+\alpha'\bar{p})(\delta N\bar{k}^2+2\bar{N}\,\bar{k}\,\delta k)\\&\quad+\frac{\delta p}{|\bar{p}|^{3/2}}\bar{N}\bar{k}^2(\alpha-\alpha'\bar{p}-\alpha''\bar{p}^2)+O(\delta(N\sqrt{|p|}))\\&\quad-\frac{\bar{N}}{6\bar{p}^{3/2}}(\alpha\beta(\beta-2)-4\beta(\alpha'\bar{p}))\nabla^2\delta p\\&\quad+\frac{\alpha\beta}{3\sqrt{|\bar{p}|}}\nabla^2\delta N+\frac{\kappa}{3}\frac{\delta H_\varphi[N]}{\delta(\delta p)}\end{aligned}\tag{38}$$

which gives the second perturbation equation equivalent to (4), the term $O(\delta(N\sqrt{|p|}))$ indicates that there are additional terms proportional to $\delta(N\sqrt{|p|})$ which are not evaluated explicitly here. They will cancel exactly in the final equations for the modes used here, but would give nonzero contributions if the lapse perturbation and the scalar mode are not identified or if other gauges are used.

Finally,

$$\dot{\bar{p}}=-\frac{\kappa}{3V_0}\frac{\partial H}{\partial\bar{k}}=2\alpha\bar{p}\,\bar{k}\tag{39}$$

relates the connection component $\bar{k}$ to the time derivative of $\bar{p}$ or the scale factor a. Together with the perturbation equation

$$\delta\dot{p}=-\frac{\kappa}{3}\frac{\delta H}{\delta(\delta k)}=2\alpha\bar{p}\delta k+2\alpha'\bar{k}\,\bar{p}\,\delta p\tag{40}$$

which relates the connection component δk to the time derivative of δp, it can be used to eliminate the extrinsic curvature components.

For the matter variables we obtain four additional equations,

$$\dot{\bar{\pi}}=-\frac{1}{V_0}\frac{\partial H}{\partial\bar{\varphi}}=-\bar{p}^2V_{,\varphi}(\bar{\varphi})\tag{41}$$

which gives the background Klein-Gordon equation,

$$\begin{aligned}\delta\dot{\pi}&=-\frac{\delta H}{\delta(\delta\varphi)}\\&=-\bar{p}(V_{,\varphi}(\bar{\varphi})\delta p+V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi-\sigma(\bar{p})\nabla^2\delta\varphi)\end{aligned}\tag{42}$$

which gives the matter perturbation equation,

$$\dot{\bar{\varphi}}=\frac{1}{V_0}\frac{\partial H}{\partial\bar{\pi}}=\frac{D(\bar{p})\bar{N}}{\bar{p}^{3/2}}\bar{\pi}\tag{43}$$

which relates $\bar{\pi}$ to the time derivative of $\bar{\varphi}$ and

$$\delta\dot{\varphi}=\frac{\delta H}{\delta(\delta\pi)}=\frac{D(\bar{p})}{\bar{p}}\Big(\delta\pi-\frac{\bar{\pi}\delta p}{\bar{p}D(\bar{p})}(2D(\bar{p})-D'(\bar{p})\bar{p})\Big)\tag{44}$$

which relates $\delta\pi$ to the time derivative of $\dot{\varphi}$.

Eqs. (39), (40), (43), and (44) will be used to eliminate momenta from the equations, rewriting some of them as second order differential equations.

B. Metric equations

We first turn to the more complicated equations obtained by varying with respect to metric modes. Here, both the gravitational and the matter part of the constraints contribute, whose variations are discussed separately. From now on, we evaluate the variation equations only for the case $\delta N^a=0$ (for longitudinal gauge without vector modes) and $\delta N=-\delta p/2\sqrt{|\bar{p}|}$ (identifying $\phi=\psi$). The latter identification implies $\delta(N\sqrt{|p|})=0$ at the linearized level which we will use from now on.

