Semiclassical limit of new path integral formulation from reduced phase space loop quantum gravity

Muxin Han*

Department of Physics, Florida Atlantic University, 777 Glades Road, Boca Raton, Florida 33431, USA and Institut für Quantengravitation, Universität Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

Hongguang Liu†

Institut für Quantengravitation, Universität Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany and Center for Quantum Computing, Pengcheng Laboratory, Shenzhen 518066, China

(Received 23 May 2020; revised 3 July 2020; accepted 14 July 2020; published 28 July 2020)

Recently, a new path integral formulation of loop quantum gravity (LQG) has been derived in M. Han and H. Liu, Phys. Rev. D **101**, 046003 (2020). from the reduced phase space formulation of the canonical LQG. This paper focuses on the semiclassical analysis of this path integral formulation. We show that dominant contributions of the path integral come from solutions of semiclassical equations of motion (EOMs), which reduce to Hamilton's equations of holonomies and fluxes $h(e)$, $p^a(e)$ in the reduced phase space $\mathcal{P}_\gamma$ of the cubic lattice γ: $\frac{\mathrm{d}h(e)}{\mathrm{d}\tau} = \{h(e), \mathbf{H}\}$, $\frac{\mathrm{d}p^a(e)}{\mathrm{d}\tau} = \{p^a(e), \mathbf{H}\}$, where $\mathbf{H}$ is the discrete physical Hamiltonian. The semiclassical dynamics from the path integral becomes an initial value problem of Hamiltonian time evolution in $\mathcal{P}_\gamma$. Moreover when we take the continuum limit of the lattice γ, these Hamilton's equations reproduce correctly classical reduced phase space EOMs of gravity coupled to dust fields in the continuum, as far as initial and final states are semiclassical. Our result proves that the new path integral formulation has the correct semiclassical limit and indicates that the reduced phase space quantization in LQG is semiclassically consistent. Based on these results, we compare this path integral formulation and the spin foam formulation, and show that this formulation has several advantages including the finiteness, the relation with canonical LQG, and the freedom from cosine and flatness problems.

DOI: 10.1103/PhysRevD.102.024083

I. INTRODUCTION

In recent developments of loop quantum gravity (LQG), tremendous progress has been obtained by the covariant path integral approach (see e.g., [1] for a summary). The covariant path integral approach of LQG focuses on transition amplitudes of LQG states (such as spin networks). These amplitudes sum all possible evolution histories of LQG states, reflecting the idea of Feynman's path integral. Moreover the path integral approach makes it possible to bypass complications from the nonpolynomial Hamiltonian constraint operator and possibly reduce difficulties in computing physical quantities in LQG. Indeed, the path integral trades the noncommutativity of quantum operators for integrals of commutative c-numbers, and thus may reduce complicated operator manipulations to computable integrals. It is the reason why most developments of quantum field theories (QFTs) are made by using path integral formulas.

A popular path integral approach in LQG is the *spin foam formulation* [1,2]. This formulation constructs transition amplitudes of LQG on four-dimensional (4D) triangulations, and all these spin foam amplitudes are made by gluing elementary building blocks called vertex amplitudes, in analogy with Feynman amplitudes made by gluing vertices and propagators. This structure of spin foam amplitudes allows them to be studied both analytically and numerically. Semiclassical behaviors of spin foam amplitudes, given by the large-j asymptotics, have been extensively studied analytically and found a close relation to the Regge calculus of discrete gravity (see e.g., [3–16]). Numerical studies of spin foam amplitudes have been developed in [17–20]. Spin foams have also been related to quantum computations recently [21–23]. However, extensive studies of spin foam amplitudes reveal several severe problems:

*hanm@fau.edu
†liu.hongguang@cpt.univ-mrs.fr

(1) *Cosine problem*: In the large-j limit, the emergent (discrete) spacetime determined by the spin foam amplitude with a fixed semiclassical boundary state is highly nonunique in general, even when the semiclassical boundary state specifies both metric and extrinsic curvature at the boundary. Different discrete spacetimes have different 4D orientations at individual 4-simplices [6,7]. Although for a single vertex amplitude the orientation can be fixed by the boundary coherent state specifying both metric and extrinsic curvature [24], it cannot be generalized to many 4-simplices. If we view the spin foam as an initial value problem, then its semiclassical time evolution from a fixed initial condition in phase space can give many different trajectories; thus it is very different from classical physics.[1]

(2) *Flatness problem*: There are evidences indicating that in the large-j limit, spin foam amplitudes dominate at the flat spacetime and miss all other curved spacetimes [27–31]. Although some other work suggests that one may modify the large-j limit and/or definitions of spin foams in order to avoid the flatness problem [10,11,32], there is still no satisfactory resolution to the problem in full generality.[2]

(3) *Relation with canonical LQG*: The spin foam approach has been developed in parallel to the canonical approach of LQG. It is not clear how to relate spin foam amplitudes to any transition amplitude or physical inner product in the canonical LQG (see e.g., [34–39] for some earlier attempts). It is not clear about the unitarity of spin foam models.

(4) *Divergence:* Spin foam amplitudes are divergent [40–42] unless the quantum Lorentz group (with real q) is employed [43,44] (the quantum group relates to cosmological constant [8,45]).

(5) *Computational complexity*: Numerical computations are currently developed only for a single vertex amplitude. Even for the vertex amplitude, the computational complexity grows very fast as the spin j increases [17]. The computational complexity grows exponentially when the number of 4-simplices increases. Quantum computing might help in this perspective, but it is still at a very preliminary stage.

(6) *Lattice dependence*: There are infinitely many spin foam amplitudes with the same boundary state. These amplitudes are defined on different triangulations (with the same boundary). It is not clear how to remove the triangulation dependence and/or how to take the continuum limit at the quantum level. The diffeomorphism invariance is difficult to be implemented in spin foam models. Group field theory (GFT) provides an interesting proposal to sum over all triangulations, but it seems still difficult to extract all semiclassical smooth spacetimes from a fixed GFT partition function (while some special cases such as black holes and cosmology can indeed be extracted from the general GFT formalism [46–48]). There are also different approaches toward the spin foam continuum limit via lattice refinement and renormalization [20,49].

As a different approach, a new path integral formulation of LQG has been proposed recently in [50]. This path integral is derived from the reduced phase space formulation of canonical LQG. The reduced phase space formulation couples gravity to matter fields such as dusts or scalar fields (clock fields), followed by a deparametrization procedure, in which gravity variables are parametrized by values of clock fields, and constraints are solved classically. Results from the deparametrization are (1) the reduced phase space $\mathcal{P}$ on which all phase space functions are Dirac observables free of gauge redundancy [except for the SU(2) gauge freedom when using connection variables], and (2) the dynamics is governed by a physical Hamiltonian $\mathbf{H}_0$ generating physical time evolution (the physical time is the value of a clock field). The reduced phase space $\mathcal{P}$ of the gravity-matter system can be quantized using the standard LQG technique and result in the physical Hilbert space $\mathcal{H}$. The physical Hamiltonian is promoted to a positive self-adjoint Hamiltonian operator $\hat{\mathbf{H}}$ on $\mathcal{H}$. The reduced phase space quantization of LQG has been proposed conceptually in [51,52] and has been made concrete in [53–58] (Sec. II provides a review of the reduced phase space formulation).

The new path integral formula in [50] equals to the transition amplitude of the unitary evolution generated by $\hat{\mathbf{H}}$:

$$A_{[g],[g']} = \langle \Psi^t_{[g]} | \exp\left[-\frac{i}{\hbar} T \hat{\mathbf{H}} \right] | \Psi^t_{[g']} \rangle \tag{1}$$

of semiclassical initial and final physical states $\Psi^t_{[g']}$ and $\Psi^t_{[g]}$. Here $\Psi^t_{[g']}$ and $\Psi^t_{[g]}$ are SU(2) gauge invariant coherent states [59,60] in $\mathcal{H}_\gamma$, the physical Hilbert space on a cubic lattice γ. $[g]$ and $[g']$ label the gauge equivalence class of initial and final data in the phase space (g is the complex coordinate of the phase space). The path integral formula is derived from $A_{[g],[g']}$ by the standard method: discretizing T

[1]There are arguments that the sum over orientations in the 3D Ponzano-Regge model is necessary to properly implement the constraints [25]. Heuristically one might argue that the spin foam model should act as a projector onto the physical Hilbert space, and thus is necessary to integrate over positive and negative lapse and shift [26]. But the semiclassical analysis of spinfoam models indicates that the lapse and shift are discrete so orientations can jump from one simplex to another. This makes semiclassical interpretations of geometries from spin foams problematic.

[2]See also a recent numerical study toward understanding the problem [33].

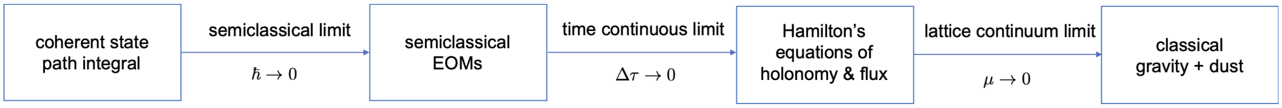

FIG. 1. The procedure of limits in this paper to reproduce classical gravity coupled to clock fields (dusts). μ is the coordinate length of lattice edges in the dust frame and used as the parameter for the lattice continuum limit.

into arbitrarily large N time steps and inserting the overcompleteness relation of coherent states. As a result, we obtain a discrete path integral on a 4D hypercubic lattice (see Sec. II for review):

$$\frac{A_{[g],[g']}}{\|\Psi^t_{[g]}\|\|\Psi^t_{[g']}\|} = \int \mathrm{d}h \prod_{i=1}^{N+1} \mathrm{d}g_i \, \nu[g] e^{S[g,h]/t}, \tag{2}$$

where we can extract a "classical action" $S[g,h]$ from the resulting path integral formula (see Sec. II B for details). $\int \mathrm{d}g_i \nu[g]$ integrates coherent states intermediating the quantum transition at different time steps $\tau_i = \frac{i}{N}T$. $t = \ell_P^2/a^2$ is a dimensionless semiclassicality parameter (it is preferred to take limits with dimensionless parameters), and a is a fixed length unit so that t is the numerical value of ℓ_P^2 measured in this unit (e.g., $t = 1.616 \times 10^{-35}$ when $a = 1m$). The semiclassical limit $\hbar \to 0$ corresponds to $t \to 0$ or $\ell_P \ll a$. Equation (2) has SU(2) integrals $\int \mathrm{d}h$ since the initial and final data have SU(2) gauge freedom.

This path integral formula is comparable to the spin foam amplitude in the coherent state representation [6] which is frequently used for analyzing the large-j behavior. On the other hand, if we choose the clock field to be a real massless scalar, Eq. (2) closely relates to the spin foam model in [61].[3] It is a matter of changing the representation basis to cast the path integral (2) into a shape similar to spin foams.

In this paper, we focus on the semiclassical analysis of the path integral formulation Eq. (2), i.e., the behavior as $t \to 0$. By stationary phase approximation, dominant contributions of the path integral come from solutions of semiclassical equations of motion (EOMs) $\delta S = 0$. These semiclassical EOMs have been derived in [50] and shown to admit time continuous limit $\Delta\tau = T/N \to 0$; i.e., all solutions can be approximated by continuous (and differentiable) trajectories $g(\tau)$ in the reduced phase space. In this paper, we show that in the time continuous limit, semiclassical EOMs derived from Eq. (2) become precisely the Hamilton's equation in the reduced phase space:

$$\frac{\mathrm{d}h(e)}{\mathrm{d}\tau} = \{h(e), \mathbf{H}\}, \qquad \frac{\mathrm{d}p^a(e)}{\mathrm{d}\tau} = \{p^a(e), \mathbf{H}\}, \tag{3}$$

where $h(e)$ and $p^a(e)$ are holonomy and gauge covariant flux associated with the edge e in γ. $h(e)$ and $p^a(e)$ relate to $g(e)$ by $g(e) = e^{-ip^a(e)\tau^a/2}h(e)$, $\tau^a = -i(\text{Pauli Matrix})^a$. $\{,\}$ is the Poisson bracket of the reduced phase space and reduces to the holonomy-flux algebra on γ. $\mathbf{H}$ is the semiclassical limit of $\hat{\mathbf{H}}$.

In addition, we show in Sec. VI that when we take the continuum limit of the lattice γ, EOMs (3) reproduce classical reduced phase space EOMs of gravity coupled to matter fields in the continuum, as far as initial and final states $\Psi^t_{[g']}$ and $\Psi^t_{[g]}$ are semiclassical in the sense that $[g'], [g]$ is within the classically allowed regime. The classically allowed regime in the phase space satisfy certain nonholonomic constraints required by the gravity-matter system. Our result proves that the path integral formulation Eq. (2) has the correct semiclassical limit and indicates that the reduced phase space quantization in LQG is semiclassically consistent. The procedure of limits in our analysis and results are summarized in Fig. 1.

Given semiclassical initial and final states and by Hamilton's equations (3), the semiclassical dynamics from $A_{[g],[g']}$ becomes an initial value problem of Hamiltonian time evolution in the reduced phase space. Fixing the initial condition $[g']$, the solution of EOMs (3), given by the Hamiltonian flow of $\mathbf{H}$, is unique up to SU(2) gauge transformation.

If semiclassical initial and final data $[g'], [g]$ are connected by the trajectory $g(\tau)$ satisfying Eq. (3), as $t \to 0$, the path integral (51) dominates at this semiclassical trajectory:

$$\frac{A_{[g],[g']}}{\|\Psi^t_{[g]}\|\|\Psi^t_{[g']}\|} = \frac{(2\pi t)^{\mathcal{N}/2}}{\sqrt{\det(-H)}} \nu[g(\tau), h] e^{S[g(\tau),h]/t}[1 + O(t)], \tag{4}$$

where $\mathcal{N}$ is the total dimension of the integral in Eq. (2) and H is the Hessian matrix at the solution. $S[g(\tau), h]$ is the action evaluated at the solution $g(\tau), h$, where the continuous trajectory $g(\tau) \simeq g_i$ approximates the discrete solution as $\Delta\tau$ small. If the initial and final data $[g'], [g]$ are not connected by the trajectory $g(\tau)$, the amplitude is suppressed exponentially as $t \to 0$.

It is interesting to make a comparison between the new path integral formulation of LQG (2) to the spin foam formulation.

(1) Our path integral formulation is free of the cosine problem. The initial state $\Psi^t_{[g']}$ determines a unique

[3] Namely Eq. (2) is the coherent state representation of the amplitude in [61], if their derivation uses graph-preserving Hamiltonian, and $\hat{\mathbf{H}}$ is the Hamiltonian in [62].

semiclassical trajectory [up to SU(e) gauge transformations] given by the Hamiltonian flow of $\mathbf{H}$. The asymptotic formula has a single exponential [integrated over SU(2) gauge transformations]. A key reason is that here all solutions of semiclassical EOMs admit a time continuous limit. Solutions with discontinuous orientations are forbidden.

(2) Our path integral formulation is free of the flatness problem. The semiclassical EOMs (3) from the path integral reproduce the classical EOMs of the gravity-matter system and admit all curved solutions that are physically interesting. For instance, Refs. [50,63] have demonstrated the homogeneous and isotropic cosmology and cosmological perturbation theory from solutions.

(3) There is a clear link between our path integral formulation and the canonical LQG.[4] The path integral (51) is rigorously derived from the canonical LQG. The unitarity is manifest because the path integral equals the transition amplitude of unitary evolution generated by $\hat{\mathbf{H}}$.

(4) The path integral formula (2) is finite for arbitrary finite N, and because of the transition amplitude $A_{[g],[g']}$ is manifestly finite. The finiteness is irrelevant to the cosmological constant.

There are open issues: Computing quantum effects within the path integral formulation (51) relies on knowledge of the matrix elements and/or expectation values of $\hat{\mathbf{H}}$ with respect to coherent states. The nonpolynomial operator $\hat{\mathbf{H}}$ may make computations highly involved. Second, the path integral is constructed on the lattice γ, and it is not clear at present if we are able to remove this lattice dependence at the quantum level. Although gauge symmetries from Hamiltonian and diffeomorphism constraints are resolved classically in the reduced phase space formulation, they lead to infinitely many classical conserved charges. But the discretization breaks these conservation laws except the conservation of $\mathbf{H}$ [57]. The limits in Fig. 1 can recover these classical conserved charges, but it is not clear how to make them conserved at the quantum level as well, due to the lattice dependence. This formulation may still share issues of computational complexity and lattice dependence with the spin foam formulation, at least at the current stage. However, studies of the new path integral formulation is still at a very preliminary stage, and research on overcoming these issues will be carried out in the future. Some discussions are given in Sec. VIII.

As a by-product from this work, we obtain an understanding of dusts or other clock fields from the LQG point of view, particularly whether dusts are valid in the quantum regime. Our attitude is that the quantum theory of LQG defined by the Hamiltonian $\hat{\mathbf{H}}$ should be the fundamental theory and starting point of discussions. Although the quantum theory is formally obtained by quantizing the classical theory, the classical theory is not fundamental but emergent from the fundamental quantum theory. From the quantum point of view, both classical gravity and dust are low-energy effective degrees of freedom produced from the quantum theory via the semiclassical approximation, as demonstrated in our work. Both classical gravity and dusts are not fundamental and not valid in the quantum regime but emergent at low energy, while what are valid in the quantum regime are $\hat{\mathbf{H}}$ defined on $\mathcal{H}$.

This work mainly focuses on scenarios with clock fields as Brown-Kuchař or Gaussian dusts. The generalization to a massless scalar clock field should be straightforward given that the formulation is defined for all three scenarios [50]. The generalization of the present formulation to include other matter fields, such as the Yang-Mills field and fermions, is based on existing quantizations of matters in the canonical LQG [66–68]. The detailed analysis is currently undergoing work.

Many computations in this work are carried out with *Mathematica* on high-performance-computing (HPC) servers. Some intermediate steps and results contain long formulas that cannot be shown in this paper. These formulas and *Mathematica* codes can be downloaded from [69].

The architecture of this paper is as follows: Section II reviews the reduced phase space formulation of LQG and the derivation of the new path integral formulation. Section III reviews semiclassical EOMs from the path integral and derives its time continuous limit in general (new results of this paper start in Sec. III B). Section IV shows that semiclassical EOMs are equivalent to Hamilton's equations (3). Section V shows that the time continuous limit of the action $S[g,h]$ gives a canonical action with the Hamiltonian $\mathbf{H}$, and demonstrates that the variational principle and time continuous limit are commutative when acting on $S[g,h]$. Section VI analyzes semiclassical EOMs in the lattice continuum limit of γ and demonstrates consistency with a classical gravity-matter system. Section VIII compares the new path integral formulation with the spin foam formulation.

