


# Gauge reduction with respect to simplicity constraint in all dimensional loop quantum gravity

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In this paper, we discuss the gauge reduction with respect to the simplicity constraint in both classical and quantum theory of all dimensional loop quantum gravity. With the gauge reduction with respect to the edge-simplicity constraint being processed and the anomalous vertex simplicity constraint being imposed weakly in holonomy-flux phase space, the simplicity reduced holonomy can be established. However, we find that the simplicity reduced holonomy cannot capture the degrees of freedom of intrinsic curvature, which leads to its failure to construct a correct scalar constraint operator in all dimensional loop quantum gravity (LQG) following the standard strategy. To tackle this problem, we establish a new type of holonomy corresponding to the simplicity reduced connection, which captures the degrees of freedom of both intrinsic and extrinsic curvature properly. Based on this new type of holonomy, we propose three new strategies to construct the scalar constraint operators, which serve as valuable candidates to study the dynamics of all dimensional LQG in the future.

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## I. INTRODUCTION

Loop quantum gravity (LQG) [1–4] as a candidate theory of quantum gravity provides a possibility of unifying general relativity (GR) and quantum mechanics. Especially, the quantum spacetime geometry is concealed in some gauge variables and described in a discrete formulation in LQG, and it is an important aspect to derive GR from the foundation of plank-scale quantum geometry. Indeed, in a broader context, LQG provides a concrete platform for exploring the relation between the continuum classical geometric variables of GR and the discretized geometric quantum data, such as the twistor theory and twisted geometry [5,6]. It has been shown that the correspondence between the field variables of GR and the quantum discrete variables of the geometry of LQG is far beyond the issue of merely taking the continuum limit and semiclassical limit, since the Hamiltonian formulation of GR is governed by a constraint system, and the correspondence could be fully revealed only for the physical degrees of freedom. By this we mean that all the constraints in LQG should be properly imposed to ensure that only all of the physical degrees of freedom remain. From the opposite direction of this view, the concrete goal of recovering the familiar Arnowitt-Deser-Misner (ADM) [7] data from LQG could provide useful

instructions in tackling the abstract issues of quantum reductions with respect to the constraints in the theory.

A series of illuminating studies in this direction has been carried out in the case of the  $SU(2)$  formulation of  $(1+3)$ -dimensional LQG. Based on the loop quantization of  $SU(2)$  connection formulation of  $(1+3)$ -dimensional GR, the kinematic structure of LQG contains the kinematic Hilbert space spanned by the spin-network states and the well-defined  $SU(2)$  holonomy-flux operators. Under the actions of holonomy-flux operators, the representations of  $SU(2)$ -valued holonomies indicate the quanta of the fluxes as the area elements dual to the graph's edges, while the intertwiners relating these representations indicate the intersection angles among these fluxes at the vertices. This discretized distribution of the two-dimensional spatial area elements with their intersection angles leads to a specific notion of quantum geometry in LQG. The classical constraints—the scalar, vector, and  $SU(2)$  Gaussian constraints—can be represented via the holonomy-flux operators for the quantum theory. More explicitly, it has been shown that the imposition of the quantum Gauss constraints on the spin-network states gives rise to a proper quantum gauge reduction, which leads to the reduced state space constituted by the gauge invariant spin-network states. Remarkably, the gauge invariant spin-network states not only describe the intrinsic spatial geometry built from the polyhedra cells dual to the network, but also carry precisely the right data to specify the extrinsic curvature of the three-hypersurface partitioned by these polyhedra [6,8,9]. Through this first stage of the gauge reduction with respect

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to the Gaussian constraint, a notion of discrete kinematic ADM data appears in the formulation of Regge geometry, upon which the further reductions with respect to the vector and scalar constraints should be carried out. However, the quantum vector and scalar constraints take much more complicated forms and the quantum algebra between them becomes no longer of first class. At least for now, since the quantum anomaly hinders the standard Dirac procedure from mirroring the classical gauge reduction, the treatment of these loop quantized vector and scalar constraints remains a crucial challenge for LQG tackled by many ongoing projects [10–12].