1. Gravitational part

Equation (39) can be rewritten as

$$\mathcal{H}:=\frac{\dot{\bar{p}}}{2\bar{p}}=\alpha\bar{k}\tag{45}$$

where $\mathcal{H}$ is the conformal Hubble rate. Inserting it in Eqs. (34) and (37) gives the first order Friedmann equation

$$\mathcal{H}^2=\frac{\alpha\kappa}{3V_0\sqrt{|\bar{p}|}}\frac{\partial H_\varphi[N]}{\partial\bar{N}}\tag{46}$$

and the second order Raychaudhuri equation

$$\dot{\mathcal{H}} = -\mathcal{H}^2\left(1 - \frac{2\alpha'\bar{p}}{\alpha}\right) + \frac{\alpha\kappa}{3V_0}\frac{\partial H_\varphi[N]|_{\bar{N}=\sqrt{\bar{p}}}}{\partial\bar{p}}$$

for the background metric. Here, as well as in any equation of motion, the lapse function is fixed prior to taking the p-derivative. In other words, any appearance of a time derivative implies that a time gauge has been chosen, i.e. the lapse function has been fixed. With this in mind, the background Raychaudhuri equation can be written

$$\dot{\mathcal{H}} = -\mathcal{H}^2\left(1 - \frac{2\alpha'\bar{p}}{\alpha}\right) + \frac{\alpha\kappa}{3V_0}\left(\frac{\partial H_\varphi[N]}{\partial\bar{p}} + \frac{\partial\bar{N}}{\partial\bar{p}}\frac{\partial H_\varphi[N]}{\partial\bar{N}}\right)\Big|_{\bar{N}=\sqrt{\bar{p}}} \tag{47}$$

Solving Eq. (40) for δk we obtain

$$\delta k = \frac{\delta\dot{p}}{2\alpha\bar{p}} - \frac{\alpha'}{\alpha}\bar{k}\delta p, \tag{48}$$

and inserting $\bar{k}$ and δk in terms of $\dot{\bar{p}}$ and $\delta\dot{p}$ in Eqs. (35), (36), and (38) gives the perturbation equations

$$-\frac{\alpha^2\beta}{3\bar{p}}\nabla^2\delta p - \mathcal{H}\frac{\delta\dot{p}}{\bar{p}} + \mathcal{H}^2(1 - \alpha'\bar{p}/\alpha)\frac{\delta p}{2\bar{p}} = \frac{\kappa\alpha}{3\sqrt{|\bar{p}|}}\frac{\delta H_\varphi[N]}{\delta(\delta N)} \tag{49}$$

$$\alpha^{-1}\partial_a(-\delta\dot{p} + \mathcal{H}\delta p(\tilde{\beta} + 2\alpha'\bar{p}/\alpha)) = \kappa\frac{\delta D_\varphi[N^a]}{\delta(\delta N^a)} \tag{50}$$

$$\frac{1}{\alpha}\delta\ddot{p} + \frac{1}{3}(\alpha\beta(\beta-1) - 4\beta(\alpha'\bar{p}))\nabla^2\delta p - \frac{\mathcal{H}}{\alpha}(1 + 2\alpha'\bar{p}/\alpha)\delta\dot{p} - \frac{\dot{\mathcal{H}}\alpha'}{\alpha^2}\delta p - \left(\frac{\mathcal{H}}{\alpha}\right)^2(2\alpha''\bar{p}^2 + \alpha'\bar{p} + \alpha - 4(\alpha'\bar{p})^2/\alpha)\delta p = \frac{2\kappa}{3}\bar{p}\frac{\delta H_\varphi[N]}{\delta(\delta p)} \tag{51}$$

for the metric mode δp.