II. REDUCED PHASE SPACE FORMULATION OF LQG

A. Classical framework

The reduced phase space formulation couples gravity to matter fields at a classical level. These matter fields are often called clock fields. In this paper, we mainly focus on two scenarios including coupling gravity to Brown-Kuchař and Gaussian dust fields [57,58,70,71]. The action of gravity coupled to Brown-Kuchař dust is given by

[4] Advantages from relating canonical and path integral formulation can be seen from loop quantum cosmology (LQC) in studying the physical inner product [64,65].

$$S = S_{\mathrm{GR}} + S_{\mathrm{BKD}}. \tag{5}$$

The gravity action is given by the Holst action

$$S_{\mathrm{GR}} = \frac{1}{16\pi G}\int_M d^4x e e_A^\mu e_B^\nu \left(\Omega_{\mu\nu}^{AB} + \frac{1}{2\beta}\epsilon^{AB}{}_{CD}\Omega_{\mu\nu}^{CD}\right) \tag{6}$$

where e_A^μ is the tetrad, e is the determinant of e_A^μ, and $\Omega_{\mu\nu}^{AB}$ is the curvature of the so(1,3) connection ω_μ^{AB}. β is the Barbero-Immirzi parameter. S_{BKD} is the action of Brown-Kuchař dust:

$$S_{\mathrm{BKD}}[\rho, g_{\mu\nu}, T, S^j, W_j] = -\frac{1}{2}\int \mathrm{d}^4x\sqrt{|\det(g)|}\rho[g^{\mu\nu}U_\mu U_\nu + 1], \tag{7}$$

$$U_\mu = -\partial_\mu T + W_j\partial_\mu S^j, \tag{8}$$

where scalars $T, S^{j=1,2,3}$ form the dust coordinates of time and space to parametrize physical fields. ρ, W_j are Lagrangian multipliers. ρ is interpreted as the dust energy density. When we couple S_{BKD} to gravity (or gravity is coupled to some other matter fields) and carry out the Hamiltonian analysis [58], we obtain the following constraints:

$$\mathcal{C}^{\mathrm{tot}} = \mathcal{C} + \frac{1}{2}\left[\frac{P^2/\rho}{\sqrt{\det(q)}} + \sqrt{\det(q)}\rho(q^{\alpha\beta}U_\alpha U_\beta + 1)\right] = 0, \tag{9}$$

$$\mathcal{C}_\alpha^{\mathrm{tot}} = \mathcal{C}_\alpha + PT_{,\alpha} - P_j S^j_{,\alpha} = 0, \tag{10}$$

$$\rho^2 = \frac{P^2}{\det(q)}(1 + q^{\alpha\beta}U_\alpha U_\beta)^{-1}, \tag{11}$$

$$W_j = P_j/P, \tag{12}$$

where α and β are spatial coordinate indices, P and P_j are momenta conjugate to T and S^j, $q_{\alpha\beta}$ is the three metric on spatial slices, and $\mathcal{C}$ and $\mathcal{C}_\alpha$ are Hamiltonian and diffeomorphism constraints of gravity (or gravity coupled to some other matter fields). First Eq. (11) can be solved by

$$\rho = \varepsilon\frac{P}{\sqrt{\det(q)}}(1 + q^{\alpha\beta}U_\alpha U_\beta)^{-1/2}, \qquad \varepsilon = \pm 1. \tag{13}$$

ε can be fixed to $\varepsilon = 1$ by a physical requirement that U is timelike and future pointing [55], so $\mathrm{sgn}(P) = \mathrm{sgn}(\rho)$. Inserting this solution into Eq. (9) and using Eq. (12) lead to

$$\mathcal{C} = -P\sqrt{1 + q^{\alpha\beta}\mathcal{C}_\alpha\mathcal{C}_\beta/P^2}. \tag{14}$$

Thus $-\mathrm{sgn}(\mathcal{C}) = \mathrm{sgn}(P) = \mathrm{sgn}(\rho)$. When we consider dust coupling to pure gravity, we must have $\mathcal{C} < 0$ and the physical dust $\rho, P > 0$ to fulfill the energy condition as in [70]. However, we may couple some additional matter fields (e.g., scalars, fermions, gauge fields) to make $\mathcal{C} > 0$, and then $\rho, P < 0$ correspond to the phantom dust as in [55,57]. The case of phantom dust may not violate the usual energy condition due to the presence of additional matter fields. We can solve P, P_j from Eqs. (9) and (10),

$$P = \begin{cases} h & \text{physical dust,} \\ -h & \text{phantom dust,} \end{cases} \qquad h = \sqrt{\mathcal{C}^2 - q^{\alpha\beta}\mathcal{C}_\alpha\mathcal{C}_\beta}, \tag{15}$$

$$P_j = -S_j^\alpha(\mathcal{C}_\alpha - hT_{,\alpha}), \tag{16}$$

which are strongly Poisson commutative constraints. S_j^α is the inverse matrix of $\partial_\alpha S^j$ ($\alpha = 1, 2, 3$). In deriving the above constraints, we find at an intermediate step that $P^2 = \mathcal{C}^2 - q^{\alpha\beta}\mathcal{C}_\alpha\mathcal{C}_\beta > 0$ constrains the argument of the square root to be positive. Moreover the physical dust requires $\mathcal{C} < 0$ due to the energy condition while the phantom dust requires $\mathcal{C} > 0$. $\mathcal{C}^2 - q^{\alpha\beta}\mathcal{C}_\alpha\mathcal{C}_\beta > 0$ and $\mathcal{C} < 0$ ($\mathcal{C} > 0$) are nonholonomic constraints for the reduced phase space.

We use $A_\alpha^a(x)$, $E_a^\alpha(x)$ to be canonical variables of gravity, where $A_\alpha^a(x)$ is the Ashtekar-Barbero connection and $E_a^\alpha(x) = \sqrt{\det q}\, e_a^\alpha(x)$ is the densitized triad. $a = 1, 2, 3$ is the Lie algebra index of su(2). Dirac observables are constructed relationally by parametrizing (A, E) with values of dust fields $T(x) \equiv \tau$, $S^j(x) \equiv \sigma^j$, i.e., $A_j^a(\sigma, \tau) = A_j^a(x)|_{T(x)\equiv\tau, S^j(x)\equiv\sigma^j}$ and $E_a^j(\sigma, \tau) = E_a^j(x)|_{T(x)\equiv\tau, S^j(x)\equiv\sigma^j}$, where σ, τ are physical space and time coordinates in the dust reference frame. Here $j = 1, 2, 3$ is the dust coordinate index (e.g., $A_j = A_\alpha S_j^\alpha$). Intuitively, $A_j^a(\sigma, \tau)$, $E_a^j(\sigma, \tau)$ depending only on values of dust fields should be independent of choices of coordinates x, i.e., should be gauge invariant. Indeed, they are proven to be invariant (on the constraint surface) under gauge transformations generated by diffeomorphism and Hamiltonian constraints [53,54,57]. Moreover $A_j^a(\sigma, \tau)$ and $E_a^j(\sigma, \tau)$ satisfy the standard Poisson bracket in the dust frame:

$$\{E_a^i(\sigma, \tau), A_j^b(\sigma', \tau)\} = \frac{1}{2}\kappa\beta\delta_j^i\delta_a^b\delta^3(\sigma, \sigma'), \tag{17}$$

where β is the Barbero-Immirzi parameter and $\kappa = 16\pi G$. $A_j^a(\sigma, \tau)$ and $E_a^j(\sigma, \tau)$ are the conjugate pair in the reduced phase space $\mathcal{P}$.

The evolution in physical time τ is generated by the classical physical Hamiltonian $\mathbf{H}_0$ given by integrating h on the constant $T = \tau$ slice $\mathcal{S}$. The constant τ slice $\mathcal{S}$ is coordinated by the value of dust scalars, and $S^j = \sigma^j$ thus is referred to as the dust space [57,58]. From Eq. (15), we find that $\mathbf{H}_0$ is negative for physical dust while it is positive for phantom dust. We flip the direction of the time flow $\tau \to -\tau$ and thus $\mathbf{H}_0 \to -\mathbf{H}_0$ for physical dust so we have a positive Hamiltonian in every case:

$$\mathbf{H}_0 = \int_{\mathcal{S}} \mathrm{d}^3\sigma \sqrt{\mathcal{C}(\sigma,\tau)^2 - \frac{1}{4}\sum_{a=1}^{3} \mathcal{C}_a(\sigma,\tau)^2}. \quad (18)$$

Here $\mathcal{C}$ and $\mathcal{C}_a = 2e_a^\alpha \mathcal{C}_\alpha$ are parametrized in the dust frame. In terms of $A_j^a(\sigma,\tau)$ and $E_a^j(\sigma,\tau)$,

$$\mathcal{C} = \frac{1}{\kappa}[F_{jk}^a - (\beta^2+1)\varepsilon_{ade}K_j^d K_k^e]\varepsilon_{abc}\frac{E_b^j E_c^k}{\sqrt{\det(q)}} + \frac{2\Lambda}{\kappa}\sqrt{\det(q)}, \quad (19)$$

$$\mathcal{C}_a = \frac{4}{\kappa\beta} F_{jk}^b \frac{E_a^j E_b^k}{\sqrt{\det(q)}}, \quad (20)$$

where all the above quantities are Dirac observables. K_j^a is the extrinsic curvature, and F_{jk}^a is the curvature of the connection A_j^a. $\tau^a = -i(\text{Pauli matrix})^a$. β is the Barbero-Immirzi parameter. Λ is the cosmological constant.

Coupling gravity to a Gaussian dust model can be analyzed similarly, so we do not present the details here (while details can be found in [58]). As a result the physical Hamiltonian has a simpler expression,

$$\mathbf{H}_0 = \int_{\mathcal{S}} \mathrm{d}^3\sigma\, \mathcal{C}(\sigma,\tau). \quad (21)$$

In order to put discussions of both the Brown-Kuchař and Gaussian dusts in a unified manner, we express the physical Hamiltonian as the following:

$$\mathbf{H}_0 = \int_{\mathcal{S}} \mathrm{d}^3\sigma\, h(\sigma,\tau), \quad (22)$$

$$h(\sigma,\tau) = \sqrt{\mathcal{C}(\sigma,\tau)^2 - \frac{\alpha}{4}\sum_{a=1}^{3}\mathcal{C}_a(\sigma,\tau)^2}, \qquad \begin{cases} \alpha = 1 & \text{Brown-Kuchař dust,} \\ \alpha = 0 & \text{Gaussian dust.} \end{cases}$$

The physical Hamiltonian $\mathbf{H}_0$ is manifestly positive in Eq. (22). When $\mathcal{C} < 0$, Eq. (22) is different from Eq. (21) by an overall minus sign, thus the time flow $\tau \to -\tau$ for the Gaussian dust is reversed compared to Brown-Kucha dust.

In both scenarios, the physical Hamiltonian $\mathbf{H}_0$ generates the τ-time evolution,

$$\frac{\mathrm{d}f}{\mathrm{d}\tau} = \{f, \mathbf{H}_0\}, \quad (23)$$

for all phase space function f of $A_j^a(\sigma,\tau)$ and $E_a^j(\sigma,\tau)$. In particular, the Hamilton's equations are

$$\frac{\mathrm{d}A_j^a(\sigma,\tau)}{\mathrm{d}\tau} = -\frac{\kappa\beta}{2}\frac{\delta\mathbf{H}_0}{\delta E_a^j(\sigma,\tau)}, \qquad \frac{\mathrm{d}E_a^j(\sigma,\tau)}{\mathrm{d}\tau} = \frac{\kappa\beta}{2}\frac{\delta\mathbf{H}_0}{\delta A_j^a(\sigma,\tau)}. \quad (24)$$

Functional derivatives on the right-hand sides of Eq. (24) can be computed by

$$\delta\mathbf{H}_0 = \int_{\mathcal{S}} \mathrm{d}^3\sigma \left(\frac{\mathcal{C}}{h}\delta\mathcal{C} - \frac{\alpha}{4}\frac{\mathcal{C}_a}{h}\delta\mathcal{C}_a\right), \quad (25)$$

where $\mathcal{C}/h$ is negative for physical dust and positive for phantom dust. Comparing $\delta\mathbf{H}$ to the variation of the Hamiltonian $H_{\mathrm{GR}} = \int \mathrm{d}^3x(N\mathcal{C} + N^\alpha\mathcal{C}_\alpha)$ of pure gravity in the absence of dust motivates us to view

$$N = \frac{\mathcal{C}}{h} \quad (26)$$

as the physical lapse function. N is negative (positive) for the physical (phantom) dust. Negative N for the physical dust relates to the flip $\tau \to -\tau$ for making the Hamiltonian positive.

In the gravity-dust models, we resolve the Hamiltonian and diffeomorphism constraints classically, while the SU(2) Gauss constraint $\mathcal{G}_a(\sigma,\tau) = D_j E_a^j(\sigma,\tau) = 0$ still has to be imposed to the phase space. In addition, nonholonomic constraints are imposed to the phase space: $\mathcal{C}(\sigma,\tau)^2 - \frac{\alpha}{4}\sum_{a=1}^{3}\mathcal{C}_a(\sigma,\tau)^2 \geq 0$ and $\mathcal{C} < 0$ for physical dust ($\mathcal{C} > 0$ for phantom dust). Recall that nonholonomic constraints come from $P^2 > 0$ and the energy condition.

These constraints are preserved by the time evolution for gravity coupled to the Brown-Kuchař dust. Indeed, first the time evolution cannot break the Gauss constraint since $\{\mathcal{G}_a(\sigma,\tau), \mathbf{H}_0\} = 0$. Second, both $h(\sigma,\tau)$ and $\mathcal{C}_j(\sigma,\tau) = \frac{1}{2}e_j^a\mathcal{C}_a(\sigma,\tau)$ are conserved densities on the Gauss constraint surface [57]:

$$\frac{\mathrm{d}h(\sigma,\tau)}{\mathrm{d}\tau} = \{h(\sigma,\tau), \mathbf{H}_0\} = 0,$$
$$\frac{\mathrm{d}\mathcal{C}_j(\sigma,\tau)}{\mathrm{d}\tau} = \{\mathcal{C}_j(\sigma,\tau), \mathbf{H}_0\} = 0. \quad (27)$$

Therefore $\mathcal{C}(\sigma,\tau)^2 - \frac{1}{4}\sum_{a=1}^3 \mathcal{C}_a(\sigma,\tau)^2 = h(\sigma,\tau)^2 \geq 0$ is conserved in the time evolution. About the other nonholonomic constraint $\mathcal{C} < 0$ ($\mathcal{C} > 0$), one can show that it is also conserved. This can be seen as the following: suppose $\mathcal{C} < 0$ ($\mathcal{C} > 0$) was violated in the time evolution; there would exist a certain time τ_0 that $\mathcal{C}(\sigma,\tau_0) = 0$, but then $\mathcal{C}(\sigma,\tau)^2 - \frac{1}{4}\sum_{a=1}^3 \mathcal{C}_a(\sigma,\tau)^2$ would become negative if $\mathcal{C}_j(\sigma,\tau) \neq 0$, contradicting the conservation of $h(\sigma,\tau)$ and the other nonholonomic constraint. If the conserved $\mathcal{C}_j(\sigma,\tau) = 0$, $h(\sigma,\tau)^2 = \mathcal{C}(\sigma,\tau)^2$ is conserved so it cannot evolve from nonzero to zero. For gravity coupled to the Gaussian dust, $\mathcal{C}_j(\sigma,\tau)$ is conserved. $h(\sigma,\tau)$ and $\mathcal{C}(\sigma,\tau)$ are conserved only when $\mathcal{C}_j(\sigma,\tau) = 0$. $\mathcal{C} < 0$ ($\mathcal{C} > 0$) may be violated in the time evolution for gravity coupled to the Gaussian dust if $\mathcal{C}_j(\sigma,\tau) \neq 0$.

In our following discussion, we focus on pure gravity coupling to dusts, thus we only work with physical dusts in order not to violate the energy condition.

B. Quantization, transition amplitude, and coherent state path integral

We construct a fixed cubic lattice γ which partitions the dust space $\mathcal{S}$. In this work, we consider $\mathcal{S}$ is compact and has no boundary so that γ is a finite lattice. We denote by $E(\gamma)$ and $V(\gamma)$ sets of (oriented) edges and vertices in γ. We assign every edge a constant coordinate length μ evaluated in the dust frame. $\mu \to 0$ relates to the lattice continuum limit. Every vertex $v \in V(\gamma)$ is six-valent. At v there are three outgoing edges $e_I(v)$ ($I = 1,2,3$) and three incoming edges $e_I(v - \mu\hat{I})$ where $\hat{I}$ is the coordinate basis vector along the Ith direction when we adapt the dust coordinate to the lattice. It is sometimes convenient to orient all six edges at v to be outgoing from v and denote six edges by $e_{v;I,s}$ ($s = \pm$):

$$e_{v;I,+} = e_I(v), \qquad e_{v;I,-} = e_I(v - \mu\hat{I})^{-1}. \tag{28}$$

These notations are illustrated in Fig. 2.

We regularize canonical variables $A_j^a(\sigma,\tau)$ and $E_a^j(\sigma,\tau)$ on the lattice γ, by defining holonomy $h(e)$ and gauge covariant flux $p^a(e)$ at every $e \in E(\gamma)$:

$$\begin{aligned} h(e) &:= \mathcal{P}\exp\int_e A, \\ p^a(e) &:= -\frac{1}{2\beta a^2}\mathrm{tr}\left[\tau^a \int_{S_e} \varepsilon_{ijk}\mathrm{d}\sigma^i \wedge \mathrm{d}\sigma^j h(\rho_e(\sigma)) E_b^k(\sigma)\tau^b h(\rho_e(\sigma))^{-1}\right], \end{aligned} \tag{29}$$

where $A = A^a\tau^a/2$ and $\tau^a = -i(\text{Pauli matrix})^a$ are two-dimensional anti-Hermitian matrices:

$$\tau^1 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \qquad \tau^2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \qquad \tau^3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{30}$$

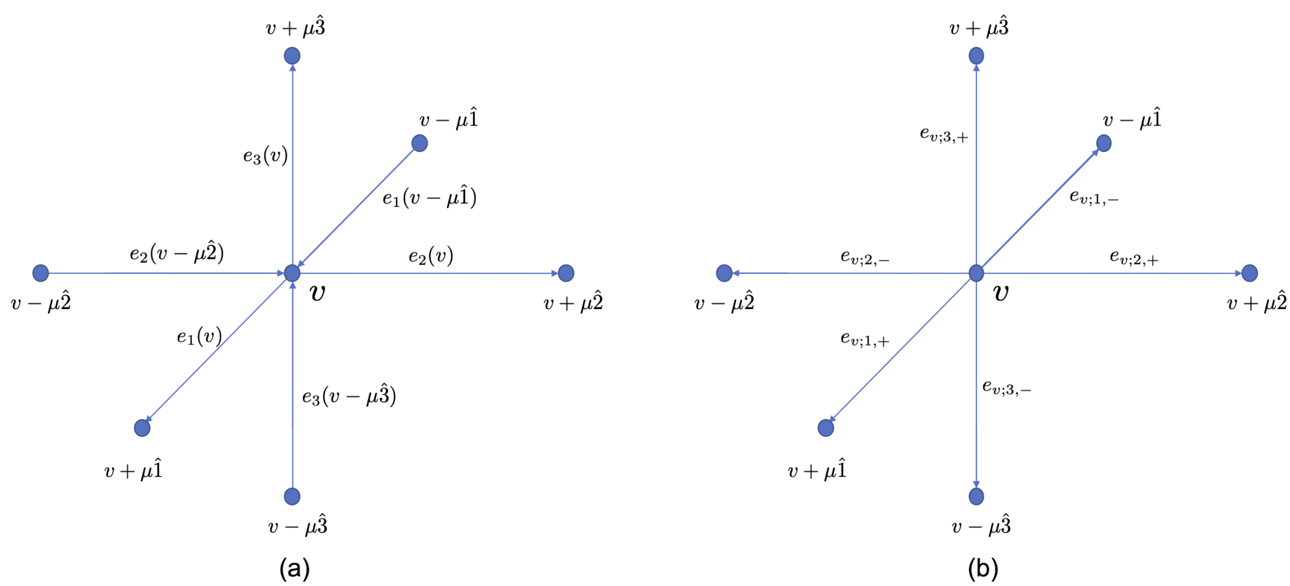

FIG. 2. (a) Notations of edges and vertices when all six edges are oriented toward positive directions of coordinates. (b) Notations of edge and vertices when all six edges are oriented outgoing from v.

S_e is a two-face intersecting e in the dual lattice γ^*. ρ_e is a path starting at the source of e, traveling along e until $e \cap S_e$, and then running in S_e until $\vec{\sigma}$. a is a length unit for making $p^a(e)$ dimensionless. Note that because $p^a(e)$ is gauge covariant flux, we have

$$p^a(e_{v;I,-}) = \frac{1}{2}\mathrm{Tr}[\tau^a h(e_{v-\hat{I};I,+})^{-1} p^b(e_{v-\hat{I};I,+})\tau^b h(e_{v-\hat{I};I,+})]. \tag{31}$$

The Poisson algebra of $h(e)$ and $p^a(e)$ is called the holonomy-flux algebra:

$$\{h(e), h(e')\} = 0, \tag{32}$$

$$\{p^a(e), h(e')\} = \frac{\kappa}{a^2}\delta_{e,e'}\frac{\tau^a}{2}h(e'), \tag{33}$$

$$\{p^a(e), p^b(e')\} = -\frac{\kappa}{a^2}\delta_{e,e'}\varepsilon_{abc}p^c(e'), \tag{34}$$

where $h(e)$ and $p^a(e)$ parametrize the reduced phase space $\mathcal{P}_\gamma$ for the theory discretized on γ.

The LQG quantization defines the Hilbert space $\mathcal{H}_\gamma$ spanned by gauge invariant (complex valued) functions of all $h(e)$'s on γ, and is a proper subspace of $\mathcal{H}^0_\gamma = \otimes_e L^2(\mathrm{SU}(2))$ of non-gauge-invariant states. $\mathcal{H}_\gamma$ is obtained by imposing the SU(2) Gauss constraint to $\mathcal{H}^0_\gamma$. $\mathcal{H}_\gamma$ is the physical Hilbert space free of constraint because it quantizes the reduced phase space. $\hat{h}(e)$ becomes multiplication operators on functions in $\mathcal{H}^0_\gamma$. $\hat{p}^a(e) = it\hat{R}^a_e/2$ where $\hat{R}^a_e$ is the right invariant vector field on SU(2): $R^a f(h) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}|_{\varepsilon=0} f(e^{\varepsilon\tau^a}h)$. $t = \ell_p^2/a^2$ is a dimensionless semiclassicality parameter ($\ell_p^2 = \hbar\kappa$). a is a fixed length unit so that t is the numerical value of ℓ_P^2 measured in this unit (e.g., $t = 1.616 \times 10^{-35}$ when $a = 1m$). The semiclassical limit $\hbar \to 0$ corresponds to $t \to 0$ or $\ell_P \ll a$.