As we mentioned above, LQG was first established as a quantum theory of GR in four-dimensional spacetime. Nevertheless, various classical and quantum gravity theories in higher-dimensional spacetimes (e.g., Kaluza-Klein theory, supergravity and superstring theories) are explored from many different kinds of perspectives. The results of these higher-dimensional theories show remarkable potentials in unifying the gravity and matter fields at the energy scale of quantum gravity. Thus, by extending the framework of loop quantum gravity to higher-dimensional spacetime, one may get a novel approach toward the higher-dimensional ideas of unification, upon the background-independent and nonperturbative construction of the discretized quantum geometry. Pioneered by Bodendorfer, Thiemann, and Thurn, the basic framework of loop quantum theory for GR in all dimensions has been developed [13–16]. The  $(1 + D)$ -dimensional LQG takes the similar framework as the standard  $(1 + 3)$ -dimensional  $SU(2)$  LQG, i.e., the formulation of Yang-Mills gauge theory and the loop quantization strategy. The key differences between these two theories include two points. The first one is that the gauge group of  $(1 + D)$ -dimensional LQG is taken as  $SO(D + 1)$ , while that of the standard  $(1 + 3)$ -dimensional LQG is  $SU(2)$ . The second key difference is that the  $(1 + D)$ -dimensional LQG contains the simplicity constraint, while the standard  $(1 + 3)$ -dimensional  $SU(2)$  LQG does not. Because of the appearance of the simplicity constraint, the challenge of loop quantum anomaly already exists at the kinematic level before the accounts of the quantum ADM constraints in all dimensional LQG. More explicitly, the all dimensional LQG is based on the connection formulation of  $(1 + D)$ -dimensional GR in the form of the  $SO(D + 1)$  Yang-Mills theory, with the phase space coordinatized by the canonical pairs  $(A_{aIJ}, \pi^{bKL})$ , consisting of the spatial  $so(D + 1)$  valued connection fields  $A_{aIJ}$  and the vector fields  $\pi^{bKL}$ . In this formulation, the theory is governed by the first class constraint system composed by the  $SO(D + 1)$  Gaussian constraint, the ADM constraints of  $(1 + D)$ -dimensional GR, and an additional constraint called the simplicity constraint. The simplicity constraint takes the form  $S_{IJKL}^{ab} := \pi^{a[IJ} \pi^{b]KL}$  [13,15], which generates extra gauge symmetries in the  $SO(D + 1)$  connection phase space.

It has been shown that the  $SO(D + 1)$  connection phase space correctly reduces to the familiar ADM phase space by proceeding with the symplectic reductions with respect to the Gaussian and simplicity constraints. Similar to the  $SU(2)$  LQG, the loop quantization of the  $SO(D + 1)$  connection formulation leads to the Hilbert space composed by the spin-network states of the  $SO(D + 1)$  holonomies, where the quantum numbers labeling these states carry the quanta of the flux operators representing the flux of  $\pi^{bKL}$  over  $(D - 1)$ -dimensional surfaces. Following the previous study for  $SU(2)$  LQG, it is expected to look for all the dimensional Regge ADM data encoded in the  $SO(D + 1)$  spin-network states, through a gauge reduction procedure with respect to both of the quantum  $SO(D + 1)$  Gaussian constraint and simplicity constraint.

However, the challenge arises in the gauge reduction procedures with respect to the quantum simplicity constraint—the quantum algebra among simplicity constraints in all dimensional LQG carries serious quantum anomaly. More explicitly, the commutative Poisson algebra among the classical simplicity constraints becomes the deformed quantum algebra among the quantum simplicity constraint which is not even close [17]. Besides, it has been shown that the “gauge” transformations induced by these anomalous quantum simplicity constraints can connect the states that are supposed to be physically distinct in terms of the semiclassical limit. Thus, strong imposition of the anomalous quantum simplicity constraint leads to overconstrained state space that are not able to capture correct physical degrees of freedom. Indeed, based on the network discretization, the quantum simplicity constraints in all dimensional LQG are divided into two kinds of local constraints, including the edge-simplicity constraint and the vertex-simplicity constraint. Specifically, the anomaly of quantum algebra only appears for the vertex-simplicity constraint, while the edge-simplicity constraint remains anomaly free in the sense of taking a weakly commutative quantum algebra. To deal with the quantum anomaly of the vertex simplicity constraint, one can focus on the discrete phase space coordinatized by  $SO(D + 1)$  holonomy-flux variables, in which the Poisson algebras of simplicity constraint are isomorphic to quantum algebras of simplicity constraint, and thus the anomaly of vertex-simplicity constraint already exists in the classical holonomy-flux phase space. Previously, based on the so-called generalized twisted geometric parametrization of the edge-simplicity constraint surface, we have proceeded with the gauge reduction with respect to the simplicity constraint in the holonomy-flux phase space [18]. Our result shows that the discretized classical Gaussian, edge-simplicity constraints and vertex-simplicity constraint which catches the anomaly of quantum vertex simplicity constraint define a constraint surface in the holonomy-flux phase space of all dimensional LQG, and the kinematical physical degrees of freedom are given by the gauge orbits in the constraint surface generated by

