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Anomaly freedom in perturbative models of Euclidean loop quantum gravity

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Euclidean gravity provides an interesting test system for an analysis of cosmological perturbations in an effective Hamiltonian constraint with holonomy modifications from loop quantum gravity. This paper presents a discussion of scalar modes, with a specific form of the holonomy modification function derived from a general expansion in a connection formulation. Compared with some previous models, the constraint brackets are deformed in a different and more restricted way. A general comparison of anomaly-free brackets in various effective and operator versions shows overall consistency between different approaches.

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I. INTRODUCTION

Loop quantum gravity [1–4], implements non-perturbative and background-independent features in an approach to quantizing general relativity. It could therefore provide models of quantum space-time structure. To this end, one should address the long-standing anomaly problem of space-time gauge transformations in order to shed light on consistent versions. Without such a derivation, assuming certain properties of solutions, for instance in the form of an effective line element, amounts to postulating a background space-time. Although overall consistency of the theory remains to be shown, there are now several encouraging results which indicate that a well-defined quantum space-time structure may be realized. If this is the case, one could potentially use the theory to derive possible effects for instance in cosmological observations.

In addition to a consistent theory, a systematic effective framework is required for a reliable evaluation of physical phenomena. In the background-independent context of loop quantum gravity, such methods have been explored by both the canonical [5–10] and the path integral perspective [11–14] in homogeneous models. For inhomogeneous modes of cosmological perturbations, one encounters new questions related to the consistency of coupled partial differential equations, or the anomaly-problem of quantum gravity.

In order to understand cosmological structure formation and anisotropies of the cosmic microwave background in models of loop quantum gravity, one needs to consider a cosmological perturbation theory with modifications including quantum-gravity effects. In the canonical setting of loop quantum gravity, quantum-gravity effects appear in an effective Hamiltonian constraint, rather than an effective action whose covariance could be checked directly. If the corrections implied by a canonical theory of quantum gravity are not covariant, Hamiltonian (and diffeomorphism) constraints obey constraint brackets which do not close but rather contain anomaly terms $\mathcal{A}_{IJ}$: Poisson brackets of two constraints would not weakly vanish but be of the form

$$\{\mathcal{C}_I, \mathcal{C}_J\} = \mathcal{K}^K_{IJ}\mathcal{C}_K + \mathcal{A}_{IJ} \tag{1}$$

with $\mathcal{A}_{IJ} \neq 0$. If there is such an anomaly, the quantum corrected perturbation equations cannot be expressed solely in terms of gauge-invariant variables [15]. Therefore, how to obtain anomaly-free constraints of cosmological perturbations including loop quantum effects has become an important question.

Several promising results have been obtained in this direction, exploring the commutators of constraint operators [16–22] or Poisson brackets of effective constraints [15, 23–30]. In models analyzed so far, it seems possible to have closed brackets ($\mathcal{A}_{IJ} = 0$), but usually with modifications of the structure functions $\mathcal{K}^K_{IJ}$ in (1), in particular for real connections. The classical brackets corresponds to a canonical version of space-time coordinate transformations, represented as deformations of spatial hypersurfaces in space-time [31]. If the brackets are modified (and not just its generators), the gauge transformations generated by the constraints are not broken but differ from coordinate transformations, so that a new space-time model is obtained. Only in some cases may it be possible to map the effective geometry to one of classical type by applying a field redefinition [32, 33]. The most dramatic effect found in this context is the possibility of signature change [34–37] at large density

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or curvature, indicated by a change of sign in some of the structure functions. Such an effect is interesting, but also dangerous owing to the indeterministic behavior that it may imply [38]. In this article, we consider a model which turns out to lead to different implications in situations that would give rise to signature change in previous models. In this respect, our results are related to those of [28–30], but qualitatively they are obtained in a different way.

In general, there are two main quantum-gravity effects in loop-quantized models, so-called inverse-triad corrections [39, 40] and holonomy modifications [41, 42]. In addition to these two, there are generic quantum back-reaction effects which occur in all interacting quantum theories but have not been explored much in inhomogeneous models of loop quantum gravity. We will continue this tradition and mostly ignore these terms in the present paper, focussing on the two types of corrections directly related to quantum geometry. (As shown in [43], under certain conditions quantum back-reaction terms from moments do not appear in structure functions of constraint brackets.) For the case of inverse-triad corrections, anomaly-free constraints and the corresponding gauge-invariant cosmological perturbation equations have been obtained for scalar modes [15, 44], vector modes [45] and tensor modes [46], respectively. (For tensor modes, anomaly-freedom of the constraints is automatically fulfilled.) A characteristic feature, shared with spherically symmetric models, is that the Poisson bracket of two Hamiltonian constraints is modified by a factor of the square of the inverse-triad correction function. As this function is positive, signature change does not happen. Some relevant applications, including potentially observable effects in the primordial power spectrum and non-Gaussianity, have already been studied [47–50].

Holonomy modifications have been implemented in consistent versions slightly more recently. The first papers used a partial gauge fixing to longitudinal gauge [51, 52] and therefore could not show all effects with full confidence. Without gauge fixing, a consistent version has been obtained in [53] for vector modes and [24] for scalar modes. A combined treatment of holonomy-modified scalar, vector and tensor perturbations has been given in [54]. Again, anomaly-free constraints can be obtained by a rather simple quantum correction for all types of perturbations. In the presence of holonomy modifications, the constraint brackets are modified in such a way that structure functions may change sign, corresponding to a transition between Lorentzian and Euclidean signature in the sense that either hyperbolic or elliptic mode equations are implied [34–36]. There is agreement with consistent constraint brackets in spherically symmetric models [23, 26, 27] even at the operator level [20]. (See [55] for a comparison.) Signature change is not always realized in self-dual variables [28–30] because the Hamiltonian constraint has a different formal structure in its dependence on spatial derivatives of the fields.

Anomaly-free constraints for both inverse-triad and holonomy modifications have been studied for all types of perturbative modes. The corresponding equations of motion are derived in [25], providing so far the most complete treatment of consistent cosmological perturbations in models of loop quantum cosmology. However, in a certain sense, holonomy modifications so far have been considered after rather than before perturbing the classical Hamiltonian constraint: One modifies the background constraint by replacing the classical quadratic dependence on the connection $\bar{q}$ (or Hubble parameter) by a bounded function, $\bar{q}^2 \mapsto \ell^{-2}\sin^2(\ell\bar{q})$, as it has been found by effective equations of isotropic models [41], and then looks for a possible anomaly-free theory of perturbative modes on such a background model. If one perturbs a modified constraint, additional terms may appear. In particular, there could be derivative corrections, even at or below the classical derivative order, which happen to be absent in the classical constraints but might be induced by quantum-geometry effects. (See [27] for a discussion in spherical symmetry.) In covariant effective actions, all quantum corrections are expected to be of higher-derivative (or higher-curvature) type, but lower-order terms may appear if the space-time structure is modified as in certain canonical approaches. An effective treatment should include all terms, up to a given order, consistent with what is known about symmetries. If the precise form of quantum space-time is unknown, one cannot assume much about symmetries and should include all possible terms in an ansatz for an effective Hamiltonian. Symmetries will then be implemented by the condition of anomaly freedom, and their possible form can be derived from the effective system rather than being assumed. By including additional derivative terms, we therefore fill in a gap in existing treatments.

In a canonical setting, the treatment of spatial and temporal derivatives is different. The former appear directly in an effective Hamiltonian while the latter would result in an adiabatic approximation of quantum back-reaction [56–58]. Although both types of derivatives should usually be considered in combination, holonomy modifications suggest a larger role for spatial derivatives because holonomies are spatially non-local functions of the connection. If holonomy modifications can be consistent in cosmological perturbation theory, one should therefore be able to find anomaly-free constraints with holonomy modifications of the background and a set of higher spatial derivative terms.

In order to explore the perturbations in a framework including holonomy modifications of loop quantum gravity, allowing for more general derivative terms than considered in [25], an effective holonomy-modified Hamiltonian in Euclidean general relativity was first proposed in [59], where the corresponding perturbative constraint brackets were studied for vector modes. The Poisson brackets between the modified Hamiltonian and diffeomorphism constraints restricted to vector modes were calculated, and a specific form of the holonomy-modification function f^i_{cd} giving rise to anomaly-free constraints was found. This result indicates that in a perturbative framework it is indeed possible to have non-trivial and anomaly-free holonomy modifications with additional derivative terms up to first order, as suggested by non-local holonomies in the full theory. In this paper, we shall extend the study to scalar modes in the same framework.

A brief review of the modification function of the full theory and some basic elements of scalar modes will be presented in section II. Then, in section III, the constraint brackets, including those between the modified Hamiltonian constraint and the diffeomorphism constraint as well as between the two modified Hamiltonian constraints, are derived. Subsequently, a specific form of the holonomy modification function is obtained from its general expression in section IV. We compare the results with those of [25] on one hand, and those of [28–30] on the other, and discuss implications for signature change in section V. Results from operator approaches are briefly discussed as well.

At a formal level, the difference between [25] and our present treatment is that we use a connection formulation and include additional derivative terms of the connection. Interestingly, the outcome does not seem to be the same. Our calculations lead to an intermediate set of deformed constraint brackets which may show a way to avoid signature change and the associated indeterministic behavior, but we have not been able to produce a fully consistent non-classical system: While the brackets of Hamiltonian and diffeomorphism constraints can be closed, the expressions are not SU(2)-covariant unless there are no holonomy corrections (while inverse-triad corrections may be possible). We interpret this result as an indication that non-local modifications are essential in SU(2)-invariant connection theories.

II. HOLONOMY MODIFICATION FUNCTIONS AND SCALAR MODES

In the connection formulation of Euclidean general relativity [3, 4], the gravitational Hamiltonian constraint can be written as

$$H[N] = \frac{1}{16\pi G}\int_\Sigma \mathrm{d}^3x N \epsilon^{\ jk}{}_i \frac{E^c_j E^d_k}{\sqrt{|\det E|}} F^i_{cd}\,, \tag{2}$$

where E^b_j is the densitized triad, and the curvature of the Ashtekar–Barbero connection $A^i_a = \Gamma^i_a + K^i_a$ is given by

$$F^i_{cd} = 2\partial_{[c}A^i_{d]} + \epsilon^i{}_{mn}A^m_c A^n_d\,. \tag{3}$$

In the expression for A^i_a, Γ^i_a is the spin connection compatible with the triad, and $K^i_a = K_{ab}E^{bi}/|\det E^c_j|$ is obtained from extrinsic curvature K_{ab}. More generally, one can define $A^i_a = \Gamma^i_a + \gamma K^i_a$ with the Barbero–Immirzi parameter γ [60, 61]. If $\gamma \neq 1$, there will be additional terms in the Hamiltonian constraint which contain spatial derivatives of the densitized triad, on whose relevance we will comment later. We use the value $\gamma = 1$ in order to work with the simplified expression (2).

In loop quantum gravity, the local dependence on the connection A^i_a is replaced by a dependence on non-local (in space) holonomies

$$h_e(A) = \mathcal{P}\exp\int_e A^i_a\tau_i \mathrm{d}x^a \tag{4}$$

for suitable choices of spatial curves e, where the symbol $\mathcal{P}$ represents path ordering, and $\tau_j = -\frac{i}{2}\sigma_j$ is a basis of the Lie-algebra su(2) with σ_j being the Pauli matrices. Holonomies, unlike connection components, can be represented as operators on the kinematical Hilbert space of loop quantum gravity, and therefore appear in candidates for the quantized Hamiltonian constraint [62, 63].

