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Anomaly freedom in perturbative loop quantum gravity

Martin Bojowald* and Golam Mortuza Hossain+
Institute for Gravitational Physics and Geometry, The Pennsylvania State University, 104 Davey Lab, University Park, Pennsylvania 16802, USA

Mikhail Kagan‡
Institute for Gravitational Physics and Geometry, The Pennsylvania State University, 104 Davey Lab, University Park, Pennsylvania 16802, USA, and Department of Science and Engineering, The Pennsylvania State University, Abington, Pennsylvania 19001, USA

S. Shankaranarayanan§
Institute of Cosmology and Gravitation, University of Portsmouth, Mercantile House, Portsmouth P01 2EG, United Kingdom
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A fully consistent linear perturbation theory for cosmology is derived in the presence of quantum corrections as they are suggested by properties of inverse volume operators in loop quantum gravity. The underlying constraints present a consistent deformation of the classical system, which shows that the discreteness in loop quantum gravity can be implemented in effective equations without spoiling space-time covariance. Nevertheless, nontrivial quantum corrections do arise in the constraint algebra. Since correction terms must appear in tightly controlled forms to avoid anomalies, detailed insights for the correct implementation of constraint operators can be gained. The procedures of this article thus provide a clear link between fundamental quantum gravity and phenomenology.

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I. INTRODUCTION

Quantum gravity is expected to play a role in the early Universe, in such a way that it may become subject to observational tests in cosmology. As is well known, a complete theory of quantum gravity is difficult to construct, and even if one would have a fully convincing candidate it would remain difficult to link such a fundamental formulation to clear-cut observational consequences. Daunting as this may seem, such a problem is not specific to quantum gravity and has been circumvented highly successfully in other areas. For instance, to date there is no complete and fully rigorous construction of interacting quantum field theories on flat space-time, and yet clear and experimentally well-tested procedures to extract predictions have been used for decades.

Quantum gravity certainly does have additional problems which do not arise in quantum field theories on flat space-time. Paramount among these issues, related to the general covariance of the theory and thus to consequences of the fully constrained nature, are the problem of time, the self-interacting nature of gravity and the notion of a physical Hilbert space. Yet, quantum field theory is a lesson that the lack of a completely formulated underlying theory should not prevent one from making trustworthy statements valid at, e.g., low energies. Not all the mathematical constructions, whose well-defined existence one may wish to prove rigorously, are required for such purposes. They are surely necessary at a fundamental level, and they have often stimulated much further research. But they do not directly relate to observables, and thus can, for some purposes, be ignored.

The key tool for extracting potentially observable consequences without being paralyzed by open issues in a fundamental framework are effective formulations. They capture quantum effects by describing relevant aspects of an evolving wave function. They allow one to focus on the relevant degrees of freedom, such as expectation values or fluctuations, rather than whole wave functions and technical issues of how they may be represented. And if applied carefully enough, they not only provide reliable self-consistent predictions but also link back to the full theory where they originate and thus provide fundamental insights.

For many purposes, almost all the information contained in a wave function is irrelevant, and a few state parameters of finite number suffice for all potentially observable consequences that can be imagined. This is what provides a much more economical derivation of physical results. One should note that effective equations are not merely an amendment of classical equations by quantum correction terms, although one can always obtain such equations in semiclassical regimes because the classical limit must be respected. However, effective equations apply more generally and constitute a systematic approximation scheme to

*bojowald@gravity.psu.edu
+hossain@gravity.psu.edu
‡kagan@gravity.psu.edu
§Shanki.Subramaniam@port.ac.uk

analyze full quantum properties such as dynamical expectation values of a state.

Best known among effective formulations are probably low-energy effective actions in particle physics [1,2]. But they are also available in canonical formulations [3–5], where they have proven fruitful for quantum cosmology [6,7]. They can be extended to constrained systems, where they provide effective constraints for the state parameters [8]. Thus, all ingredients are given which are necessary for an application to loop quantum gravity [9–11] and a derivation of its effects. Because of the complexity of the problem, there is no complete derivation of effective equations for loop quantum gravity, but several characteristic quantum effects are known and can be analyzed. Taken together, all quantum corrections provide a complicated substitute for the classical equations, but they can be separated and studied individually. As we will see in this article, this provides crucial insights into what should happen in a consistent full theory of quantum gravity. We will explicitly construct anomaly free constraints which incorporate quantum corrections of inverse metric components as they occur due to the discreteness of loop quantum gravity. A companion paper [12] will use these considerations of effective constraint algebras to provide quantum corrected cosmological perturbation equations in terms of gauge-invariant variables.

II. EFFECTIVE EQUATIONS AND EFFECTIVE CONSTRAINTS

We start by reviewing the scheme of effective equations for canonical formulations. For an unconstrained system, the quantum theory is given by a Hamiltonian operator $\hat{H}$ which is self-adjoint on a given Hilbert space. It determines evolution of states ψ by the Schrödinger equation

$$i\hbar\dot{\psi} = \hat{H}\psi \tag{1}$$

and allows one to solve, e.g., for scattering amplitudes by evolving given initial states into possible final states.

A. Effective equations of motion

Alternatively, one can view the expectation value of the Hamiltonian, $H^Q := \langle\hat{H}\rangle$, as a functional on the infinite dimensional space of states. It generates the same Schrödinger evolution by Hamiltonian equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}\rangle = \frac{\langle[\hat{O},\hat{H}]\rangle}{i\hbar} =: \{\langle\hat{O}\rangle, H^Q\}. \tag{2}$$

General expressions for the relevant Poisson brackets on the right-hand side can be computed from commutators of basic operators used in the given quantum theory.

A solution for $\langle\hat{O}\rangle(t)$ to the Hamiltonian equation of motion has the same information as the expectation value $\langle\psi|\hat{O}|\psi\rangle$ computed in a state $|\psi\rangle$ satisfying the Schrödinger equation (or as the expectation value of a Heisenberg operator). However, in general H^Q, evaluated in a given state, depends not only on expectation values of basic operators but also on fluctuations and all other moments of the state. There is thus a complicated, infinite dimensional coupled system of equations involving not only the time dependence of $\langle\hat{O}\rangle$ but also independent quantum variables such as $\langle\hat{O}^n\rangle \neq \langle\hat{O}\rangle^n$ (or expectation values of other operators) which appear in quantum theory.

Effective equations are obtained when one can self-consistently determine regimes where these infinitely many equations can be decoupled to a finite system. This usually happens in semiclassical regimes where higher moments of a state are subdominant compared to low ones, but effective equations can be applied more generally. The 1-particle irreducible low-energy effective action, for instance, can be derived in an approximation consisting of a combination of an adiabatic expansion with one in $\hbar$ [3,5]. Some rare solvable systems can be studied by exact effective equations without truncation, which in cosmology is realized for a flat isotropic model sourced by a free, massless scalar [6].

In simplest cases, the effective approximation can be truncated at the level of expectation values of the quantum operators. Such a truncation, however, can still lead to nontrivial quantum corrections. In particular, the inverse of an operator containing zero eigenvalue in its discrete spectrum cannot always be approximated merely by the inverse of the expectation value. Such classically diverging operators are conventionally expressed in terms of commutators of well-defined (nondiverging) operators prior to applying the effective techniques. The corresponding expectation values of the commutators can then be written as classical expressions multiplied by *correction functions* as discussed in Sec. II D.

B. Effective constraints

Gravity is governed by constraints rather than a true Hamiltonian. Just like the Hamiltonian before, constraint operators $\hat{C}_I$ give rise to principal effective constraints $\langle\hat{C}_I\rangle$, but with those an infinite tower of other constraints for quantum variables is generated [8]. We are thus dealing with a system of infinitely many constraints on an infinite dimensional phase space even for a single classical canonical pair. The higher constraints can be ignored in our treatment of characteristic loop quantum gravity effects appearing in the principal constraints. As we will see, this is sufficient to arrive at a consistent constraint algebra together with the cosmological perturbation equations it implies. Higher constraints would be required if we were interested in the constrained evolution of higher moments.

The principal constraints are obtained from expectation values of quantum operators and thus contain several quantum effects. In general, they depend on quantum variables and include the quantum back reaction of, e.g., fluctuations and correlations on expectation values. But especially in loop quantum gravity they also contain characteristic effects which are a consequence of the fundamental quantum representation used. In loop quantum gravity, these translate consequences of the kinematical discreteness of the loop representation into effective equations and thus show implications for dynamical states. The basic reason for properties of the loop representation is the use of SU(2)-valued holonomies of the Ashtekar-Barbero connection instead of linear functions of the connection [13]. In particular, the basic variables become complex but still have to obey certain reality conditions to ensure that the correct number of classical degrees of freedom is quantized. This is usually implemented by requiring self-adjointness or unitarity of basic operators in the quantum representation, but one advantage of effective equations is that reality conditions can be represented independently at the level of expectation values and quantum variables [6,8]. This remains true after solving the effective constraints, thus showing crucial properties of the physical Hilbert space even in cases where the physical inner product may be difficult to construct.

A further advantage of effective equations, especially for the purpose of cosmological perturbation theory, is the issue of introducing a background geometry to define perturbative expansions in gravitational variables such as inhomogeneities. While the underlying theory of loop quantum gravity is background independent in a form which does not make it straightforward to introduce a perturbative background via states, effective constraints can easily be expanded by perturbing expectation values around a background of the desired classical form. The background then enters via a selection of a class of states to compute effective constraints [14]. (See also [15] for a conceptually similar proposal based on boundary states.) Using a Friedmann-Robertson-Walker background, for instance, allows one to derive cosmological perturbation equations directly—and effectively—from a background independent quantum theory of gravity.

For the resulting set of equations to be meaningful, they must be consistent in that they derive from constraints which are anomaly free also in the presence of quantum corrections. If this fails, it will be impossible to express the quantum corrected perturbation equations solely in terms of gauge-invariant variables as they are determined by the gauge flow of the corrected constraints. In particular, as we will demonstrate in this article, *off shell anomaly freedom* is required. (The importance of the off shell anomaly problem was also emphasized in [16] based on alternative fundamental considerations.) If one has an anomaly free quantization with constraint operators such that the constraint algebra $[\hat{C}_I, \hat{C}_J]$ closes to a first class system, then the algebra of principal quantum constraints $\{\langle\hat{C}_I\rangle, \langle\hat{C}_J\rangle\}$ will also close because it derives from the commutator algebra. (If there are structure functions, higher constraints as mentioned in the beginning of this subsection will be involved.) Approximations to effective constraints then have to be done self-consistently in such a way that violations of closure of the algebra do not happen up to the order considered in an expansion.

In loop quantum gravity, however, no satisfactory form of all constraint operators is known which would satisfy the requirement of off shell closure. (The arguments in [17,18], for instance, specifically refer to partially on shell statements; the reformulation of anomaly freedom as a condition for the existence of observables in [19,20] is also on shell.) Without off shell closure, on the other hand, physical applications based on the usual form of cosmological perturbation equations are impossible. (While applications may be possible based on a complete set of quantum observables in a form of reduced quantization, this route does not seem manageable.) The final advantage of effective formulations exploited in this article is then that one can ensure off shell closure of the *effective constrained system*. Thus, one can include known quantum effects as they occur in a quantization where one has not yet taken care of anomaly freedom, obtain candidates for effective constraints with those corrections in a suitable parameterized form (reflecting either quantization ambiguities or incomplete knowledge of properties of a quantum operator), and compute their Poisson relations. In general, this algebra will exhibit anomalies, but in some cases one can adapt the correction functions used in the parametrization of quantum effects such that anomalies vanish.

If there is no such adaptation, this specific quantum correction would be ruled out. But if one can successfully remove anomalies while keeping nontrivial quantum corrections, one will learn how specifically the quantum effect has to arise in quantum operators, and how completely quantization ambiguities can be fixed by the requirement of anomaly freedom. The advantage of effective equations is then that one can do such an analysis order by order in various expansions, instead of having to face a complicated operator algebra in which all possible quantum effects are included at once. The result of completing such a program will not only be consistent sets of equations of motion which can be used for applications, but also valuable feedback on the underlying fundamental theory which in our case will be loop quantum gravity. Thus, we are providing a clear link between fundamental properties of quantum gravity and its phenomenology.

C. Cosmological perturbation equations

Linearization of Einstein's equations around Friedmann-Robertson-Walker (FRW) space-times provides cosmological perturbation equations for ten metric components. These metric perturbations are subject to coordinate (gauge) transformations parametrized by an infinitesimal 4-vector field ξ^μ ($\mu = 0, \ldots, 3$), which, in presence of matter, generically give rise to six *gauge-invariant* perturbations, i.e. combinations of metric and matter perturbations which remain unchanged under linear changes of coordinates. In the linear regime, the former decouple into three independent modes: scalar, vector, and tensor, carrying 2 degrees of freedom each. The evolution of vector and tensor modes taking into account corrections expected from loop quantum gravity was investigated in [21,22], respectively. In this paper, we focus on the scalar perturbations which, along with the background FRW-metric, take the form

$$ds^2 = a^2(\eta)(-(1+2\phi)d\eta^2 + 2\partial_a B d\eta dx^a + ((1-2\psi)\delta_{ab} + 2\partial_a\partial_b E)dx^a dx^b), \quad (3)$$

where the scale factor a is a function of the conformal time η and the spatial indices run from 1 to 3. The perturbations ϕ, ψ, B, and E are then combined into the two gauge-invariant Bardeen potentials [23]

$$\Psi = \psi - \mathcal{H}(B - \dot{E})$$
$$\Phi = \phi + (B - \dot{E})^{\cdot} + \mathcal{H}(B - \dot{E}), \quad (4)$$

whose evolution is governed by the linearized Einstein equations [24]

$$\nabla^2\Psi - 3\mathcal{H}(\mathcal{H}\Phi + \dot{\Psi}) = -4\pi G a^2 \delta T_0^{0(\mathrm{GI})}; \quad (5)$$

$$\partial_a(\mathcal{H}\Phi + \dot{\Psi}) = -4\pi G a^2 \delta T_a^{0(\mathrm{GI})}; \quad (6)$$

$$\left(\ddot{\Psi} + \mathcal{H}(2\dot{\Psi} + \dot{\Phi}) + (2\dot{\mathcal{H}} + \mathcal{H}^2)\Phi + \tfrac{1}{2}\nabla^2(\Phi - \Psi)\right)\delta_a^b - \tfrac{1}{2}\partial^b\partial_a(\Phi - \Psi) = 4\pi G a^2 \delta T_a^{b(\mathrm{GI})}. \quad (7)$$

Here a dot denotes derivative with respect to conformal time, $\mathcal{H} \equiv \frac{\dot{a}}{a}$ is the conformal Hubble parameter, and $\delta T^{(\mathrm{GI})}$ are gauge-invariant perturbations of the matter stress-energy tensor. These equations are commonly derived from the covariant field equations or by varying an action expanded to second order in the linearized fields. But Hamiltonian formulations exist for the same procedure, which is more suitable for a comparison with canonical quantum gravity (in particular in Ashtekar variables as used in [25]).

To formulate the Hamiltonian setting, the action is used to determine Poisson brackets, and thus a decomposition into configuration fields and their momenta, as well as constraint functions. The constraints serve several purposes: (i) they restrict initial values of the fields to those allowed values which make the constraints vanish, (ii) they generate gauge transformations which in the case of general relativity agree with coordinate transformations, and (iii) they provide equations of motion for the fields in any coordinate time parameter. (The latter is itself subject to the coordinate changes by transformations generated by the constraints.) All this is necessary to reproduce a covariant system even though distinguishing momenta, which are related only to time but not space derivatives of fields, invariably removes manifest covariance from the Hamiltonian formalism.

For this to be consistent, it is crucial that the constraints are preserved under the time evolution they generate. This is automatically guaranteed if they form a first class set, i.e. a set of functionals whose mutual Poisson brackets vanish when evaluated in fields satisfying the constraints. In other words, the gauge transformations and evolution generated by the constraints then define vector fields on field space which are tangent to the submanifold defined by the vanishing of constraints. Starting on the constraint surface, either changing the gauge or following evolution will then keep us on the constraint surface. This is certainly realized classically, as a reflection of the general covariance of the underlying theory.

However, if quantum aspects are implemented, one must ensure that this consistency requirement remains maintained: the quantization must be anomaly free. Otherwise the equations may show the wrong type and number of degrees of freedom if formerly gauge quantities acquire gauge-invariant meaning. Or, worse, anomalies may make the equations inconsistent to the degree that no nontrivial solution exists at all. Anomaly freedom is thus a key requirement not only for the consistency of an underlying fundamental theory but also for the possibility of applications. Quantum corrections cannot appear in arbitrary forms, but only in restricted ways such that the constraints form a closed algebra under Poisson brackets. In particular, anomaly freedom will reduce some of the arbitrariness of the form of loop quantum gravity corrections.

Moreover, as we will see explicitly, to provide quantum corrections to Eqs. (5)–(7) the algebra must close off shell, i.e. it is not enough that the Poisson brackets of constraints vanish when the constraints are satisfied but even on parts of the phase space where constraints C_I do not vanish we must produce a closed algebra of a form $\{C_I, C_J\} = f_{IJ}^K(A, E)C_K$. (Here, A and E denote the canonical fields which may appear in the coefficients of the algebra; this means that in general we have structure functions rather than structure constants.) The effective algebra may differ from the classical one, and thus be quantum corrected as well as the constraints; but it must still close. The reason is that the whole set of coupled equations must be consistent, which presents a mixture of constraint Eqs. (5) and (6) and evolution equations given by (7) together with the continuity or Klein-Gordon equation. To ensure that these equations are consistent, we must consider the constraints before they are solved. Consistency then requires an off shell closure of the constraint algebra. Practically, the consequence is that only in this case we can express all the equations solely in terms of gauge-invariant variables as they are determined by the quantum corrected constraints. Once this is achieved, the equations are consistent and can be solved and analyzed. In the absence of off shell closure, on the other hand, there would be leftover terms in the equations of motion which contain gauge-dependent quantities making such an evolution unphysical.

In this context, it is important to realize that there is no shortcut to implementing the quantum corrections of fully perturbed field equations consistently. (Notwithstanding the fact that this has been attempted on numerous occasions such as [26–28] in the context of loop quantum cosmology, including by some of the present authors [29].) Consistency even for the purposes of phenomenological applications is intimately linked to the fundamental problem of anomaly freedom once inhomogeneities enter the game. In homogeneous models of gravity there is just one constraint, which clearly has a vanishing Poisson bracket with itself and thus forms an off shell closed algebra. Thus, in homogeneous quantum cosmology there is no anomaly problem whatsoever. Here, quantum corrections can be implemented at will, only restricted by possible self-imposed conditions such as the desire to be as close to a candidate for a "full," nonsymmetric theory as possible as it is expressed in loop quantum cosmology [31]. (Some of the structures, chiefly the kinematical quantum representation, of loop quantum cosmology can be linked to loop quantum gravity and are thus more restricted [14,32–35]. But no such derivation exists yet for the constraints which are most important to see the precise role of quantum corrections on the dynamics.)

It is then sometimes proposed to implement quantum corrections only in the background evolution, for instance by effects motivated from loop quantum gravity, and then use some inhomogeneous degree of freedom such as a matter field as a measure of perturbations around the background. If just the background is quantized, one knows corrections only in its evolution but would have to keep the structure of classical perturbation equations otherwise unchanged. This is rarely consistent, and the treatment is not gauge invariant. Gauge-invariant quantities in general relativity such as (4) combine several metric perturbations and possibly matter fields. Taking only a matter field, say, as the measure of perturbations means that one is fixing the gauge (by implicitly assuming non-gauge-invariant metric perturbations to vanish) without even knowing what the gauge transformations are. The classical case of linear perturbations around Friedmann-Robertson-Walker space-times allows gauges where only the matter fields are inhomogeneous but not the metric like, for instance, the uniform density gauge. However, quantum corrections change the constraints and thus the gauge transformations they generate. The form and availability of certain gauges changes, and it is no longer possible to reexpress the gauge-fixed results in terms of the gauge-invariant quantities unless one considers the full gauge problem. This can only be done when initially all perturbations are allowed and the anomaly issue is faced head-on.

In the context of classical cosmological perturbations, the above arguments can be rephrased in the following manner. The effective corrections arising in loop quantum cosmology can formally be written as

$$G_{\mu\nu} = 8\pi G(T_{\mu\nu} + \tau_{\mu\nu}) \tag{8}$$

where $\tau_{\mu\nu}$ contains all the corrections from loop quantum cosmology and $T_{\mu\nu}$ corresponds to the stress tensor of the classical matter field. Although the matter field might be an ideal fluid, the stress tensor $\tau_{\mu\nu}$ arising due to the new physics cannot necessarily be treated as a perfect fluid. More importantly, the perturbation of the stress tensor $\delta\tau_{ab}$ will in general have some anisotropic stress and the velocity perturbation δv_a will not vanish for a standard gauge choice. Hence, it is important to study the perturbations in a gauge-invariant manner.