the first class system consisting of discretized Gaussian and edge-simplicity constraints. We found that the reduced twisted geometry describes the degrees of freedom of the  $D$ -polytopes which partition the  $D$ -hypersurface, i.e., the  $(D - 1)$ -faces' areas, the shape of each single  $D$ -polytope and the extrinsic curvature between arbitrary two adjacent  $D$ -polytopes. Finally, the discrete ADM data of the  $D$ -hypersurface in the form of Regge geometry can be identified as the degrees of freedom of the reduced generalized twisted geometry space, up to an additional condition called the shape matching condition of  $(D - 1)$ -dimensional faces. Following this result, these gauge reduction procedures can be realized in quantum theory by imposing the quantum Gaussian and edge-simplicity constraint strongly, and imposing the vertex-simplicity constraint weakly. It leads to the physical kinematic Hilbert space spanned by the spin-network states labeled by simple representations at edges and gauge invariant simple coherent intertwiners at vertices [19].

Nevertheless, the gauge reduction with respect to the simplicity constraint has not been accomplished yet, since new issues arise when one constructs the gauge invariant operators to describe the kinematic physical observables. Similar to the construction of the gauge invariant operators with respect to the Gaussian constraint, by proceeding with the regularization and quantization procedures in LQG, one may expect that a gauge invariant variable with respect to the simplicity constraint in the connection phase space can be promoted as an operator acting in the physical kinematic Hilbert space, with the gauge degrees of freedom being eliminated and the physical meaning being remained correctly. Unfortunately, these procedures fail to give a correct scalar constraint operator in all dimensional LQG. As we will show in the main part of this article, though the edge simplicity constraints only transform the pure gauge components in holonomy, the gauge reduction with respect to the simplicity constraint destroys the structure of holonomies, and it leads to the so-called simplicity reduced holonomy which cannot capture the degrees of freedom of intrinsic curvature. In other words, the simplicity reduced holonomy is not able to inherit the property of connection while the scalar constraint operator is given by regularizing and quantizing the connection formulation of scalar constraint. Hence, the appearance the simplicity reduced holonomy leads this scalar constraint operator does not have the expected geometric interpretation.

In fact, this issue arises from the inconsistency of the geometric meanings of the simplicity reduced connections and the simplicity reduced holonomies. More explicit discussions in this article will show that, by considering the matrix elements of some constraint operators in the solution space of the quantum edge simplicity constraint, one finds that the simplicity reduced holonomy operator appears inevitably. Hence, to ensure the constructed

operators possess correct geometric interpretations, it is necessary to study the specific geometric interpretation of the simplicity reduced holonomies in the holonomy-flux phase space, so that the simplicity reduced holonomies can be used as a proper building block to construct operators, e.g., the scalar constraint operator. Besides, by following the geometric interpretation of each component of holonomy given by the twisted geometry parametrization, we will introduce another type of gauge invariant holonomies with respect to the simplicity constraint, which captures the degrees of freedom of intrinsic and extrinsic curvature properly. We will show that the scalar constraint in connection formulation can be regularized and quantized based on this new type of gauge invariant holonomy, with the intrinsic and extrinsic curvatures being captured in the resulting scalar constraint operator correctly.

This paper is organized as follows. After our brief review of the classical theory of all dimensional LQG in Sec. II, we will introduce the simplicity constraint in both of the connection and holonomy-flux phase spaces. Especially, we will analyze the gauge degrees of freedom with respect to the simplicity constraint in Secs. II A and II B. Then, the simplicity reduced holonomy will be constructed, and we will also propose a new choice of the gauge (with respect to the simplicity constraint) invariant holonomy in Sec. II C. In Sec. III, we will turn to consider the gauge reduction with respect to the simplicity constraint in quantum theory of all dimensional LQG. The solution space of the quantum simplicity constraint will be introduced first, and then the simplicity reduced holonomy operator and a new choice of the gauge (with respect to simplicity constraint) invariant holonomy operator will be considered in our discussions. These operators helps us to consider the construction of the quantum scalar constraint in all dimensional LQG in Sec. IV. We will first point out that the standard strategy is problematic to construct the quantum scalar constraint in Sec. IV A, and then propose three new strategies for this construction in Sec. IV B. Finally, we will finish with a summary and discussion in Sec. V.