$\hat{h}(e)$ and $\hat{p}^a(e)$ satisfy the commutation relations:

$$\begin{aligned} &[\hat{h}(e), \hat{h}(e')] = 0, \\ &[\hat{p}^a(e), \hat{h}(e')] = it\delta_{e,e'}\frac{\tau^a}{2}h(e'), \\ &[\hat{p}^a(e), \hat{p}^b(e')] = -it\delta_{e,e'}\varepsilon_{abc}p^c(e'), \end{aligned} \tag{35}$$

as quantization of the holonomy-flux algebra.

The (non-graph-changing) physical Hamiltonian operators $\hat{\mathbf{H}}$ are given by [57]

$$\hat{\mathbf{H}} = \sum_{v\in V(\gamma)} \hat{H}_v, \qquad \hat{H}_v \coloneqq [\hat{M}^\dagger_-(v)\hat{M}_-(v)]^{1/4}, \tag{36}$$

$$\hat{M}_-(v) = \hat{C}^\dagger_v\hat{C}_v - \frac{\alpha}{4}\sum_{a=1}^{3}\hat{C}^\dagger_{a,v}\hat{C}_{a,v}, \qquad \alpha = \begin{cases} 1, & \text{Brown-Kuchař dust}, \\ 0, & \text{Gaussian dust}. \end{cases} \tag{37}$$

In our notation, $\mathbf{H}_0 = \int_S \mathrm{d}^3\sigma h$, $\mathcal{C}$, and $\mathcal{C}_a$ are the Hamiltonian, Hamiltonian constraint, and diffeomorphism constraint in the continuum. $\mathbf{H} = \sum_v H_v$, C_v, and $C_{a,v}$ are their discretizations on γ at certain vertex v, while $\hat{\mathbf{H}} = \sum_v \hat{H}_v$, $\hat{C}_v$, and $\hat{C}_{a,v}$ are quantizations of $\mathbf{H}$, C_v, and $C_{a,v}$:

$$\hat{C}_{0,v} = -\frac{1}{i\beta\kappa\ell_p^2}\sum_{s_1,s_2,s_3=\pm1} s_1s_2s_3\varepsilon^{I_1I_2I_3}\mathrm{Tr}(\hat{h}(\alpha_{v;I_1s_1,I_2s_2})\hat{h}(e_{v;I_3s_3})[\hat{h}(e_{v;I_3s_3})^{-1}, \hat{V}_v]), \tag{38}$$

$$\hat{C}_{a,v} = -\frac{2}{i\beta^2\kappa\ell_p^2}\sum_{s_1,s_2,s_3=\pm1} s_1s_2s_3\varepsilon^{I_1I_2I_3}\mathrm{Tr}(\tau^a\hat{h}(\alpha_{v;I_1s_1,I_2s_2})\hat{h}(e_{v;I_3s_3})[\hat{h}(e_{v;I_3s_3})^{-1}, \hat{V}_v]), \tag{39}$$

$$\begin{aligned} &\hat{C}_v = \hat{C}_{0,v} + \frac{1+\beta^2}{2}\hat{C}_{L,v} + \frac{2\Lambda}{\kappa}\hat{V}_v, \qquad \hat{K} = \frac{i}{\hbar\beta^2}\left[\sum_{v\in V(\gamma)}\hat{C}_{0,v}, \sum_{v\in V(\gamma)} V_v\right], \\ &\hat{C}_{L,v} = \frac{16}{\kappa(i\beta\ell_p^2)^3}\sum_{s_1,s_2,s_3=\pm1} s_1s_2s_3\varepsilon^{I_1I_2I_3} \\ &\quad\times \mathrm{Tr}(\hat{h}(e_{v;I_1s_1})[\hat{h}(e_{v;I_1s_1})^{-1}, \hat{K}]\hat{h}(e_{v;I_2s_2})[\hat{h}(e_{v;I_2s_2})^{-1}, \hat{K}]\hat{h}(e_{v;I_3s_3})[\hat{h}(e_{v;I_3s_3})^{-1}, \hat{V}_v]), \end{aligned} \tag{40}$$

where $\hat{C}_{0,v}$ and $\hat{C}_{L,v}$ are Euclidean and Lorentzian terms in Thiemann's Hamiltonian constraint operator (at the vertex v on the cubic lattice), and $\hat{V}_v$ is the volume operator at v,

$$\hat{V}_v = (\hat{Q}_v^2)^{1/4}, \tag{41}$$

$$\hat{Q}_v = -i\left(\frac{\beta\ell_P^2}{4}\right)^3 \varepsilon_{abc} \frac{R^a_{e_{v;1+}} - R^a_{e_{v;1-}}}{2} \frac{R^b_{e_{v;2+}} - R^b_{e_{v;2-}}}{2} \frac{R^c_{e_{v;3+}} - R^c_{e_{v;3-}}}{2}$$
$$= \beta^3 a^6 \varepsilon_{abc} \frac{\hat{p}^a(e_{v;1+}) - \hat{p}^a(e_{v;1-})}{4} \frac{\hat{p}^b(e_{v;2+}) - \hat{p}^b(e_{v;2-})}{4} \frac{\hat{p}^c(e_{v;3+}) - \hat{p}^c(e_{v;3-})}{4}. \tag{42}$$

In writing these operators, we have employed the notation of edges in Fig. 2(b). We have made choices in $\hat{C}_v$ and $\hat{C}_{j,v}$ that (1) they are based on discretizations on the cubic lattice γ and are non-graph-changing operators, and (2) minimal loops $\alpha_{v;I_1s_1,I_2s_2}$ (around the plaquette bounded by $e_{v;I_1,s_1}, e_{v;I_2,s_2}$) carry the fundamental representation of SU(2).

The Hamiltonian operator $\hat{\mathbf{H}}$ is positive semidefinite and self-adjoint because $\hat{M}_-^\dagger(v)\hat{M}_-(v)$ is manifestly positive semidefinite and Hermitian, and therefore admits a self-adjoint extension (Friedrich extension [72]).

Classical discrete C_v and $C_{a,v}$ are obtained from Eqs. (38)–(40) by mapping operators to their classical counterparts and $[\hat{f}_1, \hat{f}_2] \to i\hbar\{f_1, f_2\}$. Hence classical discrete physical Hamiltonian $\mathbf{H}$ is given by

$$\mathbf{H} = \sum_{v\in V(\gamma)} H_v, \qquad H_v = \sqrt{\left|C_v^2 - \frac{\alpha}{4}\sum_{a=1}^3 C_{a,v}^2\right|}. \tag{43}$$

The absolute value in the square-root results from that $\mathbf{H}$ is the classical limit of $\hat{\mathbf{H}}$ defined on the entire $\mathcal{H}_\gamma$ disregarding nonholonomic constraints in particular $\mathcal{C}^2 - \frac{\alpha}{4}\sum_{a=1}^3 \mathcal{C}_a^2 \geq 0$ for $\alpha = 1$.

An interesting quantity for quantum dynamics is the transition amplitude

$$A_{[g],[g']} = \langle \Psi^t_{[g]} | \exp\left[-\frac{i}{\hbar} T\hat{\mathbf{H}}\right] | \Psi^t_{[g']} \rangle. \tag{44}$$

For the purpose of semiclassical analysis, we focus on the semiclassical initial and final states $\Psi^t_{[g']}$, $\Psi^t_{[g]}$ which are gauge invariant coherent states [60,73]. The coherent state label parametrizes the LQG phase space, and the overlap function of these states behaves as a sharply peaked Gaussian in phase space, thus building the link with phase space dynamical variables in the semiclassical limit. $\Psi^t_{[g]}$ is expressed as

$$\Psi^t_{[g]}(h) = \int_{\mathrm{SU}(2)^{|V(\gamma)|}} \mathrm{d}h \prod_{e\in E(\gamma)} \psi^t_{h^{-1}_{s(e)} g(e) h_{t(e)}}(h(e)), \qquad \mathrm{d}h = \prod_{v\in V(\gamma)} \mathrm{d}\mu_H(h_v), \tag{45}$$

where $\mathrm{d}\mu_H(h_v)$ is the Haar measure on SU(2). The gauge invariant coherent state is labeled by gauge equivalence class $[g]$ generated by $g(e) \sim g^h(e) = h^{-1}_{s(e)} g(e) h_{t(e)}$ at all e. Here $g(e)$ is an $\mathrm{SL}(2,\mathbb{C})$ group element. $\psi^t_{g(e)}(h(e))$ is the complexifier coherent state on the edge e,

$$\psi^t_{g(e)}(h(e)) = \sum_{j_e \in \mathbb{Z}_+/2\cup\{0\}} (2j_e + 1) e^{-tj_e(j_e+1)/2} \chi_{j_e}(g(e)h(e)^{-1}), \tag{46}$$

where $g(e)$ is complex coordinate of $\mathcal{P}_\gamma$ and relates to $h(e)$, $p^a(e)$ by[5]

$$g(e) = e^{-ip_a(e)\tau_a/2} h(e) = e^{-ip^a(e)\tau^a/2} e^{\theta^a(e)\tau^a/2}, \qquad p^a(e), \quad \theta^a(e) \in \mathbb{R}^3. \tag{47}$$

Applying Eq. (45) and using a discretization of time $T = N\Delta\tau$ with large N and infinitesimal $\Delta\tau$,

$$A_{[g],[g']} = \int \mathrm{d}h \langle \psi^t_g | [e^{-\frac{i}{\hbar}\Delta\tau\hat{\mathbf{H}}}]^N | \psi^t_{g'} h \rangle, \tag{48}$$

[5]For any polynomial $\mathrm{Pol}[\hat{h}(e), \hat{p}^a(e)]$ of $\hat{h}(e)$ and $\hat{p}^a(e)$, the coherent state expectation value is semiclassical: $\langle \psi^t_{g(e)} | \mathrm{Pol}[\hat{h}(e), \hat{p}^a(e)] | \psi^t_{g(e)} \rangle = \mathrm{Pol}[h(e), p^a(e)] + O(t)$ where $h(e)$ and $p^a(e)$ on the right-hand side relate to $g(e)$ by Eq. (47) [74].

$$= \int \mathrm{d}h \prod_{i=1}^{N+1} \mathrm{d}g_i \langle \psi_g^t | \tilde{\psi}_{g_{N+1}}^t \rangle \langle \tilde{\psi}_{g_{N+1}}^t | e^{-\frac{i\Delta\tau}{\hbar}\hat{\mathbf{H}}} | \tilde{\psi}_{g_N}^t \rangle \langle \tilde{\psi}_{g_N}^t | e^{-\frac{i\Delta\tau}{\hbar}\hat{\mathbf{H}}} | \tilde{\psi}_{g_{N-1}}^t \rangle \cdots \langle \tilde{\psi}_{g_2}^t | e^{-\frac{i\Delta\tau}{\hbar}\hat{\mathbf{H}}} | \tilde{\psi}_{g_1}^t \rangle \langle \tilde{\psi}_{g_1}^t | \psi_{g'^h}^t \rangle, \tag{49}$$

where we have inserted $N+1$ overcompleteness relations of normalized coherent state $\tilde{\psi}_g^t = \otimes_e \psi_{g(e)}^t / ||\psi_{g(e)}^t||$:

$$\int \mathrm{d}g_i |\tilde{\psi}_{g_i}^t\rangle\langle\tilde{\psi}_{g_i}^t| = 1_{\mathcal{H}_\gamma^0}, \qquad \mathrm{d}g_i = \left(\frac{c}{t^3}\right)^{|E(\gamma)|} \prod_{e\in E(\gamma)} \mathrm{d}\mu_H(h_i(e))\mathrm{d}^3 p_i(e), \quad i = 1, \ldots, N-1. \tag{50}$$

A path integral formula is derived in [50] from the above expression of $A_{[g],[g']}$,

$$A_{[g],[g']} = \|\psi_g^t\| \|\psi_{g'}^t\| \int \mathrm{d}h \prod_{i=1}^{N+1} \mathrm{d}g_i \nu[g] e^{S[g,h]/t}, \tag{51}$$

where the "effective action" $S[g,h]$ is given by

$$S[g,h] = \sum_{i=0}^{N+1} K(g_{i+1}, g_i) - \frac{i\kappa}{a^2} \sum_{i=1}^{N} \Delta\tau \left[\frac{\langle \psi_{g_{i+1}}^t | \hat{\mathbf{H}} | \psi_{g_i}^t \rangle}{\langle \psi_{g_{i+1}}^i | \psi_{g_i}^t \rangle} + i\tilde{\varepsilon}_{i+1,i}\left(\frac{\Delta\tau}{\hbar}\right) \right], \tag{52}$$

$$K(g_{i+1}, g_i) = \sum_{e\in E(\gamma)} \left[z_{i+1,i}(e)^2 - \frac{1}{2} p_{i+1}(e)^2 - \frac{1}{2} p_i(e)^2 \right] \tag{53}$$

with $g_0 \equiv g'^h$, $g_{N+2} \equiv g$, and $\nu[g]$ is a measure factor. $\tilde{\varepsilon}_{i+1,i}$ contains higher order contributions in $\frac{\Delta\tau}{\hbar}$ (the exact form is given in [50]): $\tilde{\varepsilon}_{i+1,i}(\frac{\Delta\tau}{\hbar}) \to 0$ as $\Delta\tau \to 0$ and is negligible. In the above, $z_{i+1,i}(e)$ and $x_{i+1,i}(e)$ are given by

$$z_{i+1,i}(e) = \mathrm{arccosh}(x_{i+1,i}(e)), \qquad x_{i+1,i}(e) = \frac{1}{2}\mathrm{tr}[g_{i+1}(e)^\dagger g_i(e)]. \tag{54}$$

The path integral Eq. (51) is constructed with discrete time and space, and is a well-defined integration formula for the transition amplitude $A_{[g],[g']}$ as long as $\Delta\tau$ is arbitrarily small but finite. The time translation of γ with finite $\Delta\tau$ makes a hypercubic lattice in four dimensions, on which the path integral is defined. There is no issue of any divergence in this path integral formulation of LQG, since it is derived from a well-defined transition amplitude.

III. SEMICLASSICAL EQUATIONS OF MOTION

A. Discrete equations of motion

The main part of this work is to study the semiclassical limit $t \to 0$ of the transition amplitude $A_{[g],[g']}$. By Eq. (51) and the stationary phase approximation, dominant contributions to $A_{[g],[g']}$ as $t \to 0$ come from semiclassical trajectories satisfying the semiclassical equations of motion (EOMs).

Semiclassical EOMs has been derived in [50] by the variational principle $\delta S[g,h] = 0$ and expressed in the following form:

(i) The variation with respect to g_i using the holomorphic deformation

$$g_i(e) \to g_i^\varepsilon(e) = g_i(e) e^{\varepsilon_i^a(e)\tau^a}, \qquad \varepsilon_i^a(e) \in \mathbb{C}, \tag{55}$$

leads to the following equations from derivatives of $\varepsilon_i^a(e)$ and $\bar{\varepsilon}_i^a(e)$, respectively:

(a) For $i = 1, \ldots, N$, at every edge $e \in E(\gamma)$,

$$\frac{1}{\Delta\tau}\left[\frac{z_{i+1,i}(e)\mathrm{tr}[\tau^a g_{i+1}(e)^\dagger g_i(e)]}{\sqrt{x_{i+1,i}(e)-1}\sqrt{x_{i+1,i}(e)+1}} - \frac{p_i(e)\mathrm{tr}[\tau^a g_i(e)^\dagger g_i(e)]}{\sinh(p_i(e))}\right] = \frac{i\kappa}{a^2}\frac{\partial}{\partial\varepsilon_i^a(e)}\frac{\langle\psi_{g_{i+1}^\varepsilon}^t|\hat{\mathbf{H}}|\psi_{g_i^\varepsilon}^t\rangle}{\langle\psi_{g_{i+1}^\varepsilon}^t|\psi_{g_i^\varepsilon}^t\rangle}\bigg|_{\vec{\varepsilon}=0}. \tag{56}$$

(b) For $i = 2, \ldots, N+1$, at every edge $e \in E(\gamma)$,

$$\frac{1}{\Delta\tau}\left[\frac{z_{i,i-1}(e)\mathrm{tr}[\tau^a g_i(e)^\dagger g_{i-1}(e)]}{\sqrt{x_{i,i-1}(e)-1}\sqrt{x_{i,i-1}(e)+1}} - \frac{p_i(e)\mathrm{tr}[\tau^a g_i(e)^\dagger g_i(e)]}{\sinh(p_i(e))}\right] = -\frac{i\kappa}{a^2}\frac{\partial}{\partial\bar{\varepsilon}_i^a(e)}\frac{\langle\psi_{g_i^\varepsilon}^t|\hat{\mathbf{H}}|\psi_{g_{i-1}^\varepsilon}^t\rangle}{\langle\psi_{g_i^\varepsilon}^t|\psi_{g_{i-1}^\varepsilon}^t\rangle}\bigg|_{\vec{\varepsilon}=0}. \tag{57}$$

(ii) The variation with respect to h_v leads to the closure condition at every vertex $v \in V(\gamma)$ for initial data,

$$-\sum_{e,s(e)=v} p_1^a(e) + \sum_{e,t(e)=v} \Lambda^a{}_b(\vec{\theta}_1(e)) p_1^b(e) = 0, \quad (58)$$

where $\Lambda^a{}_b(\vec{\theta}) \in \mathrm{SO}(3)$ is given by $e^{\theta^c\tau^c/2}\tau^a e^{-\theta^c\tau^c/2} = \Lambda^a{}_b(\vec{\theta})\tau^b$.

The initial and final conditions are given by $g_1 = g'^h$ and $g_{N+1} = g$. Here the gauge transformation h is arbitrary. These semiclassical EOMs govern the semiclassical dynamics of LQG in the reduced phase space formulation.

Semiclassical EOMs (56)–(58) are derived with finite $\Delta\tau$. We prefer to derive EOMs from the path integral Eq. (51) with discrete time and space, because Eq. (51) is a well-defined integration formula for the transition amplitude.

The small-step transitions $\langle\tilde{\psi}^t_{g_{i+1}}|\exp(-\frac{i}{\hbar}\Delta\tau\hat{\mathbf{H}})|\tilde{\psi}^t_{g_i}\rangle$ in Eq. (49) are dominated by overlaps $\langle\tilde{\psi}^t_{g_{i+1}}|\tilde{\psi}^t_{g_i}\rangle$ as $\Delta\tau$ is arbitrarily small. $|\langle\tilde{\psi}^t_{g_{i+1}}|\tilde{\psi}^t_{g_i}\rangle|$ decays exponentially fast to zero unless g_{i+1} is within a small neighborhood at g_i of radius $\sqrt{t}$ [73] (a summary can be found in [75]). Therefore for sufficiently large N, the dominant contribution to $A_{[g],[g']}$ in Eq. (51) comes from the integral over the neighborhood where all g_{i+1} are close to g_i with a distance of $O(\sqrt{t})$. This neighborhood becomes arbitrarily small as $t \to 0$. Within this neighborhood, both quantities in square brackets in Eqs. (56) and (57) have a single isolated zero at $g_i = g_{i+1}$ (Lemma 4.1 in [50]). Therefore $\Delta\tau \to 0$ forces $g_i \to g_{i+1}$, given that the right-hand sides of Eqs. (56) and (57) are always finite [50]. So any solution of Eqs. (56) and (57) can be approximated arbitrarily well by the continuous function $g_i \simeq g(\tau)$, as $\Delta\tau$ is arbitrarily small. In the following we apply this approximation, replace all g_i by continuous function $g(\tau)$, and take the time continuous limit $\Delta\tau \to 0$ of Eqs. (56) and (57).

B. Time continuous limit

The time continuous limit leads to $g_{i+1} \to g_i = g(\tau)$, so that matrix elements $\langle\psi^t_{g_i^\varepsilon}|\hat{\mathbf{H}}|\psi^t_{g_{i-1}^\varepsilon}\rangle$ on right-hand sides of Eqs. (56) and (57) reduce to the expectation values $\langle\psi^t_{g^\varepsilon}|\hat{\mathbf{H}}|\psi^t_{g^\varepsilon}\rangle$ as $\Delta\tau \to 0$ (see [50] for proving that $g_{i+1} \to g_i$ commutes with holomorphic derivatives). Coherent state expectation values of $\hat{\mathbf{H}}$ have the correct semiclassical limit[6]

$$\lim_{t\to 0}\langle\tilde{\psi}^t_g|\hat{\mathbf{H}}|\tilde{\psi}^t_g\rangle = \mathbf{H}[g], \quad (59)$$

where $\mathbf{H}[g]$ is the classical discrete Hamiltonian (43) evaluated at $p^a(e)$, $h(e)$ determined by $g(e)$ in Eq. (47). Note that deriving the semiclassical behavior of $\langle\tilde{\psi}^t_g|\hat{\mathbf{H}}|\tilde{\psi}^t_g\rangle$ relies on a semiclassical expansion of volume operator $\hat{V}_v$ [75],

$$\hat{V}_v = \langle\hat{Q}_v\rangle^{2q}\left[1 + \sum_{n=1}^{2k+1}(-1)^{n+1}\frac{q(1-q)\cdots(n-1+q)}{n!}\left(\frac{\hat{Q}_v^2}{\langle\hat{Q}_v\rangle^2} - 1\right)^n\right], \qquad q = 1/4, \quad (60)$$

where $\langle\hat{Q}_v\rangle = \langle\psi^t_g|\hat{Q}_v|\psi^t_g\rangle$. This expansion is valid when $\langle\hat{Q}_v\rangle \gg \ell_p^6$.