If there is an anomaly free version of quantum corrected constraints and the corresponding form of covariance, one could compute complete gauge-invariant quantities to arbitrary orders in an expansion by inhomogeneities; see e.g. [36–38] or, in deparameterized form after introducing dust as a clock matter system, [39,40]. As discussed, this requires off shell anomaly freedom of the constraints which is not easy to realize in closed form. The treatment by effective constraints then provides a key advantage: one can verify anomaly freedom order by order in the expansion by inhomogeneities (which may be combined with a semiclassicality expansion in $\hbar$). This can be done with much more ease than a full anomaly analysis but still, as we will see explicitly, provides crucial feedback for the full theory.

D. Correction functions

Any quantization, such as loop quantum gravity, implies characteristic effects which change the classical behavior. Almost always, there are quantum back reaction effects by state parameters such as fluctuations and correlations on expectation values. (The only exceptions are free or solvable models such as the harmonic oscillator where moments of a state evolve independently of expectation values.) In addition, the specific quantum representation may imply further characteristic effects, which in the case of loop quantum gravity are all related to the spatial discreteness of its kinematical representation. The classical setup makes use of basic variables given by a densitized triad E^a_i, which provides the spatial metric via $E^a_i E^b_i = \det(q_{cd})q^{ab}$, and the Ashtekar connection $A^i_a = \Gamma^i_a + \gamma K^i_a$ with the spin connection Γ^i_a and extrinsic curvature $K^i_a = E^b_i K_{ab}/\sqrt{|\det(E^c_j)|}$. This canonical pair of fields is then quantized in the form of fluxes, i.e. integrations of the triad over surfaces, and holonomies or parallel transports of the connection. The resulting background independent representation has characteristic properties of spatial discreteness such as a discrete spectrum of flux operators (which contains zero). Such properties imply associated quantum corrections which appear whenever there are inverse powers of densitized triad components (some of which would classically diverge at singularities) or holonomies of a connection rather than just connection or curvature components.

All these corrections typically occur at the same time and must be combined in a complete treatment. While one type of correction might be dominant in certain regimes, this would not be known *a priori* but had to be shown by a dedicated analysis. Nevertheless, due to the complexity of general quantum corrections, it is legitimate to separate the different corrections at first, analyze individual effects and then combine results. In spirit, this is similar to the calculation of corrections to an atomic spectrum, which can be done individually for relativistic corrections, spin-orbit interaction, etc., and eventually combined in a complete spectrum. In this paper, we focus on loop quantum gravity corrections as they arise from inverse components of the triad.

These corrections are already relevant for cosmology, where they have been analyzed in preliminary forms in homogeneous and inhomogeneous contexts [26,41–49]. (Note that a subdominance of these corrections compared to those due to holonomies has been claimed based on an analysis of isotropic models [50]. However, this is based largely on an inadvertent and artificial suppression in the models used [51]; see also Appendix A. In any case, the arguments put forward in the context of [50] do not apply to inhomogeneous situations.) The precise form of such corrections as they would result in a principal constraint from the expectation value of a constraint operator cannot, at present, be computed due to the complicated form of the volume spectrum which would be required (see e.g. [52]). However, the results of Ref. [53] indicate that the behavior is known for the diagonal triads and that the classical function of triad components is multiplied by a correction function ($\alpha(E^a_i)$) which approaches the classical expectation for large values of triad components. (More precisely, the function depends on fluxes, i.e. triad components integrated over elementary plaquettes of a discrete quantum state. This makes the functional behavior independent of the choice of coordinates.)

At smaller scales, however, the function starts to deviate from one and implies quantum corrections. If the correction function is evaluated on an isotropic background [54], it has a peak at a certain characteristic scale a_* of height larger than 1, and then drops off at smaller scales to reach zero for vanishing triads. Notice that inhomogeneous contexts and states make it meaningful to speak about this behavior in terms of the scale factor a. In exactly isotropic models which are spatially flat, the absolute size of the scale factor has no meaning. However, the argument of correction functions is determined by a dimensionless ratio given by $q := \ell_0^2 a^2/\ell_{\rm P}^2 =: a^2/a_*^2$ where ℓ_0 is the size in coordinates of an elementary plaquette whose flux appears as an argument. The product $\ell_0 a$ has unambiguous meaning because it does not change under rescaling coordinates (which would change both a and ℓ_0 individually). The peak of the correction functions occurs near $q \sim 1$, i.e. $a \sim a_*$. The characteristic scale a_* can be written as $a_* = \ell_{\rm P}/\ell_0 = (\mathcal{N}/V_0)^{1/3}\ell_{\rm P}$ where $\mathcal{N}$ is the number of vertices of an underlying state contained in a region of coordinate volume V_0. The ratio $\mathcal{N}/V_0$ appearing in a_* is thus the patch density of an underlying discrete state measured in a given coordinate system. For nearly homogeneous configurations, it does not depend on the region or on V_0, but on coordinates. (The physical vertex density which would be independent of coordinates is $\mathcal{N}/(a^3V_0)$, but it would not be appropriate to determine a characteristic scale for a. Note that near $a \sim a_*$ there is one patch per Planck cube; upper bounds for the patch density can be obtained from phenomenological considerations, such as from big bang nucleosynthesis [55].) The value of a_* depends on the normalization of the scale factor. But it also depends on the vertex density which can be large. Thus, the peak of correction functions for a denser state is realized on larger scales, which increases the corresponding quantum corrections.

An additional implication of the appearance of the vertex density is that $\mathcal{N}$ is typically history dependent [14,56] if the dynamical quantum evolution refines the state as the universe grows (rather than just blowing up a fixed lattice). Thus, also the scale a_* is history dependent which contributes to the regime dependence of this type of correction. For a given background, the history dependence can always be expressed as an a-dependence, which is sometimes seen as problematic because the scale factor is not coordinate independent. However, given that the origin of the refinement lies in the inhomogeneous setting, a proper reduction introduces the correct scaling dependence via additional parameters depending on the state; see also Appendix A.

For an implementation of perturbative inhomogeneities, regimes where relevant scales fall below a_* pose difficulties because the scale of inhomogeneity would be close to the discreteness scale. In this paper, we thus assume that scales of the densitized triad are above the characteristic scale a_*, where correction functions deviate from one by terms perturbative in the Planck length:

$$\alpha(a) = 1 + c_\alpha\left(\frac{\ell_{\rm P}^2}{a^2}\right)^{n_\alpha} + \cdots \qquad (9)$$

with positive coefficients c_α and n_α. Both coefficients can be derived from a specific quantization but are subject to quantization ambiguities. The coefficient c_α, in particular, is then related to a_* (and to ℓ_0, providing the correct coordinate dependence in the presence of the scale factor). Thus, c_α may itself depend on a if the vertex number $\mathcal{N}$ in a fixed volume, and thus a_*, changes with the Universe expansion. We are assuming that the dominant a-dependence is via a power law of the given form.

Constraints for linearized perturbations will not only require the dependence of $\alpha(E^a_i)$ on the triad when the latter is diagonal, but also the dependence on off diagonal components. Classically one can always gauge the triad to be diagonal, but gauge transformations are quantum corrected and a consistency analysis of the equations must be done before a gauge is fixed. The off diagonal dependence of α is not known in explicit form, and it is difficult to derive because unlike the diagonal case it requires non-Abelian features of the quantum theory [52,57]. As we will see, the consistency analysis of constraints then relates the off diagonal dependence to the diagonal dependence via the condition of anomaly freedom. Moreover, other terms in the constraints, including matter Hamiltonians, will also require characteristic quantum corrections which, in contrast to the primary correction functions, may not obviously be expected from explicit quantizations in homogeneous models. Nevertheless, such additional corrections, called *counterterms* in what follows, are required for anomaly freedom. In this way, they are fixed in terms of the primary correction functions depending on diagonal triads. All this not only provides consistent equations ready to be applied in cosmology, but also precise feedback on what terms a full anomaly free quantum constraint must contain. As technical control on the full setting increases, these predictions will provide strong consistency checks of the whole framework.

III. CANONICAL PERTURBATION THEORY AND PRIMARY CORRECTION FUNCTIONS

In this main part of the paper we develop the ingredients of a consistent perturbation theory in the presence of quantum corrections to the classical constraints.

A. Constraints and primary corrections

We first introduce the constraints and primary correction functions which are expected to arise in the effective constraints. Formally, the corrections are introduced as multiplicative factors of some terms in the constraints which depend on the phase space variables and approach unity in the classical limit. In this paper, we restrict ourselves to correction functions resulting from the quantization of inverse-triad terms of the constraints. For the primary corrections, the functions are also assumed to depend only on the triad and to be local, i.e. independent of spatial derivatives of the triad. This reflects properties of these functions as they have been introduced in homogeneous models. The input can thus be used to formulate an initial expectation of the form of such functions. Moreover, in this section, we assume that the corrections can in principle be obtained from the full (nonperturbative) theory, and hence should depend only on the full triad $E^a_i \equiv \bar{E}^a_i + \delta E^a_i$ rather than on the background $\bar{E}^a_i$ and perturbations δE^a_i as distinct arguments. Later on we shall analyze the consistency of such assumptions. Anomaly freedom will generate additional counterterms of further corrections, which can be reinterpreted as a connection dependence or nonlocality of the primary corrections. Such a dependence is in any case expected for covariant corrections which can, e.g., be formulated as functionals of curvature invariants. Of course, we could put in such a dependence from the outset, but it would make the calculations much less tractable.

General relativity in Ashtekar variables is subject to the Gauss, diffeomorphism, and Hamiltonian constraints. The Gauss constraint is identically satisfied for scalar modes and does not need to be considered here. In the full quantum theory, the diffeomorphism constraint does not receive quantum corrections but the Hamiltonian constraint does [18]. The diffeomorphism constraint is thus taken as the classical one, $D[N^a] = D_{\rm grav}[N^a] + D_{\rm matter}[N^a]$ with a gravitational part

$$D_{\rm grav}[N^a] := \frac{1}{8\pi G\gamma}\int_\Sigma {\rm d}^3x N^a[(\partial_a A^j_b - \partial_b A^j_a)E^b_j - A^j_a\partial_b E^b_j] \quad (10)$$

and a matter part

$$D_{\rm matter}[N^a] = \int_\Sigma {\rm d}^3x N^a \pi\partial_a\varphi \quad (11)$$

for a scalar field φ.

We express the classical gravitational Hamiltonian as

$$H_{\rm grav}[N] = \frac{1}{16\pi G}\int_\Sigma {\rm d}^3x N\mathcal{H} \quad (12)$$

in terms of the Hamiltonian density

$$\mathcal{H} = \frac{E^a_i E^b_j}{\sqrt{|\det E|}}(F^k_{ab}\epsilon^{ij}{}_k - 2(1+\gamma^{-2})(A-\Gamma)^{[i}_a(A-\Gamma)^{j]}_b), \quad (13)$$

where the curvature of the Ashtekar connection is given by

$$F^k_{ab} = 2\partial_{[a}A^k_{b]} + \epsilon_{ij}{}^k A^i_a A^j_b,$$

γ is the Barbero-Immirzi parameter and the spin connection Γ^i_a is considered as a functional of the densitized triad [written explicitly in Eq. (29)]. According to the discussion in Sec. II D, the presence of an inverse of the triad determinant suggests a primary correction function of inverse-triad-type,

$$H^P_{\rm grav}[N] = \frac{1}{16\pi G}\int_\Sigma {\rm d}^3x N\alpha(E^a_i)\mathcal{H} = H_{\rm grav}[\alpha N] =: H_{\rm grav}[\tilde{N}]. \quad (14)$$

Its origin lies in deviations between the behavior of inverse-triad operators and the classical inverse of a triad. Triad operators do not have direct inverses because they have discrete spectra containing zero. Instead, they can be quantized after a classical reformulation [18] which introduces quantum corrections. These corrections enter effective Hamiltonians via expectation values of constraint operators containing the inverse-triad operators.

For the same reason, primary quantum corrections $\nu(E^a_i)$ and $\sigma(E^a_i)$ are introduced into the matter part of the Hamiltonian constraint as

$$H^P_{\rm matter}[N] = \int_\Sigma \mathrm{d}^3x N(\nu\mathcal{H}_\pi + \sigma\mathcal{H}_\nabla + \mathcal{H}_\varphi), \quad (15)$$

where

$$\mathcal{H}_\pi = \frac{\pi^2}{2\sqrt{|\det E|}}, \qquad \mathcal{H}_\nabla = \frac{E^a_i E^b_i \partial_a\varphi\partial_b\varphi}{2\sqrt{|\det E|}}, \qquad \mathcal{H}_\varphi = \sqrt{|\det E|}V(\varphi) \quad (16)$$

are the (classical) Hamiltonian densities corresponding to the kinetic, gradient, and potential terms, respectively. Note that the potential term is not expected to acquire primary quantum corrections because there is no inverse of the triad in this term. Thus, the correction does not simply amount to a rescaling of the lapse function even if ν and σ would equal α.

In Appendix B we discuss the Poisson brackets between unperturbed $H^P[N] \equiv H^P_{\rm grav}[N] + H^P_{\rm matter}[N]$ and $D[N^a] \equiv D_{\rm grav}[N^a] + D_{\rm matter}[N^a]$, as well as between $H^P[N_1]$ and $H^P[N_2]$.

B. Perturbations

Consider first an action which depends only on one scalar field φ. Generalizations to arbitrary tensor fields will be considered in the following subsection and in Appendix C. After the Legendre transform the action takes the form

$$S[\varphi] = \int \mathrm{d}^4x(\pi\dot\varphi - \mathcal{H}(\varphi,\pi)), \quad (17)$$

where $\mathcal{H}$ is the Hamiltonian density and π is the field momentum. Given a space-time slicing by constant-time surfaces, we split the fields φ and π into their homogeneous parts

$$\bar\varphi := \frac{1}{V_0}\int \mathrm{d}^3x\varphi, \qquad \bar\pi := \frac{1}{V_0}\int \mathrm{d}^3x\pi \quad (18)$$

and the inhomogeneous remainder

$$\delta\varphi := \varphi - \bar\varphi, \qquad \delta\pi := \pi - \bar\pi. \quad (19)$$

Here, V_0 is the volume of a spatial slice if it is closed, or can be thought of as a very large (but finite) infrared cutoff volume otherwise. The coordinate size V_0 will only appear in basic variables and their symplectic structure, but not in final equations of motion.

We also require the inhomogeneities $\delta\varphi$ and $\delta\pi$ to be small:

$$\left|\frac{\delta\varphi}{\bar\varphi}\right| \ll 1, \qquad \left|\frac{\delta\pi}{\bar\pi}\right| \ll 1 \quad (20)$$

for the slicing we use, so that this can be considered as perturbations around homogeneous solutions. For a generic Hamiltonian, these conditions may at some point be violated during the evolution. In fact, only a narrow class of Hamiltonians admits such a splitting, for which the inhomogeneities remain smaller than the mean fields at all times. At the moment, as is common in cosmology of the early Universe, we merely assume that (20) holds for the regime under consideration. Hence, from now on we shall refer to $\delta\varphi$ and $\delta\pi$ as perturbations and will also speak of the first, second, etc. perturbative order, denoted by superscripts (1), (2), ... in what follows. Specifically, we will be interested in the perturbations up to the second order in the Hamiltonian, which implies a linear perturbation theory in terms of equations of motion.

From the very definition of $\delta\varphi$ and $\delta\pi$ it follows that any first order quantity averages to zero. In particular,

$$\chi_1 := \int \mathrm{d}^3x\lambda_1\delta\varphi = 0, \qquad \chi_2 := \int \mathrm{d}^3x\lambda_2\delta\pi = 0, \quad (21)$$

where λ_1 and λ_2 are "smearing" constants [58]. Therefore the first term in the action (17) splits into two parts:

$$\int \mathrm{d}^4x\pi\dot\varphi \equiv \int \mathrm{d}^4x(\bar\pi + \delta\pi)(\dot{\bar\varphi} + \delta\dot\varphi) = V_0\int \mathrm{d}t\bar\pi\dot{\bar\varphi} + \int \mathrm{d}^4x\delta\pi\delta\dot\varphi, \quad (22)$$

yielding the basic Poisson brackets

$$\{\bar\varphi, \bar\pi\} = \frac{1}{V_0}, \qquad \{\delta\varphi(x), \delta\pi(y)\} = \delta^3(x-y), \quad (23)$$

and, for phase space functions, $\{,\} := \{,\}_{\bar\varphi,\bar\pi} + \{,\}_{\delta\varphi,\delta\pi}$, where

$$\{F,G\}_{\bar\varphi,\bar\pi} = \frac{1}{V_0}\left(\frac{\partial F}{\partial\bar\varphi}\frac{\partial G}{\partial\bar\pi} - \frac{\partial F}{\partial\bar\pi}\frac{\partial G}{\partial\bar\varphi}\right),$$
$$\{F,G\}_{\delta\varphi,\delta\pi} = \int \mathrm{d}^3x\left(\frac{\delta F}{\delta(\delta\varphi)}\frac{\delta G}{\delta(\delta\pi)} - \frac{\delta F}{\delta(\delta\pi)}\frac{\delta G}{\delta(\delta\varphi)}\right). \quad (24)$$

As discussed in Appendix C, these brackets are not fully general and in some cases care may be required, but they are sufficient for calculations done here.

C. Perturbed constraints

So far we have used the Ashtekar connection A^i_a as one of the canonical variables as required for holonomies. From now on we will explicitly use the spin connection and extrinsic curvature,

$$A^i_a = \Gamma^i_a + \gamma K^i_a,$$

where γ is the Barbero-Immirzi parameter. Also the canonical pair $K^i_a = \bar K^i_a + \delta K^i_a$, $E^a_i = \bar E^a_i + \delta E^a_i$ can be split into the homogeneous parts

$$\bar{K}^{\ i}_{a} = \bar{k}\delta^i_a, \qquad \bar{E}^a_i = \bar{p}\delta^a_i,$$

corresponding to the flat FRW-background, and the inhomogeneous perturbations which, for the scalar mode, are described by a pair of scalar functions each:

$$\delta K^i_a = \delta^i_a \kappa_1 + \partial_a \partial^i \kappa_2, \qquad \delta E^a_i = \delta^a_i \varepsilon_1 + \partial_i \partial^a \varepsilon_2. \tag{25}$$

Note that in the perturbed context, the independent phase space variables are $(\bar{k}, \bar{p})$ and $(\delta K^i_a, \delta E^a_i)$, and the nontrivial Poisson brackets between them are given by [59]

$$\{\bar{k}, \bar{p}\} = \frac{8\pi G}{3V_0}, \tag{26}$$
$$\{\delta K^i_a(x), \delta E^b_j(y)\} = 8\pi G \delta^i_j \delta^b_a \delta^3(x-y).$$

The Hamiltonian density (13), expressed in terms of the extrinsic curvature, becomes

$$\mathcal{H} = \epsilon_i^{jk} \frac{E^c_j E^d_k}{\sqrt{|\det E|}}[2\partial_c \Gamma^i_d + \epsilon^i_{mn}(\Gamma^m_c \Gamma^n_d - K^m_c K^n_d)] + \mathcal{H}_\gamma, \tag{27}$$

where the last term is proportional to the Barbero-Immirzi parameter,

$$\mathcal{H}_\gamma = \gamma \epsilon_i^{jk} \frac{2E^c_j E^d_k}{\sqrt{|\det E|}}(\partial_c K^i_d + \epsilon^i_{mn}\Gamma^m_c K^n_d)$$
$$\equiv \gamma \epsilon_i^{jk} \frac{2E^c_j E^d_k}{\sqrt{|\det E|}} D_c K^i_d = 2\gamma \frac{E^c_j}{\sqrt{|\det E|}} D_c \mathcal{G}^j \tag{28}$$

with the Gauss constraint $\mathcal{G}^J$, which thus vanishes. Indeed, the Gauss constraint implies that the extrinsic curvature can be written as $K^i_d = K_{db} E^{bi}/\sqrt{|\det E|}$ where $K_{dc} = K_{cd}$. Consequently,

$$\mathcal{H}_\gamma \propto \epsilon_{ijk} \frac{E^c_j E^d_k E^b_i}{\det E} D_c K_{db} = \epsilon^{bcd} D_c K_{db} = 0.$$

Thus the classical theory in (K^i_a, E^b_j) is explicitly insensitive to the Barbero-Immirzi parameter, as it should. The γ-dependence, however, will appear in the correction functions resulting from a quantization procedure (after which no unitary transformation exists to change γ without leaving a trace on observable quantities).