2. Matter part and energy-momentum

Rather than using the energy-momentum tensor as source, the primary object in a canonical analysis is the Hamiltonian combined with the diffeomorphism constraint. The matter Hamiltonian is directly related to energy density [26]

$$\rho_\varphi = \frac{1}{\sqrt{|\det E|}}\frac{\delta H_\varphi[N]}{\delta N} \tag{52}$$

while contributions to the diffeomorphism constraint give the energy flux density

$$V_{\varphi,a} = \frac{1}{\sqrt{|\det E|}}\frac{\delta D_\varphi[N^b]}{\delta N^a}. \tag{53}$$

This corresponds to time-time and time-space components of the energy-momentum tensor. The remaining components, in the absence of anisotropic stress, are pressure components which we use here only in the isotropic case. From the thermodynamical definition of pressure as $P = -\delta E_\varphi/\delta V$ with energy E_φ and volume V, pressure components can then be derived through [27]

$$P_\varphi = -\frac{1}{N}\frac{\delta H_\varphi[N]}{\delta\sqrt{|\det E|}} \tag{54}$$

from the Hamiltonian.

For the perturbative treatment, we again split these expressions into background and perturbation parts such as $\bar{\rho}$ and $\delta\rho$. By the chain rule, we have

$$\begin{aligned}\rho_\varphi(x)|p(x)|^{3/2} &= \left(\frac{\delta\bar{N}}{\delta N(x)}\frac{\partial H_\varphi[N]}{\partial\bar{N}} + \int d^3y\frac{\delta(\delta N(y))}{\delta N(x)}\frac{\delta H_\varphi[N]}{\delta(\delta N(y))}\right)\\ &= \left(\frac{1}{V_0}\frac{\partial H_\varphi[N]}{\partial\bar{N}} + \frac{\delta H_\varphi[N]}{\delta(\delta N(x))} - \frac{1}{V_0}\int d^3y\frac{\delta H_\varphi[N]}{\delta(\delta N(y))}\right)\\ &= (\bar{\rho}_\varphi + \delta\rho_\varphi(x))|p(x)|^{3/2}\end{aligned}$$

where we used

$$\frac{\delta\bar{N}}{\delta N(x)} = \frac{1}{V_0} \quad \text{and} \quad \frac{\delta(\delta N(y))}{\delta N(x)} = \delta(x,y) - \frac{1}{V_0}$$

for $\bar{N} := V_0^{-1}\int d^3xN(x)$ and $\delta N(x) = N(x) - \bar{N}$. The last term in (55) vanishes because $\delta H/\delta(\delta N(y))$ is linear (or in general odd) in perturbations and thus vanishes when integrated over space. The remaining terms then define the background energy density

$$\bar{\rho}_\varphi = \frac{1}{|\bar{p}|^{3/2}V_0}\frac{\partial H_\varphi[N]}{\partial\bar{N}} = -\bar{T}_0^0 \tag{55}$$

and the linear perturbation

$$\begin{aligned}\delta\rho_\varphi(x) &= -\frac{3\delta p}{2|\bar{p}|^{5/2}V_0}\frac{\partial H_\varphi[N]}{\partial\bar{N}} + |\bar{p}|^{-3/2}\frac{\delta H_\varphi[N]}{\delta(\delta N(x))}\\ &= -\delta T_0^0(x).\end{aligned} \tag{56}$$

Thus,

$$-\frac{\delta H_\varphi[N]}{\delta(\delta N)} = |\bar{p}|^{3/2}\delta T_0^0 + \frac{3}{2}\sqrt{|\bar{p}|}\bar{T}_0^0\delta p. \tag{57}$$

Similarly, we obtain

$$\bar{V}_{\varphi,a} = \frac{1}{\bar{N}|\bar{p}|^{3/2}} \frac{\partial D_\varphi[N^a]}{\partial \bar{N}^a} = -\bar{T}^0_a \tag{58}$$

which vanishes for a homogeneous background, and with this

$$\delta V_{\varphi,a}(x) = \frac{1}{\bar{N}|\bar{p}|^{3/2}} \frac{\delta D_\varphi[N^a]}{\delta(\delta N^a(x))} = -\delta T^0_a(x) \tag{59}$$

for the flux. Finally, we have

$$\bar{P}_\varphi = -\frac{2}{3\bar{N}\sqrt{|\bar{p}|}V_0} \frac{\partial H_\varphi[N]}{\partial \bar{p}} = \bar{T}^a_a \tag{60}$$

and

$$\delta P_\varphi(x) = \delta\left(-\frac{2}{3N\sqrt{|p|}} \frac{\delta H_\varphi[N]}{\delta(\delta p)}\right) = \delta T^a_a(x) \tag{61}$$

for pressure. Note again that the lapse is treated as an independent function at the stage of differentiation. Then using $\delta(N\sqrt{|p|}) = 0$, this gives

$$\frac{\delta H_\varphi[N]}{\delta(\delta p)} = -\frac{3}{2}|\bar{p}|\delta T^a_a. \tag{62}$$