## II. SIMPLICITY CONSTRAINT IN CLASSICAL THEORY OF $(1 + D)$ -DIMENSIONAL LQG

### A. Simplicity constraint in connection phase space of $(1 + D)$ -dimensional GR

The connection dynamics of  $(1 + D)$ -dimensional GR is based on the phase space coordinatized by the canonical field variables  $(A_{aIJ}, \pi^{bKL})$  on a spatial  $D$ -dimensional manifold  $\sigma$ , which is equipped with the kinematic constraints—Gauss constraint  $\mathcal{G}^{IJ} \approx 0$  and simplicity constraint  $S^{ab[IJKL]} \approx 0$  inducing the gauge transformation of this theory, and the dynamics constraints—vector constraint  $C_a \approx 0$  and scalar constraint  $C \approx 0$ . More explicitly, the only nontrivial Poisson bracket between the conjugate pair is given by [13]

$$\{A_{aIJ}(x), \pi^{bKL}(y)\} = 2\kappa\beta\delta_a^b\delta_{[I}^K\delta_{J]}^L\delta^{(D)}(x-y), \quad (1)$$

where  $\kappa$  is Newton's gravitational constant,  $\beta$  is the Barbero-Immirzi parameter, and we used the notation  $a, b, \dots = 1, 2, \dots, D$  for the spatial tensorial indices and  $I, J, \dots = 1, 2, \dots, D+1$  for the  $so(D+1)$  Lie algebra indices in the definition representation. The Gaussian constraint and simplicity constraint are given by

$$\mathcal{G}^{IJ} := \partial_a \pi^{aIJ} + 2A_{aK}^I \pi^{a|K|J} \approx 0 \quad (2)$$

and

$$S^{ab[IJKL]} := \pi^{a[IJ} \pi^{b|KL]} \approx 0, \quad (3)$$

respectively. It is easy to verify that

$$\{\mathcal{G}, \mathcal{G}\} \propto \mathcal{G}, \quad \{\mathcal{G}, S\} \propto S, \quad \{S, S\} = 0,$$

which means that the Gaussian and simplicity constraints obey a first class constraint algebra. It has been shown that the symplectic reduction with respect to the Gaussian and simplicity constraints reduces the connection phase space to the ADM phase space of geometry dynamics of all dimensional GR. In details, the ADM variables  $(q_{ab}, P^{cd})$  can be defined as the functionals [13]

$$q_{ab} := q_{ab}[\pi], \quad P^{cd} := P^{cd}[A, \pi]$$

in the connection phase space. It has been verified that  $q_{ab}[\pi]$  and  $P^{cd}[A, \pi]$  are weak Dirac observables with respect to Gaussian and simplicity constraints, and they obey the standard ADM Poisson brackets [13]

$$\begin{aligned} \{q_{ab}(x), P^{cd}(y)\} &= \kappa\delta_{(a}^c\delta_{b)}^d\delta^{(D)}(x-y), \\ \{q_{ab}(x), q_{cd}(y)\} &= \{P^{ab}(x), P^{cd}(y)\} = 0 \end{aligned}$$

on the constraint surface defined by simplicity and Gaussian constraints. The vector constraint and scalar constraint in the connection phase space can be defined by

$$C_a[A, \pi] := C_a(q_{cd}[\pi], P^{ef}[A, \pi])$$

and

$$C[A, \pi] := C(q_{cd}[\pi], P^{ef}[A, \pi]),$$

respectively, wherein  $C_a(q_{cd}, P^{ef})$  and  $C(q_{cd}, P^{ef})$  are the vector constraint and scalar constraint in the ADM phase space. Since  $q_{cd}[\pi]$  and  $P^{ef}[A, \pi]$  are weak Dirac observables with respect to  $S$  and are invariant under  $\mathcal{G}$ , one can immediately get that

$$\{S, C_a\} \propto S, \quad \{S, C\} \propto S, \quad \{\mathcal{G}, C_a\} = 0, \quad \{\mathcal{G}, C\} = 0.$$