The remaining part of the Hamiltonian density can be expanded straightforwardly in a perturbation series, although the spin connection requires some care. Its full expression is

$$\Gamma^i_a = -\frac{1}{2}\epsilon^{ijk} E^b_j \Big(\partial_a E^k_b - \partial_b E^k_a + E^c_k E^l_a \partial_c E^l_b - E^k_a \frac{\partial_b(\det E)}{\det E}\Big), \tag{29}$$

where E^i_a with a lower spatial index designates a cotriad of density weight minus one, whose perturbed expression reads

$$E^l_a = \frac{1}{\bar{p}}\delta^l_a - \frac{1}{\bar{p}^2}\delta E^c_k \delta_{ca}\delta^{kl}.$$

The first order part of (29),

$$\delta\Gamma^i_a = \frac{1}{2\bar{p}}(\epsilon^{ij}_c \delta^b_a - \epsilon^{ib}_c \delta^j_a + \epsilon^{ijb}\delta_{ac} + \epsilon^{ib}_a \delta^j_c)\partial_b \delta E^c_j, \tag{30}$$

is simplified significantly for a scalar perturbation of the form (25). The diagonal part of δE^c_j (in the term $\partial_b \delta E^c_j$, which is $\delta^c_j \partial_b \varepsilon_1$) contributes to the linearized spin connection

$$\delta\Gamma^{i(\mathrm{diag})}_a = \frac{1}{2\bar{p}}(0 - \epsilon^{ib}_a \partial_b \varepsilon_1 - \epsilon^{ib}_a \partial_b \varepsilon_1 + 3\epsilon^{ib}_a \partial_b \varepsilon_1)$$
$$= \frac{1}{2\bar{p}}\epsilon^{ib}_a \partial_b \varepsilon_1. \tag{31}$$

For the off diagonal perturbation, on the other hand, the expression $\partial_b \delta E^c_j \equiv \partial_b \partial^c \partial_j \varepsilon_2$ is symmetric in the indices b, c, j, implying that only one term in (30) remains:

$$\delta\Gamma^{i(\mathrm{off-diag})}_a = \frac{1}{2\bar{p}}[0 - 0 + 0 + \epsilon^{ib}_a \partial_b \Delta\varepsilon_2]$$
$$= \frac{1}{2\bar{p}}\epsilon^{ib}_a \partial_b \Delta\varepsilon_2.$$

Combining the last two expressions, we obtain the linearized spin connection

$$\delta\Gamma^i_a = \delta\Gamma^{i(\mathrm{diag})}_a + \delta\Gamma^{i(\mathrm{off-diag})}_a = \frac{1}{2\bar{p}}\epsilon^{ij}_a \partial_j(\varepsilon_1 + \Delta\varepsilon_2). \tag{32}$$

Note that this expression is diffeomorphism invariant to linear order. Remarkably, the (gradient of the) term in the parenthesis can be expressed as the divergence of the unsplit triad perturbation

$$\partial_j(\varepsilon_1 + \Delta\varepsilon_2) = \partial_a \delta E^a_j,$$

which can be easily checked by inspection. Thus, for scalar mode the linearized spin connection can be expressed as

$$\delta\Gamma^i_a = \frac{1}{2\bar{p}}\epsilon^{ij}_a \partial_b \delta E^b_j. \tag{33}$$

The second order part of the gravitational Hamiltonian constraint also contains a term quadratic in Γ^a_i. However, as such a term is necessarily multiplied with a background quantity, the term becomes proportional to the trace of the spin connection, $\delta^a_i \Gamma^i_a$. For the scalar perturbation, the latter can be shown to vanish up to at least third order using similar symmetry arguments.

In the spin connection part of the Hamiltonian, the first order term is contributed solely by the "derivative term"

$$\left[2\epsilon_i^{jk}\frac{E_j^cE_k^d}{\sqrt{|\det E|}}\partial_c\delta\Gamma_d^i\right]^{(1)}=\frac{2}{\sqrt{\bar{p}}}\partial^i\partial_a\delta E_i^a,$$

whereas the second order part comes from both the derivative and the quadratic terms:

$$\left[2\epsilon_i^{jk}\frac{E_j^cE_k^d}{\sqrt{|\det E|}}\partial_c\delta\Gamma_d^i\right]^{(2)}=\frac{1}{\bar{p}^{3/2}}\delta^{ij}\delta E_i^a\partial_a\partial_b\delta E_j^b,$$

and

$$\left[\epsilon_i^{jk}\frac{E_j^cE_k^d}{\sqrt{|\det E|}}\epsilon^i{}_{mn}\delta\Gamma_c^m\delta\Gamma_d^n\right]^{(2)}=\frac{1}{2\bar{p}^{3/2}}\delta^{ij}\partial_a\delta E_i^a\partial_b\delta E_j^b.$$

Combining the last two terms, we obtain (up to a total divergence)

$$\left[\epsilon_i^{jk}\frac{E_j^cE_k^d}{\sqrt{|\det E|}}(2\partial_c\delta\Gamma_d^i+\epsilon^i{}_{mn}\delta\Gamma_c^m\delta\Gamma_d^n)\right]^{(2)}=-\frac{1}{2\bar{p}^{3/2}}\delta^{ij}\partial_a\delta E_i^a\partial_b\delta E_j^b. \tag{34}$$

Expanding also the extrinsic curvature term, we thus arrive at the expression for the gravitational Hamiltonian density $\mathcal{H}=\mathcal{H}^{(0)}+\mathcal{H}^{(1)}+\mathcal{H}^{(2)}$ with

$$\begin{aligned}\mathcal{H}^{(0)}&=-6\bar{k}^2\sqrt{\bar{p}},\\ \mathcal{H}^{(1)}&=-4\bar{k}\sqrt{\bar{p}}\,\delta_j^c\delta K_c^j-\frac{\bar{k}^2}{\sqrt{\bar{p}}}\delta_c^j\delta E_j^c+\frac{2}{\sqrt{\bar{p}}}\partial_c\partial^j\delta E_j^c,\\ \mathcal{H}^{(2)}&=\sqrt{\bar{p}}\delta K_c^j\delta K_d^k\delta_k^c\delta_j^d-\sqrt{\bar{p}}(\delta K_c^j\delta_j^c)^2-\frac{2\bar{k}}{\sqrt{\bar{p}}}\delta E_j^c\delta K_c^j\\ &\quad-\frac{\bar{k}^2}{2\bar{p}^{3/2}}\delta E_j^c\delta E_k^d\delta_c^k\delta_d^j+\frac{\bar{k}^2}{4\bar{p}^{3/2}}(\delta E_j^c\delta_c^j)^2\\ &\quad-\frac{\delta^{jk}}{2\bar{p}^{3/2}}(\partial_c\delta E_j^c)(\partial_d\delta E_k^d).\end{aligned} \tag{35}$$

Likewise, the perturbed diffeomorphism constraint including up to quadratic order in perturbations is

$$D_{\rm grav}[N^a]=\frac{1}{8\pi G}\int_\Sigma d^3x\delta N^c[\bar{p}\partial_c(\delta_k^d\delta K_d^k)-\bar{p}(\partial_k\delta K_c^k)-\bar{k}\delta_c^k(\partial_d\delta E_k^d)]. \tag{36}$$

We now consider the contribution from the scalar matter sector. The classical Hamiltonian is given by

$$H_{\rm matter}[N]=\int_\Sigma d^3xN(\mathcal{H}_\pi+\mathcal{H}_\nabla+\mathcal{H}_\varphi), \tag{37}$$

where the kinetic, gradient, and potential terms are defined in (16). Again, we have a perturbation expansion with

$$\mathcal{H}_\pi^{(0)}=\frac{\bar{\pi}_{\bar\varphi}^2}{2\bar{p}^{3/2}},\qquad \mathcal{H}_\nabla^{(0)}=0,\qquad \mathcal{H}_\varphi^{(0)}=\bar{p}^{3/2}V(\bar{\varphi}), \tag{38}$$

$$\mathcal{H}_\pi^{(1)}=\frac{\bar{\pi}\delta\pi}{\bar{p}^{3/2}}-\frac{\bar{\pi}^2}{2\bar{p}^{3/2}}\frac{\delta_c^j\delta E_j^c}{2\bar{p}},\qquad \mathcal{H}_\nabla^{(1)}=0,\qquad \mathcal{H}_\varphi^{(1)}=\bar{p}^{3/2}\left(V_{,\varphi}(\bar{\varphi})\delta\varphi+V(\bar{\varphi})\frac{\delta_c^j\delta E_j^c}{2\bar{p}}\right), \tag{39}$$

and

$$\begin{aligned}\mathcal{H}_\pi^{(2)}&=\frac{1}{2}\frac{\delta\pi^2}{\bar{p}^{3/2}}-\frac{\bar{\pi}\delta\pi}{\bar{p}^{3/2}}\frac{\delta_c^j\delta E_j^c}{2\bar{p}}+\frac{1}{2}\frac{\bar{\pi}^2}{\bar{p}^{3/2}}\left(\frac{(\delta_c^j\delta E_j^c)^2}{8\bar{p}^2}+\frac{\delta_c^k\delta_d^j\delta E_j^c\delta E_k^d}{4\bar{p}^2}\right),\\ \mathcal{H}_\nabla^{(2)}&=\frac{1}{2}\sqrt{\bar{p}}\delta^{ab}\partial_a\delta\varphi\partial_b\delta\varphi\\ \mathcal{H}_\varphi^{(2)}&=\frac{1}{2}\bar{p}^{3/2}V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi^2+\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\delta\varphi\frac{\delta_c^j\delta E_j^c}{2\bar{p}}+\bar{p}^{3/2}V(\bar{\varphi})\left(\frac{(\delta_c^j\delta E_j^c)^2}{8\bar{p}^2}-\frac{\delta_c^k\delta_d^j\delta E_j^c\delta E_k^d}{4\bar{p}^2}\right).\end{aligned} \tag{40}$$

The perturbed diffeomorphism constraint for the scalar matter field is

$$D_{\rm matter}[N^a]=\int_\Sigma d^3x\delta N^c\bar{\pi}\partial_c\delta\varphi. \tag{41}$$

In the following two subsections we explicitly compute the Poisson brackets between the perturbed classical constraints and show that their algebra is closed. At the same time, we will be including primary correction functions and see how the algebra changes.

D. Poisson bracket between Hamiltonian and diffeomorphism constraints

We begin by considering the gravitational sector of the classical constraint algebra. We will see later that for computational purposes it is convenient to split the classical perturbed gravitational Hamiltonian as

$$H_{\rm grav}[N]=\frac{1}{16\pi G}\int_\Sigma d^3xN\mathcal{H}=H_{\rm grav}[\delta N]+H_{\rm grav}[\bar{N}]. \tag{42}$$

Here $H_{\rm grav}[\delta N]$ includes only the perturbed component of the lapse function whereas $H_{\rm grav}[\bar{N}]$ involves only the background lapse. Explicit expressions for each part of the perturbed Hamiltonian constraint are

$$H_{\rm grav}[\bar{N}]=\frac{1}{16\pi G}\int d^3x\bar{N}[\mathcal{H}^{(0)}+\mathcal{H}^{(2)}],\qquad H_{\rm grav}[\delta N]=\frac{1}{16\pi G}\int d^3x\delta N\mathcal{H}^{(1)}, \tag{43}$$

where perturbed Hamiltonian densities are given in Eqs. (35). We consider now the Poisson bracket between the gravitational Hamiltonian $H_{\rm grav}[N]$ in (43) and the gravitational diffeomorphism constraint $D_{\rm grav}[N^a]$ in (36):

$$\{H_{\rm grav}[N], D_{\rm grav}[N^a]\} = -H_{\rm grav}[\delta N^a \partial_a \delta N]. \tag{44}$$

This Poisson bracket between classical perturbed constraints (44) is very similar to its counterpart between the full classical constraints [10], also computed in Appendix B. This demonstrates the consistency of perturbed constraint expressions and elementary Poisson brackets between background and perturbed basic variables.

As in the gravitational sector, the classical perturbed Hamiltonian for the scalar matter field including up to quadratic terms in perturbations can be expressed as $H_{\rm matter}[N] = H_{\rm matter}[\delta N] + H_{\rm matter}[\bar{N}]$ where

$$\begin{aligned} H_{\rm matter}[\bar{N}] &:= \int {\rm d}^3x \bar{N}[(\mathcal{H}_\pi^{(0)} + \mathcal{H}_\varphi^{(0)}) \\ &\quad + (\mathcal{H}_\pi^{(2)} + \mathcal{H}_\nabla^{(2)} + \mathcal{H}_\varphi^{(2)})], \\ H_{\rm matter}[\delta N] &:= \int {\rm d}^3x \delta N[\mathcal{H}_\pi^{(1)} + \mathcal{H}_\varphi^{(1)}]. \end{aligned} \tag{45}$$

Perturbed Hamiltonian densities for scalar matter are given in Eqs. (38)–(40). The Poisson bracket between the matter Hamiltonian constraint and the total diffeomorphism constraint can be computed as

$$\begin{aligned} &\{H_{\rm matter}[N], D_{\rm grav}[N^a] + D_{\rm matter}[N^a]\} \\ &\quad = -H_{\rm matter}[\delta N^a \partial_a \delta N]. \end{aligned} \tag{46}$$

Combining gravitational sector (44) and matter sector (46) contributions, we can evaluate the Poisson bracket between the total Hamiltonian and diffeomorphism constraints as

$$\begin{aligned} \{H[N], D[N^a]\} &= \{H_{\rm grav}[N], D_{\rm grav}[N^a]\} \\ &\quad + \{H_{\rm matter}[N], D_{\rm grav}[N^a] + D_{\rm matter}[N^a]\} \\ &= -H_{\rm grav}[\delta N^a \partial_a \delta N] - H_{\rm matter}[\delta N^a \partial_a \delta N] \\ &= -H[\delta N^a \partial_a \delta N]. \end{aligned} \tag{47}$$

Clearly, perturbed expressions of total constraints along with elementary Poisson brackets between background and perturbed basic variables satisfy the same Poisson brackets as the full expressions.

We now analyze the situation for primary corrected constraints. As in the classical situation, we split the primary quantum corrected gravitational Hamiltonian constraint as

$$\begin{aligned} H^P_{\rm grav}[N] &= \frac{1}{16\pi G}\int {\rm d}^3x N\alpha(E^a_i)\mathcal{H} \\ &= H^P_{\rm grav}[\delta N] + H^P_{\rm grav}[\bar{N}]. \end{aligned} \tag{48}$$

The part of Hamiltonian constraint containing only the perturbed lapse function $H^P_{\rm grav}[\delta N]$ and the part of Hamiltonian constraint containing only background lapse $H^P_{\rm grav}[\bar{N}]$ are defined as

$$\begin{aligned} H^P_{\rm grav}[\bar{N}] &:= \frac{1}{16\pi G}\int {\rm d}^3x \bar{N}(\bar{\alpha}\mathcal{H}^{(0)} + \alpha^{(2)}\mathcal{H}^{(0)} \\ &\quad + \alpha^{(1)}\mathcal{H}^{(1)} + \bar{\alpha}\mathcal{H}^{(2)}), \\ H^P_{\rm grav}[\delta N] &:= \frac{1}{16\pi G}\int {\rm d}^3x \delta N(\bar{\alpha}\mathcal{H}^{(1)} + \alpha^{(1)}\mathcal{H}^{(0)}), \end{aligned} \tag{49}$$

where $\bar{\alpha} \equiv \alpha^{(0)}$. The Poisson bracket between the primary quantum corrected Hamiltonian constraint (48) and the diffeomorphism constraint (36) can be computed as

$$\{H^P_{\rm grav}[N], D_{\rm grav}[N^a]\} = -H^P_{\rm grav}[\delta N^a \partial_a \delta N] + \mathcal{A}^{HD}_{\rm grav} \tag{50}$$

where

$$\begin{aligned} \mathcal{A}^{HD}_{\rm grav} &= -\frac{1}{16\pi G}\int {\rm d}^3x(\partial_c \delta N^j)\bar{p} \\ &\quad \times \bigg[\delta N\mathcal{H}^{(0)}\frac{\partial \alpha^{(1)}}{\partial(\delta E^a_i)}(\delta^a_j\delta^c_i - \delta^c_j\delta^a_i) \\ &\quad + \bar{N}\bigg\{\mathcal{H}^{(0)}\bigg(-\frac{\alpha^{(1)}}{\bar{p}}\delta^c_j + \frac{1}{3}\frac{\partial\bar{\alpha}}{\partial\bar{p}}\frac{\delta E^c_j}{\bar{p}} \\ &\quad + \frac{\partial\alpha^{(2)}}{\partial(\delta E^a_i)}(\delta^a_j\delta^c_i - \delta^c_j\delta^a_i)\bigg) \\ &\quad + \mathcal{H}^{(1)}\frac{\partial\alpha^{(1)}}{\partial(\delta E^a_i)}(\delta^a_j\delta^c_i - \delta^c_j\delta^a_i)\bigg\}\bigg] \end{aligned} \tag{51}$$

would appear as an anomaly if primary corrected constraints were used as quantum constraints: the Poisson bracket (50) between the quantum corrected Hamiltonian constraint and diffeomorphism constraint has additional terms which cannot be expressed completely in terms of the gravitational constraints for any lapse function or shift vector. Thus, these terms in the constraint algebra are potentially anomalous.

Next we explore this issue for the quantum corrected scalar matter sector. Similarly to the classical Hamiltonian constraint, the quantum corrected matter Hamiltonian can be split as

$$\begin{aligned} H^P_{\rm matter}[N] &= \int {\rm d}^3x N[\nu(E^a_i)\mathcal{H}_\pi + \sigma(E^a_i)\mathcal{H}_\nabla + \mathcal{H}_\varphi] \\ &=: H^P_{\rm matter}[\delta N] + H^P_{\rm matter}[\bar{N}]. \end{aligned} \tag{52}$$

The two parts $H^P_{\rm matter}[\delta N]$ and $H^P_{\rm matter}[\bar{N}]$ of the matter Hamiltonian are defined as

$$H^P_{\rm matter}[\bar{N}] := \int d^3x \bar{N}[(\bar{\nu}\mathcal{H}^{(0)}_\pi + \mathcal{H}^{(0)}_\varphi) + (\nu^{(2)}\mathcal{H}^{(0)}_\pi + \nu^{(1)}\mathcal{H}^{(1)}_\pi + \bar{\nu}\mathcal{H}^{(2)}_\pi + \bar{\sigma}\mathcal{H}^{(2)}_\nabla + \mathcal{H}^{(2)}_\varphi)],$$
$$H^P_{\rm matter}[\delta N] := \int d^3x \delta N[\nu^{(1)}\mathcal{H}^{(0)}_\pi + \bar{\nu}\mathcal{H}^{(1)}_\pi + \mathcal{H}^{(1)}_\varphi], \tag{53}$$

where $\bar{\nu} \equiv \nu^{(0)}$. Here $\nu^{(0)}$, $\nu^{(1)}$, and $\nu^{(2)}$ denote zeroth, first, and second order terms in perturbations of the quantum correction function ν. The Poisson bracket between the quantum corrected scalar matter Hamiltonian (52) and the total diffeomorphism constraint $D_{\rm grav}[N^a] + D_{\rm matter}[N^a]$ can be computed as

$$\{H^P_{\rm matter}[N], D_{\rm grav}[N^a] + D_{\rm matter}[N^a]\} = -H^P_{\rm matter}[\delta N^a \partial_a \delta N] + \mathcal{A}^{HD}_{\rm matter}. \tag{54}$$

As in the gravitational sector, there are additional terms present also in the matter sector Poisson bracket which are

$$\mathcal{A}^{HD}_{\rm matter} = -\int d^3x (\partial_c \delta N^j)\bar{p} \times \Big[\delta N \mathcal{H}^{(0)}_\pi \frac{\partial \nu^{(1)}}{\partial(\delta E^a_i)}(\delta^a_j \delta^c_i - \delta^c_j \delta^a_i) + \bar{N}\Big\{\mathcal{H}^{(0)}_\pi\Big(-\frac{\nu^{(1)}}{\bar{p}}\delta^c_j + \frac{1}{3}\frac{\partial\bar{\nu}}{\partial\bar{p}}\frac{\delta E^c_j}{\bar{p}} + \frac{\partial \nu^{(2)}}{\partial(\delta E^a_i)}(\delta^a_j \delta^c_i - \delta^c_j \delta^a_i)\Big) + \mathcal{H}^{(1)}_\pi \frac{\partial \nu^{(1)}}{\partial(\delta E^a_i)}(\delta^a_j \delta^c_i - \delta^c_j \delta^a_i)\Big\}\Big]. \tag{55}$$

Matter sector anomaly terms are similar to anomaly terms in the gravitational sector, but there are important differences. In particular, matter anomaly terms involve only the kinetic sector of the matter Hamiltonian density $\mathcal{H}_\pi$. In contrast, gravitational anomaly terms contain the total gravitational Hamiltonian density $\mathcal{H}$. Thus, one cannot even hope to combine all anomaly terms to form the total Hamiltonian constraint for specific correction functions. Moreover, cancellation would require a lapse depending on correction functions. The requirement of an anomaly free constraint algebra then demands that gravitational sector and matter sector anomaly terms must vanish separately. Combining contributions from the gravitational sector (50) and the matter sector (54), we can write the Poisson bracket between the quantum corrected total Hamiltonian constraint and the total diffeomorphism constraint as

$$\{H^P[N], D[N^a]\} = -H^P[\delta N^a \partial_a \delta N] + \mathcal{A}^{HD}_{\rm grav} + \mathcal{A}^{HD}_{\rm matter}. \tag{56}$$

E. Poisson bracket between two Hamiltonian constraints

We now consider the Poisson bracket between two Hamiltonian constraints smeared with different lapse functions. It can be split into three components as follows

$$\{H[N_1], H[N_2]\} = \{H_{\rm grav}[N_1], H_{\rm grav}[N_2]\} + \{H_{\rm matter}[N_1], H_{\rm matter}[N_2]\} + [\{H_{\rm matter}[N_1], H_{\rm grav}[N_2]\} - (N_1 \leftrightarrow N_2)]. \tag{57}$$

Using the perturbed expression of the classical gravitational Hamiltonian (43) we compute the Poisson bracket between gravitational Hamiltonian constraints as

$$\{H_{\rm grav}[N_1], H_{\rm grav}[N_2]\} = \{H_{\rm grav}[\delta N_1], H_{\rm grav}[\bar{N}]\} + \{H_{\rm grav}[\bar{N}], H_{\rm grav}[\delta N_2]\} = \{H_{\rm grav}[\delta N_1 - \delta N_2], H_{\rm grav}[\bar{N}]\} = D_{\rm grav}\Big[\frac{\bar{N}}{\bar{p}}\partial^a(\delta N_2 - \delta N_1)\Big], \tag{58}$$

where we have used the property that $\{H_{\rm grav}[\delta N_1], H_{\rm grav}[\delta N_2]\} = 0$. Similarly, using the perturbed expression of the classical scalar matter Hamiltonian (45), we compute the pure matter sector contribution as

$$\{H_{\rm matter}[N_1], H_{\rm matter}[N_2]\} = D_{\rm matter}\Big[\frac{\bar{N}}{\bar{p}}\partial^a(\delta N_2 - \delta N_1)\Big]. \tag{59}$$

It is easy to show that the net contribution from the Poisson bracket between gravitational Hamiltonian and matter Hamiltonian parts in the constraint vanishes. In particular,

$$\{H_{\rm matter}[N_1], H_{\rm grav}[N_2]\} - (N_1 \leftrightarrow N_2) = 0. \tag{60}$$

Combining Eqs. (58)–(60) we evaluate the Poisson bracket between total Hamiltonian constraints as

$$\{H[N_1], H[N_2]\} = D\Big[\frac{\bar{N}}{\bar{p}}\partial^a(\delta N_2 - \delta N_1)\Big]. \tag{61}$$

Thus, the perturbed expression of the classical Hamiltonian constraint indeed satisfies the same Poisson bracket with itself as its unperturbed expression.