For a scalar field with correction terms in the Hamiltonian, these formulae yield the energy-momentum components

$$\bar{T}^0_0 = -\frac{\dot{\bar{\varphi}}^2}{2\bar{p}D} - V(\bar{\varphi}) \tag{63}$$

$$\bar{T}^0_a = 0 \tag{64}$$

$$\bar{T}^a_a = -\frac{1}{2\bar{p}D}\dot{\bar{\varphi}}^2\left(1 - \frac{2}{3}\frac{D'\bar{p}}{D}\right) + V(\bar{\varphi}) \tag{65}$$

for the background and

$$\delta T^0_0 = -\frac{\delta p \dot{\bar{\varphi}}^2}{2\bar{p}^2 D}\left(1 - \frac{D'\bar{p}}{D}\right) - V_{,\varphi}\delta\varphi - \frac{\dot{\bar{\varphi}}\delta\dot{\varphi}}{\bar{p}D} \tag{66}$$

$$\delta T^0_a = -\frac{1}{\bar{p}D}\dot{\bar{\varphi}}\delta\varphi_{,a} \tag{67}$$

$$\delta T^a_a = -\frac{\delta p \dot{\bar{\varphi}}^2}{2\bar{p}^2 D}\left(1 - \frac{7}{3}\frac{D'\bar{p}}{D} + \frac{4}{3}\left(\frac{D'\bar{p}}{D}\right)^2 - \frac{2}{3}\frac{D''\bar{p}^2}{D}\right) - \frac{\dot{\bar{\varphi}}\delta\dot{\varphi}}{\bar{p}D}\left(1 - \frac{2}{3}\frac{D'\bar{p}}{D}\right) + V_{,\varphi}\delta\varphi \tag{68}$$

for perturbations.

C. Matter equations

Solving Eq. (43) for $\bar{\pi}$ in terms of $\dot{\bar{\varphi}}$ and inserting it into Eq. (41) yields the Klein-Gordon equation

$$\ddot{\bar{\varphi}} + \frac{\dot{\bar{p}}}{\bar{p}}\dot{\bar{\varphi}}\left(1 - \frac{D'\bar{p}}{D}\right) + \bar{p}DV_{,\varphi}(\bar{\varphi}) = 0 \tag{69}$$

for the background scalar field $\bar{\varphi}$.

Taking a time derivative of Eq. (44), one gets

$$\begin{aligned}\delta\ddot{\varphi} &= \left(\frac{D}{\bar{p}}\right)^{\cdot}\left(\delta\pi + 2\bar{\pi}\frac{\delta p}{\bar{p}}\left(2 - \frac{D'\bar{p}}{D}\right)\right) + \frac{D}{\bar{p}}\left(\delta\pi - 2\bar{\pi}\frac{\delta p}{\bar{p}}\left(1 - \frac{D'\bar{p}}{2D}\right)\right)^{\cdot} \\ &= \left(\frac{D}{\bar{p}}\right)^{\cdot}\frac{\bar{p}\delta\dot{\varphi}}{D} + \dot{\bar{\varphi}}\frac{\delta p}{\bar{p}}\left(\frac{D'\bar{p}}{D}\right)^{\cdot} + \frac{D}{\bar{p}}\left(\delta\dot{\pi} - 2\left(1 - \frac{D'\bar{p}}{2D}\right)\left(\dot{\bar{\pi}}\frac{\delta p}{\bar{p}} + \frac{\bar{\varphi}}{2D}(\delta\dot{p} - 2\mathcal{H}\delta p)\right)\right)\end{aligned} \tag{70}$$