We write $g_{i+1}(e) = g_i(e)[1 + \Delta\phi^a(e)\tau^a]$ where $\Delta\phi^a(e)$ parametrizes the infinitesimal change of $g(e)$ between two time steps. Equations (56) and (57) reduce as follows (by using Lemma 4.1 in [50]):

$$-\frac{ia^2}{\kappa}M_1{}^a{}_b(g(e))\frac{\Delta\bar{\phi}^b(e)}{\Delta\tau} = \frac{\partial}{\partial\varepsilon^a(e)}\mathbf{H}[g^\varepsilon]\Big|_{\vec{\varepsilon}=0}, \quad (61)$$

$$-\frac{ia^2}{\kappa}M_2{}^a{}_b(g(e))\frac{\Delta\phi^b(e)}{\Delta\tau} = -\frac{\partial}{\partial\bar{\varepsilon}^a(e)}\mathbf{H}[g^\varepsilon]\Big|_{\vec{\varepsilon}=0}, \quad (62)$$

where $g^\varepsilon(e) = g(e)e^{\varepsilon^a(e)\tau^a}$, $(\varepsilon^a(e) \in \mathbb{C})$. The left-hand sides become time derivatives as $\Delta\tau \to 0$, and

$$M_1{}^a{}_b(g) = 2\Lambda^a{}_c(\vec{\theta})\Lambda^b{}_d(\vec{\theta})\left[\frac{p^c}{p}\frac{p^d}{p} - i\varepsilon^{cde}p^e + \frac{p\cosh(p)}{\sinh(p)}\left(\delta^{cd} - \frac{p^c}{p}\frac{p^d}{p}\right)\right], \quad (63)$$

$$M_2{}^a{}_b(g) = 2\Lambda^a{}_c(\vec{\theta})\Lambda^b{}_d(\vec{\theta})\left[\frac{p^c}{p}\frac{p^d}{p} + i\varepsilon^{cde}p^e + \frac{p\cosh(p)}{\sinh(p)}\left(\delta^{cd} - \frac{p^c}{p}\frac{p^d}{p}\right)\right], \quad (64)$$

[6] First, we can apply the semiclassical perturbation theory of [75] to $\hat{O} \equiv \hat{H}_v^4$ [recall Eq. (36)] and all $\hat{O}^n$ $(n > 1)$: $\langle\tilde{\psi}^t_g|\hat{O}^n|\tilde{\psi}^t_g\rangle = O[g]^n + O(t)$. Then by Theorem 3.6 of [74], $\lim_{t\to 0}\langle\tilde{\psi}^t_g|f(\hat{O})|\tilde{\psi}^t_g\rangle = f(O[g])$ for any Borel measurable function on $\mathbb{R}$ such that $\langle\tilde{\psi}^t_g|f(\hat{O})^\dagger f(\hat{O})|\tilde{\psi}^t_g\rangle < \infty$.

where $e^{\theta^c\tau^c/2}\tau^a e^{-\theta^c\tau^c/2} = \Lambda^a{}_b(\vec{\theta})\tau^b$. The matrices $M_1{}^a{}_b(g)$ and $M_2{}^a{}_b(g)$ are nondegenerate since

$$\det(M_{1,2}(g)) = \frac{\sinh^2(p)}{p^2} \neq 0. \tag{65}$$

We can write $\Delta\phi^a(e)$ as a linear combination of infinitesimal change of phase space variables using (47): $\Delta p^a(e) = p^a_{i+1}(e) - p^a_i(e)$ and $\Delta\theta^a(e) = \theta^a_{i+1}(e) - \theta^a_i(e)$,

$$\begin{aligned}\Delta\phi^a(e_I) &= -\frac{1}{2}\mathrm{Tr}(g_i^{-1}(e)g_{i+1}(e)\tau^a) \\ &= J_1{}^a{}_b(e)\Delta p^a(e) + J_2{}^a{}_b(e)\Delta\theta^a(e)\end{aligned} \tag{66}$$

at leading orders of $\Delta p^a(e)$ and $\Delta\theta^a(e)$. The holomorphic deformation $\varepsilon^a(e)$ has the similar expression

$$\begin{aligned}\varepsilon^a(e) &= -\frac{1}{2}\mathrm{Tr}(g^{-1}(e)g^\varepsilon(e)\tau^a) \\ &= J_1{}^a{}_b(e)\delta p^a(e) + J_2{}^a{}_b(e)\delta\theta^a(e),\end{aligned} \tag{67}$$

where $\delta p^a(e)$ and $\delta\theta^a(e)$ relate to $g^\varepsilon(e)$ by

$$g^\varepsilon(e) = e^{-i[p^a(e)+\delta p^a(e)]\tau^a/2}e^{[\theta^a(e)+\delta\theta^a(e)]\tau^a/2}. \tag{68}$$

J_1 and J_2 are 3×3 complex matrices whose elements depend on $p^a(e)$ and $\theta^a(e)$. We define 6×6 matrices J and $\tilde{J}$ as

$$J = \begin{pmatrix} J_1 & J_2 \\ \bar{J}_1 & \bar{J}_2 \end{pmatrix}, \qquad \tilde{J} = \begin{pmatrix} \bar{J}_1 & \bar{J}_2 \\ J_1 & J_2 \end{pmatrix}. \tag{69}$$

J and $\tilde{J}$ satisfy

$$\begin{pmatrix} \boldsymbol{\varepsilon}(e) \\ \bar{\boldsymbol{\varepsilon}}(e) \end{pmatrix} = J\begin{pmatrix} \delta\boldsymbol{p}(e) \\ \delta\boldsymbol{\theta}(e) \end{pmatrix} = \begin{pmatrix} J_1 & J_2 \\ \bar{J}_1 & \bar{J}_2 \end{pmatrix}\begin{pmatrix} \delta\boldsymbol{p}(e) \\ \delta\boldsymbol{\theta}(e) \end{pmatrix}, \tag{70}$$

$$\begin{pmatrix} \Delta\bar{\boldsymbol{\phi}}(e) \\ \Delta\boldsymbol{\phi}(e) \end{pmatrix} = \tilde{J}\begin{pmatrix} \Delta\boldsymbol{p}(e) \\ \Delta\boldsymbol{\theta}(e) \end{pmatrix} = \begin{pmatrix} \bar{J}_1 & \bar{J}_2 \\ J_1 & J_2 \end{pmatrix}\begin{pmatrix} \Delta\boldsymbol{p}(e) \\ \Delta\boldsymbol{\theta}(e) \end{pmatrix}. \tag{71}$$

Here the bold letters $\boldsymbol{p}$ and $\boldsymbol{\theta}$ denote the 3-vectors p^a and θ^a. Using the above matrices Eqs. (61) and (62) become

$$T(\boldsymbol{p},\boldsymbol{\theta})\begin{pmatrix} \Delta\boldsymbol{p}(e)/\Delta\tau \\ \Delta\boldsymbol{\theta}(e)/\Delta\tau \end{pmatrix} = \frac{i\kappa}{a^2}\begin{pmatrix} \partial\mathbf{H}/\partial\boldsymbol{p}(e) \\ \partial\mathbf{H}/\partial\boldsymbol{\theta}(e) \end{pmatrix}, \tag{72}$$

where

$$T(\boldsymbol{p},\boldsymbol{\theta}) = \begin{pmatrix} J_1 & J_2 \\ \bar{J}_1 & \bar{J}_2 \end{pmatrix}^T\begin{pmatrix} M_1 & 0 \\ 0 & -M_2 \end{pmatrix}\begin{pmatrix} \bar{J}_1 & \bar{J}_2 \\ J_1 & J_2 \end{pmatrix}. \tag{73}$$

It is much more convenient to compute the right-hand side of Eq. (72) than right-hand sides of Eqs. (61) and (62), since $\mathbf{H}$ is expressed in terms of holonomies and fluxes.

By the time continuous limit $\Delta\tau \to 0$, $\Delta\boldsymbol{p}(e)/\Delta\tau \to \mathrm{d}\boldsymbol{p}(e)/\mathrm{d}\tau$ and $\Delta\boldsymbol{\theta}(e)/\Delta\tau \to \mathrm{d}\boldsymbol{\theta}(e)/\mathrm{d}\tau$, so the semiclassical EOMs reduce to

$$T(\boldsymbol{p},\boldsymbol{\theta})\begin{pmatrix} \mathrm{d}\boldsymbol{p}(e)/\mathrm{d}\tau \\ \mathrm{d}\boldsymbol{\theta}(e)/\mathrm{d}\tau \end{pmatrix} = \frac{i\kappa}{a^2}\begin{pmatrix} \partial\mathbf{H}/\partial\boldsymbol{p}(e) \\ \partial\mathbf{H}/\partial\boldsymbol{\theta}(e) \end{pmatrix}. \tag{74}$$

The above computation is carried out analytically in *Mathematica*. The matrix elements of J, $\tilde{J}$, and T are lengthy. Their explicit formulas are given in [69].

As seen from Eq. (74), the approximation $g(\tau)$ of any solution g_i of Eqs. (56) and (57) is not only continuous in τ but also differentiable. Indeed, if a solution $g_i \simeq g(\tau)$ failed to be differentiable, left-hand sides of Eq. (74) or Eqs. (56) and (57) would have blown up with small $\Delta\tau$ and contradicted the finiteness of right-hand sides; i.e., g_i could not be a solution.

IV. SEMICLASSICAL DYNAMICS AS HAMILTONIAN EVOLUTION

A. Holonomy-flux Poisson algebra

Since the semiclassical EOMs are expressed in terms of variables $p^a(e)$ and $\theta^a(e)$ from the holonomy-flux algebra Eqs. (32)–(34) by the relation $h(e) = e^{\theta^a(e)\tau^a/2}$, the computation can proceed as follows: We write Eq. (33) (at $e' = e$) as

$$\{p^a(e), \theta^b(e)\}\frac{\partial h_{AB}(e)}{\partial\theta^b(e)} = \frac{\kappa}{a^2}\left[\frac{\tau^a}{2}h(e)\right]_{AB}. \tag{75}$$

Among four matrix elements $h_{AB}(e)$, there are only three independent $h_{11}(e)$, $h_{12}(e)$, $h_{21}(e)$. The above equations with $AB = 11, 12, 21$ form a matrix equation of three 3×3 matrices U, V, and W:

$$\begin{aligned} U^a{}_b V^b{}_{AB} &= \frac{\kappa}{a^2}W^a{}_{AB}, \\ \text{where } U^a{}_b &= \{p^a(e), \theta^b(e)\}, \\ V^b{}_{AB} &= \frac{\partial h_{AB}(e)}{\partial\theta^b(e)}, \\ W^a{}_{AB} &= \left[\frac{\tau^b}{2}h(e)\right]_{AB}, \end{aligned} \tag{76}$$

where $AB = 11, 12, 21$. Solving $U = \frac{\kappa}{a^2}WV^{-1}$ gives the following result:

$$\begin{aligned}\{p^a(e),\theta^b(e)\} &\equiv U^a{}_b(\boldsymbol{\theta})\\ &= \begin{pmatrix} \frac{2\theta_1^2+\theta(\theta_2^2+\theta_3^2)\cot(\frac{\theta}{2})}{2\theta^2} & -\frac{\theta_3^3+(\theta_1^2+\theta_2^2)\theta_3+\theta_1\theta_2(\theta\cot(\frac{\theta}{2})-2)}{2\theta^2} & \frac{1}{2}\left(\frac{\theta_1\theta_3(2-\theta\cot(\frac{\theta}{2}))}{\theta^2}+\theta_2\right) \\ \frac{\theta_3^3+(\theta_1^2+\theta_2^2)\theta_3+\theta_1\theta_2(2-\theta\cot(\frac{\theta}{2}))}{2\theta^2} & \frac{2\theta_2^2+\theta(\theta_1^2+\theta_3^2)\cot(\frac{\theta}{2})}{2\theta^2} & \frac{1}{2}\left(\frac{\theta_2\theta_3(2-\theta\cot(\frac{\theta}{2}))}{\theta^2}-\theta_1\right) \\ -\frac{\theta_2\theta_1^2+\theta_2(\theta_2^2+\theta_3^2)+\theta_3\theta_1(\theta\cot(\frac{\theta}{2})-2)}{2\theta^2} & \frac{\theta_1^3+(\theta_2^2+\theta_3^2)\theta_1+\theta_2\theta_3(2-\theta\cot(\frac{\theta}{2}))}{2\theta^2} & \frac{2\theta_3^2+\theta(\theta_1^2+\theta_2^2)\cot(\frac{\theta}{2})}{2\theta^2} \end{pmatrix},\end{aligned} \tag{77}$$

where $\theta_a \equiv \theta^a(e)$ and $\theta = \sqrt{\theta^a(e)\theta^a(e)}$. With this result we check that Eq. (75) with $AB = 21$ is satisfied automatically.

The holonomy-flux algebra Eqs. (32)–(34) implies the following Poisson algebra between $p^a(e)$ and $\theta^a(e)$:

$$\{\theta^a(e),\theta^b(e')\} = 0, \tag{78}$$

$$\{p^a(e),\theta^b(e')\} = \frac{\kappa}{a^2}\delta_{e,e'}U^a{}_b(\boldsymbol{\theta}), \tag{79}$$

$$\{p^a(e),p^b(e')\} = -\frac{\kappa}{a^2}\delta_{e,e'}\varepsilon_{abc}p^c(e'). \tag{80}$$

A straightforward computation demonstrates that Eqs. (78)–(80) imply the holonomy-flux algebra Eqs. (32)–(34). Thus the holonomy-flux algebra and the Poisson algebra between $p^a(e)$ and $\theta^a(e)$ in Eqs. (78)–(80) are equivalent.

B. Hamilton's equations

We would like to relate EOMs (74) to Hamilton's equations with the discrete physical Hamiltonian $\mathbf{H}$ and symplectic structure of holonomy-flux algebra. First,

$$\begin{aligned}\{p^a(e),\mathbf{H}\} &= \{p^a(e),p^b(e)\}\frac{\partial\mathbf{H}}{\partial p^b(e)}\\ &\quad+\{p^a(e),\theta^b(e)\}\frac{\partial\mathbf{H}}{\partial\theta^b(e)},\\ \{\theta^a(e),\mathbf{H}\} &= \{\theta^a(e),p^b(e)\}\frac{\partial\mathbf{H}}{\partial p^b(e)}\\ &\quad+\{\theta^a(e),\theta^b(e)\}\frac{\partial\mathbf{H}}{\partial\theta^b(e)}.\end{aligned} \tag{81}$$

We define the matrix

$$P(\boldsymbol{p},\boldsymbol{\theta}) = \begin{pmatrix}\{p^a(e),p^b(e)\} & \{p^a(e),\theta^b(e)\}\\ \{\theta^a(e),p^b(e)\} & 0\end{pmatrix}. \tag{82}$$

Applying P to the EOMs (74) gives

$$-\frac{ia^2}{\kappa}P(\boldsymbol{p},\boldsymbol{\theta})T(\boldsymbol{p},\boldsymbol{\theta})\begin{pmatrix}\mathrm{d}\boldsymbol{p}(e)/\mathrm{d}\tau\\ \mathrm{d}\boldsymbol{\theta}(e)/\mathrm{d}\tau\end{pmatrix} = \begin{pmatrix}\{\boldsymbol{p}(e),\mathbf{H}\}\\ \{\boldsymbol{\theta}(e),\mathbf{H}\}\end{pmatrix}. \tag{83}$$

By using the explicit formula of $T(\boldsymbol{p},\boldsymbol{\theta})$ and Poisson brackets in $P(\boldsymbol{p},\boldsymbol{\theta})$, we obtain the following simple result:

$$-\frac{ia^2}{\kappa}P(\boldsymbol{p},\boldsymbol{\theta})T(\boldsymbol{p},\boldsymbol{\theta}) = 1_{6\times6}. \tag{84}$$

This shows that the semiclassical EOMs from the path integral is equivalent to Hamilton's equations with the discrete physical Hamiltonian $\mathbf{H}$:

$$\frac{\mathrm{d}p^a(e)}{\mathrm{d}\tau} = \{p^a(e),\mathbf{H}\}, \qquad \frac{\mathrm{d}\theta^a(e)}{\mathrm{d}\tau} = \{\theta^a(e),\mathbf{H}\}, \tag{85}$$

where the Poisson brackets are given by Eqs. (78)–(80), or equivalently, by the holonomy-flux algebra Eqs. (32)–(34). In general, the time evolution of any phase space function $f(p^a(e),\theta^a(e))$ or $f(p^a(e),h(e))$ is governed by

$$\frac{\mathrm{d}f}{\mathrm{d}\tau} = \{f,\mathbf{H}\}. \tag{86}$$

Mathematica is employed for all the above computations, including computing $\{p^a(e),\theta^b(e)\}$, checking the equivalence between Eqs. (78)–(80) and holonomy-flux algebra, and verifying Eq. (84). The *Mathematica* files can be found in [69].

Moreover the closure condition (58) is equivalent to $\sum_{I=1}^3\sum_{s=\pm}p^a(e_{v;I,s}) = 0$. The Hamiltonian flow generated by $G_v^a \coloneqq \sum_{I=1}^3\sum_{s=\pm}p^a(e_{v;I,s})$ in a $\mathcal{P}_\gamma$ is SU(2) gauge transformation. Since $\mathbf{H}$ is SU(2) gauge invariant,

$$\frac{\mathrm{d}G_v^a}{\mathrm{d}\tau} = \{G_v^a,\mathbf{H}\} = 0. \tag{87}$$

So the closure condition (58) is preserved in the time evolution. Given a solution $p^a(\tau,e),\theta^b(\tau,e)$ satisfying Eq. (86), its gauge transformation still satisfies Eq. (86):

$$\begin{aligned}\{\{f,G_v^a\},\mathbf{H}\} &= -\{\{G_v^a,\mathbf{H}\},f\} - \{\{\mathbf{H},f\},G_v^a\}\\ &= \left\{f,\frac{\mathrm{d}G_v^a}{\mathrm{d}\tau}\right\} + \left\{\frac{\mathrm{d}f}{\mathrm{d}\tau},G_v^a\right\}\\ &= \frac{\mathrm{d}}{\mathrm{d}\tau}\{f,G_v^a\}.\end{aligned} \tag{88}$$

Recall that the initial state in Eq. (51) is labeled by the gauge equivalence class $[g']$. The trajectory in the reduced phase space determined by the Hamiltonian flow (86) is unique up to SU(2) gauge transformations, in the phase space regime where $\mathbf{H}$ is a smooth function in p^a, θ^a.

Note that due to the absolute value and square root in $\mathbf{H}$, $\mathbf{H}$ is nondifferentiable at $C_v^2 - \frac{\alpha}{4}\sum_{a=1}^3 C_{a,v}^2 = 0$, at which the uniqueness of the solution cannot be established. As it is discussed in Sec. VI, these irregularities are avoided in general if initial states $\Psi^t_{[g']}$ are semiclassical in the sense that $[g']$ is in the classically allowed regime of the phase space. The classically allowed regime satisfies nonholonomic constraints required by the classical gravity-dust theory.

V. ACTION PRINCIPLE

Here we present another routine to derive the classical EOMs [Hamilton's equation (86)]. We are first going to take the time continuous limit of the discrete action $S[g,h]$, then derive EOMs, in contrast to the above procedure in which discrete EOMs are derived first from the path integral, and then take the time continuous limit. We will show that these two methods lead to the same result, which implies the time continuous limit and variational principle are commutative when acting on $S[g,h]$.