Next, notice the fact that the Poisson algebra between  $q_{cd}[\pi]$  and  $P^{ef}[A, \pi]$  is the same as that of the ADM variables modulo  $S, \mathcal{G}$  terms, and therefore the Poisson algebra of the vector constraint and scalar constraint in the ADM phase space can be reproduced by that in the connection phase space modulo  $S, \mathcal{G}$  terms, which means that

$$\begin{aligned} \{C_a, C_b\} &\propto C_c, S, \mathcal{G}, & \{C_a, C\} &\propto C, S, \mathcal{G}, \\ \{C, C\} &\propto C_a, S, \mathcal{G}. \end{aligned}$$

Then, one can conclude that the Gaussian, simplicity, vector, and scalar constraints form a first class constraint system in the connection phase space.

As one expected, the Gaussian constraint induces the  $SO(D+1)$  gauge transformation of the connection  $A_{aIJ}$  and its momentum  $\pi^{bKL}$ , while the simplicity constraint restricts the degrees of freedom of  $\pi^{aIJ}$  to that of a D-frame  $E^{aI}$  to describe the spatial internal geometry and generates some other gauge transformation. To clarify the gauge transformation induced by simplicity constraint, let us first give the explicit relations between the connection variables and the geometric variables on the constraint surface of both Gaussian and simplicity constraints. Specifically, the solution of the simplicity constraint is given by  $\pi^{aIJ} = 2n^{[I}E^{a|J]}$ , with  $E^{aI}$  being the densitized  $D$ -frame related to double densitized dual metric by  $\tilde{q}^{ab} = E^{aI}E^b_I$  and  $n^I$  being a unit internal vector defined by  $n_I E^{aI} = 0$ . Also, one can define the spin connection  $\Gamma_{aIJ}$  satisfying  $\partial_a e_b^I - \Gamma_{ab}^c e_c^I + \Gamma_a^{IJ} e_{bJ} = 0$  as

$$\Gamma_{aIJ}[\pi] := \frac{2}{D-1} T_{aIJ} + \frac{D-3}{D-1} \bar{T}_{aIJ} + \Gamma_{ac}^b T_{bIJ} \quad (4)$$

on the simplicity constraint surface, where  $T_{aIJ} := \pi_{bK[I} \partial_a \pi^{bK}_{J]}$ ,  $T_{bIJ}^c := \pi_{bK[I} \pi^{cK}_{J]}$ ,  $\bar{T}_{aIJ} := \tilde{\eta}_I^K \tilde{\eta}_J^L T_{aKL}$ ,  $\tilde{\eta}_I^J := \delta_I^J - n_I n^J$ ,  $\Gamma_{ab}^c$  is the Levi-Civita connection of  $q_{ab}$  and  $e_{bI}$  is the  $D$ -bein defined by  $E^{aI} e_{bI} = \sqrt{q} \delta_b^a$ . Based on these conventions, the densitized extrinsic curvature of the spatial manifold  $\sigma$  can be given by

$$\tilde{K}_a^b = K_{aIJ} \pi^{bIJ} \equiv \frac{1}{\beta} (A_{aIJ} - \Gamma_{aIJ}) \pi^{bIJ} \quad (5)$$

on the constraint surface of both Gaussian and simplicity constraints. Now, it is ready to clarify the gauge transformation induced by the simplicity constraint. One can check that  $A_{aIJ}$  transforms with respect to the simplicity constraint as

$$\begin{aligned} \int_{\sigma} d^D x f_{ab[IJKL]}(x) \{S^{abIJKL}, A_{cMN}(y)\} \\ = 2\beta\kappa f_{ac[IJMN]}(y) \pi^{aIJ}(y) = 4\beta\kappa f_{ac[IJMN]}(y) n^I E^{a|J]}(y) \end{aligned} \quad (6)$$



on the simplicity constraint surface. By decomposing the connection  $A_{aIJ} = 2n_{[I}A_{|a|J]} + \bar{A}_{aIJ}$ , it is easy to see that on the simplicity constraint surface, only the component  $\bar{A}_a^{IJ}$  transforms while the component  $2n_{[I}A_{|a|J]}$  is gauge invariant with respect to the simplicity constraint. Similarly,  $K_{aIJ} := \frac{1}{\beta}(A_{aIJ} - \Gamma_{aIJ})$  can be decomposed as  $K_{aIJ} = 2n_{[I}K_{|a|J]} + \bar{K}_{aIJ}$ . One can also check that on the simplicity constraint surface, the component  $2n_{[I}K_{|a|J]}$  is invariant and only  $\bar{K}_a^{IJ}$  transforms under the gauge transformation induced by simplicity constraint. Hence, we see that the simplicity constraint fixes both  $\bar{K}_a^b$  and  $q_{ab}$  so that it exactly introduces extra gauge degrees of freedom. In fact, to give the gauge invariant variables with respect to the simplicity constraint, one can construct the simplicity reduced connection