where the previous Eqs. (42) and (43) have been used. Finally, substituting $\bar{\pi}$ and $\delta\dot{\pi}$ from (41) and (42), we arrive at the Klein-Gordon equation for the perturbed part of the scalar field

$$\begin{aligned}&\delta\ddot{\varphi} + 2\mathcal{H}\delta\dot{\varphi}\left(1 - \frac{D'\bar{p}}{D}\right) - D\sigma\nabla^2\delta\varphi + D\bar{p}V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi \\ &\quad + (D - D'\bar{p})V_{,\varphi}(\bar{\varphi})\delta p + 2\dot{\bar{\varphi}}\frac{\delta\dot{p}}{\bar{p}}\left(1 - \frac{D'\bar{p}}{2D}\right) \\ &\quad - 2\dot{\bar{\varphi}}\mathcal{H}\frac{\delta p}{\bar{p}}\left(2 + \bar{p}^2\frac{D''}{D} - \left(\frac{D'\bar{p}}{D}\right)^2\right) = 0.\end{aligned} \tag{71}$$

D. Translation to metric variables

We can now finally write our equations of motion in familiar form by replacing derivatives of the matter Hamiltonian by energy-momentum tensor components and by introducing the scalar mode $\psi = -\delta p/2\bar{p}$. We keep the variable $\bar{p}$ rather than expressing it as the scale factor squared since this is the basic quantity appearing in our corrections functions from quantum gravity.

The background Eqs. (46) and (47) become

$$\mathcal{H}^2 = \frac{\kappa}{3}\alpha\bar{p}\bar{\rho}_\varphi \tag{72}$$

and

$$\dot{\mathcal{H}} = -\mathcal{H}^2\left(1 - \frac{2\alpha'\bar{p}}{\alpha}\right) + \frac{\kappa}{6}\alpha\bar{p}(\bar{\rho}_\varphi - 3\bar{P}_\varphi) \tag{73}$$

using (55) and (60). Equation (49), resulting from (35), together with (57) yields

$$\alpha\beta\nabla^2\psi - \frac{3}{\alpha}\mathcal{H}\dot{\psi} - \frac{3}{\alpha}\mathcal{H}^2\psi\left(1 - \frac{\alpha'\bar{p}}{\alpha}\right) = -\frac{\kappa}{2}\bar{p}\delta T^0_0, \tag{74}$$

Equation (51), resulting from (38), together with (62) yields

$$\ddot{\psi} + 2\psi\dot{\mathcal{H}}\left(1 - \frac{\alpha'\bar{p}}{\alpha}\right) + 3\dot{\psi}\mathcal{H}\left(1 - \frac{2}{3}\frac{\alpha'\bar{p}}{\alpha}\right) + \frac{\alpha\beta}{3}\nabla^2\psi(\alpha(\beta - 1) - 4\alpha'\bar{p}) + \psi\mathcal{H}^2\left(1 - 5\frac{\alpha'\bar{p}}{\alpha} + 4\left(\frac{\alpha'\bar{p}}{\alpha}\right)^2 - 2\frac{\alpha''\bar{p}^2}{\alpha}\right) = \frac{\alpha\kappa}{2}\bar{p}\delta T^a_a \tag{75}$$

and from (50) together with (59) we obtain

$$\partial_a(\dot{\psi} + \mathcal{H}\psi(2 - \tilde{\beta} - 2\alpha'\bar{p}/\alpha)) = -\frac{\kappa}{2}\bar{p}\delta T^0_a. \tag{76}$$