However, it is difficult to find anomaly-free versions because the operators and their commutators are complicated expressions depending sensitively on factor orderings and other quantization choices. There has been some progress in particular but not only in $2+1$-dimensional models [16–19, 21, 22], with consistent commutators on a subset of states which partially solve the spatial diffeomorphism constraint (introduced in [64, 65]). Attempts to go beyond the restricted set of states [21, 22] in Euclidean gravity indicate that closed commutators of constraint operators may be possible more generally. Unfortunately, the complicated semiclassical limit of such theories makes it difficult to see the full implications of holonomy modifications, in particular those related to potential deformations of the constraint brackets and signature change.

An effective approach to constraints has proven to be more powerful [8, 43, 66], in which one does not directly compute commutators $[\hat{C}_I, \hat{C}_J]$ of constraint operators but rather Poisson brackets

$$\{\langle\hat{C}_I\rangle, \langle\hat{C}_J\rangle\} := \frac{\langle[\hat{C}_I, \hat{C}_J]\rangle}{i\hbar} \tag{5}$$

of effective constraints $\langle\hat{C}_I\rangle$. Methods have been developed by which one can evaluate the left-hand side in an expansion by quantum moments, which turns out to be more feasible than computing quantum commutators. These methods, applied to a fixed order in $\hbar$, cannot show whether a consistent operator version exists. But they can rule out certain choices, or provide indications of necessary deformations of the brackets when certain modifications, such as holonomy terms, are to be implemented. (For a general discussion, see [43].) So far, the expansions used in the context of cosmological perturbations have been done to lowest order in $\hbar$, which means that one ignores quantum back-reaction but allows for some quantum-geometry effects.

In order to include holonomy modifications in an effective theory of this form, we could, in general, consider the following ansatz of holonomy modifications to the

Euclidean Hamiltonian [59]

$$\delta\mathcal{H}_Q=\epsilon^{jk}{}_i\frac{E^c_jE^d_k}{\sqrt{|\det E|}}f^i_{cd}(A,\partial A,\partial^2A,\cdots,\partial^nA,\epsilon)\,,\quad(6)$$

where $f^i_{cd}(A,\partial A,\partial^2A,\cdots,\partial^nA,\epsilon)+O(\partial^{n+1}A)=\tilde{F}^i_{cd}(h_e(A))-F^i_{cd}(A)$ is a function of A^m_a and its derivatives up to order n. (If the Hamiltonian is classical, we have $f^i_{cd}=0$.) It is obtained by expanding the corresponding function $\tilde{F}^i_{cd}(h_e(A))$ that should appear in place of the classical $F^i_{cd}(A)$ in an effective Hamiltonian computed for a loop-quantized operator. There may also be a dependence on E^a_i and its spatial derivatives if there is lattice refinement [67, 68], in which case properties of the curves e used to construct a quantum Hamiltonian would depend on the spatial geometry. For simplicity, we ignore such a dependence for a first analysis.

It is sufficient to assume that the holonomy-modification function $f^i_{cd}(A^m_a,\epsilon)$ is an antisymmetric tensor, just as F^i_{cd}, because it is contracted with the antisymmetric combination $\epsilon^{jk}{}_iE^c_jE^d_k$ of triad components. We write the modified Hamiltonian constraint as

$$H_Q[N]=\frac{1}{16\pi G}\int_\Sigma \mathrm{d}^3xN(\mathcal{H}+\delta\mathcal{H}_Q)=H[N]+\delta H_Q[N]\,.(7)$$

After this modification, motivated by full loop quantum gravity, we may perturb the Hamiltonian in order to describe cosmological inhomogeneity. We use the splittings into background and inhomogeneity as given in [15] (see also [55]). Considering perturbations around a spatially flat, homogeneous and isotropic metric, the connection variables A^i_a and the densitized triad E^a_i can be expanded as

$$A^i_a=\bar{A}^i_a+\delta A^i_a:=\bar{q}\delta^i_a+\delta A^i_a\quad(8)$$
$$E^a_i=\bar{E}^a_i+\delta E^a_i:=\bar{p}\delta^a_i+\delta E^a_i\quad(9)$$

where the homogeneous mode is defined by

$$\bar{q}:=\frac{1}{3V_0}\int_\Sigma A^i_a\delta^a_i\mathrm{d}^3x\quad,\quad\bar{p}:=\frac{1}{3V_0}\int_\Sigma E^a_i\delta^i_a\mathrm{d}^3x\quad(10)$$

with $V_0=\int_\Sigma\mathrm{d}^3x$ (integrated over some fixed region, or all of space if it is compact). We will assume $\bar{p}>0$, fixing the spatial orientation. In order to avoid over-counting the degrees of freedom, the perturbations δE^a_i and δA^i_a do not have homogeneous modes:

$$\int_\Sigma\delta E^a_i\delta^i_a\mathrm{d}^3x=0\quad,\quad\int_\Sigma\delta A^i_a\delta^a_i\mathrm{d}^3x=0\,.\quad(11)$$

Therefore, the Poisson brackets of the background and perturbed variables can be constructed as

$$\{\bar{q},\bar{p}\}=\frac{8\pi G}{3V_0}\quad,\quad\{\delta A^i_a(x),\delta E^b_j(y)\}=8\pi G\delta^i_j\delta^b_a\delta^3(x-y)\,.\quad(12)$$

We note [55] that there is a single inhomogeneous perturbation δf for any field component f, instead of a whole tower $\delta^{(1)}f$, $\delta^{(2)}f$ and so on, as often used for linear perturbation equations at all orders. The latter decomposition would be convenient when one tries to solve a given set of equations of motion. In our context, however, we first need to derive consistent forms of equations of motion using canonical methods, which requires a well-defined Poisson or symplectic structure. Since linearized perturbations $\delta^{(1)}f$, $\delta^{(2)}f$ and so on would not provide independent degrees of freedom, one cannot define a Poisson structure for them. The decomposition (8), by contrast, gives a well-defined Poisson structure (12).

The background variables of the lapse function and shift vector can be chosen as

$$\bar{N}=\sqrt{\bar{p}}\quad(13)$$

for conformal background time, and

$$\bar{N}^a=0\quad(14)$$

for an isotropic background. Moreover, the perturbed lapse δN does not have homogeneous modes:

$$\int_\Sigma\delta N\mathrm{d}^3x=0\,,\quad(15)$$

just as (11).

In order to restrict attention to scalar modes, we shall parameterize the basic perturbed phase space variables $(\delta A^i_a,\delta E^b_j)$ in terms of suitable independent functions. As discussed in [15], δE^b_j and the extrinsic-curvature perturbation δK^i_a can be parameterized as

$$\delta K^i_a=\delta^i_a\kappa_1+\partial_a\partial^i\kappa_2\quad,\quad\delta E^a_i=\delta^a_i\varepsilon_1+\partial_i\partial^a\varepsilon_2\quad(16)$$

in terms of two pairs of scalar functions. In addition, the spin connection is

$$\Gamma^i_a=-\frac{1}{2}\epsilon^{ijk}E^b_j\left(2\partial_{[a}E^k_{b]}+E^c_kE^l_a\partial_cE^l_b-E^k_a\frac{\partial_b(\det E)}{\det E}\right)\,.\quad(17)$$

Perturbing this equation at the linear level, one obtains

$$\delta\Gamma^i_a=\frac{1}{2\bar{p}}\epsilon_a{}^{ij}\partial_j(\varepsilon_1+\Delta\varepsilon_2)\,,\quad(18)$$

where $\Delta\varepsilon_2:=\partial_a\partial^a\varepsilon_2$. The connection variables δA^i_a can therefore be expressed as

$$\begin{aligned}\delta A^i_a&=\delta K^i_a+\delta\Gamma^i_a\\&=\delta^i_a\kappa_1+\partial_a\partial^i\kappa_2+\frac{1}{2\bar{p}}\epsilon_a{}^{ij}\partial_j(\varepsilon_1+\Delta\varepsilon_2)\,.\quad(19)\end{aligned}$$

It is easy to see that the Gauss constraint

$$\begin{aligned}G[\Lambda]&=\frac{1}{8\pi G\gamma}\int_\Sigma\mathrm{d}^3x\Lambda^iG_i\quad(20)\\&=\frac{1}{8\pi G\gamma}\int_\Sigma\mathrm{d}^3x\Lambda^i(\partial_aE^a_i+\epsilon_{ij}{}^kA^j_aE^a_k)\end{aligned}$$

is automatically satisfied for the scalar modes. However, there is still a non-trivial gauge flow generated by the Gauss constraint, so that we will have to make sure that all expressions are invariant under SU(2) transformations of the connection and densitized triad. The latter can be done easily without computing the extended brackets including the Gauss constraint. We will therefore first focus on the brackets between Hamiltonian and diffeomorphism constraints.

III. CONSTRAINTS

We now perturb the constraints to second order in inhomogeneity, so that non-trivial constraints are obtained which govern the gauge system of linear perturbations. We will not restrict the inhomogeneity to scalar modes right away, but only when doing so entails crucial simplifications.

A. Perturbative constraints

The diffeomorphism constraint of Euclidean general relativity can be expressed as

$$\begin{aligned} D[N^a] &:= \frac{1}{8\pi G}\int_\Sigma \mathrm{d}^3x N^c(-F^k_{cd}E^d_k) \\ &\approx \frac{1}{8\pi G}\int_\Sigma \mathrm{d}^3x N^c[(-\partial_c A^k_d+\partial_d A^k_c)E^d_k + A^i_c\partial_a E^a_i]\,, \end{aligned} \tag{21}$$

where in the second line the Gauss constraint (20) has been used. Since (20) vanishes for scalar modes, we do not need to distinguish between the diffeomorphism and vector constraints, and either expression in (21) is good for our purposes. Perturbing the first expression (usually identified as the vector constraint), we have

$$D[N^a] = \frac{1}{8\pi G}\int_\Sigma \mathrm{d}^3x\delta N^c[-\bar{p}\partial_c(\delta^d_k\delta A^k_d)+\bar{p}(\partial_k\delta A^k_c)-\bar{q}\bar{p}\epsilon^d{}_{cn}\delta A^n_d-\bar{q}^2\epsilon^k{}_{cd}\delta E^d_k]\,. \tag{22}$$

The perturbative expression of the Hamiltonian density up to the second order has been derived in the appendix of [59] as $\mathcal{H}=\mathcal{H}^{(0)}+\mathcal{H}^{(1)}+\mathcal{H}^{(2)}$ with

$$\mathcal{H}^{(0)} = 6\bar{q}^2\sqrt{\bar{p}}, \tag{23}$$

$$\mathcal{H}^{(1)} = 4\bar{q}\sqrt{\bar{p}}\delta^c_j\delta A^j_c + \frac{\bar{q}^2}{\sqrt{\bar{p}}}\delta^j_c\delta E^c_j + 2\sqrt{\bar{p}}\epsilon_i{}^{cd}\partial_c\delta A^i_d, \tag{24}$$

$$\begin{aligned} \mathcal{H}^{(2)} &= -\sqrt{\bar{p}}\delta A^j_c\delta A^k_d\delta^c_k\delta^d_j + \sqrt{\bar{p}}(\delta A^j_c\delta^c_j)^2 + \frac{2\bar{q}}{\sqrt{\bar{p}}}\delta E^c_j\delta A^j_c + \frac{\bar{q}^2}{2\bar{p}^{3/2}}\delta E^c_j\delta E^d_k\delta^k_c\delta^j_d \\ &\quad -\frac{\bar{q}^2}{4\bar{p}^{3/2}}(\delta E^c_j\delta^j_c)^2 + \frac{1}{\sqrt{\bar{p}}}\left(4\epsilon_i{}^{ck}\delta E^d_k - \epsilon_i{}^{cd}\delta E^a_j\delta^j_a\right)\partial_{[c}\delta A^i_{d]}\,. \end{aligned} \tag{25}$$