Recall $S[g,h]$ in Eq. (52); we write

$$g_i = g(\tau), \qquad g_{i+1} = g(\tau + \Delta\tau), \tag{89}$$

and expand summands in $S[g,h]$ in $\Delta\tau$:

$$\frac{\langle \psi^t_{g_{i+1}} | \hat{\mathbf{H}} | \psi^t_{g_i} \rangle}{\langle \psi^i_{g_{i+1}} | \psi^t_{g_i} \rangle} + i\tilde{\varepsilon}_{i+1,i}\left(\frac{\Delta\tau}{\hbar}\right) = \langle \psi^t_{g(\tau)} | \hat{\mathbf{H}} | \psi^t_{g(\tau)} \rangle + O(\Delta\tau), \tag{90}$$

$$K(g_{i+1}, g_i) = \Delta\tau \sum_{e\in E(\gamma)} iG_{ab}(\boldsymbol{\theta}(\tau,e))p^a(\tau,e)\frac{\mathrm{d}\theta^b(\tau,e)}{\mathrm{d}\tau} + O(\Delta\tau^2). \tag{91}$$

The 3×3 real matrix $G_{ab}(\boldsymbol{\theta})$ is given by

$$\begin{pmatrix} -\frac{(\theta\theta_1^2+(\theta_2^2+\theta_3^2)\sin(\theta))}{\theta^3} & -\frac{(\theta_1\theta_2(\theta-\sin(\theta))+\theta\theta_3(\cos(\theta)-1))}{\theta^3} & \frac{(\theta_1\theta_3(\sin(\theta)-\theta)+\theta\theta_2(\cos(\theta)-1))}{\theta^3} \\ \frac{\theta\theta_3(\cos(\theta)-1)-\theta_1\theta_2(\theta-\sin(\theta))}{\theta^3} & -\frac{(\theta\theta_2^2+(\theta_1^2+\theta_3^2)\sin(\theta))}{\theta^3} & -\frac{(\theta_2\theta_3(\theta-\sin(\theta))+\theta\theta_1(\cos(\theta)-1))}{\theta^3} \\ -\frac{(\theta_1\theta_3(\theta-\sin(\theta))+\theta\theta_2(\cos(\theta)-1))}{\theta^3} & \frac{(\theta_2\theta_3(\sin(\theta)-\theta)+\theta\theta_1(\cos(\theta)-1))}{\theta^3} & -\frac{(\theta\theta_3^2+(\theta_1^2+\theta_2^2)\sin(\theta))}{\theta^3} \end{pmatrix}, \tag{92}$$

where $\theta_a \equiv \theta^a(e)$ and $\theta = \sqrt{\theta^a(e)\theta^a(e)}$.

We find that $G_{ab}(\boldsymbol{\theta})$ closely relates to $U^a{}_b(\boldsymbol{\theta}) = \{p^a(e), \theta^b(e)\}$ by

$$G(\boldsymbol{\theta})^T U(\boldsymbol{\theta}) = U(\boldsymbol{\theta})G(\boldsymbol{\theta})^T = -\frac{\kappa}{a^2}1_{3\times 3}. \tag{93}$$

We define new variables

$$X^b(\tau,e) = G_{ab}(\boldsymbol{\theta}(\tau,e))p^a(\tau,e), \tag{94}$$

and interestingly, we obtain the following result.

Theorem 1. The following (equal-time) Poisson algebra between X^a and θ^a is equivalent to the holonomy-flux algebra

$$\{X^a(e), \theta^b(e')\} = -\frac{\kappa}{a^2}\delta^{ab}\delta_{e,e'}, \qquad \{X^a(e), X^b(e')\} = \{\theta^a(e), \theta^b(e')\} = 0. \tag{95}$$

$X^a(e)$ and $\theta^a(e)$ form local Darboux coordinates on the reduced phase space of LQG.

Proof: The first relation is equivalent to Eq. (78):

$$\{X^a(e), \theta^b(e')\} = G_{ca}(\boldsymbol{\theta}(e))\{p^c(e), \theta^b(e')\} = G_{ca}(\boldsymbol{\theta}(e))U^c{}_b(\boldsymbol{\theta}(e))\delta_{e,e'} = -\frac{\kappa}{a^2}\delta^{ab}\delta_{e,e'}. \tag{96}$$

Second,

$$\begin{aligned}\{X^a(e),X^b(e')\} &= \{G_{ca}(\boldsymbol{\theta}(e))p^c(e),G_{db}(\boldsymbol{\theta}(e'))p^d(e')\}\\ &= G_{ca}(\boldsymbol{\theta}(e))G_{db}(\boldsymbol{\theta}(e'))\{p^c(e),p^d(e')\} - G_{db}(\boldsymbol{\theta}(e'))p^c(e)\frac{\partial G_{ca}(\boldsymbol{\theta}(e))}{\partial\theta^f(e)}\{p^d(e'),\theta^f(e)\}\\ &\quad + G_{ca}(\boldsymbol{\theta}(e))p^d(e')\frac{\partial G_{db}(\boldsymbol{\theta}(e'))}{\partial\theta^f(e')}\{p^c(e),\theta^f(e')\}\\ &= G_{ca}(\boldsymbol{\theta}(e))G_{db}(\boldsymbol{\theta}(e'))\{p^c(e),p^d(e')\} + \frac{\kappa}{a^2}\delta_{e,e'}p^c(e)\left[\frac{\partial G_{ca}(\boldsymbol{\theta}(e))}{\partial\theta^b(e)} - \frac{\partial G_{cb}(\boldsymbol{\theta}(e))}{\partial\theta^a(e)}\right] \end{aligned} \tag{97}$$

is vanishing because

$$\{p^c(e),p^d(e)\} = -\frac{\kappa}{a^2}G^{-1}_{ac}(\boldsymbol{\theta}(e))G^{-1}_{bd}(\boldsymbol{\theta}(e'))\left[\frac{\partial G_{ea}(\boldsymbol{\theta}(e))}{\partial\theta^b(e)} - \frac{\partial G_{eb}(\boldsymbol{\theta}(e))}{\partial\theta^a(e)}\right]p^e(e), \tag{98}$$

which can be checked straightforwardly. The *Mathematica* file for the above computation is provided in [69]. ■

Although the Poisson algebra Eq. (95) is simple, SU(2) gauge transformations of $X^a(e)$ and $\theta^a(e)$ are complicated. In contrast, the holonomy-flux algebra uses variables $p^a(e)$ and $h(e)$ that have simple SU(2) gauge transformations, but sacrifices the simplicity of Poisson brackets.

As a result we obtain the following time continuous limit $\mathcal{S}[g,h] = \lim_{\Delta\tau\to 0} S[g,h]$:

$$\begin{aligned}\mathcal{S}[g,h] &= i\int_0^T \mathrm{d}\tau\left[\sum_{e\in E(\gamma)}X^a(\tau,e)\frac{\mathrm{d}\theta^a(\tau,e)}{\mathrm{d}\tau} - \frac{\kappa}{a^2}\langle\psi^t_{g(\tau)}|\hat{\mathbf{H}}|\psi^t_{g(\tau)}\rangle\right]\\ &= i\int_0^T \mathrm{d}\tau\left[\sum_{e\in E(\gamma)}X^a(\tau,e)\frac{\mathrm{d}\theta^a(\tau,e)}{\mathrm{d}\tau} - \frac{\kappa}{a^2}(\mathbf{H}[\boldsymbol{p}(\tau),\boldsymbol{\theta}(\tau)] + O(\hbar))\right],\end{aligned} \tag{99}$$

where $\langle\psi^t_{g(\tau)}|\hat{\mathbf{H}}|\psi^t_{g(\tau)}\rangle = \mathbf{H}[\boldsymbol{p}(\tau),\boldsymbol{\theta}(\tau)] + O(\hbar)$.

The Poisson algebra Eq. (95), or equivalently the holonomy-flux algebra, can be obtained from the above $\mathcal{S}[g,h]$ by the Legendre transformation. $\mathcal{S}[g,h]$ provides an action principle for the LQG (reduced) phase space and the quantization.

By the time continuous limit, the path integral formula (51) becomes a standard phase space path integral

$$\int [DXD\theta]\mu[X,\theta]e^{\frac{i}{t}\int_0^T \mathrm{d}\tau[\sum_{e\in E(\gamma)}X^a(\tau,e)\frac{\mathrm{d}\theta^a(\tau,e)}{\mathrm{d}\tau} - \frac{i\kappa}{a^2}(\mathbf{H}+O(\hbar))]} \tag{100}$$

up to $O(\hbar)$ in the action and a measure factor $\mu[X,\theta]$ (containing $\nu[g]$ and the Jacobian for transforming $\mathrm{d}g\to\mathrm{d}X\mathrm{d}\theta$). The path integral formula becomes an infinite dimension integral, and thus may be mathematically ill-defined. This path integral relates to a starting point in [34,36].

The variational principle $\delta\mathcal{S}=0$ gives the Hamilton's equation [up to $O(\hbar)$]

$$\frac{\mathrm{d}\theta^a(e)}{\mathrm{d}\tau} = \frac{\kappa}{a^2}\frac{\partial\mathbf{H}}{\partial X^a(e)}, \qquad \frac{\mathrm{d}X^a(e)}{\mathrm{d}\tau} = -\frac{\kappa}{a^2}\frac{\partial\mathbf{H}}{\partial\theta^a(e)}. \tag{101}$$

For any phase space function $f(\boldsymbol{X},\boldsymbol{\theta})$, its time evolution is given by

$$\frac{\mathrm{d}f}{\mathrm{d}\tau} = \{f,\mathbf{H}\}, \tag{102}$$

which is identical to Eq. (86). It shows that the time continuous limit and variational principle are commutative when acting on $S[g,h]$.

We emphasize that in our analysis the time continuum limit is taken at the semiclassical level. One may want to compare Eq. (100) with the discrete time path integral (51) and understand the continuous time path integral (100) is the time continuum limit of Eq. (100) at the quantum level. It is indeed how path integrals of quantum field theories are developed. But here we take a more conservative viewpoint and hesitate to view (100) as the limit at the quantum level because the precise relation between (51) and (100) relies on the path integral measure which, however, is difficult to make sense.

VI. LATTICE CONTINUUM LIMIT

In this section, we demonstrate the relation between the semiclassical EOMs (74) [or equivalently (86)] from path integral and classical reduced phase space EOMs (24) of the gravity-dust system in the continuum. We are going to take the continuum limit of the cubic lattice γ, i.e., send the total number $|V(\gamma)|$ of vertices to infinity, and show that (74) recovers (24) in this limit. Defining $\mu\sim|V(\gamma)|^{-3}$ to be the coordinate length of every lattice edge, the lattice continuum limit is given by $\mu\to 0$. More precisely, recall that semiclassical EOMs are derived with $t=\ell_P^2/a^2\to 0$ and $\langle\hat{Q}_v\rangle\sim\mu^6\gg\ell_P^6$ [see Eq. (60)], and the lattice continuum limit takes us to the regime

$$\ell_P\ll\mu\ll a, \tag{103}$$

where a is the macroscopic unit fixed from the beginning. When keeping a fixed, the lattice continuum limit sends $\mu\to 0$ after the semiclassical limit $\ell_P\to 0$ (from which EOMs are derived) so $\ell_P\ll\mu$ is kept.

We rescale $\theta^a(e)$ and $p^a(e)$ and define variables $\mathfrak{A}_I^a(v)$ and $\mathfrak{E}_a^I(v)$,

$$\theta^a(e_I(v))=\mu\mathfrak{A}_I^a(v),\qquad p^a(e_I(v))=\frac{2\mu^2}{\beta a^2}\mathfrak{E}_a^I(v), \tag{104}$$

where $\mathfrak{A}_I^a(v)$ and $\mathfrak{E}_a^I(v)$ behave as follows in the lattice continuum limit, by relations between $h(e)$ and $p^a(e)$ in Eq. (29) and smooth fields $(\boldsymbol{A},\boldsymbol{E})$:

$$\mathfrak{A}_I^a(v)=A_I^a(v)+O(\mu),\qquad \mathfrak{E}_a^I(v)=E_a^I(v)+O(\mu). \tag{105}$$

Here $A_I^a(v)=A_j^a(v)\dot{e}_I(v)^j$ and $E_a^I(v)=E_a^j(v)\dot{e}_I(v)^j$ are smooth fields $(\boldsymbol{A},\boldsymbol{E})$ evaluated at the vertex v. $\dot{e}_I(v)$ is the tangent vector of $e_I(v)$ at v. $A_I^a(v)$ and $E_a^I(v)$ are coordinate components of $(\boldsymbol{A},\boldsymbol{E})$ when we take $\dot{e}_I(v)\equiv\partial/\partial\sigma^I$ ($I=1$, 2, 3) as the coordinate basis. σ^I is such that the coordinate length of $e_I(v)$ is μ.

Inserting the μ expansion of $\theta^a(e)$, $p^a(e)$ in $T(\boldsymbol{p},\boldsymbol{\theta})$ of Eq. (74) gives

$$T(\boldsymbol{p},\boldsymbol{\theta})=\begin{pmatrix}0&0&0&-i&0&0\\0&0&0&0&-i&0\\0&0&0&0&0&-i\\i&0&0&0&0&0\\0&i&0&0&0&0\\0&0&i&0&0&0\end{pmatrix}+O(\mu). \tag{106}$$

So the left-hand side of Eq. (74) becomes

$$T(\boldsymbol{p},\boldsymbol{\theta})\begin{pmatrix}\frac{\mathrm{d}\boldsymbol{p}(e_I(v))}{\mathrm{d}\tau}\\\frac{\mathrm{d}\boldsymbol{\theta}(e_I(v))}{\mathrm{d}\tau}\end{pmatrix}=i\begin{pmatrix}-\mu\frac{\mathrm{d}\boldsymbol{A}_I(v)}{\mathrm{d}\tau}+O(\mu^2)\\\frac{2\mu^2}{\beta a^2}\frac{\mathrm{d}\boldsymbol{E}^I(v)}{\mathrm{d}\tau}+O(\mu^3)\end{pmatrix}. \tag{107}$$

On the right-hand side of Eq. (74),

$$\frac{\partial\mathbf{H}[\boldsymbol{p},\boldsymbol{\theta}]}{\partial p^a(e_I(v))}=\frac{\beta a^2}{2\mu^2}\frac{\partial\mathbf{H}[\mathfrak{E},\mathfrak{A}]}{\partial\mathfrak{E}_a^I(v)},\qquad \frac{\partial\mathbf{H}[\boldsymbol{p},\boldsymbol{\theta}]}{\partial\theta^a(e_I(v))}=\frac{1}{\mu}\frac{\partial\mathbf{H}[\mathfrak{E},\mathfrak{A}]}{\partial\mathfrak{A}_I^a(v)}. \tag{108}$$

$\mathbf{H}[\mathfrak{E},\mathfrak{A}]$ is obtained from $\mathbf{H}[\boldsymbol{p},\boldsymbol{\theta}]$ by changing variables (104). Derivatives of $\mathbf{H}$ reduce to derivatives of C_v and $C_{a,v}$,

$$\frac{\partial\mathbf{H}}{\partial\mathfrak{E}_a^I(v')}=\sum_{v\in V(\gamma)}s_v\left[\frac{C_v}{H_v}\frac{\partial C_v}{\partial\mathfrak{E}_a^I(v')}-\frac{\alpha}{4}\sum_{b=1}^3\frac{C_{b,v}}{H_v}\frac{\partial C_{b,v}}{\partial\mathfrak{E}_a^I(v')}\right], \tag{109}$$

$$\frac{\partial\mathbf{H}}{\partial\mathfrak{A}_I^a(v')}=\sum_{v\in V(\gamma)}s_v\left[\frac{C_v}{H_v}\frac{\partial C_v}{\partial\mathfrak{A}_I^a(v')}-\frac{\alpha}{4}\sum_{b=1}^3\frac{C_{b,v}}{H_v}\frac{\partial C_{b,v}}{\partial\mathfrak{A}_I^a(v')}\right], \tag{110}$$

where $H_v=\sqrt{|C_v^2-\frac{\alpha}{4}\sum_{a=1}^3C_{a,v}^2|}$ and $s_v=\mathrm{sgn}(C_v^2-\frac{\alpha}{4}\sum_{a=1}^3C_{a,v}^2)$. We have assumed that variations of $\mathfrak{E}_a^I(v')$ and $\mathfrak{A}_I^a(v')$ (for computing above derivatives) do not make any s_v jump, so derivatives of s_v are zero. Without this assumption, Hamilton's equations (85) is ill-defined because $\mathbf{H}$ is not differentiable as s_v jumps. Semiclassial EOMs are singular at $C_v^2-\frac{\alpha}{4}\sum_{a=1}^3C_{a,v}^2=0$.

Computing explicitly Poisson brackets $h(e)\{h(e)^{-1},V_v\}$ and $h(e)\{h(e)^{-1},K\}$ makes C_v and $C_{a,v}$ as polynomials generated by the following quantities:

$$h(e_I(v))=e^{\mu\mathfrak{A}_I^a(v)},\qquad p^a(e_I(v))=\frac{2\mu^2}{\beta a^2}\mathfrak{E}_a^I(v), \tag{111}$$

$$Q_v^{-\frac{1}{2}}=\mu^{-3}\mathfrak{q}(v)^{-\frac{1}{2}},\quad \mathfrak{q}(v)=\frac{1}{6}\varepsilon_{IJK}\varepsilon^{abc}\mathfrak{E}_a^I(v)\mathfrak{E}_b^J(v)\mathfrak{E}_c^K(v), \tag{112}$$

where Q_v is the classical limit of $\hat{Q}_v$ in Eq. (42). We assume that the initial condition satisfies $Q_v>0$ at all v, and the continuous time evolution does not flip $\mathrm{sgn}(Q_v)$.[7]

[7]Evolving continuously from $Q_v>0$ to $Q_v<0$ implies $Q_v=0$ at a certain time, and violates the semiclassicality condition $Q_v\gg\ell_P^6$.

In the following we often use the shorthand notation

$$\mathfrak{F}_\alpha(v) = (\mathfrak{E}^I_a(v), \mathfrak{A}^a_I(v), \mathfrak{q}(v)^{-\frac{1}{2}}) = f_\alpha(v) + O(\mu),$$
$$f_\alpha(v) = (E^I_a(v), A^a_I(v), q(v)^{-\frac{1}{2}}), \qquad q(v) = \frac{1}{6}\varepsilon_{IJK}\varepsilon^{abc}E^I_a(v)E^J_b(v)E^K_c(v), \tag{113}$$

where α labels components in $(\cdots)$.

We apply Eqs. (111) and (112) to C_v and $C_{a,v}$ and expand in terms of μ and $\mathfrak{F}_\alpha$. C_v and $C_{a,v}$ can be written as polynomials of $\mathfrak{F}_\alpha$ and lattice derivatives $\Delta\mathfrak{F}_\alpha$ by reorganizing terms and truncating to μ^3 (see Appendix for an explanation),

$$C_v \quad \text{or} \quad C_{a,v} = \mu \sum_{\alpha,\beta,J,K,N^\pm_J,M^\pm_K} F^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(\vec{v})\Delta_{J,N^\pm_J}\mathfrak{F}_\alpha(\tilde{v}_1)\Delta_{K,M^\pm_K}\mathfrak{F}_\beta(\tilde{v}_2) + \mu^2\sum_{\alpha,J,N^\pm_J} F^\alpha_{N^\pm_J}(\vec{v})\Delta_{J,N^\pm_J}\mathfrak{F}_\alpha(\tilde{v}) + \mu^3 F(\vec{v}) + O(\mu^4), \tag{114}$$

where $F^\alpha_{N^+_J,N^-_J}(\vec{v})$ and $F(\vec{v})$ are polynomials of $\mathfrak{F}_\alpha$ (explained below). $\Delta_{J,N^\pm_J}\mathfrak{F}_\alpha(\tilde{v})$ is the lattice derivative at $\tilde{v}$ in the J direction, by the difference between $\mathfrak{F}_\alpha$ at two vertices $\tilde{v}+N^+_J\mu\hat{J}$ and $\tilde{v}-N^-_J\mu\hat{J}$ ($N^\pm \in \mathbb{Z}$),

$$\Delta_{J,N^\pm_J}\mathfrak{F}_\alpha(\tilde{v}) = \mathfrak{F}_\alpha(\tilde{v}+N^+_J\mu\hat{J}) - \mathfrak{F}_\alpha(\tilde{v}-N^-_J\mu\hat{J}). \tag{115}$$

$\vec{v} = (v_1, v_2, \ldots)$ and $\tilde{v}, \tilde{v}_1, \tilde{v}_2$ are some vertices whose distance from v are of $O(\mu)$. $-3 \le N^\pm_J \le 3$ ($N^+_J \ne -N^-_J$) are integers and $\hat{J}$ is the lattice vector along the Jth direction. Nonzero $N^\pm_J$ reflect interactions among variables at neighboring vertices in C_v and $C_{a,v}$. Interactions are not only among nearest neighbors. $F^\alpha_{N^+_J,N^-_J}(\vec{v})$ and $F(\vec{v})$ [with $\vec{v} = (v_1, v_2, \ldots)$ a finite sequence of vertices v_i] are polynomials of $\mathfrak{F}_\alpha(v_i)$ where $v_i = v + \sum_J N_i(J)\mu\hat{J}_i$ ($J_i \in \{1,2,3\}$ and integer $N_i \in [-3,3]$) are vertices at or near v. Parameters α, β, $N^\pm$, $M^\pm$, J, $\vec{v}$, and $\tilde{v}, \tilde{v}_1, \tilde{v}_2$ are determined by patterns of variables and Poisson brackets in C_v,$C_{a,v}$, and thus are independent of v.