Now using the perturbed expression of the primary quantum corrected Hamiltonian (48) we compute the Poisson bracket between quantum corrected gravitational Hamiltonian constraints as

$$\{H^P_{\rm grav}[N_1], H^P_{\rm grav}[N_2]\} = \{H_{\rm grav}[\delta N_1 - \delta N_2], H_{\rm grav}[\bar{N}]\} = D_{\rm grav}\Big[\bar{\alpha}^2\frac{\bar{N}}{\bar{p}}\partial^a(\delta N_2 - \delta N_1)\Big] + \mathcal{A}^{HH}_{\rm grav} \tag{62}$$

with

$$\mathcal{A}^{HH}_{\rm grav} = \frac{1}{8\pi G}\int d^3x \bar{N}(\delta N_1 - \delta N_2)\bigg[(\bar{\alpha}\bar{k}^2\bar{p}\delta K^j_c)\bigg\{-2\frac{\partial\bar{\alpha}}{\partial\bar{p}}\delta^c_j + \frac{\partial\alpha^{(1)}}{\partial(\delta E^a_i)}(\delta^c_j\delta^a_i + 3\delta^c_i\delta^a_j)\bigg\} + (2\bar{\alpha}\,\bar{k}\,\partial_c\partial^j\delta E^c_j)\bigg\{\frac{\partial\bar{\alpha}}{\partial\bar{p}} - \frac{\partial\alpha^{(1)}}{\partial(\delta E^a_i)}\delta^a_i\bigg\} + (6\bar{\alpha}\bar{k}^3\bar{p})\bigg\{\frac{\partial\alpha^{(2)}}{\partial(\delta E^a_i)}\delta^a_i - \frac{\partial\alpha^{(1)}}{\partial\bar{p}}\bigg\} + (6\alpha^{(1)}\bar{k}^3\bar{p})\bigg\{\frac{\partial\bar{\alpha}}{\partial\bar{p}} - \frac{\partial\alpha^{(1)}}{\partial(\delta E^a_i)}\delta^a_i\bigg\} + (\bar{\alpha}\bar{k}^3\delta E^c_j)\frac{\partial\alpha^{(1)}}{\partial(\delta E^a_i)}\{\delta^j_c\delta^a_i - 3\delta^a_c\delta^j_i\}\bigg]. \quad (63)$$

Similarly, using Eq. (52) we compute the Poisson bracket between primary quantum corrected scalar matter Hamiltonians as

$$\{H^P_{\rm matter}[N_1], H^P_{\rm matter}[N_2]\} = D_{\rm matter}\bigg[\bar{\nu}\,\bar{\sigma}\frac{\bar{N}}{\bar{p}}\partial^a(\delta N_2 - \delta N_1)\bigg]. \quad (64)$$

Equation (64) is analogous to its classical counterpart except that the new shift vector for the resulting diffeomorphism constraint now contains quantum correction functions $\bar{\nu}$ and $\bar{\sigma}$. Net contributions from the Poisson bracket between quantum corrected gravitational Hamiltonian and matter Hamiltonian constraints are

$$\{H^P_{\rm matter}[N_1], H^P_{\rm grav}[N_2]\} - (N_1 \leftrightarrow N_2) = \mathcal{A}^{HH}_m \quad (65)$$

with

$$\mathcal{A}^{HH}_{\rm matter} = \int d^3x \bar{N}(\delta N_1 - \delta N_2)\bigg[\frac{\bar{\pi}^2}{2\bar{p}^{3/2}}(\sqrt{\bar{p}}\delta K^j_c)\bigg\{-\frac{2}{3}\frac{\partial\bar{\nu}}{\partial\bar{p}}\delta^c_j + \frac{\partial\nu^{(1)}}{\partial(\delta E^a_i)}(\delta^c_j\delta^a_i - \delta^c_i\delta^a_j)\bigg\} + \frac{\bar{\pi}\delta\pi}{\bar{p}^{3/2}}(2\bar{k}\sqrt{\bar{p}})\bigg\{\frac{\partial\bar{\nu}}{\partial\bar{p}} - \frac{\partial\nu^{(1)}}{\partial(\delta E^a_i)}\delta^a_i\bigg\} - \frac{\bar{\pi}^2}{2\bar{p}^{3/2}}(2\bar{k}\sqrt{\bar{p}})\bigg\{\frac{\partial\nu^{(2)}}{\partial(\delta E^a_i)}\delta^a_i - \frac{\partial\nu^{(1)}}{\partial\bar{p}}\bigg\} + \frac{\bar{\pi}^2}{2\bar{p}^{3/2}}\bigg(\frac{\bar{k}}{\sqrt{\bar{p}}}\delta E^c_j\bigg)\bigg\{-\frac{4}{3}\frac{\partial\bar{\nu}}{\partial\bar{p}}\delta^j_c + \frac{\partial\nu^{(1)}}{\partial(\delta E^a_i)}(\delta^j_c\delta^a_i + \delta^a_c\delta^j_i)\bigg\}\bigg]. \quad (66)$$

Using Eqs. (62), (64), and (65) we can combine contributions from the gravitational and matter sectors to express the Poisson bracket between primary quantum corrected total Hamiltonians:

$$\{H^P[N_1], H^P[N_2]\} = D\bigg[\bar{\alpha}^2\frac{\bar{N}}{\bar{p}}\partial^a(\delta N_2 - \delta N_1)\bigg] + D_{\rm matter}\bigg[(\bar{\nu}\,\bar{\sigma} - \bar{\alpha}^2)\frac{\bar{N}}{\bar{p}}\partial^a(\delta N_2 - \delta N_1)\bigg] + \mathcal{A}^{HH}_{\rm grav} + \mathcal{A}^{HH}_{\rm matter}.$$

F. Conditions for an anomaly free constraint algebra

In contrast to the classical situation, we have seen that primary quantum corrected constraints fail to form a first class constraint algebra for arbitrary correction functions. To interpret this properly, we recall that quantum correction functions that we have used as a guideline in the Hamiltonian constraint are not completely known. In particular, one can compute only zeroth order terms using homogeneous models [54,60,61] (as well as some partially gauge-fixed inhomogeneous cases using lattice states [53]). Linear and quadratic terms in perturbations of quantum correction functions can in principle be computed using the machinery of the full theory [52]. However such computations are not yet available. In this section, we will analyze whether there are conditions on quantum correction functions that we must impose based solely on the requirement of an anomaly free constraint algebra.

First, we note that the explicit appearance of the matter diffeomorphism constraint in Eq. (67), drops out if the quantum correction functions satisfy

$$\bar{\alpha}^2 = \bar{\nu}\,\bar{\sigma}. \quad (67)$$

This requirement may be seen as a consistency relation between gravitational and matter correction functions, which has important physical implications: For instance, it ensures that gravitational waves and massless scalar fields propagate with the same group velocity given by the physical speed of light [22].

Furthermore, in order for the constraint algebra to be closed, $\mathcal{A}^{HD}_{\rm grav}$ should vanish irrespective of the choice of lapse function. In other words, anomaly terms involving background lapse $\bar{N}$ and perturbed lapse δN must vanish independently. This requirement leads to

$$\alpha^{(1)} = 0 \quad \text{and} \quad \frac{1}{3}\frac{\partial\bar{\alpha}}{\partial\bar{p}}\frac{\delta E^c_j}{\bar{p}} + \frac{\partial\alpha^{(2)}}{\partial(\delta E^a_i)}(\delta^a_j\delta^c_i - \delta^c_j\delta^a_i) = 0. \quad (68)$$

On the other hand, from Eq. (63) the conditions

$$\frac{1}{3}\frac{\partial\bar{\alpha}}{\partial\bar{p}}\delta_i^a = \frac{\partial\alpha^{(1)}}{\partial(\delta E_i^a)} \quad \text{and} \quad \frac{\partial\alpha^{(1)}}{\partial\bar{p}} = \frac{\partial\alpha^{(2)}}{\partial(\delta E_i^a)}\delta_i^a \tag{69}$$

are required to make $\mathcal{A}^{HH}_{\rm grav}$ vanish. Clearly, the requirement of an anomaly free constraint algebra imposes restrictions on the first and second order terms of the quantum correction functions. However, it is evident that Eqs. (68) and (69) are overcomplete for the unknown functions $\alpha^{(1)}$ and $\alpha^{(2)}$. Importantly, these conditions are incompatible with each other for nontrivial primary corrections and admit only trivial solutions of $\bar{\alpha} = $ constant, $\alpha^{(1)} = 0$, and $\alpha^{(2)} = 0$ which is just the classical situation without quantum corrections. The situation for the scalar matter sector is very similar. Using Eq. (55) it is easy to see that $\mathcal{A}^{HD}_{\rm grav} = 0$ requires

$$\nu^{(1)} = 0 \quad \text{and} \quad \frac{1}{3}\frac{\partial\bar{\nu}}{\partial\bar{p}}\frac{\delta E_j^c}{\bar{p}} + \frac{\partial\nu^{(2)}}{\partial(\delta E_i^a)}(\delta_j^a\delta_i^c - \delta_j^c\delta_i^a) = 0, \tag{70}$$

while

$$\frac{1}{3}\frac{\partial\bar{\nu}}{\partial\bar{p}}\delta_i^a = \frac{\partial\nu^{(1)}}{\partial(\delta E_i^a)} \quad \text{and} \quad \frac{\partial\nu^{(1)}}{\partial\bar{p}} = \frac{\partial\nu^{(2)}}{\partial(\delta E_i^a)}\delta_i^a, \tag{71}$$

solves $\mathcal{A}^{HH}_{\rm matter} = 0$. As in the gravitational sector, anomaly free requirements on matter quantum correction functions admit only trivial solutions of $\bar{\nu} = $ constant, $\nu^{(1)} = 0$, and $\nu^{(2)} = 0$. There are no additional requirements on the quantum correction function σ as only its background component appears in the perturbed Hamiltonian. However, Eq. (67) then requires that also $\bar{\sigma}$ must be constant.

At this stage, we could only conclude that inverse-triad corrections leave no trace whatsoever in effective constraints of an anomaly free quantization. This would be extremely puzzling given the crucial role played by the corresponding operators for well-defined fundamental constraints of loop quantum gravity. Fortunately, what we have shown is, in fact, a weaker statement since we assumed the primary correction function to depend only locally on the triad in algebraic form. What we have shown is that this pure triad dependence is insufficient, and we will now relax this assumption by introducing additional corrections which we call counterterms. These terms are not directly motivated by simple expressions computed from a constraint operator, but they will be fixed in terms of primary correction functions by anomaly freedom. In the conclusions, we will comment on the expectations for the presence of such terms based on a loop quantization.

IV. ANOMALY FREE QUANTUM CONSTRAINTS

In the previous section, we have shown that the presence of only primary quantum correction functions does not lead to an anomaly free perturbed constraint algebra. It is, however, possible that the chosen form of quantum correction functions, as they have been used in all studies so far, does not capture all possible quantum effects. Naturally, one is then led to ask whether there are "counterterms" to the chosen form of the correction functions that should be included in quantum corrected expressions of the Hamiltonian constraint to make the constraint algebra anomaly free. We show here that such expectations are indeed realized. In particular, it is possible to arrive at a quantum corrected constraint algebra which is anomaly free by including specific counterterms to the primary quantum corrected Hamiltonian constraint.

A. Gravitational sector

For a nontrivial primary quantum correction function it is not possible for both $\mathcal{A}^{HD}_{\rm grav}$ and $\mathcal{A}^{HH}_{\rm grav}$ to vanish simultaneously. However, it turns out that one can perform partial anomaly cancellation in the constraint algebra even for nontrivial quantum correction functions by relaxing some of the conditions imposed so far to result in manageable computations. We approach this by adding counterterms, i.e. further potential quantum corrections, ensuring first that the quantum corrected Hamiltonian constraint is covariant under spatial diffeomorphisms, i.e. $\mathcal{A}^{HD}_{\rm grav} = 0$. At this point, it is important that the diffeomorphism constraint should not receive quantum corrections of the type studied here. Counterterms thus appear only in the Hamiltonian constraint. We have seen that condition (68) on the quantum correction function, in particular $\alpha^{(1)} = 0$, precisely ensures this requirement and we can simplify the primary gravitational constraint (45) to

$$\begin{aligned} H^P_{\rm grav}[\bar{N}] &:= \frac{1}{16\pi G}\int {\rm d}^3x\bar{N}[\bar{\alpha}\mathcal{H}^{(0)} \\ &\quad + (\alpha^{(2)}\mathcal{H}^{(0)} + \bar{\alpha}\mathcal{H}^{(2)})], \\ H^P_{\rm grav}[\delta N] &:= \frac{1}{16\pi G}\int {\rm d}^3x\delta N[\bar{\alpha}\mathcal{H}^{(1)}]. \end{aligned} \tag{72}$$

Similarly, we simplify the expression of $\mathcal{A}^{HH}_{\rm grav}$ (59), which we then refer to as

$$\mathcal{A}^P_{\rm grav} = \frac{1}{8\pi G}\int {\rm d}^3x\bar{N}(\delta N_1 - \delta N_2)(2\bar{\alpha}\,\bar{p})\frac{\partial\bar{\alpha}}{\partial\bar{p}} \times\left[\frac{\bar{k}}{\bar{p}}(\partial_c\partial^j\delta E_j^c) - \bar{k}^2(\delta_j^c\delta K_c^j) + \bar{k}^3\frac{(\delta_c^j\delta E_j^c)}{2\bar{p}}\right]. \tag{73}$$

As we have already seen, canceling this anomaly based solely on primary corrections could be achieved only for the trivial case of constant α. To cancel the anomaly terms (73) without having to require constant $\bar{\alpha}$, we need to generate additional terms which take a form similar to primary anomaly terms. In fact, additional corrections not considered so far can easily arise in an effective

Hamiltonian constraint. Adding additional terms into the Hamiltonian constraint however can potentially generate new anomaly terms in the Poisson bracket $\{H^P_{\rm grav}[N], D_{\rm grav}[N^a]\}$. To avoid this we should ensure that the counterterms being added to the Hamiltonian constraint commute with the diffeomorphism constraint. Moreover, counterterms should not affect the background dynamics as there are no anomalies in the constraint algebra when one turns off inhomogeneity. Thus, counterterms should be constructed using only those terms which contain inhomogeneous perturbations.

We notice that while we describe the emergence of counterterms in a constructive manner, all this reflects requirements which fundamental anomaly freedom would pose. To that end, we consider a minimal approach for constructing counterterms. In particular, we require that counterterms should generate only those three kinds of terms which are already present in the anomaly expression (73). With this requirement, the allowed form of counterterms that can be included in the quantum corrected Hamiltonian is given by $H^C_{\rm grav}[N] = H^C_{\rm grav}[\delta N] + H^C_{\rm grav}[\bar{N}]$ where

$$H^C_{\rm grav}[\delta N] = \frac{1}{16\pi G}\int {\rm d}^3x \delta N \bar{\alpha}\bigg[-4f(\bar{p})\bar{k}\sqrt{\bar{p}}(\delta^c_j \delta K^j_c) - g(\bar{p})\frac{\bar{k}^2}{\sqrt{\bar{p}}}(\delta^j_c \delta E^c_j)\bigg] \tag{74}$$

and

$$H^C_{\rm grav}[\bar{N}] = \frac{1}{16\pi G}\int {\rm d}^3x \bar{N}\,\bar{\alpha} \times\bigg[-h(\bar{p})\frac{\delta^{jk}}{2\bar{p}^{3/2}}(\partial_c \delta E^c_j)(\partial_d \delta E^d_k)\bigg]. \tag{75}$$

Here we have introduced three dimensionless scalar functions f, g and h which depend on the quantum correction functions and are to be determined through anomaly cancellation conditions. Only background components of these functions are relevant as the counterterms are already quadratic in perturbations.

The new terms can be interpreted as resulting from a dependence of the primary α on extrinsic curvature components and spatial derivatives of the triad as a general functional. Thus, the introduction of counterterms relaxes some of the conditions imposed earlier on α. The Poisson bracket between counterterms and the diffeomorphism constraint can be computed as

$$\{H^C_{\rm grav}[N], D[N^a]\} = \frac{1}{8\pi G}\int {\rm d}^3x \bar{\alpha}(\partial_c \delta N^c) \times \delta N[-(2f+g)(\bar{k}^2\sqrt{\bar{p}})]. \tag{76}$$

Thus, the requirement that counterterms commute with the diffeomorphism constraint leads to the simple condition

$$2f + g = 0 \tag{77}$$

on the coefficient functions. Out of three unknown coefficient functions only two remain to be determined. Using Eqs. (74) and (75) we compute contributions from counterterms to the Poisson bracket between Hamiltonian constraints

$$\begin{aligned}\mathcal{A}^C_{\rm grav} &= \{H^C_{\rm grav}[N_1], H^P_{\rm grav}[N_2]\} - (N_1 \leftrightarrow N_2) = \{H^C_{\rm grav}[\delta N_1 - \delta N_2], H^P_{\rm grav}[\bar{N}]\} + \{H^P_{\rm grav}[\delta N_1 - \delta N_2], H^C_{\rm grav}[\bar{N}]\} \\ &= \frac{1}{8\pi G}\int {\rm d}^3x \bar{N}(\delta N_1 - \delta N_2)\bar{\alpha}^2\bigg[\bar{k}^2(\delta^c_j \delta K^j_c)\bigg(f - g - 4\bar{p}\frac{\partial f}{\partial \bar{p}}\bigg) + \bar{k}^3\frac{(\delta^j_c \delta E^c_j)}{2\bar{p}}\bigg(-f + g - 2\bar{p}\frac{\partial g}{\partial \bar{p}}\bigg) \\ &\quad + \frac{\bar{k}}{\bar{p}}(\partial_c \partial^j \delta E^c_j)(-h - f)\bigg].\end{aligned} \tag{78}$$

Since the perturbed classical constraint algebra is closed without counterterms, the quantum counterterms must vanish in the classical limit, i.e. when all primary correction functions are unity. Counterterms can then depend on primary correction functions only through their derivatives. Given the expanded form (9) of primary quantum correction functions used here, terms such as $(\partial \bar{\alpha}/\partial \bar{p})^2$ can be neglected compared to the terms $\partial \bar{\alpha}/\partial \bar{p}$. For the same reason the contributions from the Poisson bracket between counterterms $\{H^C_{\rm grav}[N_1], H^C_{\rm grav}[N_2]\}$ can be neglected compared to the contributions considered in (78).