For a Hamiltonian constraint of the form (6), we write

$$f^i_{cd} = f^{i(0)}_{cd} + f^{i(1)}_{cd} + f^{i(2)}_{cd} \tag{26}$$

expanded up to second order in inhomogeneity, and obtain the modification terms

$$\delta\mathcal{H}^{(0)}_Q = \sqrt{\bar{p}}f^{i(0)}_{cd}\epsilon_i{}^{cd}\,, \tag{27}$$

$$\delta\mathcal{H}^{(1)}_Q = \sqrt{\bar{p}}f^{i(1)}_{cd}\epsilon_i{}^{cd} + \frac{f^{i(0)}_{cd}}{\sqrt{\bar{p}}}\left(2\epsilon_i{}^{ck}\delta E^d_k - \frac{1}{2}\epsilon_i{}^{cd}\delta E^a_j\delta^j_a\right), \tag{28}$$

$$\begin{aligned} \delta\mathcal{H}^{(2)}_Q &= \sqrt{\bar{p}}f^{i(2)}_{cd}\epsilon_i{}^{cd} + \frac{f^{i(1)}_{cd}}{\sqrt{\bar{p}}}\left(2\epsilon_i{}^{ck}\delta E^d_k - \frac{1}{2}\epsilon_i{}^{cd}\delta E^a_j\delta^j_a\right) \\ &\quad + \frac{f^{i(0)}_{cd}}{\bar{p}^{3/2}}\left[\epsilon_i{}^{jk}\delta E^c_j\delta E^d_k - \epsilon_i{}^{ck}\delta E^d_k\delta E^a_j\delta^j_a + \frac{1}{8}\epsilon_i{}^{cd}(\delta E^a_j\delta^j_a)^2 + \frac{1}{4}\epsilon_i{}^{cd}\delta E^a_j\delta E^b_k\delta^j_b\delta^k_a\right]\,. \end{aligned} \tag{29}$$

For later convenience, we denote $\mathcal{F}^{(0)}=f^{i(0)}_{cd}\epsilon_i{}^{cd}$, $\mathcal{F}^{(1)}=f^{i(1)}_{cd}\epsilon_i{}^{cd}$ and $\mathcal{F}^{(2)}=f^{i(2)}_{cd}\epsilon_i{}^{cd}$.

At this stage, we pause and compare the parameterization with the one used in [25] and related work. In these papers, δK_a^i was used instead of δA_a^i, and the derivative term present in the classical constraint (25) could be eliminated using the Gauss constraint. The Hamiltonian constraint then contains no derivatives of the field conjugate to δE_i^a. However, even if such terms can be eliminated from the classical Hamiltonian, they may appear in an effective constraint with a derivative expansion of non-local holonomy modifications. Here, we assume that they may be induced via the terms $f_{cd}^{i(1)}$ and $f_{cd}^{i(2)}$, up to a certain order in derivatives.

B. Brackets

For computational purposes, it is convenient to split the perturbed Hamiltonian and its modification terms into two parts each,

$$H[N] = \frac{1}{16\pi G}\int \mathrm{d}^3x N\mathcal{H} = H[\bar{N}] + H[\delta N]\,, \tag{30}$$

$$\delta H_Q[N] = \frac{1}{16\pi G}\int \mathrm{d}^3x N\delta\mathcal{H}_Q = \delta H_Q[\bar{N}] + \delta H_Q[\delta N] \tag{31}$$

According to Eqs. (11) and (15), the integrals $\int_\Sigma \mathrm{d}^3x\bar{N}\mathcal{H}^{(1)}$, $\int_\Sigma \mathrm{d}^3x\delta N\mathcal{H}^{(0)}$, $\int_\Sigma \mathrm{d}^3x\bar{N}\delta\mathcal{H}_Q^{(1)}$ and $\int_\Sigma \mathrm{d}^3x\delta N\delta\mathcal{H}_Q^{(0)}$ are zero. Therefore, the explicit expressions for the perturbed Hamiltonian constraint are [15]

$$H[\bar{N}] = \frac{1}{16\pi G}\int \mathrm{d}^3x\bar{N}[\mathcal{H}^{(0)} + \mathcal{H}^{(2)}] \tag{32}$$

$$H[\delta N] = \frac{1}{16\pi G}\int \mathrm{d}^3x\delta N\mathcal{H}^{(1)}\,, \tag{33}$$

$$\delta H_Q[\bar{N}] = \frac{1}{16\pi G}\int \mathrm{d}^3x\bar{N}[\delta\mathcal{H}_Q^{(0)} + \delta\mathcal{H}_Q^{(2)}] \tag{34}$$

$$\delta H_Q[\delta N] = \frac{1}{16\pi G}\int \mathrm{d}^3x\delta N\delta\mathcal{H}_Q^{(1)}\,. \tag{35}$$

In a perturbative treatment, one may fix the background gauge so that $H[\bar{N}]$ would generate equations of motion of background and perturbation variables, while $H[\delta N]$ generates gauge transformations for the modes. However, for consistency in the form of a closed set of gauge-invariant observables, the constraints must be preserved by evolution. Both types of generators must then come from a closed bracket of constraints $H[\bar{N}+\delta N]$ together with $D[N^a]$. As we have the explicit expression for the perturbed Hamiltonian constraint at hand, we can calculate the Poisson brackets between Hamiltonian and diffeomorphism constraints and between two Hamiltonian constraints, and check whether they can be closed.

Before proceeding, we shall assume that the holonomy-modification function f_{cd}^i is a function of the connection variable A_a^m up to first-order derivative, that is $f_{cd}^i \equiv f_{cd}^i(A,\partial A,\epsilon)$, as used for vector modes in [59]. Higher spatial derivatives require a more-involved treatment by a systematic expansion as developed and applied to spherically symmetric systems in [27]. Here we assume the classical derivative order but allow for all coefficients to be modified, thereby extending the treatment of [25]. In this case, the holonomy-modification function can be expanded as

$$\begin{aligned}
&f_{cd}^i(A,\partial A,\epsilon)\\
&= f_{cd}^i(A,\partial A,\epsilon)\big|_{\bar{A}_a^m} + \left.\frac{\partial f_{cd}^i(A,\partial A,\epsilon)}{\partial A_a^m}\right|_{\bar{A}_a^m}\delta A_a^m\\
&\quad+ \left.\frac{\partial f_{cd}^i(A,\partial A,\epsilon)}{\partial(\partial_e A_a^m)}\right|_{\bar{A}_a^m}\partial_e\delta A_a^m\\
&\quad+\frac{1}{2}\left.\frac{\partial^2 f_{cd}^i(A,\partial A,\epsilon)}{\partial A_a^m\partial A_b^n}\right|_{\bar{A}_a^m}\delta A_a^m\delta A_b^n\\
&\quad+ \left.\frac{\partial^2 f_{cd}^i(A,\partial A,\epsilon)}{\partial A_a^m\partial(\partial_e A_b^n)}\right|_{\bar{A}_a^m}\delta A_a^m\partial_e\delta A_b^n\\
&\quad+\frac{1}{2}\left.\frac{\partial^2 f_{cd}^i(A,\partial A,\epsilon)}{\partial(\partial_e A_a^m)\partial(\partial_f A_b^n)}\right|_{\bar{A}_a^m}\partial_e\delta A_a^m\partial_f\delta A_b^n+\cdots\\
&= f_{cd}^{i(0)}(\bar{q},\epsilon) + \mathcal{A}_{cd}^{i(1)}(\bar{q},\delta A,\epsilon) + \mathcal{B}_{cd}^{i(1)}(\bar{q},\partial\delta A,\epsilon)\\
&\quad+\mathcal{A}_{cd}^{i(2)}(\bar{q},\delta A,\epsilon) + \mathcal{B}_{cd}^{i(2)}(\bar{q},\delta A,\partial\delta A,\epsilon)\\
&\quad+\mathcal{C}_{cd}^{i(2)}(\bar{q},\partial\delta A,\epsilon)+\cdots
\end{aligned} \tag{36}$$

For later convenience, we have denoted $f_{cd}^{i(1)} \equiv \mathcal{A}_{cd}^{i(1)} + \mathcal{B}_{cd}^{i(1)}$ and $f_{cd}^{i(2)} \equiv \mathcal{A}_{cd}^{i(2)} + \mathcal{B}_{cd}^{i(2)} + \mathcal{C}_{cd}^{i(2)}$, where superscripts indicate orders of inhomogeneity, and $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$ derivative orders. We note that specific expressions for coefficients in a derivative expansion could be derived, for instance, by using expectation values in coherent states as done for spherically symmetric models in [69]. This paper also shows that the Lorentzian constraint may have further derivative corrections compared with the Euclidean term.

Since we expand the Hamiltonian and diffeomorphism constraints up to second order in inhomogeneity, higher-order terms in a power-series expansion by A_a^i of the holonomy-modification function will not provide independent contributions of products of δA_a^i but just modify the background dependence of coefficients included here. Therefore, it is enough to consider the holonomy-modification function up to the second order in inhomogeneity, even if it may come from non-polynomial functions such as the sine used in the usual background modification. As already stated, our only assumption is that no spatial derivatives of A_a^i of orders higher than the classical one appear.

We first consider the Poisson bracket between Hamiltonian and diffeomorphism constraints,

$$\{H[N],D[N^a]\} = \{H[\bar{N}],D[N^a]\} + \{H[\delta N],D[N^a]\} \tag{37}$$

It is straightforward to show that the Poisson bracket $\{H[\bar{N}],D[N^a]\}$ vanishes, and hence we have

$$\{H[N],D[N^a]\} = \{H[\delta N],D[N^a]\} = H[\delta N^c\partial_c\delta N]\,. \tag{38}$$

Note that in Euclidean signature one commonly employs the diffeomorphism constraint with a sign opposite to that in Lorentzian general relativity, so that there is a sign difference between the above Poisson bracket and corresponding one in Lorentzian signature. There are similar results in the following Poisson brackets, including the classical case and that with holonomy modifications. Thus the Poisson bracket between perturbed classical Hamiltonian and diffeomorphism constraints agrees with the bracket between the original classical constraints. This indicates the consistency between the perturbed constraint expressions and elementary Poisson brackets including the background and perturbed basic variables.

We shall now derive the Poisson bracket between the Hamiltonian and the diffeomorphism constraints when the former includes holonomy modifications. It should be noted that for vector modes in [59], there is no lapse perturbation, that is $\delta N = 0$, and $\delta H_Q[\delta N]$ vanishes. But for scalar modes we have $\delta N \neq 0$, so that we need to calculate both Poisson brackets, $\{\delta H_Q[\bar{N}], D[N^a]\}$ and $\{\delta H_Q[\delta N], D[N^a]\}$.