Recall that $f_\alpha(v)$ are smooth fields, and the continuum limit of (114) is of $O(\mu^3)$,

$$C_v \quad \text{or} \quad C_{a,v} = \mu^3 \sum_{\alpha,\beta,J,K}\left[\sum_{N^\pm_J,M^\pm_K}(N^+_J+N^-_J)(M^+_K+M^-_K)\mathcal{F}^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(v)\right]\partial_J f_\alpha(v)\partial_K f_\beta(v) + \mu^3\sum_{\alpha,J}\left[\sum_{N^\pm_J}(N^+_J+N^-_J)\mathcal{F}^\alpha_{N^\pm_J}(v)\right]\partial_J f_\alpha(v) + \mu^3\mathcal{F}(v) + O(\mu^4). \tag{116}$$

$\mathcal{F}^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(v)$, $\mathcal{F}^\alpha_{N^+_J,N^-_J}(v)$, and $\mathcal{F}(v)$ denote continuum limits of $F^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(\vec{v})$, $F^\alpha_{N^+_J,N^-_J}(\vec{v})$, and $F(\vec{v})$, respectively:

$$F^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(\vec{v}) = \mathcal{F}^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(v) + O(\mu),$$
$$F^\alpha_{N^+_J,N^-_J}(\vec{v}) = \mathcal{F}^\alpha_{N^+_J,N^-_J}(v) + O(\mu),$$
$$F(\vec{v}) = \mathcal{F}(v) + O(\mu). \tag{117}$$

They are given by $F^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(\vec{v})$, $F^\alpha_{N^+_J,N^-_J}(\vec{v})$, and $F(\vec{v})$ with all $v_i \to v$ and applying Eq. (105). $\mathcal{F}^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(v)$, $\mathcal{F}^\alpha_{N^+_J,N^-_J}(v)$, and $\mathcal{F}(v)$ are polynomials of $E^I_a(v)$, $A^a_I(v)$, $q(v)^{-\frac{1}{2}}$. Let us take an example for illustration,

$$\mathfrak{q}(v_1)^{-\frac{1}{2}}\mathfrak{E}^2_1(v_2)\mathfrak{E}^1_2(v_3) = q(v)^{-\frac{1}{2}}E^2_1(v)E^1_2(v) + O(\mu). \tag{118}$$

The leading term on the right-hand side corresponds to a term in $\mathcal{F}^{\alpha,\beta}_{N^\pm_J,M^\pm_K}(v)$, $\mathcal{F}^\alpha_{N^+_J,N^-_J}(v)$, or $\mathcal{F}(v)$.

We check that C_v, $C_{a,v}$, $\mathbf{H}$, and G^a_v have correct continuum limits [i.e., Eq. (116) recovers continuum expressions of scalar and vector constraints $\mathcal{C}(v)$ and $\mathcal{C}_a(v)$ up to a prefactor μ^3],

$$C_v = \mu^3\mathcal{C}(v) + O(\mu^4), \tag{119}$$

$$C_{a,v} = \mu^3\mathcal{C}_a(v) + O(\mu^4), \tag{120}$$

$$H_v = \mu^3 h(v) + O(\mu^4) = \mu^3 \sqrt{\left|\mathcal{C}(v)^2 - \frac{\alpha}{4}\sum_{a=1}^{3}\mathcal{C}_a(v)^2\right|} + O(\mu^4), \tag{121}$$

$$\mathbf{H} = \sum_v \mu^3 \sqrt{\left|\mathcal{C}(v)^2 - \frac{\alpha}{4}\sum_{a=1}^{3}\mathcal{C}_a(v)^2\right|} + O(\mu^4) \simeq \int_{\mathcal{S}} \mathrm{d}^3\sigma \sqrt{\left|\mathcal{C}(\sigma)^2 - \frac{\alpha}{4}\sum_{a=1}^{3}\mathcal{C}_a(\sigma)^2\right|}, \tag{122}$$

$$G_v^a = \frac{2\mu^3}{\beta a^2} D_j E_a^j(v) + O(\mu^3). \tag{123}$$

The prefactor μ^3 is desired for correct continuum limits. *Mathematica* codes for deriving Eqs. (119) and (120) are given in [69]. The last relation indicates that the closure condition (58) reduces to the Gauss constraint in the lattice continuum limit.

The continuum limit of s_v is given by

$$s_v = \mathrm{sgn}\left(C_v^2 - \frac{\alpha}{4}\sum_{a=1}^{3} C_{a,v}^2\right) = \mathrm{sgn}\left(\mathcal{C}(v)^2 - \frac{\alpha}{4}\sum_{a=1}^{3}\mathcal{C}_a(v)^2 + O(\mu)\right). \tag{124}$$

$\mathcal{C}$ and $\mathcal{C}_a$ are smooth fields in the continuum.

Given $v' \in V(\gamma)$, we assume v' is inside a neighborhood $U \subset \mathcal{S}$, such that $s_v = s_U$ is a constant for all $v \in U$ and the coordinate distance $r(v', \partial U)$ between v' and any point in ∂U satisfies $r(v', \partial U) \gg \mu$. This is an assumption for phase space points at which derivatives in Eqs. (109) and (110) are computed. This assumption is necessary for the lattice continuum limit of Eqs. (109) and (110), because otherwise as $\mu \to 0$, v' approaches the boundary where $C_v^2 - \frac{\alpha}{4}\sum_{a=1}^{3} C_{a,v}^2 = 0$, and then $s_{v'}$ jumps by variations for computing derivatives of $\mathbf{H}$ thus invalidate Eqs. (109) and (110).

We compute the following term in Eq. (109): the sum in $\sum_{v\in V(\gamma)} s_v \frac{C_v}{H_v}\frac{\partial C_v}{\partial \mathfrak{E}_a^I(v')}$ is nontrivial only inside the neighborhood U [because C_v that depends on $\mathfrak{E}(v')$ is located at v whose distance to v' is a multiple of μ], so s_v can be moved outside the sum by the above assumption:

$$\begin{aligned}
\sum_{v\in V(\gamma)} s_v \frac{C_v}{H_v}\frac{\partial C_v}{\partial \mathfrak{E}_a^I(v')} &= \mu s_U \sum_{v\in U}\frac{C_v}{H_v}\sum_{\alpha,\beta,J,K,N_J^\pm,M_K^\pm}\sum_i \frac{\partial F^{\alpha,\beta}_{N_J^\pm,M_K^\pm}(\vec{v})}{\partial \mathfrak{E}_a^I(v_i)}\delta_{v',v_i}\Delta_{J,N_J^\pm}\mathfrak{F}_\alpha(\tilde{v}_1)\Delta_{K,M_K^\pm}\mathfrak{F}_\beta(\tilde{v}_2)\\
&+\mu s_U \sum_{v\in U}\frac{C_v}{H_v}\sum_{\alpha,\beta,J,K,N_J^\pm,M_K^\pm} F^{\alpha,\beta}_{N_J^\pm,M_K^\pm}(\vec{v})\left[\frac{\partial \mathfrak{F}_\alpha(v')}{\partial \mathfrak{E}_a^I(v')}\delta_{v',\tilde{v}_1+N_J^+\mu\hat{J}} - \frac{\partial \mathfrak{F}_\alpha(v')}{\partial \mathfrak{E}_a^I(v')}\delta_{v',\tilde{v}_1-N_J^-\mu\hat{J}}\right]\Delta_{K,M_K^\pm}\mathfrak{F}_\beta(\tilde{v}_2)\\
&+\mu s_U \sum_{v\in U}\frac{C_v}{H_v}\sum_{\alpha,\beta,J,K,N_J^\pm,M_K^\pm} F^{\alpha,\beta}_{N_J^\pm,M_K^\pm}(\vec{v})\Delta_{J,N_J^\pm}\mathfrak{F}_\alpha(\tilde{v}_1)\left[\frac{\partial \mathfrak{F}_\beta(v')}{\partial \mathfrak{E}_a^I(v')}\delta_{v',\tilde{v}_2+M_K^+\mu\hat{K}} - \frac{\partial \mathfrak{F}_\beta(v')}{\partial \mathfrak{E}_a^I(v')}\delta_{v',\tilde{v}_2-M_K^-\mu\hat{K}}\right]\\
&+\mu^2 s_U \sum_{v\in U}\frac{C_v}{H_v}\sum_{\alpha,J,N_J^\pm}\sum_i \frac{\partial F^{\alpha}_{N_J^\pm}(\vec{v})}{\partial \mathfrak{E}_a^I(v_i)}\delta_{v',v_i}\Delta_{J,N_J^\pm}\mathfrak{F}_\alpha(\tilde{v})\\
&+\mu^2 s_U \sum_{v\in U}\frac{C_v}{H_v}\sum_{\alpha,J,N_J^\pm} F^{\alpha}_{N_J^\pm}(\vec{v})\left[\frac{\partial \mathfrak{F}_\alpha(v')}{\partial \mathfrak{E}_a^I(v')}\delta_{v',\tilde{v}+N_J^+\mu\hat{J}} - \frac{\partial \mathfrak{F}_\alpha(v')}{\partial \mathfrak{E}_a^I(v')}\delta_{v',\tilde{v}-N_J^-\mu\hat{J}}\right] + \mu^3 s_U \sum_{v\in U}\frac{C_v}{H_v}\sum_i \frac{\partial F(\vec{v})}{\partial \mathfrak{E}_a^I(v_i)}\delta_{v',v_i}\\
&+O(\mu^4).
\end{aligned} \tag{125}$$

Two sums $\sum_v$ and $\sum_{\alpha,\beta,J,K,N_J^\pm,M_K^\pm}$ (or $\sum_{\alpha,J,N_J^\pm}$ and $\sum_i$) can be interchanged since α, J, N_J^+, N_J^-, N_i are independent of v. Kronecker deltas in Eq. (125) are nonzero only if v is inside U by the assumption $r(v', \partial U) \gg \mu$, since distances from v_i, $\tilde{v}$, $\tilde{v}_{1,2}$ to v are of $O(\mu)$. $\sum_{v\in U}$ in the result can be freely extended to $\sum_v$ over all $v \in V(\gamma)$, because v outside U has no contribution.

In the first term in the result of Eq. (125), $\delta_{v_i,v'}$ restricts $v = v' - \delta_i$, where $\delta_i = v_i - v = \sum_J N_i(J)\mu\hat{J}_i$. We denote by $\tilde{\delta}_{1,2} = \tilde{v}_{1,2} - v \sim O(\mu)$ that δ_i and $\tilde{\delta}_{1,2}$ are independent of v. Carrying out $\sum_v$, the first term in Eq. (125) becomes

$$\mu s_U \sum_{\alpha,\beta,J,K,N_J^\pm,M_K^\pm} \sum_i \frac{C_{v'-\delta_i}}{H_{v'-\delta_i}} \frac{\partial F^{\alpha\beta}_{N_J^\pm,M_K^\pm}(\overrightarrow{v'-\delta_i})}{\partial \mathfrak{E}^I_a(v')} \Delta_{J,N_J^\pm}\mathfrak{F}_\alpha(v'-\delta_i+\tilde{\delta}_1)\Delta_{K,M_K^\pm}\mathfrak{F}_\beta(v'-\delta_i+\tilde{\delta}_2)$$
$$= \mu^3 s_U \sum_{\alpha,\beta,J,K,N_J^\pm,M_J^\pm} \frac{\mathcal{C}(v')}{h(v')} \frac{\partial \mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}(v')}{\partial E^I_a(v')} (N_J^+ + N_J^-)(M_K^+ + M_K^-)\partial_J f_\alpha(v')\partial_K f_\beta(v') + O(\mu^4), \tag{126}$$

where $F^{\alpha\beta}_{N_J^\pm,M_K^\pm}(\overrightarrow{v'-\delta_i})$ is from the expansion of $C_{v'-\delta_i}$. Note that all vertices in $\overrightarrow{v'-\delta_i}$ are inside U. $F^{\alpha\beta}_{N_J^\pm,M_K^\pm}(\vec{v})$ is a polynomial of $\mathfrak{F}_\alpha(v_i)$. Derivatives $\partial F^{\alpha\beta}_{N_J^\pm,M_K^\pm}/\partial \mathfrak{E}^I_a$ have continuum limit $\partial \mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}/\partial E^I_a$. Thanks to summing over all $v \in U$, $\sum_i$ in Eq. (126) sums over vertices $v'-\delta_i$ at which $\partial F^{\alpha\beta}_{N_J^\pm,M_K^\pm}(\overrightarrow{v'-\delta_i})/\partial \mathfrak{E}^I_a(v')$ are nonzero, and reduces to the Leibniz rule of $\partial \mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}(v')/\partial E^I_a(v')$.

In the second term in the result of Eq. (125), $\delta_{v',\tilde{v}_1 \pm N_J^\pm \mu \hat{J}}$ restricts $v = v' - \tilde{\delta}_1 \mp N_J^\pm \mu \hat{J} \equiv v_J^\pm$. Carrying out $\sum_v$ in the second term in Eq. (125) gives

$$\mu s_U \sum_{\alpha,\beta,J,K,N_J^\pm,M_K^\pm} \left[\frac{C_{v_J^+}}{H_{v_J^+}} F^{\alpha\beta}_{N_J^\pm,M_K^\pm}(\vec{v_J^+})\Delta_{K,M_K^\pm}\mathfrak{F}_\beta(v_J^+ + \tilde{\delta}_2) - \frac{C_{v_J^-}}{H_{v_J^-}} F^{\alpha\beta}_{N_J^\pm,M_K^\pm}(\vec{v_J^-})\Delta_{K,M_K^\pm}\mathfrak{F}_\beta(v_J^- + \tilde{\delta}_2)\right] \frac{\partial \mathfrak{F}_\alpha(v')}{\partial \mathfrak{E}^I_a(v')}$$
$$= -\mu^3 s_U \sum_{\alpha,\beta,J,K,N_J^+,N_J^-} (N_J^+ + N_J^-)(M_K^+ + M_K^-)\partial_J\left[\frac{\mathcal{C}}{h}\mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}\partial_K f_\beta\right](v')\frac{\partial f_\alpha(v')}{\partial E^I_a(v')} + O(\mu^4). \tag{127}$$

The third and fifth terms in Eq. (125) are treated similar to the second term, while the fourth and sixth terms are treated similar to the first term. As results,

$$\text{3rd term} = -\mu^3 s_U \sum_{\alpha,\beta,J,K,N_J^+,N_J^-} (N_J^+ + N_J^-)(M_K^+ + M_K^-)\partial_K\left[\frac{\mathcal{C}}{h}\mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}\partial_J f_\alpha\right](v')\frac{\partial f_\beta(v')}{\partial E^I_a(v')} + O(\mu^4),$$
$$\text{4th term} = \mu^3 s_U \sum_{\alpha,J,N_J^+,N_J^-} \frac{\mathcal{C}(v')}{h(v')}\frac{\partial \mathcal{F}^\alpha_{N_J^+,N_J^-}(v')}{\partial E^I_a(v')}(N_J^+ + N_J^-)\partial_J f_\alpha(v') + O(\mu^4),$$
$$\text{5th term} = -\mu^3 s_U \sum_{\alpha,J,N_J^+,N_J^-} (N_J^+ + N_J^-)\partial_J\left[\frac{\mathcal{C}(v')}{h(v')}\mathcal{F}^\alpha_{N_J^+,N_J^-}(v')\right]\frac{\partial f_\alpha(v')}{\partial E^I_a(v')} + O(\mu^4),$$
$$\text{6th term} = \mu^3 \frac{\mathcal{C}(v')}{h(v')}\frac{\partial \mathcal{F}(v')}{\partial E^I_a(v')} + O(\mu^4). \tag{128}$$

On the other hand, we apply the functional derivative to $\mathcal{C}$ using Eq. (116),

$$\begin{aligned}\int_U \mathrm{d}^3\sigma \frac{\mathcal{C}(\sigma)}{h(\sigma)}\frac{\delta\mathcal{C}(\sigma)}{\delta E^I_a(v')} =& \sum_{\alpha,\beta,J,K,N_J^\pm,M_J^\pm} \frac{\mathcal{C}(v')}{h(v')}\frac{\partial \mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}(v')}{\partial E^I_a(v')}(N_J^+ + N_J^-)(M_K^+ + M_K^-)\partial_J f_\alpha(v')\partial_K f_\beta(v') \\ &- \sum_{\alpha,\beta,J,K,N_J^+,N_J^-}(N_J^+ + N_J^-)(M_K^+ + M_K^-)\partial_J\left[\frac{\mathcal{C}}{h}\mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}\partial_K f_\beta\right](v')\frac{\partial f_\alpha(v')}{\partial E^I_a(v')} \\ &- \sum_{\alpha,\beta,J,K,N_J^+,N_J^-}(N_J^+ + N_J^-)(M_K^+ + M_K^-)\partial_K\left[\frac{\mathcal{C}}{h}\mathcal{F}^{\alpha\beta}_{N_J^\pm,M_K^\pm}\partial_J f_\alpha\right](v')\frac{\partial f_\beta(v')}{\partial E^I_a(v')} \\ &+ \sum_{\alpha,J,N_J^+,N_J^-}\frac{\mathcal{C}(v')}{h(v')}\frac{\partial\mathcal{F}^\alpha_{N_J^+,N_J^-}(v')}{\partial E^I_a(v')}(N_+ + N_-)\partial_J f_\alpha(v') \\ &- \sum_{\alpha,J,N_J^+,N_J^-}(N_+ + N_-)\partial_J\left[\frac{\mathcal{C}(v')}{h(v')}\mathcal{F}^\alpha_{N_J^+,N_J^-}(v')\right]\frac{\partial f_\alpha(v')}{\partial E^I_a(v')} + \frac{\mathcal{C}(v')}{h(v')}\frac{\partial\mathcal{F}(v')}{\partial E^I_a(v')}. \end{aligned} \tag{129}$$

Comparing Eq. (129) with (126)–(128), we obtain the following result:

$$\sum_{v\in V(\gamma)} s_v \frac{C_v}{H_v}\frac{\partial C_v}{\partial \mathfrak{E}^I_a(v')} = \mu^3\int_U \mathrm{d}^3\sigma s_U \frac{\mathcal{C}(\sigma)}{h(\sigma)}\frac{\delta\mathcal{C}(\sigma)}{\delta E^I_a(v')} + O(\mu^4). \tag{130}$$

The derivation of Eq. (130) only uses general patterns of C_v and $C_{j,v}$ in Eq. (114) and their continuum limit, so it can easily be generalized to $\sum_v \frac{C_{b,v}}{H_v}\frac{\partial C_{b,v}}{\partial\mathfrak{E}^I_a(v')}$ and derivatives with respect to $\mathfrak{A}^a_I(v')$. Therefore

$$\begin{aligned}\frac{\partial\mathbf{H}}{\partial\mathfrak{E}^I_a(v')} &= \mu^3\int_U \mathrm{d}^3\sigma s_U\left[\frac{\mathcal{C}(\sigma)}{h(\sigma)}\frac{\delta\mathcal{C}(\sigma)}{\delta E^I_a(v')} - \frac{\alpha}{4}\sum_{b=1}^3\frac{\mathcal{C}_b(\sigma)}{h(\sigma)}\frac{\delta\mathcal{C}_b(\sigma)}{\delta E^I_a(v')}\right] + O(\mu^4) \\ &= \mu^3\frac{\delta}{\delta E^I_a(v')}\int_{\mathcal{S}}\mathrm{d}^3\sigma\sqrt{\left|\mathcal{C}(\sigma)^2 - \frac{\alpha}{4}\sum_{b=1}^3\mathcal{C}_b(\sigma)^2\right|} + O(\mu^4), \end{aligned} \tag{131}$$

$$\frac{\partial\mathbf{H}}{\partial\mathfrak{A}^a_I(v')} = \mu^3\int_U \mathrm{d}^3\sigma s_U\left[\frac{\mathcal{C}(\sigma)}{h(\sigma)}\frac{\delta\mathcal{C}(\sigma)}{\delta A^a_I(v')} - \frac{\alpha}{4}\sum_{b=1}^3\frac{\mathcal{C}_b(\sigma)}{h(\sigma)}\frac{\delta\mathcal{C}_b(\sigma)}{\delta A^a_I(v')}\right] + O(\mu^4) \tag{132}$$

$$= \mu^3\frac{\delta}{\delta A^a_I(v')}\int_{\mathcal{S}}\mathrm{d}^3\sigma\sqrt{\left|\mathcal{C}(\sigma)^2 - \frac{\alpha}{4}\sum_{b=1}^3\mathcal{C}_b(\sigma)^2\right|} + O(\mu^4). \tag{133}$$

$\int_U$ can be replaced by $\int_{\mathcal{S}}$ because the functional derivative is local. This result shows that the lattice continuum limit of partial derivatives in discrete variables gives the functional derivatives in smooth fields.