Combining all contributions from the original anomaly (73) and from counterterms (78) one can express the total gravitational anomaly $\mathcal{A}_{\rm grav} := \mathcal{A}^P_{\rm grav} + \mathcal{A}^C_{\rm grav}$ as

$$\mathcal{A}_{\rm grav} = \frac{1}{8\pi G}\int {\rm d}^3x \bar{N}(\delta N_1 - \delta N_2)\bar{\alpha}^2\bigg[\frac{\bar{k}}{\bar{p}}(\partial_c \partial^j \delta E^c_j)\mathcal{G}_1 + \bar{k}^2(\delta^c_j \delta K^j_c)\mathcal{G}_2 + \bar{k}^3\frac{(\delta^j_c \delta E^c_j)}{2\bar{p}}\mathcal{G}_3\bigg], \tag{79}$$

where

$$\mathcal{G}_1 = -h - f + \frac{2\bar{p}}{\bar{\alpha}}\frac{\partial\bar{\alpha}}{\partial\bar{p}}, \tag{80}$$

$$\mathcal{G}_2 = f - g - 4\bar{p}\frac{\partial f}{\partial\bar{p}} - \frac{2\bar{p}}{\bar{\alpha}}\frac{\partial\bar{\alpha}}{\partial\bar{p}}, \tag{81}$$

$$\mathcal{G}_3 = -f + g - 2\bar{p}\frac{\partial g}{\partial\bar{p}} + \frac{2\bar{p}}{\bar{\alpha}}\frac{\partial\bar{\alpha}}{\partial\bar{p}}. \tag{82}$$

Anomaly cancellation will require coefficients of $(\partial_c\partial^j\delta E^c_j)$, $(\delta^c_j\delta K^j_c)$ and $(\delta^j_c\delta E^c_j)$ to vanish. This in turn implies that the coefficient functions f, g and h should be such that they satisfy three equations $\mathcal{G}_1 = 0$, $\mathcal{G}_2 = 0$ and $\mathcal{G}_3 = 0$. On the other hand, f and g also need to satisfy Eq. (77). Thus, the set of equations for f, g and h may appear to be over-complete. However, it is remarkable to note that Eq. (77) along with Eq. (81) solves the Eq. (82) identically. In particular using Eq. (77), it is easy to see that

$$\mathcal{G}_3 = -\mathcal{G}_2. \tag{83}$$

Thus for a given quantum correction function α, there are unambiguous solutions for f, g and h such that the constraint algebra is anomaly free. In particular, for a background quantum correction function α given in (9),

$$f = -\frac{g}{2} = \frac{2}{4n_\alpha + 3}\frac{\bar{p}}{\bar{\alpha}}\frac{\partial\bar{\alpha}}{\partial\bar{p}}, \qquad h = 4\frac{2n_\alpha + 1}{4n_\alpha + 3}\frac{\bar{p}}{\bar{\alpha}}\frac{\partial\bar{\alpha}}{\partial\bar{p}}, \tag{84}$$

solve Eq. (77) and ensure vanishing of Eqs. (80)–(82).

B. Cosmological constant

For obtaining anomaly freedom in the gravitational sector by adding appropriate counterterms, it was crucial that coefficients $\mathcal{G}_2$ and $\mathcal{G}_3$ are related through Eq. (83). Thus, one should consider the robustness of this relation under the inclusion of additional classical terms. Including a nonzero cosmological constant to the gravitational sector provides a definite test to see whether such a relation can still be satisfied. Counterterms in the gravitational sector would now generate additional contributions due to the presence of the cosmological constant term. We now show that a nonzero cosmological constant does not spoil the nontrivial consistency condition (83).

Contributions to the gravitational Hamiltonian constraint from a nonzero cosmological constant Λ are

$$H_\Lambda[N] = \frac{1}{8\pi G}\int \mathrm{d}^3x N\sqrt{|\det E|}\Lambda =: H_\Lambda[\delta N] + H_\Lambda[\bar{N}]. \tag{85}$$

As with the matter potential term, no primary inverse-triad corrections are expected. The perturbed expressions of $H_\Lambda[\delta N]$ and $H_\Lambda[\bar{N}]$, including up to quadratic terms in perturbations are given by

$$H_\Lambda[\bar{N}] = \frac{1}{16\pi G}\int \mathrm{d}^3x\bar{N}[\mathcal{H}^{(0)}_\Lambda + \mathcal{H}^{(2)}_\Lambda], \qquad H_\Lambda[\delta N] = \frac{1}{16\pi G}\int \mathrm{d}^3x\,\delta N\mathcal{H}^{(1)}_\Lambda. \tag{86}$$

The explicit expressions of perturbed densities $\mathcal{H}^{(0)}_\Lambda$, $\mathcal{H}^{(1)}_\Lambda$ and $\mathcal{H}^{(2)}_\Lambda$ are

$$\mathcal{H}^{(0)}_\Lambda = 2\Lambda\bar{p}^{3/2}, \qquad \mathcal{H}^{(1)}_\Lambda = 2\Lambda\bar{p}^{3/2}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}, \tag{87}$$

$$\mathcal{H}^{(2)}_\Lambda = 2\Lambda\bar{p}^{3/2}\left(\frac{(\delta^j_c\delta E^c_j)^2}{8\bar{p}^2} - \frac{(\delta^k_c\delta^j_d\delta E^c_j\delta E^d_k)}{4\bar{p}^2}\right). \tag{88}$$

Contributions to the anomaly expression arising from the Poisson bracket between counterterms and cosmological constant terms are

$$\mathcal{A}_\Lambda = \{H^C_{\rm grav}[N_1], H_\Lambda[N_2]\} - (N_1 \leftrightarrow N_2) = \frac{1}{8\pi G}\int \mathrm{d}^3x\bar{N}(\delta N_1 - \delta N_2)\bar{\alpha}(\Lambda\bar{p}) \times\left[-(\delta^c_j\delta K^j_c)f - \bar{k}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(f+g)\right]. \tag{89}$$

Combining contributions from counterterms and the original anomaly in the presence of a nonzero cosmological constant, one can evaluate the total gravitational anomaly $\mathcal{A}_{\rm grav} := \mathcal{A}^P_{\rm grav} + \mathcal{A}^C_{\rm grav} + \mathcal{A}_\Lambda$ as

$$\mathcal{A}_{\rm grav} = \frac{1}{8\pi G}\int \mathrm{d}^3x\bar{N}(\delta N_1 - \delta N_2)\bar{\alpha}^2\left[\frac{\bar{k}}{\bar{p}}(\partial_c\partial^j\delta E^c_j)\mathcal{G}^\Lambda_1 + \bar{k}^2(\delta^c_j\delta K^j_c)\mathcal{G}^\Lambda_2 + \bar{k}^3\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\mathcal{G}^\Lambda_3\right], \tag{90}$$

where new coefficients in the anomaly expression are

$$\mathcal{G}^\Lambda_1 = \mathcal{G}_1, \qquad \mathcal{G}^\Lambda_2 = \mathcal{G}_2 - f\frac{\Lambda\bar{p}}{\bar{\alpha}\bar{k}^2}, \qquad \mathcal{G}^\Lambda_3 = \mathcal{G}_3 - (f+g)\frac{\Lambda\bar{p}}{\bar{\alpha}\bar{k}^2}. \tag{91}$$

(The Λ-dependence cancels upon using the background Friedmann equation.) Using Eq. (77), which remains unchanged, we again note that the new coefficients satisfy the same nontrivial consistency relation

$$\mathcal{G}^\Lambda_3 = -\mathcal{G}^\Lambda_2. \tag{92}$$

Thus, also in the presence of a nonzero cosmological constant there are unambiguous solutions for f, g and h such that the constraint algebra is anomaly free. This demonstrates that anomaly freedom of the quantum corrected constraint algebra including appropriate counterterms is a robust feature.

C. Scalar matter

For cosmological applications, we must ensure the existence of consistent equations in the presence of matter. Similarly to the gravitational sector we ensure first that the quantum corrected scalar matter Hamiltonian is covariant under spatial diffeomorphism, i.e. $\mathcal{A}^{HD}_{\rm matter}=0$. This requirement implies that we should impose conditions (71) on the quantum correction function ν and simplify the expression of the primary quantum corrected matter Hamiltonian as

$$H^P_{\rm matter}[\bar N] := \int d^3x \bar N[(\bar\nu \mathcal{H}^{(0)}_\pi + \mathcal{H}^{(0)}_\varphi) + (\nu^{(2)}\mathcal{H}^{(0)}_\pi + \bar\nu\mathcal{H}^{(2)}_\pi + \bar\sigma\mathcal{H}^{(2)}_\nabla + \mathcal{H}^{(2)}_\varphi)]$$
$$H^P_{\rm matter}[\delta N] := \int d^3x \delta N[\bar\nu\mathcal{H}^{(1)}_\pi + \mathcal{H}^{(1)}_\varphi]. \tag{93}$$

This also simplifies the matter anomaly term $\mathcal{A}^{HH}_{\rm matter}$ which we then refer to as

$$\mathcal{A}^P_{\rm matter} = \int d^3x \bar N(\delta N_1 - \delta N_2)\Big[\frac{\bar\nu\,\bar\pi\,\delta\pi}{\bar p^{3/2}}\frac{\bar\alpha\,\bar k}{\sqrt{\bar p}}\Big(\frac{2\bar p}{\bar\nu}\frac{\partial\bar\nu}{\partial\bar p}\Big) + \frac{\bar\nu\bar\pi^2}{2\bar p^{3/2}}(\delta^c_j\delta K^j_c)\frac{\bar\alpha}{\sqrt{\bar p}}\Big(-\frac{2\bar p}{3\bar\nu}\frac{\partial\bar\nu}{\partial\bar p}\Big) + \frac{\bar\nu\bar\pi^2}{2\bar p^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar p}\frac{\bar\alpha\,\bar k}{\sqrt{\bar p}}\Big(-\frac{10\bar p}{3\bar\nu}\frac{\partial\bar\nu}{\partial\bar p}\Big)\Big].$$

For computational convenience we consider the construction of counterterms for the kinetic and potential sectors separately.

1. Kinetic sector

To cancel anomalies in the kinetic sector of scalar matter, we start with a general form of possible counterterms as $H^C_{\pi\nabla}[N] := H^C_\pi[\delta N] + H^C_\nabla[\delta N] + H^C_\pi[\bar N] + H^C_\nabla[\bar N]$ where

$$H^C_\pi[\delta N] = \int d^3x \delta N\Big[f_1(\bar p)\frac{\bar\nu\,\bar\pi\,\delta\pi}{\bar p^{3/2}} - f_2(\bar p)\frac{\bar\nu\bar\pi^2}{2\bar p^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar p}\Big],\qquad H^C_\nabla[\delta N] = 0 \tag{94}$$

and

$$H^C_\pi[\bar N] = \int d^3x \bar N\Big[g_1(\bar p)\frac{\bar\nu\delta\pi^2}{2\bar p^{3/2}} - g_2(\bar p)\frac{\bar\nu\,\bar\pi\,\delta\pi}{\bar p^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar p}\frac{\bar\nu\bar\pi^2}{2\bar p^{3/2}}\Big(g_3(\bar p)\frac{(\delta^j_c\delta E^c_j)^2}{8\bar p^2} + g_4(\bar p)\frac{(\delta^k_c\delta^j_d\delta E^c_j\delta E^d_k)}{4\bar p^2}\Big)\Big],$$
$$H^c_\nabla[\bar N] = \int d^3x \bar N\Big[g_5(\bar p)\frac{\bar\sigma\sqrt{\bar p}}{2}\delta^{ab}\partial_a\delta\varphi\partial_b\delta\varphi\Big]. \tag{95}$$

The general guidelines followed for the gravitational sector led us to introduce seven dimensionless unknown functions f_1, f_2, g_1, g_2, g_3, g_4 and g_5 which should be related to primary quantum correction functions as it will be determined through anomaly cancellation conditions.

The Poisson bracket between counterterms (94) and (95) and the total diffeomorphism constraint is

$$\{H^C_{\pi\nabla}[N], D[N^a]\} = \int d^3x\Big[(\partial_c\delta N^j)\bar N\Big(g_4\frac{\bar\nu\bar\pi^2}{2\bar p^{3/2}}\frac{\delta E^c_j}{2\bar p}\Big) + (\partial_c\delta N^c)\Big\{\delta N(2f_1 - f_2)\frac{\bar\nu\bar\pi^2}{2\bar p^{3/2}} + \bar N(g_1 - g_2)\frac{\bar\nu\,\bar\pi\,\delta\pi}{\bar p^{3/2}} - \bar N(2g_2 - g_3 + g_4)\frac{\bar\nu\bar\pi^2}{2\bar p^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar p}\Big\}\Big]. \tag{96}$$

Requiring that counterterms commute with the diffeomorphism constraint leads to the conditions

$$2f_1 = f_2,\qquad g_1 = g_2,\qquad 2g_2 = g_3,\qquad g_4 = 0. \tag{97}$$

Given that g_4 is required to vanish, we will drop the corresponding term from the set of counterterms in our further evaluation. We began with seven unknown functions in the counterterms for the kinetic sector. Requiring that counterterms commute with the diffeomorphism constraint imposes four conditions. This in turn allows only three more conditions to be imposed on these functions from anomaly cancellation in the remaining Poisson bracket of Hamiltonian constraints.

There are some subtleties in finding anomaly cancellation conditions for the matter sector. Inclusion of counterterms to the gravitational sector has generated additional contributions both in the gravitational as well as the matter sector. Thus, matter sector counterterms need to cancel the original anomaly expression (94) but also contributions from gravitational counterterms. Contributions from gravitational counterterms to anomaly expressions of the matter kinetic sector are

$$\mathcal{A}^{C}_{\mathrm{grav}\pi\nabla} := \{H^C_{\mathrm{grav}}[N_1], H^P_{\pi\nabla}[N_2]\} - (N_1 \leftrightarrow N_2) = \int \mathrm{d}^3x \bar{N}(\delta N_1 - \delta N_2)\Big[\frac{\bar{\nu}\,\bar{\pi}\,\delta\pi}{\bar{p}^{3/2}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}(3f) + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}(\delta^c_j\delta K^j_c)\frac{\bar{\alpha}}{\sqrt{\bar{p}}}(f) + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}(g-5f)\Big]. \tag{98}$$

Similarly, contributions from counterterms of the matter kinetic sector to the Poisson bracket between total Hamiltonians can be computed as

$$\mathcal{A}^{C}_{\pi\nabla} := \{H^C_{\pi\nabla}[N_1], H^P_{\mathrm{grav}}[N_2] + H^P_{\pi\nabla}[N_2]\} - (N_1 \leftrightarrow N_2) = \int \mathrm{d}^3x \bar{N}(\delta N_1 - \delta N_2)\Big[\frac{\bar{\nu}\,\bar{\pi}}{\bar{p}}\bar{\sigma}\nabla^2\delta\varphi(f_1+g_5) + \frac{\bar{\nu}\,\bar{\pi}\,\delta\pi}{\bar{p}^{3/2}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\Big(2\bar{p}\frac{\partial f_1}{\partial\bar{p}} - 3f_1 + 3g_2\Big) + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}(\delta^c_j\delta K^j_c)\frac{\bar{\alpha}}{\sqrt{\bar{p}}}(-f_2) + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\Big(-2\bar{p}\frac{\partial f_2}{\partial\bar{p}} + 4f_2 - 3g_3\Big)\Big]. \tag{99}$$

We then combine the original anomaly (94) with contributions (98) from gravitational counterterms and contributions from matter kinetic sector counterterms (99) to express the total anomaly $\mathcal{A}_{\pi\nabla} := \mathcal{A}^P_{\mathrm{matter}} + \mathcal{A}^C_{\mathrm{grav}\pi\nabla} + \mathcal{A}^C_{\pi\nabla}$ in the kinetic sector of scalar matter as

$$\mathcal{A}_{\pi\nabla} = \int \mathrm{d}^3x \bar{N}(\delta N_1 - \delta N_2)\Big[\frac{\bar{\nu}\,\bar{\pi}\,\delta\pi}{\bar{p}^{3/2}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\mathcal{B}_1 + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}(\delta^c_j\delta K^j_c)\frac{\bar{\alpha}}{\sqrt{\bar{p}}}\mathcal{B}_2 + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\mathcal{B}_3 + \frac{\bar{\nu}\,\bar{\pi}}{\bar{p}}\bar{\sigma}\nabla^2\delta\varphi\mathcal{B}_4\Big], \tag{100}$$

where

$$\mathcal{B}_1 = \frac{2\bar{p}}{\bar{\nu}}\frac{\partial\bar{\nu}}{\partial\bar{p}} + 3f + 2\bar{p}\frac{\partial f_1}{\partial\bar{p}} - 3f_1 + 3g_2, \tag{101}$$

$$\mathcal{B}_2 = -\frac{2\bar{p}}{3\bar{\nu}}\frac{\partial\bar{\nu}}{\partial\bar{p}} + f - f_2, \tag{102}$$

$$\mathcal{B}_3 = -\frac{10\bar{p}}{3\bar{\nu}}\frac{\partial\bar{\nu}}{\partial\bar{p}} - 5f + g - 2\bar{p}\frac{\partial f_2}{\partial\bar{p}} + 4f_2 - 3g_3, \tag{103}$$

$$\mathcal{B}_4 = f_1 + g_5. \tag{104}$$

In the presence of a nonzero scalar matter potential, the imposition of background and perturbed Hamiltonian constraints does not determine matter kinetic terms in terms of gravitational terms in the Hamiltonian constraint. In such situations anomalies in the kinetic sector of scalar matter must vanish independently of the gravitational sector anomaly. From, Eq. (100) it is evident that anomaly freedom in the kinetic sector requires four conditions to be satisfied, i.e. $\mathcal{B}_1 = 0$, $\mathcal{B}_2 = 0$, $\mathcal{B}_3 = 0$ and $\mathcal{B}_4 = 0$. However as we mentioned, after imposing Eqs. (97) we have only three undetermined functions in kinetic sector counterterms. Thus it may appear once again that there is over-determination of counterterms. However, similarly to the gravitational sector, coefficients of the anomaly expression (100) satisfy a nontrivial consistency relation. In particular, using relations (77) and (97), one notes that

$$\mathcal{B}_3 = -2\mathcal{B}_1 - \mathcal{B}_2. \tag{105}$$

Thus, cancellation of kinetic sector anomalies requires only three equations to be satisfied by counterterm coefficients. In other words, counterterms for kinetic sector are unambiguously determined by anomaly cancellation conditions.

2. *Potential sector*

We recall that the potential sector did not involve any primary quantum correction functions and did not contribute to the matter sector anomaly. However, including counterterms in the gravitational and matter kinetic sectors leads to new anomaly terms involving the scalar matter potential. Such new anomaly contributions from gravitational counterterms to the Poisson bracket between Hamiltonians can be computed as

$$\mathcal{A}^C_{\mathrm{grav}\varphi} := \{H^C_{\mathrm{grav}}[N_1], H^P_\varphi[N_2]\} - (N_1 \leftrightarrow N_2)$$
$$= \int \mathrm{d}^3x \bar{N}(\delta N_1 - \delta N_2)\Big[\frac{\bar{\alpha}}{\sqrt{\bar{p}}}\bar{p}^{3/2}V(\bar{\varphi})(\delta^c_j\delta K^j_c)(-f) + \frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\delta\varphi(-3f)$$
$$+ \frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\bar{p}^{3/2}V(\bar{\varphi})\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(-f-g)\Big]. \tag{106}$$

Similar anomaly contributions from counterterms of the matter kinetic sector are

$$\mathcal{A}^C_{\varphi\pi} := \{H^C_{\pi\nabla}[N_1], H^P_\varphi[N_2]\} - (N_1 \leftrightarrow N_2)$$
$$= \int \mathrm{d}^3x \bar{N}(\delta N_1 - \delta N_2)\Big[\frac{\bar{\nu}\,\bar{\pi}}{\bar{p}^{3/2}}\bar{p}^{3/2}V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi(-f_1) + \frac{\bar{\nu}\delta\pi}{\bar{p}^{3/2}}\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})(-f_1+g_1)$$
$$+ \frac{\bar{\nu}\,\bar{\pi}}{\bar{p}^{3/2}}\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(f_2-f_1-g_2)\Big]. \tag{107}$$

Thus, counterterms of the matter kinetic sector generate a new anomaly term involving $V_{,\varphi\varphi}(\bar{\varphi})$. Gravitational counterterms on the other hand, do not lead to such a term. For nonvanishing f_1, not all terms can cancel by combining Eqs. (106) and (107). Even though we did not consider primary quantum corrections in the potential sector, for anomaly freedom we need to allow counterterms even here. As in the kinetic sector, we begin with a general expression of possible counterterms in the potential sector $H^C_\varphi[N] := H^C_\varphi[\delta N] + H^C_\varphi[\bar{N}]$ where

$$H^C_\varphi[\delta N] = \int \mathrm{d}^3x\delta N\Big[f_3(\bar{p})\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\delta\varphi + f_4(\bar{p})\bar{p}^{3/2}V(\bar{\varphi})\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\Big], \tag{108}$$

and

$$H^C_\varphi[\bar{N}] = \int \mathrm{d}^3x\bar{N}\Big[g_6(\bar{p})\frac{1}{2}\bar{p}^{3/2}V_{\varphi\varphi}(\bar{\varphi})\delta\varphi^2 + g_7(\bar{p})\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\delta\varphi\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}$$
$$+ \bar{p}^{3/2}V(\bar{\varphi})\Big(g_8(\bar{p})\frac{(\delta^j_c\delta E^c_j)^2}{8\bar{p}^2} - g_9(\bar{p})\frac{\delta^k_c\delta^j_d\delta E^c_j\delta E^d_k}{4\bar{p}^2}\Big)\Big]. \tag{109}$$