We calculate the first Poisson bracket:

$$
\begin{aligned}
&\{\delta H_Q[\bar{N}], D[N^a]\} \\
&= \frac{1}{16\pi G}\int \mathrm{d}^3x\delta N^c\Big[-\frac{1}{2}\bar{q}\delta^i_c\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\partial_a(\delta E^d_k\delta^k_d) + f^{i(0)}_{bc}\epsilon_i{}^{bj}\partial_j(\delta E^d_k\delta^k_d) - \frac{2}{3}\mathcal{F}^{(0)}\delta^k_c(\partial_d\delta E^d_k) \\
&-2f^{i(0)}_{cd}\epsilon_i{}^{jk}\partial_j\delta E^d_k + 2\bar{q}\frac{\partial\mathcal{A}^{j(1)}_{bd}}{\partial(\delta A^i_a)}\epsilon_j{}^{bk}\delta^i_c\partial_a\delta E^d_k + \frac{\bar{q}}{2}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\delta^i_c\partial_a\partial_e(\delta E^d_k\delta^k_d) \\
&-2\bar{q}\frac{\partial\mathcal{B}^{j(1)}_{bd}}{\partial(\partial_e\delta A^i_a)}\epsilon_j{}^{bk}\delta^i_c\partial_a\partial_e\delta E^d_k + \frac{1}{3}\bar{p}\frac{\partial\mathcal{F}^{(0)}}{\partial\bar{q}}\partial_k\delta A^k_c + \bar{q}\bar{p}\delta^i_c\partial_a\frac{\partial\mathcal{A}^{(2)}}{\partial(\delta A^i_a)} + \bar{q}\bar{p}\delta^i_c\partial_a\frac{\partial\mathcal{B}^{(2)}}{\partial(\delta A^i_a)} \\
&-\bar{q}\bar{p}\delta^i_c\partial_a\partial_e\frac{\partial\mathcal{B}^{(2)}}{\partial(\partial_e\delta A^i_a)} - \bar{q}\bar{p}\delta^i_c\partial_a\partial_e\frac{\partial\mathcal{C}^{(2)}}{\partial(\partial_e\delta A^i_a)} + \bar{p}\partial_c\mathcal{A}^{(1)} + \bar{p}\partial_c\mathcal{B}^{(1)} \\
&-2\bar{p}\epsilon_i{}^{bj}\partial_j\mathcal{A}^{i(1)}_{bc} - 2\bar{p}\epsilon_i{}^{bj}\partial_j\mathcal{B}^{i(1)}_{bc} - \frac{\bar{p}}{3}\frac{\partial\mathcal{F}^{(0)}}{\partial\bar{q}}\partial_c(\delta^d_k\delta A^k_d)\Big]\,. \qquad (39)
\end{aligned}
$$

Hence in contrast to the classical case, the Poisson bracket $\{H_Q[\bar{N}], D[N^a]\}$ does not vanish identically due to the introduction of holonomy effects. The second Poisson bracket is

$$
\begin{aligned}
\{\delta H_Q[\delta N], D[N^a]\} \;=\; &\frac{1}{16\pi G}\int \mathrm{d}^3x\Big[(\delta N^i\partial_a\delta N)\left(\bar{q}\sqrt{\bar{p}}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)} - 2\sqrt{\bar{p}}f^{k(0)}_{di}\epsilon_k{}^{da}\right) \\
&+(\delta N^c\partial_c\delta N)\sqrt{\bar{p}}\mathcal{F}^{(0)} - (\delta N^i\partial_a\partial_e\delta N)\bar{q}\sqrt{\bar{p}}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\Big]\,. \qquad (40)
\end{aligned}
$$

The Poisson bracket we are looking for is the sum of Eqs. (38), (39) and (40),

$$
\{H_Q[N], D[N^a]\} = \{H[\delta N], D[N^a]\} + \{H_Q[\bar{N}], D[N^a]\} + \{H_Q[\delta N], D[N^a]\}\,. \qquad (41)
$$

We will discuss possible anomaly-free versions in the next section.

We now calculate the Poisson bracket between two Hamiltonian constraints, smeared with different functions $N_1 = \bar{N} + \delta N_1$ and $N_2 = \bar{N} + \delta N_2$. We have $\{H[\delta N_1], H[\delta N_2]\} = 0$ because the absence of a background term in the diffeomorphism constraint implies that the leading non-zero contribution would be of third order, which is eliminated in our second-order expansion. We therefore have

$$
\begin{aligned}
\{H[N_1], H[N_2]\} \;&=\; \{H[\delta N_1], H[\bar{N}]\} + \{H[\bar{N}], H[\delta N_2]\} \\
&=\; \{H[\delta N_1 - \delta N_2], H[\bar{N}]\} = -D\left[\frac{\bar{N}}{\bar{p}}\partial^c(\delta N_2 - \delta N_1)\right]\,. \qquad (42)
\end{aligned}
$$

Again, Eq. (42) confirms the consistency between the perturbed constraint expressions and elementary Poisson brackets including the background and perturbed basic variables.

With holonomy modifications, we similarly have

$$
\begin{aligned}
\{H_Q[N_1], H_Q[N_2]\} \;&=\; \{H_Q[\delta N_1 - \delta N_2], H_Q[\bar{N}]\} \\
&=\; \{H[\delta N_1 - \delta N_2], H[\bar{N}]\} + \{H[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\} \\
&\quad+\{\delta H_Q[\delta N_1 - \delta N_2], H[\bar{N}]\} + \{\delta H_Q[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\} \qquad (43)
\end{aligned}
$$

where

$$
\begin{aligned}
\{H[\delta N_1-\delta N_2],\delta H_Q[\bar N]\} &= \frac{1}{8\pi G}\int \mathrm{d}^3x(\delta N_1-\delta N_2)\Big\{\Big[\frac{\bar q}{24\sqrt{\bar p}}\left(8\mathcal{F}^{(0)}+\bar q\frac{\partial\mathcal{F}^{(0)}}{\partial\bar q}\right)+\frac{\bar q^2}{8\sqrt{\bar p}}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\delta^i_a\Big]\delta E^d_k\delta^k_d\\
&\quad -\Big[\frac{\bar q}{\sqrt{\bar p}}f^{i(0)}_{cd}\epsilon_i{}^{ck}+\frac{\bar q^2}{2\sqrt{\bar p}}\frac{\partial\mathcal{A}^{j(1)}_{cd}}{\partial(\delta A^i_a)}\delta^i_a\epsilon_j{}^{ck}\Big]\delta E^d_k+\frac{\sqrt{\bar p}}{6}\left(\mathcal{F}^{(0)}-\bar q\frac{\partial\mathcal{F}^{(0)}}{\partial\bar q}\right)\delta A^k_d\delta^d_k\\
&\quad +\frac{1}{2}\bar q\sqrt{\bar p}\mathcal{F}^{(1)}-\frac{\bar q^2\sqrt{\bar p}}{4}\delta^i_a\left(\frac{\partial\mathcal{A}^{(2)}}{\partial(\delta A^i_a)}+\frac{\partial\mathcal{B}^{(2)}}{\partial(\delta A^i_a)}\right)\Big\}\\
&\quad +\frac{1}{8\pi G}\int \mathrm{d}^3x\partial_e(\delta N_1-\delta N_2)\Big\{\Big[\frac{1}{2\sqrt{\bar p}}f^{i(0)}_{cb}\epsilon_i{}^{cj}\epsilon_j{}^{eb}+\frac{\bar q^2}{8\sqrt{\bar p}}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\delta^i_a\Big]\delta E^d_k\delta^k_d\\
&\quad +\frac{1}{\sqrt{\bar p}}\Big[-\frac{\mathcal{F}^{(0)}}{4}-f^{i(0)}_{bd}\epsilon_i{}^{jk}\epsilon_j{}^{eb}+\frac{\bar q^2}{2}\delta^i_a\epsilon_j{}^{ck}\frac{\partial\mathcal{B}^{j(1)}_{cd}}{\partial(\partial_e\delta A^i_a)}\Big]\delta E^d_k+\frac{\sqrt{\bar p}}{12}\frac{\partial\mathcal{F}^{(0)}}{\partial\bar q}\epsilon_i{}^{ed}\delta A^i_d\\
&\quad -f^{i(1)}_{db}\epsilon_i{}^{dj}\epsilon_j{}^{eb}+\frac{\sqrt{\bar p}\bar q^2}{4}\left(\frac{\partial\mathcal{B}^{(2)}}{\partial(\partial_e\delta A^i_a)}+\frac{\partial\mathcal{C}^{(2)}}{\partial(\partial_e\delta A^i_a)}\right)\delta^i_a\Big\} \qquad (44)
\end{aligned}
$$

for the first non-classical bracket,

$$
\begin{aligned}
\{\delta H_Q[\delta N_1-\delta N_2],H[\bar N]\} &= \frac{1}{8\pi G}\int \mathrm{d}^3x(\delta N_1-\delta N_2)\Big\{-\frac{\bar q^2}{8\sqrt{\bar p}}\left(\frac{\partial\mathcal{F}^{(0)}}{\partial\bar q}+\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\delta^i_a\right)\delta E^d_k\delta^k_d-\frac{\sqrt{\bar p}}{2}\mathcal{F}^{(0)}\delta A^k_d\delta^d_k\\
&\quad +\Big[\frac{\bar q}{\sqrt{\bar p}}\left(f^{i(0)}_{cd}+\frac{\bar q}{4}\frac{\partial f^{i(0)}_{cd}}{\partial\bar q}\right)+\frac{\bar q^2}{4\sqrt{\bar p}}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\delta^k_a\delta^i_d\Big]\delta E^d_k+\left(\frac{1}{2}\bar q\sqrt{\bar p}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}+\sqrt{\bar p}f^{j(0)}_{ca}\epsilon_j{}^{cd}\delta^a_k\right)\delta A^k_d\\
&\quad +\frac{\bar q\sqrt{\bar p}}{4}\left(\bar q\frac{\partial\mathcal{F}^{(1)}}{\partial\bar q}-2\mathcal{F}^{(1)}\right)\Big\}\\
&\quad +\frac{1}{8\pi G}\int \mathrm{d}^3x\partial_e(\delta N_1-\delta N_2)\Big\{\Big[\frac{\bar q^2}{8\sqrt{\bar p}}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\delta^i_a+\frac{1}{2\sqrt{\bar p}}f^{j(0)}_{ba}\epsilon_j{}^{bi}\epsilon_i{}^{ea}\Big]\delta E^d_k\delta^k_d\\
&\quad +\Big[-\frac{\bar q^2}{4\sqrt{\bar p}}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\delta^k_a\delta^i_d+\frac{1}{4\sqrt{\bar p}}\mathcal{F}^{(0)}\epsilon_d{}^{ek}-\frac{1}{\sqrt{\bar p}}f^{j(0)}_{bd}\epsilon_j{}^{bi}\epsilon_i{}^{ek}+\frac{1}{\sqrt{\bar p}}f^{j(0)}_{ba}\epsilon_j{}^{bi}\epsilon_i{}^{ak}\delta^e_d\Big]\delta E^d_k\\
&\quad +\frac{1}{4\sqrt{\bar p}}\frac{\partial\mathcal{A}^{(1)}}{\partial\delta A^i_a}\epsilon_a{}^{ed}\delta A^i_d+\frac{1}{4\sqrt{\bar p}}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\epsilon_a{}^{cd}\partial_c\delta A^i_d\Big\} \qquad (45)
\end{aligned}
$$