$$A_{aIJ}^S := A_{aIJ} - \beta \bar{K}_{aIJ}. \quad (7)$$

Then, the symplectic reduction with respect to the simplicity constraint in the connection phase space can be illustrated as

$$(A_{aIJ}, \pi^{bKL}) \xrightarrow{\text{reduction}} (A_{aIJ}^S, \pi^{bKL})|_{S^{abIJKL}=0},$$

which gives the gauge invariant variables  $(A_{aIJ}^S, \pi^{bKL})$  with respect to simplicity constraint on the constraint surface defined by  $S^{abIJKL} = 0$ .

## B. Simplicity constraint in discrete phase space of (1 + D)-dimensional GR

Apart from the different gauge group which, however, is compact and the additional simplicity constraint, the  $SO(D+1)$  connection formulation of (1 + D)-dimensional GR is precisely the same as the  $SU(2)$  connection formulation of (1 + 3)-dimensional GR, and the quantization of the  $SO(D+1)$  connection formulation is therefore in complete analogy with (1 + 3)-dimensional  $SU(2)$  LQG [1–4,20]. By following any standard text on LQG such as [3,4], the loop quantization of the  $SO(D+1)$  connection formulation of (1 + D)-dimensional GR leads to a kinematical Hilbert space  $\mathcal{H}$  [15], which can be regarded as a union of the Hilbert spaces  $\mathcal{H}_\gamma = L^2((SO(D+1))^{|E(\gamma)|}, d\mu_{\text{Haar}}^{|E(\gamma)|})$  on all possible graphs  $\gamma$  embedded in  $\sigma$ , where  $E(\gamma)$  denotes the set composed by the independent edges of  $\gamma$  and  $d\mu_{\text{Haar}}^{|E(\gamma)|}$  denotes the product of the Haar measure on  $SO(D+1)$ . In this sense, on each given  $\gamma$  there is a discrete phase space  $(T^*SO(D+1))^{|E(\gamma)|}$ , which is coordinatized by the elementary discrete variables—holonomies and fluxes. The holonomy of  $A_{aIJ}$  along an edge  $e \in \gamma$  is defined by

$$\begin{aligned} h_e[A] &:= \mathcal{P} \exp \left( \int_e A \right) \\ &= 1 + \sum_{n=1}^{\infty} \int_0^1 dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 A(t_1) \cdots A(t_n), \end{aligned} \quad (8)$$

where  $A(t) := \frac{1}{2} \dot{e}^a A_{aIJ} \tau^{IJ}$ ,  $\dot{e}^a$  is the tangent vector field of  $e$ ,  $\tau^{IJ}$  is a basis of  $so(D+1)$  given by  $(\tau^{IJ})_{KL}^{\text{def.}} = 2\delta_K^I \delta_L^J$  in definition representation space of  $SO(D+1)$ , and  $\mathcal{P}$  denotes the path-ordered product. The flux  $F_e^{IJ}$  of  $\pi^{aIJ}$  through the  $(D-1)$ -dimensional face dual to edge  $e$  is defined by

$$F_e^{IJ} := -\frac{1}{4} \text{tr} \left( \tau^{IJ} \int_{e^*} \epsilon_{aa_1 \dots a_{D-1}} h(\rho_e^s(\sigma)) \pi^{aKL}(\sigma) \tau_{KL} h(\rho_e^s(\sigma)^{-1}) \right), \quad (9)$$

where  $e^*$  is the  $(D-1)$ -face traversed by  $e$  in the dual lattice of  $\gamma$ ,  $\rho_e^s(\sigma): [0, 1] \rightarrow \Sigma$  is a path connecting the source point  $s_e \in e$  to  $\sigma \in e^*$  such that  $\rho_e^s(\sigma): [0, \frac{1}{2}] \rightarrow e$  and  $\rho_e^s(\sigma): [\frac{1}{2}, 1] \rightarrow e^*$ . Similarly, we can define the dimensionless flux  $X_e^{IJ}$  as