We have introduced six new unknown functions f_3, f_4, g_6, g_7, g_8 and g_9 in the counterterms of the potential sector. To ensure invariance of the potential sector counterterms under diffeomorphism constraint we compute the Poisson bracket between counterterms and the diffeomorphism constraint:

$$\{H^C_\varphi[N], D[N^a]\} = \int \mathrm{d}^3x\bar{p}(\partial_c\delta N^c\delta^a_i - \partial_i\delta N^a)$$
$$\times\Big[\delta N\bar{p}^{3/2}f_4V(\bar{\varphi})\frac{\delta^i_a}{2\bar{p}} + \bar{N}\bar{p}^{3/2}\Big\{g_7V_{,\varphi}(\bar{\varphi})\delta\varphi\frac{\delta^i_a}{2\bar{p}} + V(\bar{\varphi})\Big(g_8\frac{(\delta^j_c\delta E^c_j)\delta^i_a}{4\bar{p}^2} - g_9\frac{\delta^i_c\delta^j_a\delta E^c_j}{2\bar{p}^2}\Big)\Big\}\Big]. \tag{110}$$

It is then easy to see that counterterms commute with the diffeomorphism constraint only if the coefficients satisfy

$$f_4 = 0, \qquad g_7 = 0, \qquad g_8 = 0, \qquad g_9 = 0. \tag{111}$$

Thus diffeomorphism invariance of the counterterms allows just two independent functions in the potential sector. The nonvanishing counterterms in the potential sector reduce to

$$H^C_\varphi[N] = \int \mathrm{d}^3x\Big[\delta Nf_3\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\delta\varphi + \bar{N}\frac{1}{2}g_6\bar{p}^{3/2}V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi^2\Big]. \tag{112}$$

Contributions from counterterms of the potential sector to the Poisson bracket between total Hamiltonians can be computed as

$$\mathcal{A}^C_\varphi := \{H^C_\varphi[N_1], H^P_{\rm grav}[N_2] + H^Q_{\rm matter}[N_2]\} - (N_1 \leftrightarrow N_2) = \int d^3x \bar{N}(\delta N_1 - \delta N_2)\bigg[\frac{\bar{\nu}\,\bar{\pi}}{\bar{p}^{3/2}}\bar{p}^{3/2}V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi(f_3 - g_6) + \frac{\bar{\nu}\delta\pi}{\bar{p}^{3/2}}\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})(f_3) + \frac{\bar{\nu}\,\bar{\pi}}{\bar{p}^{3/2}}\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(-f_3) + \frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\bar{p}^{3/2}V_{,\varphi}(\bar{\varphi})\delta\varphi\Big(2\bar{p}\frac{\partial f_3}{\partial\bar{p}} + 3f_3\Big)\bigg]. \tag{113}$$

Combining (106), (107), and (113) we form the total anomaly term $\mathcal{A}_\varphi := \mathcal{A}^C_{{\rm grav}\varphi} + \mathcal{A}^C_{\varphi\pi} + \mathcal{A}^C_\varphi$ in the scalar matter potential sector:

$$\mathcal{A}_\varphi = \int d^3x\bar{N}(\delta N_1 - \delta N_2)\bigg[\bar{\nu}\,\bar{\pi}\,V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi\mathcal{D}_1 + V_{,\varphi}(\bar{\varphi})\Big\{\bar{\nu}\delta\pi\mathcal{D}_2 + \bar{\nu}\,\bar{\pi}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\mathcal{D}_3\Big\} + (\bar{\alpha}\,\bar{k}\,\bar{p})V_{,\varphi}(\bar{\varphi})\delta\varphi\mathcal{D}_4 - (\bar{\alpha}\,\bar{p})V(\bar{\varphi})\Big\{(\delta^c_j\delta K^j_c)f + \bar{k}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(f+g)\Big\}\bigg] \tag{114}$$

where

$$\begin{aligned}\mathcal{D}_1 &= f_3 - f_1 - g_6,\\ \mathcal{D}_2 &= f_3 - f_1 + g_1,\\ \mathcal{D}_3 &= -f_3 + f_2 - f_1 - g_2,\\ \mathcal{D}_4 &= 2\bar{p}\frac{\partial f_3}{\partial\bar{p}} + 3f_3 - 3f.\end{aligned} \tag{115}$$

As in the gravitational and matter kinetic sectors, coefficients of the potential sector anomaly satisfy a nontrivial consistency relation

$$\mathcal{D}_3 = -\mathcal{D}_2 \tag{116}$$

using (97). We recall that counterterms (113) of the potential sector have only two unknown functions f_3 and g_6 which would be determined by choosing, say, $\mathcal{D}_1 = 0$ and $\mathcal{D}_2 = 0$. Then, we would automatically have $\mathcal{D}_3 = 0$, but there are still nonvanishing terms in the anomaly (114) of the potential sector. In particular, the last two terms in (114) are similar to the anomaly terms due to cosmological constant (89) and can be absorbed into anomaly terms of the gravitational and matter kinetic sectors by subtracting the total Hamiltonian constraint with suitable lapse function from it. Vanishing of total anomaly terms from the potential sector then requires that $\mathcal{D}_4$ should also vanish *i.e.* $\mathcal{D}_4 = 0$ [62]. However, requiring $\mathcal{D}_4$ to vanish imposes additional restriction on counterterms which in turn requires primary correction functions α, ν and σ to satisfy another consistency requirement [see Eq. (134)] in presence of a nonzero scalar potential, apart from the relation (67). After imposing $\mathcal{D}_1 = 0$, $\mathcal{D}_2 = 0$, $\mathcal{D}_3 = 0$ and $\mathcal{D}_4 = 0$, we can express the remaining terms in Eq. (114) as

$$\mathcal{A}^{\rm rem}_\varphi = \mathcal{A}_{{\rm grav}\varphi} + \mathcal{A}_{\pi\nabla\varphi} - H^P\bigg[\bar{N}(\delta N_1 - \delta N_2)\frac{\bar{\alpha}}{\sqrt{\bar{p}}} \times\Big\{(\delta^c_j\delta K^j_c)f + \bar{k}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(f+g)\Big\}\bigg], \tag{117}$$

where part of the potential sector anomaly to be included in the gravitational sector anomaly can be expressed as

$$\mathcal{A}_{{\rm grav}\varphi} = \frac{1}{8\pi G}\int d^3x\bar{N}(\delta N_1 - \delta N_2)\bar{\alpha}^2\bigg[\bar{k}^2(\delta^c_j\delta K^j_c)(-3f) + \bar{k}^3\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(-3f - 3g)\bigg], \tag{118}$$

and another part that needs to be included in the anomaly expression of the matter kinetic sector is

$$\mathcal{A}_{\pi\nabla\varphi} = \int d^3x\bar{N}(\delta N_1 - \delta N_2)\bigg[\frac{\bar{\alpha}}{\sqrt{\bar{p}}}\frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}(\delta^c_j\delta K^j_c)(f) + \frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}(f+g)\bigg]. \tag{119}$$

We have seen earlier that the presence of a nonzero cosmological constant modifies the anomaly cancellation conditions as reflected in Eq. (91). Similarly, the presence of a nontrivial scalar matter potential leads to changes in the anomaly cancellation conditions for both the gravitational sector as well as the kinetic sector of matter. In particular, we can combine Eqs. (79) and (118) to express the total gravitational anomaly $\mathcal{A}_{\rm grav} := \mathcal{A}^P_{\rm grav} + \mathcal{A}^C_{\rm grav} + \mathcal{A}_{{\rm grav}\varphi}$ as

$$\mathcal{A}_{\rm grav} = \frac{1}{8\pi G}\int d^3x\bar{N}(\delta N_1 - \delta N_2)\bar{\alpha}^2\bigg[\frac{\bar{k}}{\bar{p}}(\partial_c\partial^j\delta E^c_j)\mathcal{G}^\varphi_1 + \bar{k}^2(\delta^c_j\delta K^j_c)\mathcal{G}^\varphi_2 + \bar{k}^3\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\mathcal{G}^\varphi_3\bigg], \tag{120}$$

where the new coefficients are

$$\mathcal{G}^\varphi_1 = \mathcal{G}_1, \qquad \mathcal{G}^\varphi_2 = \mathcal{G}_2 - 3f, \qquad \mathcal{G}^\varphi_3 = \mathcal{G}_3 - 3f - 3g. \tag{121}$$

Using Eq. (77), we again note that the new coefficients satisfy the same nontrivial consistency relation

$$\mathcal{G}_3^{\varphi} = -\mathcal{G}_2^{\varphi}. \tag{122}$$

Thus also in the presence of a nontrivial scalar matter potential, there are unambiguous solutions for f, g and h such that the gravitational sector of constraint algebra is anomaly free. Similarly, for the matter kinetic sector we can combine the original anomaly (94), contributions (98) from gravitational counterterms, contributions (99) from kinetic sector counterterms and contributions (119) from the potential sector to express the total anomaly in the kinetic sector of scalar matter as

$$\begin{aligned}\mathcal{A}_{\pi\nabla} &:= \mathcal{A}^P_{\rm matter} + \mathcal{A}^C_{{\rm grav}\pi\nabla} + \mathcal{A}^C_{\pi\nabla} + \mathcal{A}_{\pi\nabla\varphi} \\ &= \int {\rm d}^3x\bar{N}(\delta N_1 - \delta N_2) \\ &\quad\times\Big[\frac{\bar{\nu}\,\bar{\pi}\,\delta\pi}{\bar{p}^{3/2}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\mathcal{B}_1^{\varphi} + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}(\delta^c_j\delta K^j_c)\frac{\bar{\alpha}}{\sqrt{\bar{p}}}\mathcal{B}_2^{\varphi} \\ &\quad + \frac{\bar{\nu}\bar{\pi}^2}{2\bar{p}^{3/2}}\frac{(\delta^j_c\delta E^c_j)}{2\bar{p}}\frac{\bar{\alpha}\,\bar{k}}{\sqrt{\bar{p}}}\mathcal{B}_3^{\varphi} + \frac{\bar{\nu}\,\bar{\pi}}{\bar{p}}\bar{\sigma}\nabla^2\delta\varphi\mathcal{B}_4^{\varphi}\Big],\end{aligned} \tag{123}$$

with new coefficients

$$\begin{aligned}\mathcal{B}_1^{\varphi} = \mathcal{B}_1, &\qquad \mathcal{B}_2^{\varphi} = \mathcal{B}_2 + f, \\ \mathcal{B}_3^{\varphi} = \mathcal{B}_3 + f + g, &\qquad \mathcal{B}_4^{\varphi} = \mathcal{B}_4\end{aligned} \tag{124}$$

in the matter kinetic sector anomaly expression. Also here, the new coefficients satisfy a consistency relation

$$\mathcal{B}_3^{\varphi} = -2\mathcal{B}_1^{\varphi} - \mathcal{B}_2^{\varphi} \tag{125}$$

using (77) and (97). This relation is analogous to Eq. (105) and likewise it ensures that anomaly cancellation conditions lead to unambiguous expressions for counterterms in the kinetic sector of scalar matter when there is a nontrivial potential.

D. Quantum corrected total Hamiltonian constraint

We now combine all primary correction functions and the counterterms to form the quantum corrected total Hamiltonian constraint $H^Q[N] := H^P[N] + H^C[N]$ for the system consisting of a scalar matter field with arbitrary potential:

$$\begin{aligned}H^Q_{\rm grav}[\bar{N}] &:= \frac{1}{16\pi G}\int {\rm d}^3x\bar{N}[\bar{\alpha}\mathcal{H}^{Q(0)} + \alpha^{(2)}\mathcal{H}^{Q(0)} \\ &\qquad + \bar{\alpha}\mathcal{H}^{Q(2)}], \\ H^Q_{\rm grav}[\delta N] &:= \frac{1}{16\pi G}\int {\rm d}^3x\delta N[\bar{\alpha}\mathcal{H}^{Q(1)}],\end{aligned} \tag{126}$$

where the background density is unchanged except for the explicit factor of the primary correction, i.e. $\mathcal{H}^{Q(0)} \equiv \mathcal{H}^{(0)}$. However the perturbed densities now involve counterterms:

$$\begin{aligned}\mathcal{H}^{Q(1)} &= -4(1+f)\bar{k}\sqrt{\bar{p}}\,\delta^c_j\delta K^j_c - (1+g)\frac{\bar{k}^2}{\sqrt{\bar{p}}}\delta^j_c\delta E^c_j \\ &\quad + \frac{2}{\sqrt{\bar{p}}}\partial_c\partial^j\delta E^c_j, \\ \mathcal{H}^{Q(2)} &= \sqrt{\bar{p}}\delta K^j_c\delta K^k_d\delta^c_k\delta^d_j - \sqrt{\bar{p}}(\delta K^j_c\delta^c_j)^2 - \frac{2\bar{k}}{\sqrt{\bar{p}}}\delta E^c_j\delta K^j_c \\ &\quad - \frac{\bar{k}^2}{2\bar{p}^{3/2}}\delta E^c_j\delta E^d_k\delta^k_c\delta^j_d + \frac{\bar{k}^2}{4\bar{p}^{3/2}}(\delta E^c_j\delta^j_c)^2 \\ &\quad - (1+h)\frac{\delta^{jk}}{2\bar{p}^{3/2}}(\partial_c\delta E^c_j)(\partial_d\delta E^d_k).\end{aligned} \tag{127}$$

It should be noted here that the terms in gravitational Hamiltonian which involve counterterms, contain either trace or divergence of perturbed basic variables. Thus, inclusion of counterterms does not affect the earlier results for vector and tensor modes [21,22]. The complete quantum corrected matter Hamiltonian constraint is given by

$$\begin{aligned}H^Q_{\rm matter}[\bar{N}] &= \int_\Sigma {\rm d}^3x\bar{N}[(\bar{\nu}\mathcal{H}^{Q(0)}_\pi + \mathcal{H}^{Q(0)}_\varphi) \\ &\quad + (\nu^{(2)}\mathcal{H}^{Q(0)}_\pi + \bar{\nu}\mathcal{H}^{Q(2)}_\pi + \bar{\sigma}\mathcal{H}^{Q(2)}_\nabla \\ &\quad + \mathcal{H}^{Q(2)}_\varphi)] \\ H^Q_{\rm matter}[\delta N] &= \int {\rm d}^3x\delta N[\bar{\nu}\mathcal{H}^{Q(1)}_\pi + \mathcal{H}^{Q(1)}_\varphi],\end{aligned} \tag{128}$$

where background densities are again unchanged, i.e. $\mathcal{H}^{Q(0)}_\pi \equiv \mathcal{H}^{(0)}_\pi$ and $\mathcal{H}^{Q(0)}_\varphi \equiv \mathcal{H}^{(0)}_\varphi$. As in the gravitational sector, perturbed matter densities include counterterms and are given by

$$\begin{aligned}\mathcal{H}^{Q(1)}_\pi &= (1+f_1)\frac{\bar{\pi}\delta\pi}{\bar{p}^{3/2}} - (1+f_2)\frac{\bar{\pi}^2}{2\bar{p}^{3/2}}\frac{\delta^j_c\delta E^c_j}{2\bar{p}}; \\ \mathcal{H}^{Q(1)}_\varphi &= \bar{p}^{3/2}\Big((1+f_3)V_{,\varphi}(\bar{\varphi})\delta\varphi + V(\bar{\varphi})\frac{\delta^j_c\delta E^c_j}{2\bar{p}}\Big); \\ \mathcal{H}^{Q(2)}_\pi &= (1+g_1)\frac{\delta\pi^2}{2\bar{p}^{3/2}} - (1+g_2)\frac{\bar{\pi}\delta\pi}{\bar{p}^{3/2}}\frac{\delta^j_c\delta E^c_j}{2\bar{p}} \\ &\quad + \frac{1}{2}\frac{\bar{\pi}^2}{\bar{p}^{3/2}}\Big((1+g_3)\frac{(\delta^j_c\delta E^c_j)^2}{8\bar{p}^2} + \frac{\delta^k_c\delta^j_d\delta E^c_j\delta E^d_k}{4\bar{p}^2}\Big); \\ \mathcal{H}^{Q(2)}_\nabla &= \frac{1}{2}(1+g_5)\sqrt{\bar{p}}\delta^{ab}\partial_a\delta\varphi\partial_b\delta\varphi; \\ \mathcal{H}^{Q(2)}_\varphi &= \bar{p}^{3/2}\Big[(1+g_6)\frac{1}{2}V_{,\varphi\varphi}(\bar{\varphi})\delta\varphi^2 + V_{,\varphi}(\bar{\varphi})\delta\varphi\frac{\delta^j_c\delta E^c_j}{2\bar{p}} \\ &\quad + V(\bar{\varphi})\Big(\frac{(\delta^j_c\delta E^c_j)^2}{8\bar{p}^2} - \frac{\delta^k_c\delta^j_d\delta E^c_j\delta E^d_k}{4\bar{p}^2}\Big)\Big].\end{aligned} \tag{129}$$

To summarize the conditions on nonvanishing coefficients of the counterterms, we note that there are three such functions in the gravitational sector (127), six in the kinetic sector and two in the potential sector of scalar matter (129).

Thus for the system under consideration we have a total of 11 correction functions contained in all counterterms. Invariance of counterterms under diffeomorphisms, (77) and (97), led to four conditions

$$g = -2f, \qquad f_2 = 2f_1, \qquad g_2 = g_1, \qquad g_3 = 2g_2 \tag{130}$$

among the nonvanishing coefficients. These equations trivially lead to the solutions for g, f_2, g_2 and g_3, leaving seven functions to be determined.

Cancellation of anomaly terms from the Poisson bracket between Hamiltonian constraints led to three conditions (121) from the gravitational sector

$$\mathcal{G}_1^{\varphi} = 0, \qquad \mathcal{G}_2^{\varphi} = 0, \qquad \mathcal{G}_3^{\varphi} = 0, \tag{131}$$

among which only two are independent due to (122). These two independent equations explicitly solve f and h in terms of the primary correction function α. Thus, there are only five remaining functions that need to be determined. Anomaly cancellation from matter kinetic sector (124) leads to four conditions

$$\mathcal{B}_1^{\varphi} = 0, \qquad \mathcal{B}_2^{\varphi} = 0, \qquad \mathcal{B}_3^{\varphi} = 0, \qquad \mathcal{B}_4^{\varphi} = 0. \tag{132}$$

Given the relation (125), there are only three independent equations which leads to explicit solutions for f_1, g_1 and g_5 in terms of primary correction functions α and ν. The remaining two free functions f_3 and g_6 are constrained by requiring cancellation of anomalies from the potential sector which gives four conditions

$$\mathcal{D}_1 = 0, \qquad \mathcal{D}_2 = 0, \qquad \mathcal{D}_3 = 0, \qquad \mathcal{D}_4 = 0. \tag{133}$$

Using Eq. (115), one notes that $\mathcal{D}_1 = 0$ and $\mathcal{D}_2 = 0$ already determines both f_3 and g_6 in terms of other counterterms coefficients which are already fixed.

While $\mathcal{D}_3 = 0$ is not an independent equation, $\mathcal{D}_4 = 0$ imposes a nontrivial restriction on counterterms. Since all of them have been determined at this stage, consistency requires the primary correction functions to satisfy

$$\frac{\bar{\alpha}'\bar{p}}{\bar{\alpha}} + \frac{\bar{p}}{3}\left(\frac{\bar{\alpha}'\bar{p}}{\bar{\alpha}}\right)' - \frac{\bar{\nu}'\bar{p}}{\bar{\nu}} - \frac{\bar{p}}{9}\left(\frac{\bar{\nu}'\bar{p}}{\bar{\nu}}\right)' + \frac{2\bar{p}^2}{9}\left(\frac{\bar{\nu}'\bar{p}}{\bar{\nu}}\right)'' = 0. \tag{134}$$

Note that this relation ties the matter correction function to the gravitational correction function, but it is independent of the matter fields. Finally, from (67) we have the relation $\bar{\alpha}^2 = \bar{\nu}\,\bar{\sigma}$ to be satisfied by the primary correction functions.

To summarize, the requirement of anomaly freedom in the constraint algebra tightly controls the allowed forms of primary correction functions. For primary corrections of the form (9), for instance, one can easily see that solutions exist provided certain relations between the coefficients c_α, c_ν and powers n_α, n_ν in the two primary correction functions α and ν are satisfied. Thus, quantization ambiguities are nontrivially reduced, which allows stringent consistency tests by direct calculations from a full representation of the underlying operators. These restrictions indirectly help to eliminate some of the quantization ambiguities encountered in quantizing inverse-triad operators.

V. CONCLUSIONS

In this paper we have analyzed quantum corrected constraints at the perturbative effective level. The key issue has been whether they form a closed Poisson algebra, which would ensure consistency of the equations of motion they generate. There are correction functions α, ν, and σ whose expressions are well known in homogeneous models. A direct extension of the functions as scalars of density weight zero correcting inhomogeneous constraints would suggest that they (i) depend only on the triad E^a_i (but not on the extrinsic curvature K^i_a), (ii) depend on the triad algebraically (i.e. do not contain spatial derivatives of E^a_i), and (iii) in the perturbed context, depend on the background triad $\bar{E}^a_i$ and its perturbation δE^a_i only in the combination $E^a_i = \bar{E}^a_i + \delta E^a_i$. However, as we have found, this would allow a closed algebra only if corrections are trivial.