for the second non-classical bracket, and

$$
\begin{aligned}
&\{\delta H_Q[\delta N_1-\delta N_2],\delta H_Q[\bar N]\}\\
&= \frac{1}{8\pi G}\int \mathrm{d}^3x(\delta N_1-\delta N_2)\Big\{-\frac{1}{24\sqrt{\bar p}}\mathcal{F}^{(0)}\frac{\partial\mathcal{F}^{(0)}}{\partial\bar q}\delta E^d_k\delta^k_d+\Big[\frac{1}{12\sqrt{\bar p}}\mathcal{F}^{(0)}\frac{\partial f^{i(0)}_{cd}}{\partial\bar q}\epsilon_i{}^{ck}+\frac{1}{12\sqrt{\bar p}}f^{i(0)}_{cd}\frac{\partial\mathcal{F}^{(0)}}{\partial\bar q}\epsilon_i{}^{ck}\\
&\quad +\frac{1}{8\sqrt{\bar p}}\mathcal{F}^{(0)}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\delta^i_d\delta^k_a-\frac{1}{4\sqrt{\bar p}}f^{j(0)}_{cd}\epsilon_j{}^{ck}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\delta^i_a+\frac{1}{2\sqrt{\bar p}}f^{j(0)}_{ad}\epsilon_j{}^{ik}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\\
&\quad -\frac{1}{2\sqrt{\bar p}}\left(-\frac{1}{2}\mathcal{F}^{(0)}\delta^i_a+2f^{k(0)}_{ca}\epsilon_k{}^{ci}\right)\frac{\partial\mathcal{A}^{j(1)}_{cd}}{\partial(\delta A^i_a)}\epsilon_j{}^{ck}\Big]\delta E^d_k+\frac{\sqrt{\bar p}}{24}\left(\mathcal{F}^{(0)}\frac{\partial\mathcal{F}^{(1)}}{\partial\bar q}-\mathcal{F}^{(1)}\frac{\partial\mathcal{F}^{(0)}}{\partial\bar q}\right)\\
&\quad -\frac{\sqrt{\bar p}}{8}\mathcal{F}^{(1)}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}\delta^i_a+\frac{\sqrt{\bar p}}{2}f^{k(1)}_{ca}\epsilon_k{}^{ci}\frac{\partial\mathcal{A}^{(1)}}{\partial(\delta A^i_a)}-\frac{\sqrt{\bar p}}{4}\left(-\frac{1}{2}\mathcal{F}^{(0)}\delta^i_a+2f^{k(0)}_{ca}\epsilon_k{}^{ci}\right)\left(\frac{\partial\mathcal{A}^{(2)}}{\partial(\delta A^i_a)}+\frac{\partial\mathcal{B}^{(2)}}{\partial(\delta A^i_a)}\right)\Big\}\\
&\quad +\frac{1}{8\pi G}\int \mathrm{d}^3x\partial_e(\delta N_1-\delta N_2)\Big\{\frac{\sqrt{\bar p}}{4}\left(-\frac{1}{2}\mathcal{F}^{(0)}\delta^i_a+2f^{k(0)}_{ca}\epsilon_k{}^{ci}\right)\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\\
&\quad +\Big[-\frac{1}{8\sqrt{\bar p}}\mathcal{F}^{(0)}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\delta^i_d\delta^k_a+\frac{1}{4\sqrt{\bar p}}f^{j(0)}_{cd}\epsilon_j{}^{ck}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\delta^i_a-\frac{1}{2\sqrt{\bar p}}f^{j(0)}_{ad}\epsilon_j{}^{ik}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\\
&\quad -\frac{1}{2\sqrt{\bar p}}\left(-\frac{1}{2}\mathcal{F}^{(0)}\delta^i_a+2f^{l(0)}_{ba}\epsilon_l{}^{bi}\right)\epsilon_j{}^{ck}\frac{\partial\mathcal{B}^{j(1)}_{cd}}{\partial(\partial_e\delta A^i_a)}\Big]\delta E^d_k+\frac{\sqrt{\bar p}}{8}\mathcal{F}^{(1)}\delta^i_a\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}\\
&\quad -\frac{\sqrt{\bar p}}{2}f^{k(1)}_{ca}\epsilon_k{}^{ci}\frac{\partial\mathcal{B}^{(1)}}{\partial(\partial_e\delta A^i_a)}-\frac{\sqrt{\bar p}}{4}\left(-\frac{1}{2}\mathcal{F}^{(0)}\delta^i_a+2f^{l(0)}_{ba}\epsilon_l{}^{bi}\right)\left(\frac{\partial\mathcal{B}^{(2)}}{\partial(\partial_e\delta A^i_a)}+\frac{\partial\mathcal{C}^{(2)}}{\partial(\partial_e\delta A^i_a)}\right)\Big\} \qquad (46)
\end{aligned}
$$

for the last bracket.

IV. HOLONOMY MODIFICATION FUNCTION AND ANOMALY FREEDOM

We can now check whether there are some specific forms of the holonomy modification function which imply that the constraints are anomaly free. The general form [59]

$$
\begin{aligned}
f^i_{cd} \;=\;& \sigma(\bar q)\epsilon^i{}_{cd} + \not\phi(\bar q)\epsilon^i{}_{cd}A^j_a\delta^a_j + \mu(\bar q)A^i_b\epsilon^b{}_{cd} \\
&+\nu(\bar q)(\epsilon^i{}_{md}A^m_c + \epsilon^i{}_{cn}A^n_d) + \widetilde{\not\phi}(\bar q)\epsilon^i{}_{cd}(A^j_a\delta^a_j)^2 \\
&+\not\mu(\bar q)A^i_b\epsilon^b{}_{cd}A^j_a\delta^a_j + \not\psi(\bar q)(\epsilon^i{}_{md}A^m_c + \epsilon^i{}_{cn}A^n_d)A^j_a\delta^a_j \\
&+\rho(\bar q)\epsilon^i{}_{mn}A^m_c A^n_d + \tau(\bar q)\partial_{[c}A^i_{d]}\,, \qquad (47)
\end{aligned}
$$

of holonomy modification functions satisfies our previous assumptions: antisymmetry in c and d as well as up to first-order derivatives of A^i_a. At this point, there is no term of the form $A^i_a\partial_b A^j_c$ because on shell A^i_a appears as a first-order (time) derivative. The omitted term would therefore be considered to be of second total derivative order and should not be included in a first-order derivative expansion. This treatment of derivatives has been shown to be consistent in [27]. The dependence of coefficients on the background connection $\bar q$ is unrestricted, as it may result from an expansion of a non-quadratic function of the connection. However, if f^i_{cd} is expected to result from a function of holonomies, expanded up to n-th order in a dependence on A^i_a, the perturbation expansion implies that $\sigma(\bar q)$ is a polynomial of the same degree n, while $\not\phi(\bar q)$, $\mu(\bar q)$, $\nu(\bar q)$ and $\tau(\bar q)$ are polynomials of degree $n-1$, and $\widetilde{\not\phi}(\bar q)$, $\not\mu(\bar q)$, $\not\psi(\bar q)$ and $\rho(\bar q)$ are polynomials of degree $n-2$.

In the notation of (36), the expressions of the holonomy modification function f^i_{cd} up to first order can be found as

$$
\begin{aligned}
f^{i(0)}_{cd} \;=\;& (\sigma + 3\not\phi\bar q + \mu\bar q + 2\nu\bar q + \rho\bar q^2 + 9\widetilde{\not\phi}\bar q^2 \\
&+3\not\mu\bar q^2 + 6\not\psi\bar q^2)\epsilon^i{}_{cd}\,, \\
\mathcal{A}^{i(1)}_{cd} \;=\;& (\nu + \rho\bar q + 3\not\psi\bar q)(\epsilon^i{}_{md}\delta A^m_c + \epsilon^i{}_{cn}\delta A^n_d) \\
&+(\not\phi + 6\widetilde{\not\phi}\bar q + \not\mu\bar q + 2\not\psi\bar q)\delta A^j_a\delta^a_j\epsilon^i{}_{cd} \\
&+(\mu + 3\not\mu\bar q)\delta A^i_b\epsilon^b{}_{cd}\,, \\
\mathcal{B}^{i(1)}_{cd} \;=\;& \tau\partial_{[c}\delta A^i_{d]}\,, \\
\mathcal{A}^{i(2)}_{cd} \;=\;& \rho\epsilon^i{}_{mn}\delta A^m_c\delta A^n_d + \widetilde{\not\phi}(\delta A^j_a\delta^a_j)^2\epsilon^i{}_{cd} \\
&+\not\psi(\epsilon^i{}_{md}\delta A^m_c + \epsilon^i{}_{cn}\delta A^n_d)\delta A^j_a\delta^a_j + \not\mu\delta A^i_b\epsilon^b{}_{cd}\delta A^j_a\delta^a_j\,, \\
\mathcal{B}^{i(2)}_{cd} \;=\;& 0\,, \\
\mathcal{C}^{i(2)}_{cd} \;=\;& 0\,. \qquad (48)
\end{aligned}
$$

Note that for vector modes, with $\delta^b_j\delta A^j_b = 0$, these equations reduce to Eq. (35) in [59]. We list the following relations for later convenience,

$$
\begin{aligned}
\mathcal{F}^{(0)} \;=\;& 6(\sigma + 3\not\phi\bar q + \mu\bar q + 2\nu\bar q + \rho\bar q^2 + 9\widetilde{\not\phi}\bar q^2 + 3\not\mu\bar q^2 + 6\not\psi\bar q^2)\,, \\
\mathcal{A}^{(1)} \;=\;& (4\nu + 6\not\phi + 2\mu + 4\rho\bar q + 24\not\psi\bar q + 36\widetilde{\not\phi}\bar q + 12\not\mu\bar q)\delta A^k_d\delta^d_k\,, \\
\mathcal{A}^{(2)} \;=\;& (\rho + 6\widetilde{\not\phi} + 2\not\psi + 2\not\mu)(\delta A^k_d\delta^d_k)^2 - \rho\delta A^m_c\delta A^n_d\delta^c_n\delta^d_m\,, \\
f^{i(0)}_{cd} \;=\;& \frac{\mathcal{F}^{(0)}}{6}\epsilon^i{}_{cd}\,, \\
\mathcal{B}^{(1)} \;=\;& \tau\partial_c(\delta A^i_d\epsilon_i{}^{cd})\,. \qquad (49)
\end{aligned}
$$