Here, the energy-momentum tensor components are

$$\delta T^0_0 = -\frac{\dot{\bar{\varphi}}^2\psi}{2\bar{p}D}\left(1 - \frac{D'\bar{p}}{D}\right) - V_{,\varphi}\delta\varphi - \frac{\dot{\bar{\varphi}}\delta\dot{\varphi}}{\bar{p}D} \tag{77}$$

$$\delta T^0_a = -\frac{1}{\bar{p}D}\dot{\bar{\varphi}}\delta\varphi_{,a} \tag{78}$$

$$\delta T^a_a = -\frac{\dot{\bar{\varphi}}^2\psi}{2\bar{p}D}\left(1 - \frac{7}{3}\frac{D'\bar{p}}{D} + \frac{4}{3}\left(\frac{D'\bar{p}}{D}\right)^2 - \frac{2}{3}\frac{D''\bar{p}^2}{D}\right) - \frac{\dot{\bar{\varphi}}\delta\dot{\varphi}}{\bar{p}D}\left(1 - \frac{2}{3}\frac{D'\bar{p}}{D}\right) + V_{,\varphi}\delta\varphi \tag{79}$$

and φ is subject to the Klein-Gordon equation

$$\ddot{\bar{\varphi}} + 2\mathcal{H}\dot{\bar{\varphi}}\left(1 - \frac{D'\bar{p}}{D}\right) + \bar{p}DV_{,\varphi}(\bar{\varphi}) = 0 \tag{80}$$

for the background and

$$\delta\ddot{\varphi} + 2\mathcal{H}\delta\dot{\varphi}\left(1 - \frac{D'\bar{p}}{D}\right) - D\sigma\nabla^2\delta\varphi + D\bar{p}V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi + 2(D - D'\bar{p})\bar{p}V_{,\varphi}(\bar{\varphi})\psi - 4\dot{\bar{\varphi}}\dot{\psi}\left(1 - \frac{D'\bar{p}}{2D}\right) + 4\dot{\bar{\varphi}}\psi\mathcal{H}\left(\frac{D'\bar{p}}{D} + \frac{D''\bar{p}^2}{D} - \left(\frac{D'\bar{p}}{D}\right)^2\right) = 0 \tag{81}$$

for the perturbation, obtained by expressing (71) in terms of ψ.

Comparison with Eqs. (3)–(5), (7), (9), and (10) shows that the classical equations are indeed reproduced when all correction functions equal one. As the classical perturbation equations, the corrected ones are scale invariant when the background is flat. This is manifest in the written form since ψ is scale invariant and, although the background scale factor $a^2 = |\bar{p}|$ appears explicitly, any combination such as $\alpha'\bar{p}$ where the prime denotes a derivative by $\bar{p}$ is scale invariant, too. Although the correction functions depend on $\bar{p}$, the derivation shows that they do so only in combinations which are scale invariant, taking into account normalizations provided by a quantum state [14,15].

IV. COVARIANCE

We have derived corrected perturbation equations in a fixed gauge, which simplified quantum and classical calculations. Their spacetime covariance is thus not obvious, just as the classical equations in the form (3)–(5) are not manifestly covariant. When classical equations are modified by quantum corrections, in particular, in a canonical scheme, it is not clear whether covariance will be broken. Canonically, spacetime covariance is realized if the lapse function N and shift vector N^a are not restricted by equations of motion but can be specified freely as a gauge choice. This is always the case if the Hamiltonian and diffeomorphism constraints form a first-class set, i.e. their Poisson brackets among each other vanish when the constraints are satisfied. With arbitrary modifications in their terms, this is unlikely to remain true, suggesting a breakdown of general covariance.

The situation in quantum gravity is, however, more general because new quantum degrees of freedom arise, which can absorb some of the restrictions which would otherwise be imposed on N and N^a. In fact, for an effective description of a canonical quantum theory [28] one derives effective constraints such as $H_{\rm eff} = \langle\hat{H}\rangle$ and $D_{\rm eff} = \langle\hat{D}\rangle$ as expectation values in suitable states. Since states are described by many, in fact infinitely many, more variables (or fields in a field theory) than just the classical ones the effective constraints are imposed on all these parameters. Additional variables include, e.g., the spread or deformations of wave packets in addition to expectation values identified with classical variables. If the quantum constraints preserve the first-class nature of the classical constraints, one has by definition $\{H_{\rm eff}, D_{\rm eff}\} = \frac{1}{i\hbar}\langle[\hat{H}, \hat{D}]\rangle$ as a first-class set of constraints. General covariance is thus preserved.