$$X_e^{IJ} = -\frac{1}{4\beta a^{D-1}} \text{tr} \left( \tau^{IJ} \int_{e^*} \epsilon_{aa_1 \dots a_{D-1}} h(\rho_e^s(\sigma)) \pi^{aKL}(\sigma) \tau_{KL} h(\rho_e^s(\sigma)^{-1}) \right), \quad (10)$$

where  $a$  is an arbitrary but fixed constant with the dimension of length. Since  $SO(D+1) \times so(D+1) \cong T^*SO(D+1)$ , this new discrete phase space  $\times_{e \in \gamma} (SO(D+1) \times so(D+1))_e$ , called the phase space of  $SO(D+1)$  loop quantum gravity on the fixed graph  $\gamma$ , is a direct product of  $SO(D+1)$  cotangent bundles. Finally, the complete phase space of the theory is given by taking the union over the phase spaces of all possible graphs. In the discrete phase space associated with  $\gamma$ , the constraints are expressed by the smeared variables. The discretized Gauss constraints are given by

$$G_v := \sum_{b(e)=v} X_e - \sum_{t(e')=v} h_{e'}^{-1} X_{e'} h_{e'} \approx 0. \quad (11)$$

The discretized simplicity constraints are separated as two sets. The first one is the edge-simplicity constraint  $S_e^{IJKL} \approx 0$  which takes the form [15,16]

$$S_e^{IJKL} \equiv X_e^{[IJ} X_e^{KL]} \approx 0, \quad \forall e \in \gamma, \quad (12)$$

and the second one is the vertex-simplicity constraint  $S_{v,e,e'}^{IJKL} \approx 0$  which is given by [15,16]

$$S_{v,e,e'}^{IJKL} \equiv X_e^{[IJ} X_{e'}^{KL]} \approx 0, \quad \forall e, e' \in \gamma, s(e) = s(e') = v. \quad (13)$$

The symplectic structure of the discrete phase space can be expressed by the Poisson algebra between the elementary variables  $(h_e, X_e^{IJ})$ , which reads

$$\begin{aligned} \{h_e, h_{e'}\} &= 0, & \{h_e, X_{e'}^{IJ}\} &= \delta_{e,e'} \frac{\kappa}{a^{D-1}} \frac{d}{dt} (e^{\lambda \tau^{IJ}} h_e)|_{\lambda=0}, \\ \{X_e^{IJ}, X_{e'}^{KL}\} &= \delta_{e,e'} \frac{\kappa}{a^{D-1}} (\delta^{IK} X_e^{JL} + \delta^{JL} X_e^{IK} \\ &\quad - \delta^{IL} X_e^{JK} - \delta^{JK} X_e^{IL}). \end{aligned} \quad (14)$$

Based on these Poisson algebras, one can check that the Gaussian constraint generates the  $SO(D+1)$  gauge transformation in  $SO(D+1)$  Yang-Mills theory, and the edge simplicity constraint induces the transformation

$$\{X_e^{[IJ} X_e^{KL]}, h_e\} = 2X_e^{[IJ} \{X_e^{KL]}, h_e\} = -\frac{2\kappa}{a^{D-1}} X_e^{[IJ} (\tau^{KL]} h_e). \quad (15)$$

Besides, one can evaluate the algebra among the discretized Gauss constraints, edge-simplicity constraints, and vertex-simplicity constraints. It turns out that  $G_v \approx 0$  and  $S_e \approx 0$  form a first class constraint system, with the algebra

$$\begin{aligned} \{S_e, S_e\} &\propto S_e, \{S_e, S_v\} \propto S_e, \{G_v, G_v\} \propto G_v, \\ \{G_v, S_e\} &\propto S_e, \{G_v, S_v\} \propto S_v, \quad b(e) = v, \end{aligned} \quad (16)$$

where the brackets within  $G_v \approx 0$  are isomorphic to the  $so(D+1)$  algebra, and the ones involving  $S_e \approx 0$  weakly vanish. Especially, since the commutative momentum Poisson algebra in connection phase space is instead by the noncommutative flux Poisson algebra in the holonomy-flux phase space, the simplicity constraint becomes anomalous at the vertex of the graphs in the holonomy-flux phase space. In other words, the algebras among the vertex-simplicity constraint are the problematic ones, with the open anomalous brackets [17]

$$\{S_{v,e,e'}, S_{v,e,e''}\} \propto \text{anomaly terms}, \quad (17)$$

where the anomaly terms are not proportional to any of the existing constraints in the phase space.