A. Hamiltonian and diffeomorphism constraints

Substituting Eq. (48) into the expression of the Poisson bracket (39) and using the relations in Eq. (49), we have

$$
\begin{aligned}
\{\delta H_Q[\bar N], D[N^a]\} \;=\;& \frac{1}{16\pi G}\int \mathrm{d}^3x\,\delta N^c\Big[-2\left(\frac{\sigma}{\bar q} + 3\not\phi + 2\mu + \nu + 9\bar q\widetilde{\not\phi} + 6\bar q\not\mu + 3\bar q\not\psi\right)\bar q\delta^k_c(\partial_d\delta E^d_k) \\
&+2\Bigg(\frac{\partial\sigma}{\partial\bar q} + 3\bar q\frac{\partial\not\phi}{\partial\bar q} + \bar q\frac{\partial\mu}{\partial\bar q} + 2\bar q\frac{\partial\nu}{\partial\bar q} + 3\bar q^2\frac{\partial\not\mu}{\partial\bar q} + \bar q^2\frac{\partial\rho}{\partial\bar q} + 9\bar q^2\frac{\partial\widetilde{\not\phi}}{\partial\bar q} + 6\bar q^2\frac{\partial\not\psi}{\partial\bar q} \\
&+3\not\phi + 2\mu + \nu + 18\bar q\widetilde{\not\phi} + 9\bar q\not\mu + 9\bar q\not\psi\Bigg)\bar p\partial_k\delta A^k_c \\
&-2\Bigg(\frac{\partial\sigma}{\partial\bar q} + 3\bar q\frac{\partial\not\phi}{\partial\bar q} + \bar q\frac{\partial\mu}{\partial\bar q} + 2\bar q\frac{\partial\nu}{\partial\bar q} + 3\bar q^2\frac{\partial\not\mu}{\partial\bar q} + \bar q^2\frac{\partial\rho}{\partial\bar q} + 9\bar q^2\frac{\partial\widetilde{\not\phi}}{\partial\bar q} + 6\bar q^2\frac{\partial\not\psi}{\partial\bar q} \\
&+2\not\phi + \mu + \nu + 3\bar q\not\mu + 5\bar q\not\psi + 6\bar q\widetilde{\not\phi}\Bigg)\bar p\partial_c(\delta^d_k\delta A^k_d) \\
&+(\not\phi + 6\bar q\widetilde{\not\phi} + \mu + 4\bar q\not\mu + 2\bar q\not\psi)\bar q\partial_c(\delta E^d_k\delta^k_d)\Big]\,. \qquad (50)
\end{aligned}
$$

For scalar modes (16) and (19), we have the relations

$$
\begin{aligned}
&\delta^k_c(\partial_d \delta E^d_k) = \partial_c\varepsilon_1 + \partial_c(\Delta\varepsilon_2),\\
&\partial_c(\delta E^d_k \delta^k_d) = 3\partial_c\varepsilon_1 + \partial_c(\Delta\varepsilon_2),\\
&\partial_k \delta A^k_c = \partial_c\kappa_1 + \partial_c(\Delta\kappa_2),\\
&\partial_c(\delta A^k_d \delta^d_k) = 3\partial_c\kappa_1 + \partial_c(\Delta\kappa_2),\\
&\epsilon^k{}_{cd}\delta E^d_k = 0,\\
&\epsilon^d{}_{cn}\delta A^n_d = -\frac{1}{\bar{p}}\partial_c\varepsilon_1 - \frac{1}{\bar{p}}\partial_c(\Delta\varepsilon_2)
\end{aligned}
\tag{51}
$$

The diffeomorphism constraint in term of the scalar functions $(\varepsilon_1, \varepsilon_2)$ and (κ_1, κ_2) is

$$
D[N^a] = \frac{1}{8\pi G}\int_\Sigma \mathrm{d}^3x \delta N^c[-2\bar{p}\partial_c\kappa_1 + \bar{q}\partial_c\varepsilon_1 + \bar{q}\partial_c(\Delta\varepsilon_2)] \tag{52}
$$

Using these relations, the Poisson bracket (50) is

$$
\begin{aligned}
\{\delta H_Q[\bar{N}], D[N^a]\} \;=\; & \frac{1}{16\pi G}\int \mathrm{d}^3x \delta N^c \Big\{-\left(2\frac{\sigma}{\bar{q}} + 3\phi + \mu + 2\nu\right)\bar{q}\partial_c\varepsilon_1\\
& -\left(2\frac{\sigma}{\bar{q}} + 5\phi + 3\mu + 2\nu + 12\tilde{\phi} + 8\bar{q}\not{\mu} + 4\bar{q}\not{\psi}\right)\bar{q}\partial_c(\Delta\varepsilon_2)\\
& -2\Big[2\left(\frac{\partial\sigma}{\partial\bar{q}} + 3\bar{q}\frac{\partial\phi}{\partial\bar{q}} + \bar{q}\frac{\partial\mu}{\partial\bar{q}} + 2\bar{q}\frac{\partial\nu}{\partial\bar{q}} + 3\bar{q}^2\frac{\partial\not{\mu}}{\partial\bar{q}} + \bar{q}^2\frac{\partial\rho}{\partial\bar{q}} + 9\bar{q}^2\frac{\partial\tilde{\phi}}{\partial\bar{q}} + 6\bar{q}^2\frac{\partial\not{\psi}}{\partial\bar{q}}\right)\\
& +3\phi + \mu + 2\nu + 6\bar{q}\not{\psi}\Big]\bar{p}\partial_c\delta\kappa_1 + 2(\phi + \mu + 12\bar{q}\tilde{\phi} + 6\bar{q}\not{\mu} + 4\bar{q}\not{\psi})\bar{p}\partial_c(\Delta\kappa_2)\Big\}.
\end{aligned}
\tag{53}
$$

This contribution would vanish classically, but may be non-zero here as long as the scalar modes can be combined in the right form to produce a multiple of the diffeomorphism constraint (52). Comparing the Poisson bracket (53) with the expression of the diffeomorphism constraint (52), we observe that the conditions

$$
\phi = -\mu - 2\bar{q}\not{\mu}\,, \tag{54}
$$

$$
\tilde{\phi} = -\frac{1}{3}(\not{\mu} + \not{\psi})\,, \tag{55}
$$

$$
\begin{aligned}
&\frac{\partial\sigma}{\partial\bar{q}} + 3\bar{q}\frac{\partial\phi}{\partial\bar{q}} + \bar{q}\frac{\partial\mu}{\partial\bar{q}} + 2\bar{q}\frac{\partial\nu}{\partial\bar{q}} + 3\bar{q}^2\frac{\partial\not{\mu}}{\partial\bar{q}} + \bar{q}^2\frac{\partial\rho}{\partial\bar{q}}\\
&+9\bar{q}^2\frac{\partial\tilde{\phi}}{\partial\bar{q}} + 6\bar{q}^2\frac{\partial\not{\psi}}{\partial\bar{q}}\\
&= -\frac{\sigma}{\bar{q}} - 6\phi - 4\mu - 2\nu - 27\bar{q}\tilde{\phi} - 15\bar{q}\not{\mu} - 12\bar{q}\not{\psi}
\end{aligned}
\tag{56}
$$

imply a closed Poisson bracket:

$$
\{H_Q[\bar{N}], D[N^a]\} = -\left(\frac{\sigma}{\bar{q}} - \mu + \nu - 3\bar{q}\not{\mu}\right)D[N^a]\,. \tag{57}
$$

Substituting Eqs. (54) and (55) into Eq. (56),

$$
\begin{aligned}
&\frac{\partial\sigma}{\partial\bar{q}} - 2\bar{q}\frac{\partial\mu}{\partial\bar{q}} + 2\bar{q}\frac{\partial\nu}{\partial\bar{q}} - 6\bar{q}^2\frac{\partial\not{\mu}}{\partial\bar{q}} + \bar{q}^2\frac{\partial\rho}{\partial\bar{q}} + 3\bar{q}^2\frac{\partial\not{\psi}}{\partial\bar{q}}\\
&= -\frac{\sigma}{\bar{q}} + 2\mu - 2\nu + 12\bar{q}\not{\mu} - 3\bar{q}\not{\psi}\,.
\end{aligned}
\tag{58}
$$

Similarly to the case of vector modes [59], we find that the form of the Poisson bracket $\{H_Q[\bar{N}], D[N^a]\}$ may be modified by holonomy terms. One of the conditions for scalar modes, Eq. (56), is the same as that for vector modes (Eq. (38) in [59]). For scalar modes, however, we need the additional conditions (54) and (55). The requirement of having anomaly-free constraints therefore imposes tighter restrictions on the parameters of the holonomy-modification function (47) when we consider scalar modes.

Moreover, for the contribution (40) to the Poisson bracket, we have

$$
\begin{aligned}
&\{\delta H_Q[\delta N], D[N^a]\} = \delta H_Q[\delta N^c\partial_c\delta N]\\
&-\frac{1}{16\pi G}\int \mathrm{d}^3x(\delta N^c\partial_c\delta N)4\bar{q}\sqrt{\bar{p}}\left(\frac{\sigma}{\bar{q}} - \mu + \nu - 3\not{\mu}\bar{q}\right)
\end{aligned}
\tag{59}
$$

using Eqs. (54) and (55). The condition of anomaly-free constraints requires

$$
\frac{\sigma}{\bar{q}} - \mu + \nu - 3\not{\mu}\bar{q} = 0\,, \tag{60}
$$

so that $\{\delta H_Q[N], D[N^a]\}$ in (57) vanishes. Therefore, when the conditions (54), (55), (58) and (60) are satisfied, the Poisson bracket between the holonomy-modified Hamiltonian and diffeomorphism constraints becomes

$$
\{\delta H_Q[N], D[N^a]\} = \delta H_Q[\delta N^c\partial_c\delta N], \tag{61}
$$

which is identical to the classical case. The conditions (54), (55), (58) and (60) can be combined as

$$
\begin{aligned}
&\sigma = \bar{q}\mu - \bar{q}\nu + 3\bar{q}^2\not{\mu}\,,\\
&\phi = -\mu - 2\bar{q}\not{\mu}\,,\\
&\tilde{\phi} = -\frac{1}{3}(\not{\mu} + \not{\psi})\,,\\
&-\bar{q}\frac{\partial\mu}{\partial\bar{q}} + \bar{q}\frac{\partial\nu}{\partial\bar{q}} - 3\bar{q}^2\frac{\partial\not{\mu}}{\partial\bar{q}} + \bar{q}^2\frac{\partial\rho}{\partial\bar{q}} + 3\bar{q}^2\frac{\partial\not{\psi}}{\partial\bar{q}} = 3\bar{q}\not{\mu} - 3\bar{q}\not{\psi}\,.
\end{aligned}
\tag{62}
$$

B. Two Hamiltonian constraints

We now turn to the study of the Poisson bracket between two holonomy-modified Hamiltonian constraints. Using Eq. (62), the terms of the holonomy modification function (48) can be rewritten as

$$
\begin{aligned}
f^{i(0)}_{cd} &= (-\mu\bar{q} + \nu\bar{q} - 3\not{\mu}\bar{q}^2 + 3\not{\nu}\bar{q}^2 + \rho\bar{q}^2)\epsilon^i{}_{cd}\,,\\
\mathcal{A}^{i(1)}_{cd} &= (\nu + \rho\bar{q} + 3\not{\nu}\bar{q})(\epsilon^i{}_{md}\delta A^m_c + \epsilon^i{}_{cn}\delta A^n_d) - (\mu + 3\not{\mu}\bar{q})\delta A^j_a\delta^a_j\epsilon^i{}_{cd} + (\mu + 3\not{\mu}\bar{q})\delta A^i_b\epsilon^b{}_{cd}\,,\\
\mathcal{B}^{i(1)}_{cd} &= \tau\partial_{[c}\delta A^i_{d]}\,,\\
\mathcal{A}^{i(2)}_{cd} &= \rho\epsilon^i{}_{mn}\delta A^m_c\delta A^n_d - \frac{1}{3}(\not{\mu} + \not{\nu})(\delta A^j_a\delta^a_j)^2\epsilon^i{}_{cd} + \not{\nu}(\epsilon^i{}_{md}\delta A^m_c + \epsilon^i{}_{cn}\delta A^n_d)\delta A^j_a\delta^a_j + \not{\mu}\delta A^i_b\epsilon^b{}_{cd}\delta A^j_a\delta^a_j\,,\\
\mathcal{B}^{i(2)}_{cd} &= 0\,,\\
\mathcal{C}^{i(2)}_{cd} &= 0\,.
\end{aligned}
\tag{63}
$$