At the same time, from the constructive point of view, it is not surprising that the three conditions cannot be met together. Indeed, the only scalar quantity that can be constructed from the triad alone is its determinant—a density-weight-one object—leaving no possibility of cancelling the density weight. One could relax any of these conditions and see whether that would allow nontrivial corrections. For instance, by allowing correction functions to depend on spatial curvature, which would require spatial derivatives of the triad, we could alleviate the problem of zero density weight since this would make available the quantity

$$\frac{E^a_i}{\sqrt{|\det E|}}\,\partial_a\left(\frac{\partial_b E^b_i}{\sqrt{|\det E|}}\right).$$

On the other hand, if we relax the first condition, quantities of the form $E^a_i K^i_a/\sqrt{|\det E|}$ would be allowed.

We were therefore led to conclude that expectations from homogeneous models did not capture all possible quantum effects, and turned to investigating what quantum corrections of inhomogeneous constraints would be allowed in principle, and which ones should be ruled out. In this process, we have generated several counterterms in addition to the primary corrections suggested by homogeneous models. The resulting counterterms admit nontrivial quantum corrections, and their presence and form can be related to fundamental aspects of loop quantum gravity. For instance, we have seen that quantum corrections must be connection dependent even when they come from inverse-triad corrections. This can be interpreted as meaning that the computation of effective constraints, based on expectation values of constraint operators, must be done in coherent states such that a holonomy dependence of inverse-triad expressions results. Correction functions must also depend on spatial derivatives of the triad, which can be seen as leading terms in a derivative expansion of nonlocal expressions involving fluxes, i.e. 2-dimensionally integrated triads. There are also quite unexpected effects, such as counterterms in the matter sector involving derivatives of the potential. Not all of them are simply realized as a consequence of the expansion of $V(\bar{\varphi} + \delta\varphi)$ by inhomogeneities. This suggests that the matter potential must be quantized in a nonlocal way to ensure anomaly freedom. This form of nonlocality is currently not realized in quantizations of scalar matter in loop quantum gravity. It suggests concrete ways to change full constructions so as to provide an (off shell) anomaly free formulation.

From the perturbed second order constraints one can directly derive Hamiltonian equations of motion for the perturbed variables as well as gauge transformations on them. Both equations of motion and gauge transformations will be corrected by quantum gravity terms, which has to be combined for equations of motion of gauge-invariant variables of the form (5)–(7). Imposing the conditions found for an anomaly free constraint algebra must, on general grounds, result in a consistent set of equations. This has already been verified for vector and tensor modes (see [21,22], respectively). In a companion paper [12], we explicitly derive gauge transformations and construct gauge-invariant variables taking into account quantum corrections, which we will then use to derive gauge-invariant equations of motion describing cosmological perturbations.

We have provided one consistent set of equations by a process which demonstrates that the possibilities of nontrivial quantum corrections are rather tight. In fact, existing proposals for primary correction functions are nontrivially restricted. Yet, different versions may be available, which could in principle be compared with full derivations of effective Hamiltonians to fix remaining ambiguities. But there may also be quantization ambiguities which cannot be removed based solely on consistency considerations; they would have to be restricted phenomenologically instead. It is thus important also for a fundamental understanding to evaluate cosmological implications of the quantum corrected perturbation equations.

In addition to other choices regarding one type of quantum corrections, which in this paper is inverse-triad corrections, there are different general types of corrections. In loop quantum gravity, we have two additional classes: corrections of higher powers of the connection or extrinsic curvature due to the use of holonomies, and genuine quantum back reaction effects which include the influence of the whole wave function on its expectation values. (It is the latter which underlies constructions such as the low-energy effective action used in particle physics.) These corrections turn out to be more difficult to compute in consistent form, which is still in progress. Our consistent equations are thus not to be considered as complete effective equations, and including the corresponding terms of one type may add to the effects of another type or decrease them (in a way which is regime dependent). But it is unlikely that complete cancellations happen because corrections of the different types take such different forms. Moreover, a complete cancellation would mean that the characteristic fundamental representation of loop quantum gravity would leave no trace on the physics of the theory.

While quantitative results are expected to depend on the specific form of corrections and the interplay of different types, the occurrence of qualitative effects signalling deviations from classical relativity is more robust. This differs from other results of loop quantum cosmology, such as bounces in homogeneous models where a sharp zero result for the time derivative of a scale factor is required. Such sharp conditions can easily be destroyed when additional quantum corrections are included; see e.g. [7]. Compared to that, the complete elimination of qualitative effects of one type of correction by including another type is highly unlikely.

The consistent constraint algebra shows that nontrivial quantum corrections which reflect the underlying discreteness of spatial geometry are possible. In this sense, general covariance is preserved. However, we have shown that the classical constraint algebra, while consistently deformed, is not represented exactly but receives quantum corrections from the corrected constraints. One can see this directly from (62), for instance, which carries a factor of $\bar{\alpha}^2$ in the smearing function of the diffeomorphism constraint. This is required by consistency since the classical algebra cannot be realized with nontrivial quantum corrections. Thus, an effective action of loop quantum gravity cannot be simply of higher-curvature type. (Nonlocal features, for instance, would then be essential.) Nevertheless, we expect that some of the corrections can be formulated by effective higher-curvature actions which applies even to the inverse-triad corrections used here. Some of the counterterms, which depend on extrinsic curvature components as well as spatial derivatives of the triad, can in fact be interpreted as bringing the corrected constraints in a form amenable to being formulated as a higher-curvature action. In this context, we emphasize that the absence of new degrees of freedom in this Hamiltonian framework is not in conflict with the higher-derivative nature of higher-curvature effective actions as also discussed in [5]: a perturbative interpretation of higher-derivative actions, which is the only appropriate way in quantum gravity, does not give rise to more solutions than expected classically [63].

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APPENDIX A: COMPARISON WITH ISOTROPIC MODELS

An important measure for the size of quantum corrections is the characteristic scale a_* which signals the onset of nonperturbative effects. As a critical value for the scale factor, it does not have absolute meaning because it can be rescaled by a choice of coordinates. It is ratios such as a/a_* which have physical meaning related to the patch density of a quantum gravity state. For a denser state features of correction functions based on inverse-triad components are realized on larger scales, which increases the corresponding quantum corrections.

These effects are also important if one tries to include the behavior in homogeneous models, even though an exactly homogeneous model provides only limited means of referring to spatial discreteness of an underlying state and its refinement. For this reason, care is needed if one tries to address possibilities of refinement schemes and the size of quantum corrections in purely homogeneous settings, as is often done due to the simplicity of homogeneous models. Quantum corrections in a fully inhomogeneous situation must be expected to be larger than in a naive isotropic quantization which ignores the factor $\mathcal{N}$ of the patch density and implicitly assumes $\mathcal{N}^{1/3} \sim 1$ as in [64]. This is the reason why some minisuperspace considerations artificially suppress those corrections. Corrections from holonomies, on the other hand, increase with decreasing vertex density such that they would appear to be more pronounced. It is possible to mimic the enhancement of inverse-triad corrections even in exact homogeneous models by computing their correction function for operators based on higher representations of SU(2) instead of the fundamental one [60]. The corresponding spin label is then related to the vertex density.

In addition to the size of corrections, there is also the issue of the correct scaling behavior of correction terms. To have independence of the coordinate size V_0 of the region whose patches are counted, we must have $\mathcal{N} \propto V_0$. However, this provides coordinate independent quantum corrections only if we multiply by another function which can absorb the coordinate dependence of V_0. The simplest possibility in isotropic models is to use $\mathcal{N} \propto a^3 V_0$ for which corrections depend neither on the size of the volume nor on coordinates. This behavior is indeed well motivated based on lattice refinements (where the physical vertex density is constant) and was introduced in [65] based on scaling arguments. If $\mathcal{N}$ is allowed to depend directly only on the scale factor (and not on $\dot{a}/a$, say), and there is no other parameter which rescales under changing coordinates other than V_0, this is indeed the only consistent choice. In this sense, the behavior proposed in [65] is unique in isotropic models up to a single constant which determines the absolute number of patches.

This uniqueness is, however, contingent on conditions which are too strong for reliably modelling what happens in inhomogeneous situations. If the model is no longer exactly homogeneous, the refinement of underlying states is history dependent in ways which do not simply amount to a dependence on a. One can always express the refinement as a dependence on scaling-independent observables such as $\dot{a}/a$ which provide an equally good measure for the history of different phases of the Universe. For a given background solution, one can then express this as a dependence on a alone, given that all observables depend on a. In general, however, this provides more complicated functions than just $\mathcal{N}(a) \propto a^3 V_0$ for the patch density. Some phases can, for instance, be described by a power-law form $\mathcal{N}(a) = \mathcal{N}_0 a^x V_0$ where $\mathcal{N}_0$ arises in a complicated process by expressing the refinement via a function only of a. In particular, because the original refinement is history dependent only via observable quantities, this constant will automatically be equipped with a scaling dependence such that $\mathcal{N}_0 a^x V_0$ is coordinate independent even if $x \neq 3$. The emergence of such a parameter can only be seen in the proper inhomogeneous context, invalidating considerations based solely on homogeneous models.

APPENDIX B: POISSON BRACKETS BETWEEN UNPERTURBED CONSTRAINTS

It is instructive to compute Poisson brackets between primary quantum corrected constraints without expanding by inhomogeneities. We first consider the gravitational Hamiltonian constraint (14). As $H^P_{\rm grav}$ commutes with matter diffeomorphism $D_{\rm matter}$, it is sufficient to compute $\{H^P_{\rm grav}[N], D_{\rm grav}[N^a]\}$. Classically, this Poisson bracket is

$$\{H_{\rm grav}[N], D_{\rm grav}[N^a]\} = -H_{\rm grav}[N^a \partial_a N]. \tag{B1}$$

The (gravitational) diffeomorphism constraint acts as a Lie derivative on a (gravitational) phase space function

$$\{F(A, E), D_{\rm grav}[N^a]\} = \mathcal{L}_{N^a} F. \tag{B2}$$

The Poisson bracket between $H^P_{\rm grav}[N]$ and $D_{\rm grav}[N^a]$ then is

$$\begin{aligned}\{H^P_{\rm grav}[N], D_{\rm grav}[N^a]\} &\equiv \left\{\int_\Sigma {\rm d}^3x N\alpha\mathcal{H}, D_{\rm grav}[N^a]\right\} \\ &= \int_\Sigma {\rm d}^3x N \mathcal{L}_{N^a}(\alpha\mathcal{H}) \\ &= \int_\Sigma {\rm d}^3x N(N^a\partial_a(\alpha\mathcal{H}) \\ &\quad + (\partial_a N^a)\alpha\mathcal{H}) \\ &= \int_\Sigma {\rm d}^3x(-N^a\partial_a N)\alpha\mathcal{H} \\ &\equiv -H^P_{\rm grav}[N^a\partial_a N].\end{aligned} \tag{B3}$$

Where we have used the fact that the quantity $\alpha\mathcal{H}$ has density weight one to expand the Lie derivative and integrated by parts in the next line. By the same token, we would not obtain the correct algebra if α would not be of density weight zero. Clearly, any functional of the (gravitational) variables defined by integration must be an integral of a density-weight-one function. Thus the only restriction on the correction function, obtained so far, is that it must be of zero density weight. In fact, only this condition makes the spatial integrals well defined.

The matter Hamiltonian constraint has nonzero Poisson brackets with both gravitational and matter parts of the diffeomorphism constraint. However, the total diffeomorphism constraint acts as a Lie derivative on any function of *all* phase space variables

$$\{F(A, E, \varphi, \pi), D[N^a]\} = \mathcal{L}_{N^a} F. \tag{B4}$$

Hence its Poisson bracket with the (gravitational) diffeomorphism constraint should boil down to an expression analogous to (B3). Again, the only condition on the correction functions is that they have zero density weight. In that case not only are the quantum corrected constraints first class, but also form an algebra identical to the classical one.

In what follows we will make extensive use of *lemma 1:* Consider a functional

$$F[N] = \int d^3x N(x) f(\varphi, \pi) \tag{B5}$$

of two canonically conjugate scalar [66] fields φ and π. If f does not depend on spatial derivatives of the fields, the Poisson bracket

$$\{F[N_1], F[N_2]\}_{(\varphi,\pi)} = 0 \tag{B6}$$

vanishes.

Proof: Since the integrand does not contain spatial derivatives, we have the functional derivative $\delta F[N]/\delta\varphi = N\partial f/\partial\varphi$ and

$$\begin{aligned}\{F[N_1], F[N_2]\} &\equiv \int d^3x\Big(\frac{\delta F[N_1]}{\delta\varphi}\frac{\delta F[N_2]}{\delta\pi} - (N_1 \leftrightarrow N_2)\Big)\\ &= \int d^3x\Big(N_1\frac{\partial f}{\partial\varphi}N_2\frac{\partial f}{\partial\pi} - (N_1 \leftrightarrow N_2)\Big)\\ &= 0.\end{aligned}$$

On the contrary, if spatial derivatives of the fields are present in the integrand, the relevant functional derivative involves derivatives of the smearing function which implies a nonvanishing final expression for the Poisson bracket after antisymmetrization over N_1 and N_2.

Using this result, let us analyze the expression

$$\begin{aligned}\{H^P[N_1], H^P[N_2]\} &\equiv \{H^P_{\rm grav}[N_1] + H^P_{\rm matter}[N_1], H^P_{\rm grav}[N_2] + H^P_{\rm matter}[N_2]\}\\ &= \{H^P_{\rm grav}[N_1], H^P_{\rm grav}[N_2]\} + \{H^P_{\rm matter}[N_1], H^P_{\rm matter}[N_2]\} + (\{H^P_{\rm grav}[N_1], H^P_{\rm matter}[N_2]\} - (N_1 \leftrightarrow N_2))\end{aligned} \tag{B7}$$

term by term. The gravitational constraints yield

$$\begin{aligned}\{H^P_{\rm grav}[N_1], H^P_{\rm grav}[N_2]\} &= \int_\Sigma d^3x\Big(\frac{\delta H_{\rm grav}[\tilde{N}_1]}{\delta A^i_a}\frac{\delta H_{\rm grav}[\tilde{N}_2]}{\partial E^a_i} - (N_1 \leftrightarrow N_2)\Big) + \int_\Sigma d^3x\Big(\frac{\delta H_g[\tilde{N}_1]}{\delta A^i_a}\frac{\partial\alpha}{\partial E^a_i}N_2\mathcal{H} - (N_1 \leftrightarrow N_2)\Big)\\ &= D_{\rm grav}[\tilde{N}_1\partial^a\tilde{N}_2 - \tilde{N}_2\partial^a\tilde{N}_1] + \mathcal{A}_{\rm grav\,grav},\end{aligned} \tag{B8}$$

where we have used the fact that if $\tilde{N}_{1,2}$ were independent of phase space variables then we would simply have the classical constraint algebra but with new lapse functions $\tilde{N}_1$ and $\tilde{N}_2$. However, since $\tilde{N}_{1,2}$ do depend on the densitized triad there is an extra (potentially anomalous) term in the Poisson bracket which is the second term $\mathcal{A}_{\rm grav\,grav}$, proportional to the derivatives of the correction function. The nontrivial contributions to the anomaly

$$\begin{aligned}\mathcal{A}_{\rm grav\,grav} &= -\int_\Sigma d^3x\Big\{N_1\frac{\partial\alpha}{\partial E^a_{i'}}\mathcal{H}\frac{\delta}{\delta A^{i'}_a}\Big(\int_\Sigma d^3y N_2\alpha\frac{2E^c_iE^d_j}{\sqrt{\det E}}\partial_c A^k_d\epsilon_{ijk}\Big) - (N_1 \leftrightarrow N_2)\Big\}\\ &= \int_\Sigma d^3x\mathcal{H}\frac{\partial\alpha}{\partial E^a_k}\epsilon_{ijk}\Big\{N_1\partial_c\Big(\alpha N_2\frac{2E^c_iE^a_j}{\sqrt{\det E}}\Big) - (N_1 \leftrightarrow N_2)\Big\}\end{aligned} \tag{B9}$$

come from the gradient terms of the Hamiltonians. Note that, for convenience, we switched the order of terms in the first line of (B9). In the second line, the only term in the parenthesis that survives the antisymmetrization is the one proportional to the gradient of the lapse function $\partial_c N_2$. Thus the anomaly simply boils down to

$$\mathcal{A}_{\rm grav\,grav} = H^P_{\rm grav}[M_\alpha] \quad \text{with } M_\alpha := 2\epsilon_{ijk}\frac{E^c_iE^a_j}{\sqrt{\det E}}\frac{\partial\alpha}{\partial E^a_k}(N_1\partial_c N_2 - N_2\partial_c N_1). \tag{B10}$$

It is easy to see that the symmetricity condition

$$E^a_j \frac{\partial \alpha}{\partial E^a_k} = E^a_k \frac{\partial \alpha}{\partial E^a_j} \tag{B11}$$

is sufficient to make the anomaly (B10) vanish due the contraction with ϵ_{ijk}. We should point out that (B11) is definitely satisfied for any triad-dependent scalar function, which has all internal indices contracted.

The cross Poisson bracket $\{H^P_{\rm grav}[N_1], H^P_{\rm matter}[N_2]\} - (N_1 \leftrightarrow N_2)$ can be computed similarly. In the absence of curvature couplings, such that the matter Hamiltonian contains neither connection nor spatial derivatives of the triad, this Poisson bracket is given by

$$\begin{aligned}&\{H^P_{\rm grav}[N_1], H^P_{\rm matter}[N_2]\} - (N_1 \leftrightarrow N_2)\\ &\quad= \int_\Sigma {\rm d}^3x\bigg(\frac{\delta H_{\rm grav}[\tilde{N}_1]}{\delta A^i_a}\frac{\partial \nu}{\partial E^a_i} N_2 \mathcal{H}_\pi - (N_1 \leftrightarrow N_2)\bigg)\\ &\qquad+ \int_\Sigma {\rm d}^3x\bigg(\frac{\delta H_{\rm grav}[\tilde{N}_1]}{\delta A^i_a}\frac{\partial \sigma}{\partial E^a_i} N_2 \mathcal{H}_\nabla - (N_1 \leftrightarrow N_2)\bigg)\\ &\quad= H^P_\pi[M_\nu] + H^P_\nabla[M_\sigma],\end{aligned} \tag{B12}$$

where

$$H^P_\pi[M_\nu] = \int_\Sigma {\rm d}^3x M_\nu \mathcal{H}_\pi, \qquad H^P_\nabla[M_\sigma] = \int_\Sigma {\rm d}^3x M_\sigma \mathcal{H}_\nabla \tag{B13}$$

with the effective lapse functions

$$\begin{aligned}M_\nu &:= 2\epsilon_{ijk}\frac{E^c_i E^a_j}{\sqrt{\det E}}\frac{\partial \nu}{\partial E^a_k}(N_1\partial_c N_2 - N_2\partial_c N_1),\\ M_\sigma &:= 2\epsilon_{ijk}\frac{E^c_i E^a_j}{\sqrt{\det E}}\frac{\partial \sigma}{\partial E^a_k}(N_1\partial_c N_2 - N_2\partial_c N_1)\end{aligned} \tag{B14}$$

similar to (B10). These vanish if the correction functions satisfy

$$E^a_j \frac{\partial \nu}{\partial E^a_k} = E^a_k \frac{\partial \nu}{\partial E^a_j}, \qquad E^a_j \frac{\partial \sigma}{\partial E^a_k} = E^a_k \frac{\partial \sigma}{\partial E^a_j}. \tag{B15}$$

Finally, the Poisson bracket between two matter Hamiltonians involves only functional derivatives with respect to the matter variables φ and π. By virtue of lemma 1, the nontrivial contribution comes from

$$\bigg\{\int_\Sigma {\rm d}^3x N_1 \nu \mathcal{H}_\pi, \int_\Sigma {\rm d}^3x N_2 \sigma \mathcal{H}_\nabla\bigg\}_{(\varphi,\pi)} - (N_1 \leftrightarrow N_2).$$

Since the correction functions do not depend on the matter variables, they act as constant factors, i.e.

$$\begin{aligned}&\{H^P_{\rm matter}[N_1], H^P_{\rm matter}[N_2]\}\\ &\quad= D_{\rm matter}[\nu\sigma(N_1\partial^a N_2 - N_2\partial^a N_1)],\end{aligned} \tag{B16}$$

Combining (B8), (B12), and (B16) and assuming (B11) and (B15) we obtain

$$\begin{aligned}\{H^P[N_1], H^P[N_2]\} &= D_{\rm grav}[\alpha^2(N_1\partial^a N_2 - N_2\partial^a N_1)]\\ &\quad+ D_{\rm matter}[\nu\sigma(N_1\partial^a N_2 - N_2\partial^a N_1)].\end{aligned} \tag{B17}$$

It is easy to see that the constraint algebra closes, if $\alpha^2 = \nu\sigma$ in addition to the requirement that α, ν, and σ are all scalars of vanishing density weight. In that case the right-hand side of (B17) reduces to the total diffeomorphism constraint

$$\begin{aligned}\{H^P[N_1], H^P[N_2]\} &= D[\alpha^2(N_1\partial^a N_2 - N_2\partial^a N_1)]\\ &\equiv D[\tilde{N}_1\partial^a\tilde{N}_2 - \tilde{N}_2\partial^a\tilde{N}_1)].\end{aligned} \tag{B18}$$

So far in this appendix, we have worked nonperturbatively which gives only a few conditions on quantum correction functions. The anomaly freedom conditions (68) and (69) obtained in the main part of this paper, where the condition of vanishing density weight turns out to be quite nontrivial, appear much more restrictive compared with the relatively mild-looking requirement derived in the context of the unperturbed system in this appendix. It is therefore pertinent to comment on this apparent discrepancy.