However, effective descriptions not only entail taking expectation values but also a truncation of the infinitely many quantum variables to a finite set (which means finitely many fields in a field theory). This corresponds, in some sense, to the derivative expansion done in effective actions to arrive at a finite sum of local correction terms. In particular, in this paper we completely ignored, as a first approximation, all quantum variables and correction terms they imply. Such truncations usually lead to effective constraints which do not exactly preserve covariance. Nevertheless, in perturbative regimes of quantum corrections the equations are consistent: One can choose a classically motivated gauge, fixing N and N^a, and compute corresponding perturbative corrections as we did for the longitudinal gauge. However, the gauge should not be too special as assumptions could implicitly be used which will no longer hold with quantum corrections. This would be the case if one used conditions on spatial metric components to achieve a certain gauge, obtained by solving gauge transformation equations for lapse and shift. Since gauge transformations change themselves when constraints are corrected, such a gauge would not be safe for the derivation of corrected equations. Specifying lapse and shift directly, such as $N^a = 0$ in longitudinal gauge, is safer because it can be done in the same way with any corrected constraints. This gauge is not complete, but after having computed the corrected constraints one can combine the remaining variables to gauge-invariant quantities.

Nonperturbative regimes, such as those to the left of the peaks of our correction functions, have to be treated with more care since the classical background geometry is strongly modified there. Usually, additional quantum variables are required to describe the situation and to discuss gauge issues fully. (The homogeneous background evolution, on the other hand, is safe even in this regime since it is subject to only one constraint. This will automatically commute with itself, thus being first class.)

V. DISCUSSION

We have presented in detail the Hamiltonian derivation of cosmological perturbation equations for scalar modes in longitudinal gauge around a flat isotropic background. The same scheme, of course, applies to other gauges and also under inclusion of vector and tensor modes and for perturbations around different backgrounds. As in the case of scalar modes, due care has to be taken in deciding when a gauge or mode selection is to be specified.

Since our main interest is to compute corrections from a canonical quantization of gravity, typical such correction functions have been included. We have seen how simple modifications of the constraints can propagate to more involved corrections of equations of motion. We emphasize that we have not presented a complete set of effective equations including all possible correction terms. Alternative corrections can arise, and moreover gauge issues have to be studied.

For applications, it is important to note that not only coefficients in evolution equations are corrected, but also constraints are modified. Since constraints generate gauge transformations, the form of gauge-invariant variables changes, too. For instance, it is not sufficient to take the classical expression of the gauge-invariant curvature perturbation $\mathcal{R} = \psi + \mathcal{H}\delta\varphi/\dot{\varphi}$ and use corrected equations of motion for all variables involved. A complete treatment requires correction terms in matter and metric equations as derived above, as well as in expressions for the relevant quantities to be related to observations. Ignoring any of the ingredients in general can lead to misleading conclusions. Nevertheless, some qualitative conclusions can be drawn. For instance, a modified evolution equation for $\mathcal{R}$ can be derived which implies correction terms leading to a slight nonconservation of this curvature perturbation [29]. While the quantity $\mathcal{R}$ itself will have to be corrected as the relevant gauge-invariant quantity, implying additional corrections to the evolution of curvature perturbations, this is unlikely to happen in such a way that all corrections from equations of motion and gauge invariance properties conspire to cancel each other. For the precise form of nonconservation, however, all these effects have to be taken into account. Still, interesting qualitative effects for cosmological phenomenology have already materialized.

We have started here a program to derive effects systematically and presented a first set of corrected constraints as well as evolution equations. A systematic study of different gauges and of observable implications is still to be done. The derivation in a Hamiltonian formulation as well as the use of Ashtekar variables are crucial for the inclusion of effective quantum gravity effects in modified perturbation equations if canonical quantum gravity, in particular, loop quantum gravity, is employed.