In terms of

$$
\begin{aligned}
&\mathcal{F}^{(0)} = 6(-\mu\bar{q} + \nu\bar{q} - 3\not{\mu}\bar{q}^2 + 3\not{\nu}\bar{q}^2 + \rho\bar{q}^2)\,,\\
&\mathcal{A}^{(1)} = (-4\mu + 4\nu - 12\not{\mu}\bar{q} + 12\not{\nu}\bar{q} + 4\rho\bar{q})\delta A^k_d\delta^d_k = \frac{2}{3}\frac{\mathcal{F}^{(0)}}{\bar{q}}\delta A^k_d\delta^d_k\,,\\
&\mathcal{A}^{(2)} = \rho(\delta A^k_d\delta^d_k)^2 - \rho\delta A^m_c\delta A^n_d\delta^c_n\delta^d_m\,,\\
&\frac{\partial\mathcal{F}^{(0)}}{\partial\bar{q}} = 6(-\mu + \nu - 3\not{\mu}\bar{q} + 3\not{\nu}\bar{q} + 2\rho\bar{q}) = \frac{\mathcal{F}^{(0)}}{\bar{q}} + 6\rho\bar{q}\,,\\
&f^{i(0)}_{cd} = \frac{\mathcal{F}^{(0)}}{6}\epsilon^i{}_{cd} \quad , \quad \mathcal{B}^{(1)} = \tau\partial_c\delta A^i_d\epsilon_i{}^{cd}\,,\\
&\frac{\partial\mathcal{A}^{(1)}}{\partial\bar{q}} = 4\rho\delta A^k_d\delta^d_k\,,
\end{aligned}
\tag{64}
$$

the sum of the holonomy-modified Poisson brackets, (44), (45) and (46) is

$$
\begin{aligned}
&\{H[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\} + \{\delta H_Q[\delta N_1 - \delta N_2], H[\bar{N}]\} + \{\delta H_Q[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\}\\
=\; &\frac{1}{8\pi G}\int \mathrm{d}^3x\,\partial^c(\delta N_2 - \delta N_1)\frac{\bar{N}}{\bar{p}}\Big\{-(\frac{1}{4}\tau^2 + \tau)\left[\bar{p}\partial_k\delta A^k_c - \bar{p}\partial_c(\delta A^k_d\delta^d_k)\right]\\
&+\left[-\frac{1}{24}(\mathcal{F}^{(0)} + 6\bar{q}^2)\frac{\partial\tau}{\partial\bar{q}} + (1 + \frac{\tau}{2})(\mu + 3\not{\mu}\bar{q}) + \frac{1}{6}\frac{\mathcal{F}^{(0)}}{\bar{q}} + \frac{1}{2}\tau\bar{q} + \frac{1}{4}\tau^2\bar{q}\right]\bar{p}\delta A^n_d\epsilon^d{}_{cn}\\
&-\frac{1}{12}(\tau\mathcal{F}^{(0)} + 2\mathcal{F}^{(0)} + 6\tau\bar{q}^2)\epsilon^k{}_{cd}\delta E^d_k\Big\}\\
&+\frac{1}{8\pi G}\int \mathrm{d}^3x(\delta N_2 - \delta N_1)\frac{1}{72}(\mathcal{F}^{(0)} + 6\bar{q}^2)(\mathcal{F}^{(0)} - 6\rho\bar{q}^2)\left(\frac{1}{\bar{q}\sqrt{\bar{p}}}\delta E^d_k\delta^k_d - 2\frac{\sqrt{\bar{p}}}{\bar{q}^2}\delta A^k_d\delta^d_k\right)\,.
\end{aligned}
\tag{65}
$$

By using Eqs. (51), we express the Poisson bracket (65) in terms of the scalar modes $(\varepsilon_1, \varepsilon_2)$ and (κ_1, κ_2) as

$$
\begin{aligned}
&\{H[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\} + \{\delta H_Q[\delta N_1 - \delta N_2], H[\bar{N}]\} + \{\delta H_Q[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\}\\
=\; &\frac{1}{8\pi G}\int \mathrm{d}^3x\,\partial^c(\delta N_2 - \delta N_1)\frac{\bar{N}}{\bar{p}}\Big\{(\frac{1}{2}\tau^2 + 2\tau)\bar{p}\partial_c\kappa_1\\
&-\left[-\frac{1}{24}(\mathcal{F}^{(0)} + 6\bar{q}^2)\frac{\partial\tau}{\partial\bar{q}} + (1 + \frac{\tau}{2})(\mu + 3\not{\mu}\bar{q}) + \frac{1}{6}\frac{\mathcal{F}^{(0)}}{\bar{q}} + \frac{1}{2}\tau\bar{q} + \frac{1}{4}\tau^2\bar{q}\right]\partial_c(\varepsilon_1 + \Delta\varepsilon_2)\Big\}\\
&+\frac{1}{8\pi G}\int \mathrm{d}^3x(\delta N_2 - \delta N_1)\frac{1}{72}(\mathcal{F}^{(0)} + 6\bar{q}^2)(\mathcal{F}^{(0)} - 6\rho\bar{q}^2)\left[\frac{1}{\bar{q}\sqrt{\bar{p}}}(3\varepsilon_1 + \Delta\varepsilon_2) - 2\frac{\sqrt{\bar{p}}}{\bar{q}^2}(3\kappa_1 + \Delta\kappa_2)\right]\,.
\end{aligned}
\tag{66}
$$

Equation (66) implies that, in order to have a closed Poisson bracket, we should impose the conditions

$$
\begin{aligned}
&(\rho + 1)\bar{q}\frac{\partial\tau}{\partial\bar{q}} - 4\left(1 + \frac{\tau}{2}\right)\left(\frac{\mu}{\bar{q}} + 3\not{\mu}\right) + 2\tau - 4\rho = 0,\\
&\mu = \nu - 3\not{\mu}\bar{q} + 3\not{\nu}\bar{q}\,.
\end{aligned}
\tag{67}
$$

The Poisson bracket (66) can then be expressed as

$$
\begin{aligned}
&\{H[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\} + \{\delta H_Q[\delta N_1 - \delta N_2], H[\bar{N}]\}\\
&+\{\delta H_Q[\delta N_1 - \delta N_2], \delta H_Q[\bar{N}]\}\\
=\; &-\left(\frac{1}{4}\tau^2 + \tau\right)D[\bar{N}\bar{p}^{-1}\partial^c(\delta N_2 - \delta N_1)]\,.
\end{aligned}
\tag{68}
$$

Using (67), we obtain

$$-\bar{q}\frac{\partial\mu}{\partial\bar{q}}+\bar{q}\frac{\partial\nu}{\partial\bar{q}}=\bar{q}\frac{\partial}{\partial\bar{q}}\left(3\bar{q}(\not\mu-\not\psi)\right)=3\bar{q}^2\frac{\partial(\not\mu-\not\psi)}{\partial\bar{q}}+3\bar{q}(\not\mu-\not\psi) \tag{69}$$

such that (62) simplifies to $\bar{q}^2\partial\rho/\partial\bar{q}=0$. We arrive at the conditions

$$\begin{aligned}
&\rho=c_1\,,\\
&(c_1+1)\bar{q}\frac{\partial\tau}{\partial\bar{q}}-4\left(1+\frac{\tau}{2}\right)\left(\frac{\mu}{\bar{q}}+3\not\mu\right)+2\tau-4c_1=0\,,\\
&\sigma=3\bar{q}^2\not\psi\,,\\
&\not\phi=-\nu+\bar{q}\not\mu-3\bar{q}\not\psi\,,\\
&\widetilde{\not\phi}=-\frac{1}{3}(\not\mu+\not\psi)\,,\\
&\mu=\nu-3\not\mu\bar{q}+3\not\psi\bar{q}\,,
\end{aligned} \tag{70}$$

on anomaly-free constraints, where $\rho=c_1$ is now a constant independent of $\bar{q}$. In these conditions, there are three free functions of $\bar{q}$: ν, $\not\mu$ and $\not\psi$.

In [59], a different-looking equation, (38), has been derived for anomaly-freedom of vector modes. Slightly adapted to our notation, this condition reads

$$\begin{aligned}
0\;=\;&\frac{\partial\sigma}{\partial\bar{q}}+3\bar{q}\frac{\partial\not\phi}{\partial\bar{q}}+9\bar{q}^2\frac{\partial\widetilde{\not\phi}}{\partial\bar{q}}+\bar{q}\frac{\partial\mu}{\partial\bar{q}}+2\bar{q}\frac{\partial\nu}{\partial\bar{q}}+3\bar{q}^2\frac{\partial\not\mu}{\partial\bar{q}}\\
&+6\bar{q}^2\frac{\partial\not\psi}{\partial\bar{q}}+\bar{q}^2\frac{\partial\rho}{\partial\bar{q}}+\frac{\sigma}{\bar{q}}+6\not\phi+27\bar{q}\widetilde{\not\phi}+4\mu+15\bar{q}\not\mu\\
&+2\nu+12\bar{q}\not\psi\,.
\end{aligned} \tag{71}$$

If we insert (70), this equation is identically satisfied, such that the formulations for scalar and vector modes are consistent with each other.

We have found a candidate for a non-trivial holonomy-modified function f^i_{cd}, which satisfies anomaly-free constraint brackets for both scalar and vector modes up to second order. This non-trivial function can be written as

$$\begin{aligned}
f^i_{cd}\;=\;&3\bar{q}^2\not\psi\epsilon^i{}_{cd}+(-\nu+\bar{q}\not\mu-3\bar{q}\not\psi)\epsilon^i{}_{cd}A^j_a\delta^a_j\\
&+(\nu-3\not\mu\bar{q}+3\bar{q}\not\psi)A^i_b\epsilon^b{}_{cd}+\nu(\epsilon^i{}_{md}A^m_c+\epsilon^i{}_{cn}A^n_d)\\
&-\frac{1}{3}(\not\mu+\not\psi)\epsilon^i{}_{cd}(A^j_a\delta^a_j)^2+\not\mu A^i_b\epsilon^b{}_{cd}A^j_a\delta^a_j\\
&+\not\psi(\epsilon^i{}_{md}A^m_c+\epsilon^i{}_{cn}A^n_d)A^j_a\delta^a_j+c_1\epsilon^i{}_{mn}A^m_cA^n_d\\
&+\tau\partial_{[c}A^i_{d]}\,.
\end{aligned} \tag{72}$$

Here, τ is determined by the second equation in Eq. (70). When $\nu=\not\mu=\not\psi=0$, $\tau=2c_1$, the modification function returns to the form of classical curvature as $f^i_{cd}=c_1F^i_{cd}$, in which $\rho=c_1$ is a constant and can be absorbed in the definition of G.