Note that the conditions on the three correction functions imply the same functional form of α, ν, and σ. Thus we shall restrict our consideration to only one of them. In Sec. III A, we had made the following assumptions concerning the primary correction function α:

(i) α depends only on the triad E^a_i (but not on the extrinsic curvature K^i_a or the connection),

(ii) α depends only algebraically on the triad E^a_i (but not its spatial derivatives)

(iii) in the perturbed context, α depends on the background triad $\bar{E}^a_i$ and its perturbation δE^a_i only in the combination $\bar{E}^a_i + \delta E^a_i \equiv E^a_i$ (i.e. α is expected to originate from a full unperturbed expression).

One can check by inspection that assumption (iii) implies that (69) is automatically satisfied. Indeed, using the Taylor expansion

$$\begin{aligned}\alpha(E^a_i) &= \alpha(\bar{E}^a_i) + \frac{\partial\alpha(E^a_i)}{\partial E^a_i}\bigg|_{\bar{E}^a_i}\delta E^a_i\\ &\quad+ \frac{1}{2}\frac{\partial^2\alpha(E^a_i)}{\partial E^a_i\partial E^b_j}\bigg|_{\bar{E}^a_i}\delta E^a_i\delta E^b_i + \cdots\\ &\equiv \bar{\alpha} + \alpha^{(1)} + \alpha^{(2)} + \cdots\end{aligned} \tag{B19}$$

it is easy to see that the terms on the right-hand side are not entirely independent. Clearly the relations between $\bar{\alpha}$, $\alpha^{(1)}$, and $\alpha^{(2)}$ are exactly written in Eq. (69).

However, of greater concern is the other condition, Eq. (68). In particular, the requirement $\alpha^{(1)} = 0$ [along with (69)] rules out all possible nontrivial solutions. In order to understand its origin let us revisit the seemingly trivial restriction on the correction function to be of zero density weight. We start by formulating the following *lemma 2:* A scalar $\alpha(E^a_i)$ of density weight zero satisfying the three assumptions above must be a constant function.

Proof: Consider a scalar $\alpha(E^a_i)$ of density weight w satisfying the aforementioned assumptions. Its Lie derivative along an arbitrary shift vector N^a is given by

$$\mathcal{L}_{\vec{N}}\alpha = N^b\partial_b\alpha + w\alpha\partial_b N^b.$$

On the other hand,

$$\mathcal{L}_{\vec{N}}\alpha = \frac{\partial\alpha}{\partial E^a_i}\mathcal{L}_{\vec{N}}E^a_i = \frac{\partial\alpha}{\partial E^a_i}(N^b\partial_b E^a_i - E^b_i\partial_b N^a + E^a_i\partial_b N^b).$$

These equations are valid for any N^a. In the context of cosmological perturbation theory, $\bar{N}^a = 0$, hence $N^a = \delta N^a$. In the perturbative expansion of the right-hand side of the equations there is no contribution from the background part. Equating the corresponding linear order terms, we obtain

$$w\bar{\alpha}\partial_b\delta N^b = \left(\frac{\partial\alpha}{\partial E^a_i}\right)^{(0)}(\bar{E}^a_i\partial_b\delta N^b - \bar{E}^b_i\partial_b\delta N^a).$$

Using $\bar{E}^a_i = \bar{p}\delta^a_i$, the derivative $(\partial\alpha/\partial E^a_i)^{(0)} \equiv (\partial\alpha/\partial\bar{E}^a_i)|_{\bar{E}^a_i}$ can be rewritten as $\frac{1}{3}\delta^a_i\partial\bar{\alpha}/\bar{p}$, which yields

$$\frac{2\bar{p}}{3}\frac{\partial\bar{\alpha}}{\partial\bar{p}}\partial_b\delta N^b = w\bar{\alpha}\partial_b\delta N^b.$$

The divergence of a generic shift vector does not vanish, and therefore the derivative of the background correction function is $\partial\bar{\alpha}/\partial\bar{p} = \frac{2}{3}\bar{p}w\alpha$. Requiring $w = 0$ results in $\partial\bar{\alpha}/\partial\bar{p} = 0$ and consequently from (69), $\alpha^{(1)} = 0$, $\alpha^{(2)} = 0$, and so on. This concludes the proof of the lemma.

In light of this, we are led to the following conclusion. The three assumptions that we made on the functional form of the correction functions are incompatible with the conditions for anomaly freedom, unless α, ν, and σ are constants. Therefore, to allow a nontrivial solution we have to relax one or more of the assumptions which makes the algebra much more involved. In the main text of this paper, we organize these calculations by the method of counterterms.

APPENDIX C: POISSON BRACKETS OF PERTURBED VARIABLES

A direct application of the Poisson brackets given by (24) can sometimes be problematic. For instance, the Poisson bracket between the two original fields $\{\varphi, \pi\}$, given by

$$\{\bar{\varphi} + \delta\varphi(x), \bar{\pi} + \delta\pi(x)\}_{\bar{\varphi},\bar{\pi},\delta\varphi,\delta\pi} = \{\bar{\varphi}, \bar{\pi}\}_{\bar{\varphi},\bar{\pi}} + \{\delta\varphi(x), \delta\pi(y)\}_{\delta\varphi,\delta\pi} = \frac{1}{V_0} + \delta(x-y), \tag{C1}$$

does not agree with the original expression $\{\varphi(x), \pi(y)\} = \delta(x-y)$. This can be traced to the fact that (24) provides Poisson brackets for the fields $(\bar{\varphi}, \bar{\pi}, \delta\varphi, \delta\pi)$ only if the conditions (21) are used in (22) to identify $\bar{\varphi}$ and $\bar{\pi}$ with the sole zero modes of inhomogeneous fields. The constraints (21) clearly have a nonzero Poisson bracket $\{\chi_1, \chi_2\}$, which makes them of the second class.

According to Dirac [67], second-class constraints correspond to nonphysical degrees of freedom and can be dealt with in the following way. (i) One should take linear combinations of (all) the constraints, in order to bring as many of them into first-class form as possible, and (ii) redefine the Poisson bracket to

$$\{F, G\}^*_{\delta\varphi,\delta\pi} = \{F, G\}_{\delta\varphi,\delta\pi} - \{F, \chi_a\}_{\delta\varphi,\delta\pi}C^{ab}\{\chi_b, G\}_{\delta\varphi,\delta\pi}, \tag{C2}$$

where

$$C^{ab}\{\chi_b, \chi_c\} = \delta^a_c$$

so as to remove the variations with respect to the nonphysical degrees of freedom. Using (21) we obtain

$$C^{11} = C^{22} = 0, \qquad C^{21} = -C^{12} = (V_0\lambda_1\lambda_2)^{-1},$$

which implies

$$\{F, G\}^*_{\delta\varphi,\delta\pi} = \{F, G\}_{\delta\varphi,\delta\pi} - \frac{1}{V_0}\left(\int d^3z\frac{\delta F}{\delta(\delta\varphi)}\int d^3z'\frac{\delta G}{\delta(\delta\pi)} - (F\leftrightarrow G)\right). \tag{C3}$$

Let us first point out the basic properties of the Dirac bracket (C3). For the field perturbations

$$\{\delta\varphi(x), \delta\pi(y)\}^*_{\bar{\varphi},\bar{\pi},\delta\varphi,\delta\pi} = \delta(x-y) - \frac{1}{V_0}.$$

Clearly the last term would remove the extra contribution in (C1) yielding the expected result

$$\{\varphi, \pi\}^*_{\bar{\varphi},\bar{\pi},\delta\varphi,\delta\pi} = \{\bar{\varphi}, \bar{\pi}\}_{\bar{\varphi},\bar{\pi}} + \{\delta\varphi(x), \delta\pi(y)\}^*_{\delta\varphi,\delta\pi} = \frac{1}{V_0} + \delta(x-y) - \frac{1}{V_0} = \{\varphi, \pi\}_{\varphi,\pi}.$$

Thus the Dirac bracket ensures a correct transition from the full theory to the perturbed one. By construction, the constraints (21) now commute, $\{\chi_1, \chi_2\}^* = 0$, and we can impose χ_1 and χ_2 strongly. Moreover, Dirac brackets between a first order functional and a functional of arbitrary order vanish, which can be seen by inspection using (C3). Thus for any two functionals, their linear terms do not contribute to the Dirac bracket [68].

We will now address an issue directly related to closure of the constraints algebra. When computing Poisson brackets in the context of perturbation theory, one has a choice between two methods:

(1) calculate the Poisson bracket of the constraints with respect to the full fields and expand the resulting expression in orders of perturbations, or
(2) expand the constraints first and then compute their Poisson (Dirac) brackets in terms of the expanded fields.

It is, in general, not guaranteed that the two approaches agree for arbitrary functionals which depend on the fields and their first derivatives. However, we have
lemma 3: If the fields $\bar{\varphi}$, $\bar{\pi}$, $\delta\varphi$, and $\delta\pi$ enter the functionals

$$F = \int d^3x f(\varphi, \nabla\varphi, \pi, \nabla\pi), \qquad G = \int d^3x g(\varphi, \nabla\varphi, \pi, \nabla\pi) \tag{C4}$$

only as a combination $\varphi \equiv \bar{\varphi} + \delta\varphi$ or $\pi \equiv \bar{\pi} + \delta\pi$, then the two procedures described above yield the same result for $\{F, G\}$.

Proof: We shall show that the second procedure is equivalent to the first one. First of all, as linear terms do not contribute to (C3), we can rewrite the Dirac bracket between two expanded constraints as

$$\{F^{(0)} + F^{(2)}, G^{(0)} + G^{(2)}\}^*_{\bar{\varphi},\bar{\pi},\delta\varphi,\delta\pi} = \{F^{(0)} + F^{(1)} + F^{(2)}, G^{(0)} + G^{(1)} + G^{(2)}\}^*_{\bar{\varphi},\bar{\pi},\delta\varphi,\delta\pi} \equiv \{F, G\}^*_{\bar{\varphi},\bar{\pi},\delta\varphi,\delta\pi}.$$

According to (C3), we have

$$\begin{aligned}
\{F, G\}^*_{\bar{\varphi},\bar{\pi},\delta\varphi,\delta\pi} &= \frac{1}{V_0}\left(\frac{\partial F}{\partial\bar{\varphi}}\frac{\partial G}{\partial\bar{\pi}} - \frac{\partial F}{\partial\bar{\pi}}\frac{\partial G}{\partial\bar{\varphi}}\right) + \int d^3x\left(\frac{\delta F}{\delta(\delta\varphi)}\frac{\delta G}{\delta(\delta\pi)} - \frac{\delta F}{\delta(\delta\pi)}\frac{\delta G}{\delta(\delta\varphi)}\right) \\
&\quad - \frac{1}{V_0}\left(\int d^3z \frac{\delta F}{\delta(\delta\varphi)}\int d^3z' \frac{\delta G}{\delta(\delta\pi)} - \int d^3z \frac{\delta F}{\delta(\delta\pi)}\int d^3z' \frac{\delta G}{\delta(\delta\varphi)}\right) \\
&= \frac{1}{V_0}\int d^3z \frac{\partial f}{\partial\varphi}\int d^3z' \frac{\partial g}{\partial\pi} + \int d^3x \frac{\delta F}{\delta\varphi}\frac{\delta G}{\delta\pi} - (\varphi \leftrightarrow \pi) \\
&\quad - \frac{1}{V_0}\int d^3z\left(\frac{\partial f}{\partial\varphi} - \partial_a\frac{\partial f}{\partial(\partial_a\varphi)}\right)\int d^3z'\left(\frac{\partial g}{\partial\pi} - \partial_a\frac{\partial g}{\partial(\partial_a\pi)}\right) - (\varphi \leftrightarrow \pi) \\
&= \int d^3x \frac{\delta F}{\delta\varphi}\frac{\delta G}{\delta\pi} - (\varphi \leftrightarrow \pi) \equiv \{F, G\}_{\varphi,\pi}.
\end{aligned}$$

In the second equality, we have used

$$\frac{\partial f}{\partial\bar{\varphi}} = \frac{\partial f}{\partial\varphi}, \qquad \frac{\delta F}{\delta(\delta\varphi)} = \frac{\delta F}{\delta\varphi} = \frac{\partial f}{\partial\varphi} - \partial_a\frac{\partial f}{\partial(\partial_a\varphi)}$$

and dropped the surface integrals originating from integration of the total divergence terms. It is now easy to see that if higher-derivative terms were present in the functionals, they would have merely led to additional surface terms and would not have affected the final conclusion.

Since linear functionals do not contribute to Dirac brackets, they can be omitted, and one can restrict consideration to terms of the zeroth and second order only. Moreover, for functionals of an even order, the second term in the Dirac bracket (C3) vanishes, and one can simply use the Poisson bracket (24).

A somewhat similar consistency issue arises when it comes to equations of motion, generated e.g. by a (Hamiltonian) constraint

$$H = \int d^3x h(\varphi, \nabla\varphi, \pi, \nabla\pi). \tag{C5}$$

There are again two approaches: (i) either derive the equations of motion for the original fields and then split into the background and (linear) perturbation, or (ii) expand the constraint and obtain separately equations of motion for the homogeneous and inhomogeneous parts of the field. In other words, one needs to compare

$$\{\varphi, H\} \quad \text{with } \{\bar{\varphi}, H\}^* \quad \text{and} \quad \{\delta\varphi, H\}^*. \tag{C6}$$

We start by noting that

$$\dot{\varphi} = \{\varphi, H\}_{\varphi,\pi} = \frac{\delta H}{\delta\pi} = \frac{\partial h}{\partial\pi} - \partial_a\frac{\partial h}{\partial(\partial_a\pi)}, \tag{C7}$$

whereas the equation of motion for the background field

$$\dot{\bar{\varphi}} = \{\bar{\varphi}, H\}_{\bar{\varphi},\bar{\pi}} = \frac{1}{V_0}\int \mathrm{d}^3x \frac{\partial h}{\partial \bar{\pi}} = \frac{1}{V_0}\int \mathrm{d}^3x \frac{\partial h}{\partial \pi}$$
$$= \frac{1}{V_0}\int \mathrm{d}^3x \left(\frac{\partial h}{\partial \pi} - \partial_a \frac{\partial h}{\partial(\partial_a \pi)}\right) = \frac{1}{V_0}\int \mathrm{d}^3x \frac{\delta h}{\delta \pi}$$

coincides with the background part of the equation of motion (C7) for the total field, $(\delta H/\delta\pi)^{(0)}$. At the same time, the equation of motion for the perturbation

$$\delta\dot{\varphi}(x) = \{\delta\varphi(x), H\}^*_{\delta\varphi,\delta\pi}$$
$$= \frac{\delta H}{\delta(\delta\pi(x))} - \frac{1}{V_0}\int \mathrm{d}^3y \frac{\delta H}{\delta(\delta\pi(y))}$$
$$= \int \mathrm{d}^3y \left(\delta(x-y) - \frac{1}{V_0}\right)\frac{\delta H}{\delta\pi(y)} = \left(\frac{\delta H}{\delta\pi}\right)^{(1)}$$

is nothing else but the perturbed part of the Eq. (C7). In fact, one can think of the kernel $\delta(x-y) - 1/V_0$ as cutting off the background part of the function, with which it is integrated. It is again pertinent to mention that the linear (as well as the background) part of the functional does not contribute to the perturbed equation of motion, that is

$$\delta\dot{\varphi}(x) = \{\delta\varphi(x), H\}^*_{\delta\varphi,\delta\pi} = \{\delta\varphi(x), H^{(2)}\}_{\delta\varphi,\delta\pi}. \quad \text{(C8)}$$

Note that in the second equality the Poisson bracket is used, not the Dirac bracket.

To summarize, we have shown that in order to proceed to the perturbation theory, the Dirac bracket (C3) in terms of the background and perturbed variables should be used. Nevertheless, when dealing with already expanded functionals, containing only even order terms, the Dirac bracket reduces to the Poisson bracket (24).

So far we have considered perturbations of a scalar field. Generalization to tensorial fields is rather straightforward for any rank. In particular, we need the canonical pair of loop quantum gravity, i.e. the extrinsic curvature and densitized triad whose perturbations have Dirac brackets

$$\{F, G\}^*_{\delta K^i_a,\delta E^a_i} = \{F, G\}_{\delta K^i_a,\delta E^a_i} - \frac{1}{V_0}\left(\int \mathrm{d}^3z\mathrm{d}^3z' \frac{\delta F}{\delta(\delta K^i_a(z))}\frac{\delta G}{\delta(\delta E^a_i(z'))} - (F \leftrightarrow G)\right), \quad \text{(C9)}$$

where F and G are arbitrary functionals of K^i_a and E^a_i.

Of interest is also a generalization of the Dirac brackets to the case of local second-class constraints. Let us split the triad and extrinsic curvature into the diagonal and traceless parts

$$K^i_a = \kappa\delta^i_a + \kappa^i_a, \qquad E^a_i = \varepsilon\delta^a_i + \varepsilon^a_i, \quad \text{(C10)}$$

such that

$$\chi_1 := \mathrm{tr}\varepsilon^a_i = 0, \qquad \chi_2 := \mathrm{tr}\kappa^i_a = 0. \quad \text{(C11)}$$

It is easy to see that the pairs (κ, ε) and $(\kappa^i_a, \epsilon^a_i)$ are symplectically orthogonal. Indeed, the symplectic structure takes the form

$$\int \mathrm{d}^3x(\dot{\varepsilon}\delta^i_a + \dot{\varepsilon}^i_a)(\kappa\delta^i_a + \kappa^i_a) = \int \mathrm{d}^3x(3\dot{\varepsilon}\kappa + \dot{\varepsilon}^i_a\kappa^i_a).$$

However the constraints (C11) are second class under the tentative Poisson bracket

$$\{F, G\}_{\kappa,\varepsilon,\kappa^i_a,\varepsilon^a_i} = \frac{1}{3}\int \mathrm{d}^3x\left(\frac{\delta F}{\delta\kappa}\frac{\delta G}{\delta\varepsilon} - \frac{\delta F}{\delta\varepsilon}\frac{\delta G}{\delta\kappa}\right) + \int \mathrm{d}^3x\left(\frac{\delta F}{\delta\kappa^i_a}\frac{\delta G}{\delta\varepsilon^a_i} - \frac{\delta F}{\delta\varepsilon^a_i}\frac{\delta G}{\delta\kappa^i_a}\right). \quad \text{(C12)}$$

Specifically,

$$\{\chi_2(x), \chi_1(y)\}_{\kappa^i_a,\varepsilon^a_i} = 3\delta(x-y). \quad \text{(C13)}$$

As before, we define the Dirac brackets

$$\{F, G\}^* = \{F, G\} - \int \mathrm{d}^3z\mathrm{d}^3z'\{F, \chi_a(z)\}C^{ab}(z, z') \times \{\chi_b(z), G\}, \quad \text{(C14)}$$

where the matrix $C^{ab}(x, y)$ is now space dependent and satisfies

$$\int \mathrm{d}^3y C^{ab}(x, y)\{\chi_b(y), \chi_c(z)\} = \delta^a_c\delta(x-z). \quad \text{(C15)}$$

Using the constraints (C11) in the equation above, we find that

$$C^{11}(x, y) = C^{22}(x, y) = 0; \quad \text{(C16)}$$

$$C^{12}(x, y) = -C^{21}(x, y) = \frac{1}{3}\delta(x-y). \quad \text{(C17)}$$

Therefore the Dirac bracket reads

$$\{F, G\}^*_{\kappa^i_a,\varepsilon^a_i} = \int \mathrm{d}^3z \frac{\delta F}{\delta\kappa^i_a(z)}\frac{\delta G}{\delta\varepsilon^a_i(z)} - \frac{1}{3}\int \mathrm{d}^3z\left(\frac{\delta^j_b\delta F}{\delta\kappa^j_b(z)}\frac{\delta^c_k\delta G}{\delta\varepsilon^c_k(z)}\right) - (F \leftrightarrow G). \quad \text{(C18)}$$

It is easy to see by inspection that the constraints (C11) indeed commute under this Dirac bracket, $\{\chi_1, \chi_2\}^* = 0$, so these constraints may be imposed strongly. Also, the Dirac bracket between the original canonical variables has the correct expression

$$\{K^i_a(x), E^b_j(y)\}^*_{\kappa,\varepsilon,\kappa^k_c,\varepsilon^c_k} = \delta^b_a\delta^i_j\delta(x-y) = \{K^i_a(x), E^b_j(y)\}_{K^k_c,E^k_c}.$$

Earlier on we have seen that one can still use the Poisson bracket rather than the corresponding Dirac bracket if one removes from the original constraints (that is before splitting the canonical variables) all the terms proportional to the second-class constraints arising because of the splitting. This still holds for local second-class constraints. In the case at hand, as soon as all the terms containing traces of the extrinsic curvature and the densitized triad are omitted, the remaining constraints form the correct algebra under the Poisson bracket (C12).

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