Primary dynamical objects are then the constraints, rather than Lagrangians, which are modified by quantum effects. Without regarding gravitational parts and all matter energy-momentum terms, changes to the classical behavior in an inflationary context have been considered in [30–32] in a strongly modified regime of background correction functions and in [33] in a perturbative regime. Ignoring corrections in gravitational parts of the equations corresponds to choosing a flat gauge in which no metric perturbations are present. The availability of this gauge choice is based on classical reasoning, and has to be reconsidered with gauge transformations generated by the quantum corrected constraints. Our treatment is more general since we allowed metric perturbations ψ and matter perturbations $\delta\varphi$ to be independent before they are to be combined to a quantity gauge invariant under the quantum corrected transformations. This allowed us to discuss nonconservation of curvature perturbations as a new effect.

Following the lines of derivations in this paper, basic effects in the constraints then translate unambiguously into effects in perturbation equations. Since several of the variational equations have to be combined in different manners, even simple modifications in the constraints can have complex implications at the level of perturbation equations. Modifications one expects on general grounds are regular versions of any inverse power of metric variables such as those of p in the Hamiltonian constraint, the spin connection and the matter Hamiltonian [18,19,21,34,35], higher order corrections as powers of k [36–38] and higher derivative terms in space as well as in time [28]. All this gives rise to characteristic correction functions which can be computed at least qualitatively. In the perturbation equations, coefficients as well as the derivative order of the equations can then change and differ considerably from the classical ones in strong quantum regimes.

We have illustrated this throughout the paper with corrections which are expected from inverse power modifications. Those corrections are easiest to implement and to deal with because they change only coefficients but not the type of perturbation equations. They are also expected to be stronger in inhomogeneous situations [14]. One expects four different correction functions, two for the gravitational Hamiltonian and two for the matter Hamiltonian. When they equal one, classical behavior is reproduced, while on small scales they can differ considerably from one and lead to modified and new coefficients. On very small scales, i.e. in regimes where correction functions are not Taylor expandable around the value one, cosmological perturbation theory is more difficult to apply.

There are many effects from quantum gravity in combination, and even different implementations depending on the quantization scheme used for constraints. An effective analysis shows which of the terms are most crucial for physical consequences and should be fixed. Other corrections on which the behavior does not depend so sensitively can then first be ignored. We can clearly see this from our example, where the correction functions β from the spin connection and σ from the matter gradient term do not play as important roles as the functions α and D. This is fortunate, in particular, for β because there is no tight prescription for its behavior in the full theory. Also the function $\tilde{\beta}$, which could equal β or simply one depending on how one deals with the diffeomorphism constraint, only appears once in the final Eqs. (76) and in a way which does not significantly change the behavior given by α-corrections. (For large $\bar{p}$, $1-\tilde{\beta}$ is negative while $-\alpha'\bar{p}/\alpha$ is positive. Because of the perturbative form (23) of the functions as a power series in $\ell_{\rm P}^2/\bar{p}$, however, the correction from α is dominant in this regime and determines the sign of the correction. For small $\bar{p}$, on the other hand, effects from $\tilde{\beta}$ can be more pronounced but perturbation theory is more complicated.) The most sensitive corrections at the level of linearized perturbations around flat space are thus those coming from α and D. A phenomenological analysis then shows which behavior of these functions is preferred.

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[17] The spin connection is in general more complicated as obtained directly from (11). However, the spin connection is not quantized in the full theory because it is not a covariant object and does not have physical meaning without gauge fixing. There is thus no tight prescription on how to obtain correction terms in perturbative situations. A further difference between our perturbative treatment here and the full theory is that we treat extrinsic curvature and the spin connection separately as it has been proven useful in homogeneous [18] and midi-superspace models [12,19]. This is not done in the full theory where one rather quantizes extrinsic curvature components in the constraint using $K_a^i \propto \{A_a^i, \{\int d^3x \epsilon^{ijk} F_{ab}^i \frac{E_j^a E_k^b}{\sqrt{|\det E|}}, \int \sqrt{|\det E|} d^3x\}\}$ [20]. Such a treatment is also possible to analyze in our situation but would be more complicated. We will later see that corrections from the spin connection are much less important than corrections from the inverse determinant explicit in the Hamiltonian constraint. Thus,

the precise treatment of extrinsic curvature and the spin connection does not seem crucial for phenomenology.
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