C. SU(2)-covariance

It remains to check the SU(2)-covariance of the holonomy-modification function f^i_{cd} in (72). To this end, we calculate the Poisson bracket between the holonomy modifications of the Hamiltonian constraint, $\delta H_Q[N]$, and the Gauss constraint $G[\Lambda]$:

$$\begin{aligned}
\{\delta H_Q[N],G[\Lambda]\}\;=\;&\frac{1}{16\pi G}\int d^3xN\sqrt{|\det E|}\Big[4\bar{q}\not\psi(3-A^k_b\delta^b_k)D_l\Lambda^l+(\tau-2c_1)(A^k_be^b_kD_l\Lambda^l-A^k_be^b_lD_k\Lambda^l)\\
&+2\Lambda^l\Big((2\nu-3\not\mu\bar{q}+3\bar{q}\not\psi)A^k_b\epsilon^b{}_{lk}+(\not\mu+\not\psi)A^j_a\delta^a_jA^k_b\epsilon^b{}_{lk}+\left(c_1-\frac{1}{2}\tau\right)\epsilon^d{}_{mn}A^m_cA^n_de^c_l\Big)\Big]\,.
\end{aligned} \tag{73}$$

We have introduced the covariant derivative defined as

$$D_av^i=\partial_av^i-\epsilon^i{}_{jk}A^j_av^k\,. \tag{74}$$

From Eq. (73), it is easy to conclude that the Poisson bracket $\{\delta H_Q[N],G[\Lambda]\}$ vanishes only if the parameters satisfy $\nu=\not\mu=\not\psi=0$, $\tau=2c_1$. The modification function then returns to the classical case of $f^i_{cd}\propto F^i_{cd}$. Therefore, if we now combine the constraint brackets with the condition that all expressions be invariant under SU(2) transformations, the system turns out to be strongly restricted: In (72), only the last two terms (with coefficients ρ and τ) can appear in an SU(2)-covariant expression, as is well known from the possible covariant combinations of connection components. Moreover, the combination of the last two terms is covariant only if $\tau=2\rho=2c_1$. All other terms in (72) which are quadratic in δA^i_a must be zero, so that $\not\mu=\not\psi=\nu=0$, and also the first background contribution is ruled out. In particular, background holonomy modifications are ruled out in this model, which would give rise to a function $\not\psi(\bar{q})=(\ell\bar{q})^{-2}\sin^2(\ell\bar{q})-1\neq 0$. This result is in contrast to [25], where a consistent version with background holonomy modifications has been found using an extrinsic-curvature formulation instead of a connection formulation. (If there were background holonomy modifications similar to [25], they should contribute to (68) a factor of $\partial^2\not\psi/\partial\bar{q}^2$ in addition to τ^2.) The only allowed correction here is a function τ which would multiply the classical F^i_{cd}. Such a modification resembles the results from inverse-triad rather than holonomy modifications.

The appearance of this modification, however, shows an interesting analogy with the results of [25]: A crucial factor in the deformation function found in this paper is called $1+\tau_3$ there, which is the coefficient of $\partial_c\partial^j\delta E^c_j$

in the linear term of the Hamiltonian constraint. Such a second derivative of the triad perturbation also appears here, when one writes $\partial_{[c}\delta A^i_{d]}$ in terms of the spin connection and extrinsic curvature, and this term in (72) has the coefficient that appears in the deformation function in (68). Also the deformed brackets (68) resemble those found for inverse-triad corrections: The deformation function in the full contraint $H + \delta H_Q$ is one plus a correction function which does not necessarily change sign. There is an indication that signature change may be avoided in the presence of holonomy modifications because the deformation function in (68) does not depend on ψ, but then holonomy modifications are ruled out altogether in this model.

V. CONCLUSIONS

We have extended the investigation of inhomogeneous perturbations of the effective Hamiltonian constraint with holonomy modifications in Euclidean models of loop quantum gravity to include scalar modes. The Poisson brackets between a holonomy-modified Hamiltonian constraint and the diffeomorphism constraint as well as that between the two holonomy-modified Hamiltonian constraints have been calculated. It turns out that anomaly-free scalar modes impose stronger restrictions on the parameters of the holonomy-modification function than vector modes, but non-trivial modifications remain possible such that the Poisson brackets of Hamiltonian and diffeomorphism constraints are anomaly-free. If SU(2)-covariance is implemented, however, the modifications are much more tightly restricted, even ruling out background holonomy modifications. These results have several new implications and help to clarify relationships between previous studies.

A. Spatial derivatives

The main new ingredient used here, compared with existing models which allow background holonomy modifications, is the possibility of new corrections even at the classical form of at most first-order derivatives of the connection. We have motivated these new terms by starting with a connection rather than extrinsic-curvature formulation, in which case the derivative structure of the Hamiltonian constraint is different. The appearance of derivatives, in turn, affects possible modifications of constraint brackets derived using integration by parts.

If one does not implement SU(2)-covariance, one does not obtain a physical model but may still consider algebraic aspects of the system of Hamiltonian and diffeomorphism constraints, which turns out to be quite nontrivial. In this case, there are several free coefficients in (72), including background holonomy modifications ψ. However, the resulting bracket (68) does not show the characteristic form found in other such cases, which have led to signature change at high density: Structure functions in the classical bracket would be multiplied by $\frac{1}{2}\partial^2\psi/\partial\bar{q}^2$ for this form to be realized, but we have seen no such factor.

Although our results do not provide a physical model in this case, they may indicate that it is possible to avoid signature change and the associated indeterministic behavior, provided one starts with a connection formulation. The appearance of spatial derivatives in the Hamiltonian constraint is then different from an extrinsic-curvature formulation, which can affect the constraint brackets when integrating by parts. An extrinsic-curvature formulation has a classical Hamiltonian constraint without derivatives of the extrinsic curvature, while the densitized triad appears with up to second-order derivatives. In a connection formulation, the connection appears with up to first-order derivatives, while the densitized triad does not have derivative terms in the version used here, that is with $\gamma = 1$. The fact that signature change appears in the former but not in the latter case is consistent with the simple 1-dimensional model of [38].

In a comparison with results from self-dual variables [28–30], we see similar properties in that signature change or, more generally, modifications of the constraint brackets do not seem generic. Also at a formal level there are similarities, in particular the appearance of spatial derivatives of the connection in the constraint, which do not appear in extrinsic-curvature versions, and a more important role played by the Gauss constraint. The latter is usually solved explicitly in extrinsic-curvature formulations, which automatically ensures compatibility with its flow but also leads to less ambiguity in identifying the Hamiltonian constraint. In a connection formulation, by contrast, the Hamiltonian constraint is defined only up to multiples of the Gauss constraint. The form (2) used here is conventional, but not unique. One could use the Gauss constraint in order to eliminate spatial deirvatives of the connection, which may bring the structure closer to an extrinsic-curvature formulation. Such brackets, however, are beyond the scope of the present paper.

Since SU(2)-covariance leads to significant restrictions of the allowed modifications, the form of holonomies as covariant functionals of the connection gives further indications as to how a fully anomaly-free system could be found in a connection formulation. Holonomies are nonlocal in space because they are computed by integrating the connection over a curve. In an effective theory, such an expression appears in the form of a derivative expansion that does not end at any finite order. Therefore, SU(2)-covariant formulations may require higher spatial derivatives beyond the classical order. Holonomies as used in kinematical constructions of loop quantum gravity suggest that higher spatial derivatives are unaccompanied by higher time derivatives because one uses only spatial curves in holonomies. However, this picture suggests problems with space-time covariance because it is difficult to maintain different orders of space and time derivatives in a covariant formulation or, alternatively, because a spatial curve embedded in space-time may no longer be spatial after a general coordinate transformation.

B. Comparison between effective and operator approaches

The preceding arguments provide intuitive reasons why it seems difficult to have space-time covariance and SU(2) covariance in the same holonomy-based theory. At a formal level, these difficulties have been confirmed in spherically symmetric models [27]. On the other hand, [21, 22] suggest that very careful routings of loops used to construct holonomies for a quantization of the Hamiltonian constraint could lead to a full anomaly-free quantum theory. A comparison between these results therefore seems useful.

The operator constructions of [21, 22] so far have not given indications about possible deformations of the constraint brackets. Since they have been obtained in Euclidean gravity, our present results help to reconcile this outcome with those of effective derivations based on real variables, which generically lead to deformed constraint brackets. In the present paper, we used Euclidean gravity with a derivative structure of the Hamiltonian constraint that is more similar to the constraints quantized in [21, 22] than those of effective approaches in real variables. And here, as in the case of self-dual connections [28–30], the constraint brackets are subject to different modifications compared with Lorentzian models in real variables, and no deformations are possible if SU(2)-covariance is imposed.

While these are qualitative similarities, we emphasize that a comparison of constraint brackets in effective and operator approaches is not straightforward. Effective approaches, by construction, lead to constraints and brackets of classical type, and therefore implicitly assume that there is an underlying semiclassical state in which one has taken expectation values. Using the systematic treatment of canonical effective constraints [8, 43, 56, 57, 66], one can derive properties of such a semiclassical state within the effective formalism, but not much has been done in this direction in spherically symmetric or perturbed cosmological models. The operator treatment, on the other hand, results in commutators instead of brackets. A detailed comparison would therefore require an understanding of the semiclassical limit of loop quantum gravity, perhaps with input from effective results about semiclassical states. Consistent versions of effective constraint brackets should then be compared with expectation values of consistent commutators of constraint operators computed in a semiclassical state. Only the latter step of computing semiclassical expectation values would give unambiguous results about possible deformations of constraint brackets in operator approaches. Unfortunately, no such results are available owing to the complicated nature of the semiclassical limit of loop quantum gravity.

C. Space-time structure

The question whether it is possible to avoid indeterministic behavior in effective models of loop quantum gravity remains open, but at least the present results have confirmed the indications of [28–30] pointing to an affirmative answer. The form of signature change appears to depend on the specific formulation used, so that its absence would provide an additional restrictive condition together with anomaly-freedom alone. However, existing results need to be extended in several directions before a firm conclusion can be drawn. First, the derivative nature of the Hamiltonian constraint and therefore the constraint brackets are different for $\gamma \neq 1$, even if one still considers Euclidean gravity. Second, spatial derivatives in an effective constraint may be generated by quantum corrections even if they are absent from the classical constraint. All such derivatives should be included unless they are prohibited by symmetries. In background-independent quantum theories of gravity, symmetries of space-time are to be derived and do not restrict the terms in effective constraints used before anomaly-free brackets have been obtained. For the same reason, our calculations should be extended by including a general derivative expansion not just of A_a^i but also of E_j^b. In the same vein, one should extend our setup in this paper to the Lorentzian case, where the construction of the effective holonomy-modified Hamiltonian of full loop quantum gravity and the calculation of constraint brackets would be more complicated, as even the classical constraint would contain spatial derivatives of E_j^b via Γ_a^i. Matter terms added in an anomaly-free way provide another large question, as do the possible forms of higher-derivative corrections in both space and time.

There are therefore several extensions of existing calculations which should be completed before reliable conclusions about the potential consistency of loop quantum gravity can be drawn. Our present results differ in some crucial respects from previous calculations and should therefore help to provide a better estimate of the options realized in models of cosmological perturbations within this framework.

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