Recall Eqs. (107) and (108), where we obtain the lattice continuum limit of discrete semiclassical EOMs (74),

$$-\frac{\mathrm{d}A^a_I(v)}{\mathrm{d}\tau} = \frac{\kappa\beta}{2}\frac{\delta}{\delta E^I_a(v)}\int_{\mathcal{S}}\mathrm{d}^3\sigma\sqrt{\left|\mathcal{C}(\sigma)^2 - \frac{\alpha}{4}\sum_{a=1}^3\mathcal{C}_a(\sigma)^2\right|} + O(\mu), \tag{134}$$

$$\frac{\mathrm{d}E^I_a(v)}{\mathrm{d}\tau} = \frac{\kappa\beta}{2}\frac{\delta}{\delta A^a_I(v)}\int_{\mathcal{S}}\mathrm{d}^3\sigma\sqrt{\left|\mathcal{C}(\sigma)^2 - \frac{\alpha}{4}\sum_{a=1}^3\mathcal{C}_a(\sigma)^2\right|} + O(\mu). \tag{135}$$

The result recovers the classical EOMs (24) of the gravity-dust system in the continuum when $\mathcal{C}(\sigma)^2 - \frac{\alpha}{4}\sum_{a=1}^3\mathcal{C}_a(\sigma)^2 > 0$.

The above derivation replies on the assumption that $v'\in U$, $r(v',\partial U)\gg\mu$, and $s_v = s_U$ is constant on U. But if we violate this assumption, i.e., let $v'\in U$, $r(v',\partial U)\sim\mu$, and s_v changes sign outside U, then in the lattice continuum limit

$\mu\to 0$, v' belongs to the boundary where s_v jumps and $\mathcal{C}(\sigma)^2-\frac{\alpha}{4}\sum_{a=1}^3\mathcal{C}_a(\sigma)^2=0$. Semiclassical EOMs at this v' cannot relate to Eqs. (134) and (135) by the lattice continuum limit, because the functional derivative is ill-defined at v'.

In our quantization, nonholonomic constraints $\mathcal{C}(\sigma)^2-\frac{\alpha}{4}\sum_{a=1}^3\mathcal{C}_a(\sigma)^2>0$ and $\mathcal{C}<0$ are not imposed to the Hilbert space $\mathcal{H}_\gamma$. Therefore $\mathbf{H}$ are defined on the entire phase space $\mathcal{P}_\gamma$, and thus the continuum limit Eqs. (134) and (135) extend the continuum theory to the regime where nonholonomic constraints are not valid. The relation between Eqs. (134) and (135) and the classical EOMs (24) is sensitive to the choice of initial condition. Here the initial condition is given by $[g']$ at which the initial coherent state $\Psi^t_{[g']}$ is peaked. $\Psi^t_{[g']}$ is semiclassical if $[g']$ is in the classical allowed regime of the phase space, while the classical allowed regime satisfies the nonholonomic constraints required by the classical gravity-dust system. Equations (134) and (135) indeed coincide with classical EOMs (24) of the continuum theory, if the initial data g' satisfies (discretized) nonholonomic constraints:

(i) For gravity coupled to Brown-Kuchař dust, if the initial data g' at $\tau=0$ satisfies $C_v^2-\frac{1}{4}\sum_{a=1}^3 C_{a,v}^2>0$ and $C_v<0$ at all $v\in V(\gamma)$, these two nonholonomic constraints are still going to be satisfied by the solution to EOMs (134) and (135) within a finite time period $\tau\in[0,T_0]$, simply because the solution is a continuous function in τ. Therefore $||$ in (134) and (135) can be removed at least within this time period.

On the other hand, although $C_v^2-\frac{1}{4}\sum_{a=1}^3 C_{a,v}^2$ is not exactly conserved in (74) [or (86)] due to the anomaly from discretization [57], it is approximately conserved up to $O(\mu)$ because its continuum limit $\mathcal{C}^2-\frac{1}{4}\sum_{a=1}^3\mathcal{C}_a^2$ is conserved by the continuum limit Eqs. (134) and (135). C_v cannot flip sign by a similar reason. Therefore $C_v^2-\frac{1}{4}\sum_{a=1}^3 C_{a,v}^2>0$ and $C_v<0$ can continuously be satisfied by the solution at and even after T_0. By adding another time period $[T_0,2T_0]$, repeating the argument iteratively, we can extend the time period to entire $[0,T]$ in which $C_v^2-\frac{1}{4}\sum_{a=1}^3 C_{a,v}^2>0$ and $C_v<0$ are satisfied, when μ is sufficiently small.[8] Then semiclassical EOMs from $A_{[g],[g']}$ reproduce classical EOMs (24) for gravity coupled to Brown-Kuchař dust in the continuum limit,

$$-\frac{\mathrm{d}A^a_I(v)}{\mathrm{d}\tau}=\frac{\kappa\beta}{2}\frac{\delta}{\delta E^I_a(v)}\int_S \mathrm{d}^3\sigma\sqrt{\mathcal{C}(\sigma)^2-\frac{1}{4}\sum_{a=1}^3\mathcal{C}_a(\sigma)^2}+O(\mu), \tag{136}$$

$$\frac{\mathrm{d}E^I_a(v)}{\mathrm{d}\tau}=\frac{\kappa\beta}{2}\frac{\delta}{\delta A^a_I(v')}\int_S \mathrm{d}^3\sigma\sqrt{\mathcal{C}(\sigma)^2-\frac{1}{4}\sum_{a=1}^3\mathcal{C}_a(\sigma)^2}+O(\mu). \tag{137}$$

(ii) A similar reasoning applies to gravity coupled to Gaussian dust, when the initial data g' of $A_{[g],[g']}$ satisfy $C_v<0$ and $C_{a,v}=0$; both C_v and $C_{a,v}$ are approximately conserved if μ is sufficiently small, since they are conserved in the continuum limit, and thus $C_v<0$ is preserved by the time evolution for sufficiently small μ. Then semiclassical EOMs of reduced phase space LQG with Gaussian dust reproduce classical EOMs (24) in the continuum limit up to a flip of time direction

$$\frac{\mathrm{d}A^a_I(v)}{\mathrm{d}\tau}=\frac{\kappa\beta}{2}\frac{\delta}{\delta E^I_a(v)}\int_S \mathrm{d}^3\sigma\,\mathcal{C}(\sigma)+O(\mu), \tag{138}$$

$$-\frac{\mathrm{d}E^I_a(v)}{\mathrm{d}\tau}=\frac{\kappa\beta}{2}\frac{\delta}{\delta A^a_I(v')}\int_S \mathrm{d}^3\sigma\,\mathcal{C}(\sigma)+O(\mu). \tag{139}$$

Recall that time direction has been flipped to flow backward in Sec. II in order to obtain a positive Hamiltonian.

(iii) If the initial data do not satisfy nonholonomic constraints, $\Psi^t_{[g']}$ is not semiclassical anymore. The continuum limit of semiclassical EOMs derived from $A_{[g],[g']}$ cannot be related to classical EOMs (24) of the gravity-dust system. The existence of nonclassical solutions has been anticipated in [57] and viewed as analogs of negative energy states in relativistic QFT, because when Eq. (15) is viewed as constraint, it can be written as $P^2+(\mathcal{C}-q^{\alpha\beta}\mathcal{C}_\alpha\mathcal{C}_\beta)=0$ whose quantization would be an analog of the Klein-Gordon operator. But whether

[8] $T\to\infty$ is more subtle because accumulating errors of $O(\mu)$ over an infinite amount of time might cause a finite change of $C_v^2-\frac{1}{4}\sum_{a=1}^3 C_{a,v}^2$ and flip the sign.

nonclassical solutions appear or disappear is determined by initial conditions, similar to the situation of negative energy states in QFT.

Some examples of solutions of semiclassical EOMs and their continuum limit are studied in cosmological perturbation theory in [63].

VII. ASYMPTOTICS OF TRANSITION AMPLITUDE

Assuming initial and final states $\Psi^t_{[g']}$ and $\Psi^t_{[g]}$ are both semiclassical in the sense that both $[g']$ and $[g]$ are within the classical allowed regime, if $[g], [g']$ are connected by the trajectory $g(\tau)$ satisfying Eq. (85), as $t \to 0$, the path integral (51) dominates at this semiclassical trajectory,

$$\frac{A_{[g],[g']}}{\|\Psi^t_{[g]}\|\|\Psi^t_{[g']}\|} = \frac{(2\pi t)^{\mathcal{N}/2}}{\sqrt{\det(-H)}} \nu[g(\tau), h] e^{S[g(\tau),h]/t}[1 + O(t)], \tag{140}$$

where $\mathcal{N}$ is the total dimension of the integral in Eq. (51) and H is the Hessian matrix at the solution. $S[g(\tau), h]$ is the action evaluated at the solution $g(\tau), h$, where the continuous trajectory $g(\tau) \simeq g_i$ approximates the discrete solution as $\Delta\tau$ small. We can set for the solution $h = 1$ by setting representatives g and g' such that $g(T) = g$ and $g(0) = g'$.

If the initial and final data $[g'], [g]$ are not connected by any trajectory $g(\tau)$ satisfying Eq. (85), the amplitude is suppressed as $t \to 0$,

$$\frac{A_{[g],[g']}}{\|\Psi^t_{[g]}\|\|\Psi^t_{[g']}\|} = O(t^M), \quad \forall\ M > 0. \tag{141}$$

VIII. COMPARISON WITH SPIN FOAM FORMULATION AND OUTLOOK

The above analysis demonstrates the semiclassical consistency of the new path integral formulation from reduced phase space LQG. If we compare our results to the spin foam formulation, we find the following advantages of our path integral formulation:

(1) Our path integral formulation is free of the cosine problem. The initial condition $[g']$ given by the semiclassical initial state $\Psi^t_{[g']}$ determines a unique solution of semiclassical EOMs up to SU(2) gauge freedom. Therefore the asymptotic formula (140) has only a single exponential in the integrand.

A key reason why we obtain a unique solution and avoid the cosine problem is that all solutions of discrete EOMs (56) and (57) admit the time continuous limit. If spin foam formulation admitted the time continuous limit or anything similar, the continuous time EOMs (critical equations) would have forbidden the 4D orientation to jump and suppressed contributions from orientation-changing evolutions to spin foam amplitude.

(2) Our path integral formulation is free of the flatness problem. The semiclassical analysis of the path integral has been shown to reproduce the classical EOMs (24), which are Einstein equation formulated in the reduced phase space. Semiclassical EOMs (86) admit all curved solutions that are physically interesting. For instance, [50] has demonstrated the homogeneous and isotropic cosmology as a solution, while [63] obtains cosmological perturbation theory from solutions. Note that the flat spacetime is not a solution of semiclassical EOMs because of the presence of a physical dust field with positive energy density.

(3) There is a clear link between our path integral formulation and the canonical LQG. The path integral (51) is rigorously derived from the canonical formulation in the reduced phase space. The unitarity is manifest because the path integral is the transition amplitude of unitary evolution generated by the Hamiltonian $\hat{\mathbf{H}}$.

(4) The path integral formula (51) is clearly finite (irrelevant to the cosmological constant), because the transition amplitude $A_{[g],[g']} = \langle \Psi^t_{[g]} | \exp[-\frac{i}{\hbar} T \hat{\mathbf{H}}] | \Psi^t_{[g']} \rangle$ is finite. All ingredients $\Psi^t_{[g]}$, $\Psi^t_{[g']}$, $\exp[-\frac{i}{\hbar} T \hat{\mathbf{H}}]$, and $\langle \cdot | \cdot \rangle$ are well-defined.

Our formulation may still have issues of computational complexity and lattice dependence similar to the spin foam formulation, at least at the present stage. However, studies of the new path integral formulation are still at a very preliminary stage, and research on overcoming these issues will be carried out in the future. Research in progress and in the near future focus on generalizing the present work to other matter couplings, investigating quantum corrections, and studying various physical situations such as cosmology and black holes:

(1) The generalization to include standard matter couplings can be carried out by following the existing quantization of matters in the canonical LQG [66–68]. It is straightforward to construct $\hat{\mathbf{H}}$ for LQG coupled to all standard model matters (and it has been done [57,67]). The only gap of deriving a coherent state path integral formula is computing the overlap of Yang-Mills coherent states with a higher-rank gauge group. This task is currently in progress. Once the path integral formula is obtained, the semiclassical limit will be studied to contact with the standard model.

(2) At the level of discrete path integral (51), the action $S[g, h]$ depends on the nonpolynomial operator $\hat{\mathbf{H}}$ and its matrix element, which is hard to compute. However, because $\Delta\tau$ is arbitrarily small, we may

consider a formal time continuous limit at the level of the path integral, as in the standard QFT. The resulting path integral formula integrates over continuous paths, and then the matrix element of $\hat{\mathbf{H}}$ in $S[g,h]$ reduces to the coherent state expectation value $\langle\psi_g^t|\hat{\mathbf{H}}|\psi_g^t\rangle$, which is computable as a perturbative expansion in t by using the method in [75]. Therefore perturbative techniques in QFT (more precisely, the lattice perturbation theory) should be applied to our path integral formulation to compute quantities such as correlation functions and quantum effective action as power expansions in t. Contributions of higher order in t give quantum corrections predicted from LQG.

(3) Our path integral formulation depends on the cubic lattice γ even after taking the time continuous limit. Currently the lattice continuum limit at the quantum level is not clear for our formulation (in Sec. VI, the lattice continuum limit $\mu\to 0$ is taken after the semiclassical limit $l_P\to 0$). We expect to see the effects of the lattice continuum limit at the quantum level order by order in t in perturbative computations. It is also interesting to apply the refinement and renormalization techniques [20,49] to our path integral formulation.

(4) Another interesting direction is to study solutions of semiclassical EOMs from the path integral and extract physical consequences. In [50,63], we have applied the EOMs to cosmology and cosmological perturbation theory. The research in progress is to apply the EOMs to other situations, and in particular black holes. The studies are likely to be done numerically.

ACKNOWLEDGMENTS

This work receives support from the National Science Foundation through Grant No. PHY-1912278. *Mathematica* computations in this work are carried out on the HPC server at Fudan University and the KoKo HPC server at Florida Atlantic University. The authors acknowledge Ling-Yan Hung for sharing the computational resource at Fudan University.

APPENDIX: PROOF OF EQ. (114)

There are two useful properties of C_v and $C_{a,v}$:

(i) C_v and $C_{a,v}$ are polynomials of $h(e)$, $p^a(e)$, and $Q_v^{1/2}$. By applying Eq. (111) and expanding in μ, C_v and $C_{a,v}$ become series of μ and $\mathfrak{F}_\alpha(v)$.

(ii) In the continuum limit $C_v=\mu^3\mathcal{C}(v)+O(\mu^4)$, $C_{a,v}=\mu^3\mathcal{C}_a(v)+O(\mu^4)$ where the leading order is of $O(\mu^3)$ and both $\mathcal{C}$ and $\mathcal{C}_a$ are polynomials of f_α and their first order derivatives.[9] Each term in $\mathcal{C}$ and $\mathcal{C}_a$ contain no more than two derivatives.

We extract arbitrarily two terms at $O(\mu^n)$ in the expansion of C_v and $C_{a,v}$. Generically they may be written as

$$\begin{aligned}&\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)\\ \text{and}\quad &\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\mathfrak{F}'_{n+1}(v_{n+1}')\cdots\mathfrak{F}'_q(v_q').\end{aligned}\tag{A2}$$

They may share $\mathfrak{F}_1,\ldots,\mathfrak{F}_n$ although locations of $\mathfrak{F}_1,\ldots,\mathfrak{F}_n$, v_i, and v_i' may be different between these two terms. Distances from v to v_i, v_i' are of $O(\mu)$. $\mathfrak{F}_i$ and $\mathfrak{F}_i'$ are factors not shared by these two terms. If the relative sign between these two terms is negative, we can perform the following reduction:

$$\begin{aligned}&\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)-\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\mathfrak{F}'_{n+1}(v_{n+1}')\cdots\mathfrak{F}'_q(v_q')\\
&\quad=\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)-\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)\\
&\qquad+\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)-\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\mathfrak{F}'_{n+1}(v_{n+1}')\cdots\mathfrak{F}'_q(v_q')\\
&\quad=[\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)-\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')]\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)\\
&\qquad+\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')[\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)-\mathfrak{F}'_{n+1}(v_{n+1}')\cdots\mathfrak{F}'_q(v_q')].\end{aligned}\tag{A3}$$

The quantity in the first square bracket of the above result is the difference of two monomials $\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)$ and $\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')$ sharing the same set of $\mathfrak{F}_{1,\ldots,n}$, and can be further reduced

[9] F^a_{IJ} has only first order derivatives of A^a_I. $\beta K^a_I=A^a_I-\Gamma^a_I$ where

$$\Gamma^a_I=\frac{1}{2}\epsilon^{abc}E^J_c[E^b_{I,J}-E^b_{J,I}+E^K_bE^d_IE^d_{K,J}]+\frac{1}{4}\epsilon^{abc}E^J_c\left[2E^b_I\frac{(\det(E))_{,J}}{\det(E)}-E^b_J\frac{(\det(E))_{,I}}{\det(E)}\right].\tag{A1}$$

Here $\det(E(v))=q(v)$, the inverse $E^a_I(v)=\det(E(v))^{-1}$ (quadatic polynomial of $E^I_a(v)$), and $\det(E)\frac{(\det(E))_{,J}}{\det(E)}=\frac{-2}{q}\partial_I q^{1/2}$ [we assume $q(v)>0$].

$$\begin{aligned}
&\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)-\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\\
&\quad=\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)-\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')+\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')-\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\\
&\quad=\mathfrak{F}_1(v_1)[\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)-\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')]+[\mathfrak{F}_1(v_1)-\mathfrak{F}_1(v_1')]\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\\
&\quad=\cdots\\
&\quad=\sum_{i=1}^{n}\mathfrak{F}_1(v_1)\cdots\mathfrak{F}_{i-1}(v_{i-1})[\mathfrak{F}_i(v_i)-\mathfrak{F}_i(v_i')]\mathfrak{F}_{i+1}(v_{i+1}')\cdots\mathfrak{F}_n(v_n'). \qquad (A4)
\end{aligned}$$

Inserting this result back into Eq. (A3) gives

$$\begin{aligned}
&\mathfrak{F}_1(v_1)\mathfrak{F}_2(v_2)\cdots\mathfrak{F}_n(v_n)\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)-\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')\mathfrak{F}'_{n+1}(v_{n+1}')\cdots\mathfrak{F}'_q(v_q')\\
&\quad=\sum_{i=1}^{n}\mathfrak{F}_1(v_1)\cdots\mathfrak{F}_{i-1}(v_{i-1})[\mathfrak{F}_i(v_i)-\mathfrak{F}_i(v_i')]\mathfrak{F}_{i+1}(v_{i+1}')\cdots\mathfrak{F}_n(v_n')\\
&\qquad+\mathfrak{F}_1(v_1')\mathfrak{F}_2(v_2')\cdots\mathfrak{F}_n(v_n')[\mathfrak{F}_{n+1}(v_{n+1})\cdots\mathfrak{F}_m(v_m)-\mathfrak{F}'_{n+1}(v_{n+1}')\cdots\mathfrak{F}'_q(v_q')], \qquad (A5)
\end{aligned}$$

while there is no reduction for the second square bracket. Here the point of this reduction is to manifest the difference $\mathfrak{F}_i(v_i)-\mathfrak{F}_i(v_i')$ in the formula.

We insert the above result back into C_v and $C_{v,a}$ so that they become polynomials of $\mathfrak{F}_\alpha$ and $\Delta\mathfrak{F}_\alpha(v,v')\equiv\mathfrak{F}_\alpha(v)-\mathfrak{F}_\alpha(v')$. We make a further similar reduction as above, by including $\Delta\mathfrak{F}_\alpha$ as one of generators of the polynomial. As a result from iteration, we obtain at $O(\mu^n)$

$$\begin{aligned}
&\mu^n\left[\mathrm{Pol}_n(\mathfrak{F}_\alpha)+\sum_{p>0}\mathrm{Pol}_n^p(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha)+\sum_{k\geq 0,l>0}\mathrm{Pol}_n^{k,l}(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha,\Delta^2\mathfrak{F}_\alpha)\right]\\
&\quad=\mu^n\left[\mathrm{Pol}_n(\mathfrak{F}_\alpha)+\sum_{p>0}\mu^p\mathrm{Pol}_n^p(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha/\mu)+\sum_{k\geq 0,l>0}\mu^{k+2l}\mathrm{Pol}_n^{k,l}(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha/\mu,\Delta^2\mathfrak{F}_\alpha/\mu^2)\right]. \qquad (A6)
\end{aligned}$$

$\Delta^2\mathfrak{F}_\alpha=\Delta\mathfrak{F}_\alpha(v,v')-\Delta\mathfrak{F}_\alpha(\tilde{v},\tilde{v}')$ and $\Delta\mathfrak{F}_\alpha/\mu$, $\Delta^2\mathfrak{F}_\alpha/\mu^2$ are lattice derivatives. $\mathrm{Pol}_n(\mathfrak{F}_\alpha)$ is a polynomial of $\mathfrak{F}_\alpha$. $\mathrm{Pol}_n^p(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha)$ is a polynomial homogeneous in $\Delta\mathfrak{F}_\alpha$ of degree p. $\mathrm{Pol}_n^{k,l}(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha,\Delta^2\mathfrak{F}_\alpha)$ is a polynomial homogeneous in $\Delta\mathfrak{F}_\alpha$ and $\Delta^2\mathfrak{F}_\alpha$ of degree k and l, respectively. We stop the reduction at $\Delta^2\mathfrak{F}_\alpha$ and do not try to get $\Delta^3\mathfrak{F}_\alpha$ (even if we get $\Delta\mathfrak{F}_\alpha$, its coefficient vanishes as $\mu\to 0$ since C_v and $C_{v,a}$ do not contain a third derivative).

Importantly, we assume that when $\mathrm{Pol}_n(\mathfrak{F}_\alpha)$, $\mathrm{Pol}_n^p(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha)$, and $\mathrm{Pol}_n^{k,l}(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha,\Delta^2\mathfrak{F}_\alpha)$ are nonzero, $\mathrm{Pol}_n(\mathfrak{F}_\alpha)$ and the coefficients of $\Delta\mathfrak{F}_\alpha$ and $\Delta^2\mathfrak{F}_\alpha$ (as polynomials of $\mathfrak{F}_\alpha$) in $\mathrm{Pol}_n^p(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha)$,$\mathrm{Pol}_n^{k,l}(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha,\Delta^2\mathfrak{F}_\alpha)$ do not vanish as $\mu\to 0$, because otherwise they can be further reduced to higher order in $\Delta\mathfrak{F}_\alpha$.

We are interested in expansions of C_v and $C_{v,a}$ truncated up to $O(\mu^3)$ to be relevant to their continuum limit. So we focus on

$$n\leq 3,\qquad n+p\leq 3,\qquad n+k+2l\leq 3. \qquad (A7)$$

Continuum limits of C_v and $C_{v,a}$ contain no terms of three derivatives, so it imposes in addition

$$k=0,\qquad l=1,\qquad p\leq 2. \qquad (A8)$$

Moreover $C_v, C_{v,a}\sim\mu^3$ in the continuum limit. So at $n=0$, $\mathrm{Pol}_0(\mathfrak{F}_\alpha)$, $\mathrm{Pol}_0^p(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha)$, and $\mathrm{Pol}_0^{k,l}(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha,\Delta^2\mathfrak{F}_\alpha)$ have to vanish, since otherwise they produce a nonzero continuum limit at $O(\mu^0)$, $O(\mu^1)$, $O(\mu^2)$,

$$\mathrm{Pol}_0(f_\alpha)+\sum_{p=1}^{2}\mu^p\mathrm{Pol}_0^p(f_\alpha,\partial f_\alpha)+\mu^2\mathrm{Pol}_0^{0,1}(f_\alpha,\partial f_\alpha,\partial^2 f_\alpha). \qquad (A9)$$

By similar arguments, $\mathrm{Pol}_1(\mathfrak{F}_\alpha)$ and $\mathrm{Pol}_1^1(\mathfrak{F}_\alpha,\Delta\mathfrak{F}_\alpha)$ have to vanish at $n=1$, and $\mathrm{Pol}_2(\mathfrak{F}_\alpha)$ has to vanish at $n=2$. As a result, C_v and $C_{v,a}$ can be written as

$$\mu[\mathrm{Pol}_1^2(\mathfrak{F}_\alpha, \Delta\mathfrak{F}_\alpha) + \mathrm{Pol}_1^{0,1}(\mathfrak{F}_\alpha, \Delta\mathfrak{F}_\alpha, \Delta^2\mathfrak{F}_\alpha)] + \mu^2\mathrm{Pol}_2^1(\mathfrak{F}_\alpha, \Delta\mathfrak{F}_\alpha) + \mu^3\mathrm{Pol}_3(\mathfrak{F}_\alpha) + O(\mu^4)$$
$$\to \mu^3[\mathrm{Pol}_1^2(f_\alpha, \partial f_\alpha) + \mathrm{Pol}_1^{0,1}(f_\alpha, \partial f_\alpha, \partial^2 f_\alpha) + \mathrm{Pol}_2^1(f_\alpha, \partial f_\alpha) + \mathrm{Pol}_3(f_\alpha)] + O(\mu^4). \tag{A10}$$

Recall that continuum limits of C_v and $C_{v,a}$, $\mathcal{C}$ and $\mathcal{C}_a$, contain no second order derivative. So $\mathrm{Pol}_1^{0,1}(\mathfrak{F}_\alpha, \Delta\mathfrak{F}_\alpha, \Delta^2\mathfrak{F}_\alpha)$ has to vanish. Finally we obtain

$$C_v \quad \text{or} \quad C_{v,a} = \mu\mathrm{Pol}_1^2(\mathfrak{F}_\alpha, \Delta\mathfrak{F}_\alpha) + \mu^2\mathrm{Pol}_2^1(\mathfrak{F}_\alpha, \Delta\mathfrak{F}_\alpha) + \mu^3\mathrm{Pol}_3(\mathfrak{F}_\alpha) + O(\mu^4). \tag{A11}$$

Given any v_1, v_2 of $O(\mu)$ distance from v ($\mu\hat{J}$ with $J = 1, 2, 3$ are lattice vectors),

$$v_1 = v + M_1\mu\hat{1} + N_1\mu\hat{2} + P_1\mu\hat{3}, \qquad v_2 = v + M_2\mu\hat{1} + N_2\mu\hat{2} + P_2\mu\hat{3}, \tag{A12}$$

where $M_{1,2}$, $N_{1,2}$, $P_{1,2} \in \mathbb{Z}$, we define

$$v_3 = v + M_1\mu\hat{1} + N_1\mu\hat{2} + P_2\mu\hat{3}, \qquad v_4 = v + M_1\mu\hat{1} + N_2\mu\hat{2} + P_2\mu\hat{3}, \tag{A13}$$

so that

$$v_1 - v_2 = (v_1 - v_3) + (v_3 - v_4) + (v_4 - v_2), \tag{A14}$$

$$\Delta\mathfrak{F}_\alpha(v_1, v_2) = \Delta_3\mathfrak{F}_\alpha(v_1, v_3) + \Delta_2\mathfrak{F}_\alpha(v_3, v_4) + \Delta_1\mathfrak{F}_\alpha(v_4, v_2), \tag{A15}$$

where $\Delta_3\mathfrak{F}_\alpha(v_1, v_3)$, $\Delta_2\mathfrak{F}_\alpha(v_3, v_4)$, $\Delta_1\mathfrak{F}_\alpha(v_4, v_2)$ are differences along the 3,2,1 directions, respectively. Inserting Eq. (A15) and expanding, Eq. (A11) can be rewritten as

$$C_v \quad \text{or} \quad C_{v,a} = \mu\mathrm{Pol}_2^{\prime 1}(\mathfrak{F}_\alpha, \Delta_J\mathfrak{F}_\alpha) + \mu^2\mathrm{Pol}_2^{\prime 1}(\mathfrak{F}_\alpha, \Delta_J\mathfrak{F}_\alpha) + \mu^3\mathrm{Pol}_3(\mathfrak{F}_\alpha) + O(\mu^4), \tag{A16}$$

where every difference Δ_J is along the $J = 1, 2, 3$ direction.

[1] C. Rovelli and F. Vidotto, *Covariant Loop Quantum Gravity: An Elementary Introduction to Quantum Gravity and Spinfoam Theory*, *Cambridge Monographs on Mathematical Physics* (Cambridge University Press, Cambridge, 2014), https://doi.org/10.1017/CBO9781107706910.

[2] A. Perez, The spin foam approach to quantum gravity, Living Rev. Relativity **16**, 3 (2013).

[3] F. Conrady and L. Freidel, On the semiclassical limit of 4d spin foam models, Phys. Rev. D **78**, 104023 (2008).

[4] J. W. Barrett, R. Dowdall, W. J. Fairbairn, F. Hellmann, and R. Pereira, Lorentzian spin foam amplitudes: Graphical calculus and asymptotics, Classical Quantum Gravity **27**, 165009 (2010).

[5] J. W. Barrett, R. Dowdall, W. J. Fairbairn, H. Gomes, and F. Hellmann, Asymptotic analysis of the EPRL four-simplex amplitude, J. Math. Phys. (N.Y.) **50**, 112504 (2009).

[6] M. Han and M. Zhang, Asymptotics of spinfoam amplitude on simplicial manifold: Lorentzian theory, Classical Quantum Gravity **30**, 165012 (2013).

[7] M. Han and M. Zhang, Asymptotics of spinfoam amplitude on simplicial manifold: Euclidean theory, Classical Quantum Gravity **29**, 165004 (2012).

[8] H. M. Haggard, M. Han, W. Kaminski, and A. Riello, SL(2,C) Chern-Simons theory, a non-planar graph operator, and 4D loop quantum gravity with a cosmological constant: Semiclassical geometry, Nucl. Phys. **B900**, 1 (2015).

[9] H. Liu and M. Han, Asymptotic analysis of spin foam amplitude with timelike triangles, Phys. Rev. D **99**, 084040 (2019).

[10] M. Han, Einstein equation from covariant loop quantum gravity in semiclassical continuum limit, Phys. Rev. D **96**, 024047 (2017).

[11] M. Han, Z. Huang, and A. Zipfel, Emergent four-dimensional linearized gravity from a spin foam model, Phys. Rev. D **100**, 024060 (2019).

[12] B. Bahr, S. Kloser, and G. Rabuffo, Towards a Cosmological subsector of Spin Foam Quantum Gravity, Phys. Rev. D **96**, 086009 (2017).

[13] E. Alesci, Graviton propagator as a tool to test spinfoam models, in *Proceedings of the 3rd Stueckelberg Workshop on Relativistic Field Theories, Pescara, Italy, 2008* (2009), http://www.icra.it/ICRA_Networkshops/INW25_Stueckelberg3/Welcome.html.

[14] E. Bianchi and Y. Ding, Lorentzian spinfoam propagator, Phys. Rev. D **86**, 104040 (2012).
[15] M. Han, Z. Huang, and A. Zipfel, Spin foam propagator: A new perspective to include the cosmological constant, Phys. Rev. D **97**, 084055 (2018).
[16] E. Bianchi, E. Magliaro, and C. Perini, LQG propagator from the new spin foams, Nucl. Phys. **B822**, 245 (2009).
[17] P. Donà, M. Fanizza, G. Sarno, and S. Speziale, Numerical study of the Lorentzian Engle-Pereira-Rovelli-Livine spin foam amplitude, Phys. Rev. D **100**, 106003 (2019).
[18] P. Donà, F. Gozzini, and G. Sarno, Searching for classical geometries in spin foam amplitudes: A numerical method, Classical Quantum Gravity **37**, 094002 (2020).
[19] P. Dona and G. Sarno, Numerical methods for EPRL spin foam transition amplitudes and Lorentzian recoupling theory, Gen. Relativ. Gravit. **50**, 127 (2018).
[20] B. Bahr and S. Steinhaus, Numerical Evidence for a Phase Transition in 4d Spin Foam Quantum Gravity, Phys. Rev. Lett. **117**, 141302 (2016).
[21] L. Cohen, A. J. Brady, Z. Huang, H. Liu, D. Qu, J. P. Dowling, and M. Han, Simulation of loop quantum gravity—A scalable linear-optical approach, arXiv:2003.03414.
[22] K. Li, Y. Li, M. Han, S. Lu, J. Zhou, D. Ruan, G. Long, Y. Wan, D. Lu, B. Zeng, and R. Laflamme, Quantum spacetime on a quantum simulator, Commun. Phys. **2**, 122 (2019).
[23] J. Mielczarek, Spin foam vertex amplitudes on quantum computer—Preliminary results, Universe **5**, 179 (2019).
[24] E. Bianchi, E. Magliaro, and C. Perini, Spinfoams in the holomorphic representation, Phys. Rev. D **82**, 124031 (2010).
[25] K. Noui and A. Perez, Three-dimensional loop quantum gravity: Physical scalar product and spin foam models, Classical Quantum Gravity **22**, 1739 (2005).
[26] D. Oriti, The Feynman Propagator for Spin Foam Quantum Gravity, Phys. Rev. Lett. **94**, 111301 (2005).
[27] V. Bonzom, Spin foam models for quantum gravity from lattice path integrals, Phys. Rev. D **80**, 064028 (2009).
[28] C. Perini, Holonomy-flux spinfoam amplitude, arXiv: 1211.4807.
[29] F. Hellmann and W. Kaminski, Holonomy spin foam models: Asymptotic geometry of the partition function, J. High Energy Phys. 10 (2013) 165.
[30] M. Han, Covariant loop quantum gravity, low energy perturbation theory, and Einstein gravity with high curvature UV corrections, Phys. Rev. D **89**, 124001 (2014).
[31] M. Han, On spinfoam models in large spin regime, Classical Quantum Gravity **31**, 015004 (2014).
[32] E. Magliaro and C. Perini, Emergence of gravity from spinfoams, Europhys. Lett. **95**, 30007 (2011).
[33] P. Dona, F. Gozzini, and G. Sarno, Numerical analysis of spin foam dynamics and the flatness problem, arXiv: 2004.12911.
[34] M. Han and T. Thiemann, On the relation between operator constraint–, master constraint–, reduced phase space–, and path integral quantisation, Classical Quantum Gravity **27**, 225019 (2010).
[35] M. Han and T. Thiemann, On the relation between rigging inner product and master constraint direct integral decomposition, J. Math. Phys. (N.Y.) **51**, 092501 (2010).
[36] M. Han, Canonical path-integral measures for Holst and Plebanski gravity. II. Gauge invariance and physical inner product, Classical Quantum Gravity **27**, 245015 (2010).
[37] J. Engle, M. Han, and T. Thiemann, Canonical path integral measures for Holst and Plebanski gravity. I. Reduced phase space derivation, Classical Quantum Gravity **27**, 245014 (2010).
[38] E. Alesci, T. Thiemann, and A. Zipfel, Linking covariant and canonical LQG: New solutions to the Euclidean scalar constraint, Phys. Rev. D **86**, 024017 (2012).
[39] T. Thiemann and A. Zipfel, Linking covariant and canonical LQG II: Spin foam projector, Classical Quantum Gravity **31**, 125008 (2014).
[40] P. Dona, Infrared divergences in the EPRL-FK Spin Foam model, Classical Quantum Gravity **35**, 175019 (2018).
[41] L.-Q. Chen, Bulk amplitude and degree of divergence in 4d spin foams, Phys. Rev. D **94**, 104025 (2016).
[42] A. Riello, Self-energy of the Lorentzian Engle-Pereira-Rovelli-Livine and Freidel-Krasnov model of quantum gravity, Phys. Rev. D **88**, 024011 (2013).
[43] M. Han, 4-dimensional spin-foam model with quantum Lorentz group, J. Math. Phys. (N.Y.) **52**, 072501 (2011).
[44] W. J. Fairbairn and C. Meusburger, Quantum deformation of two four-dimensional spin foam models, J. Math. Phys. (N.Y.) **53**, 022501 (2012).
[45] M. Han, Cosmological constant in loop quantum gravity vertex amplitude, Phys. Rev. D **84**, 064010 (2011).
[46] D. Oriti, D. Pranzetti, and L. Sindoni, Black holes as quantum gravity condensates, Phys. Rev. D **97**, 066017 (2018).
[47] S. Gielen and D. Oriti, Cosmological perturbations from full quantum gravity, Phys. Rev. D **98**, 106019 (2018).
[48] D. Oriti, L. Sindoni, and E. Wilson-Ewing, Bouncing cosmologies from quantum gravity condensates, Classical Quantum Gravity **34**, 04LT01 (2017).
[49] B. Dittrich, The continuum limit of loop quantum gravity—A framework for solving the theory, in *Loop Quantum Gravity: The First 30 Years*, edited by A. Ashtekar and J. Pullin (World Scientific, 2017), pp. 153–179, https://doi.org/10.1142/10445.
[50] M. Han and H. Liu, Effective dynamics from coherent state path integral of full loop quantum gravity, Phys. Rev. D **101**, 046003 (2020).
[51] C. Rovelli, What is observable in classical and quantum gravity? Classical Quantum Gravity **8**, 297 (1991).
[52] C. Rovelli, Partial observables, Phys. Rev. D **65**, 124013 (2002).
[53] B. Dittrich, Partial and complete observables for Hamiltonian constrained systems, Gen. Relativ. Gravit. **39**, 1891 (2007).
[54] T. Thiemann, Reduced phase space quantization and Dirac observables, Classical Quantum Gravity **23**, 1163 (2006).
[55] K. Giesel, S. Hofmann, T. Thiemann, and O. Winkler, Manifestly gauge-invariant general relativistic perturbation theory. I. Foundations, Classical Quantum Gravity **27**, 055005 (2010).
[56] K. Giesel, S. Hofmann, T. Thiemann, and O. Winkler, Manifestly gauge-invariant general relativistic perturbation theory. II. FRW background and first order, Classical Quantum Gravity **27**, 055006 (2010).

[57] K. Giesel and T. Thiemann, Algebraic quantum gravity (AQG). IV. Reduced phase space quantisation of loop quantum gravity, Classical Quantum Gravity **27**, 175009 (2010).

[58] K. Giesel and T. Thiemann, Scalar material reference systems and loop quantum gravity, Classical Quantum Gravity **32**, 135015 (2015).

[59] A. Ashtekar, J. Lewandowski, D. Marolf, J. Mourao, and T. Thiemann, Coherent state transforms for spaces of connections, J. Funct. Anal. **135**, 519 (1996).

[60] T. Thiemann, Gauge field theory coherent states (GCS): 1. General properties, Classical Quantum Gravity **18**, 2025 (2001).

[61] M. Kisielowski and J. Lewandowski, Spin-foam model for gravity coupled to massless scalar field, Classical Quantum Gravity **36**, 075006 (2019).

[62] M. Assanioussi, J. Lewandowski, and I. Makinen, New scalar constraint operator for loop quantum gravity, Phys. Rev. D **92**, 044042 (2015).

[63] M. Han, H. Li, and H. Liu, Manifestly gauge-invariant cosmological perturbation theory from full loop quantum gravity, arXiv:2005.00883.

[64] A. Ashtekar, M. Campiglia, and A. Henderson, Casting loop quantum cosmology in the spin foam paradigm, Classical Quantum Gravity **27**, 135020 (2010).

[65] A. Henderson, C. Rovelli, F. Vidotto, and E. Wilson-Ewing, Local spinfoam expansion in loop quantum cosmology, Classical Quantum Gravity **28**, 025003 (2011).

[66] T. Thiemann, QSD 5: Quantum gravity as the natural regulator of matter quantum field theories, Classical Quantum Gravity **15**, 1281 (1998).

[67] K. Giesel and T. Thiemann, Algebraic quantum gravity (AQG). I. Conceptual setup, Classical Quantum Gravity **24**, 2465 (2007).

[68] H. Sahlmann and T. Thiemann, Towards the QFT on curved space-time limit of QGR. 1. A general scheme, Classical Quantum Gravity **23**, 867 (2006).

[69] M. Han and H. Liu, https://github.com/LQG-Florida-Atlantic-University/Classical-EOM (2020).

[70] J. D. Brown and K. V. Kuchar, Dust as a standard of space and time in canonical quantum gravity, Phys. Rev. D **51**, 5600 (1995).

[71] K. V. Kuchar and C. G. Torre, Gaussian reference fluid and interpretation of quantum geometrodynamics, Phys. Rev. D **43**, 419 (1991).

[72] M. Reed and B. Simon, *II: Fourier Analysis, Self-Adjointness, Methods of Modern Mathematical Physics* (Academic Press, London, 1975).

[73] T. Thiemann and O. Winkler, Gauge field theory coherent states (GCS). 2. Peakedness properties, Classical Quantum Gravity **18**, 2561 (2001).

[74] T. Thiemann and O. Winkler, Gauge field theory coherent states (GCS): 3. Ehrenfest theorems, Classical Quantum Gravity **18**, 4629 (2001).

[75] K. Giesel and T. Thiemann, Algebraic quantum gravity (AQG). III. Semiclassical perturbation theory, Classical Quantum Gravity **24**, 2565 (2007).