The anomalous Poisson algebra of the vertex simplicity constraint in discrete phase space destroys the first class

constraint system in continuum phase space. Thus, the gauge reduction in discrete phase space cannot be a simple copy of the corresponding reduction in continuum phase space. The main obstacle to explore the gauge reduction in discrete phase space is how to deal with the anomaly of the vertex simplicity constraint to reduce correct gauge degrees of freedom. This problem is solved based on the generalized twisted geometric parametrization of the discrete phase space, where the twisted geometry covers the degrees of freedom of the Regge geometries so that it can get back to the connection phase space in some continuum limit [18]. Let us give a brief introduction of this parametrization as follows.

From now on, let us focus on a graph  $\gamma$  whose dual lattice gives a partition of  $\sigma$  constituted by  $D$ -dimensional polytopes, and the elementary edges in  $\gamma$  refer to such a kind of edges that only pass through one  $(D-1)$ -dimensional face in the dual lattice of  $\gamma$ . The discrete phase space related to the give graph  $\gamma$  is given by  $\times_{e \in \gamma} T^*SO(D+1)_e$  with  $e$  being the elementary edges of  $\gamma$ . Then, the edge simplicity constraint surface that we are interested in can be given as [18]

$$\begin{aligned} \times_{e \in \gamma} T_s^*SO(D+1)_e &:= \{(h_e, X_e) \in \times_{e \in \gamma} T^*SO(D+1)_e \\ &\quad | X_e^{[IJ} X_e^{KL]} = 0\}. \end{aligned} \quad (18)$$

Without loss of generality, we can focus on the edge simplicity constraint surface  $T_s^*SO(D+1)_e$  related to one single elementary edge  $e \in \gamma$ . This space can be parametrized by using the generalized twisted-geometry variables

$$\begin{aligned} (V_e, \tilde{V}_e, \xi_e, \eta_e, \bar{\xi}_e^\mu) \in P_e &:= Q_{D-1}^e \times Q_{D-1}^e \times T^*S_e \\ &\quad \times SO(D-1)_e, \end{aligned} \quad (19)$$

where  $\eta_e \in \mathbb{R}$ ,  $Q_{D-1}^e := SO(D+1)/(SO(2) \times SO(D-1))$  is the space of unit bivectors  $V_e$  or  $\tilde{V}_e$  where  $SO(2) \times SO(D-1)$  is the maximum subgroup fixing the bivector  $\tau_o := 2\delta_1^{[I} \delta_2^{J]}$  in  $SO(D+1)$ ,  $\xi_e \in [-\pi, \pi)$ ,  $e^{\bar{\xi}_e^\mu \bar{\tau}_\mu} := \bar{u}_e$ , and  $\bar{\tau}_\mu$  where  $\mu \in \{1, \dots, \frac{(D-1)(D-2)}{2}\}$  is the basis of the Lie algebra of the subgroup  $SO(D-1)$  fixing both  $\delta_1^I, \delta_2^J$  in  $SO(D+1)$ . To capture the intrinsic curvature, we specify one pair of the  $SO(D+1)$  valued Hopf sections  $u_e := u(V_e)$  and  $\tilde{u}_e := \tilde{u}(\tilde{V}_e)$  which satisfies  $V_e = u_e \tau_o u_e^{-1}$  and  $\tilde{V}_e = -\tilde{u}_e \tau_o \tilde{u}_e^{-1}$ . Then, the parametrization associated with each edge is given by the map

$$\begin{aligned} (V_e, \tilde{V}_e, \xi_e, \eta_e, \bar{\xi}_e^\mu) \mapsto (h_e, X_e) \in T_s^*SO(D+1)_e: & \quad X_e = \frac{1}{2} \eta_e V_e = \frac{1}{2} \eta_e u(V_e) \tau_o u(V_e)^{-1}, \\ & \quad h_e = u(V_e) e^{\bar{\xi}_e^\mu \bar{\tau}_\mu} e^{\xi_e \tau_o} \tilde{u}(\tilde{V}_e)^{-1}. \end{aligned} \quad (20)$$

Now we can get back to the discrete phase space of all dimensional LQG on the whole graph  $\gamma$ . Notice that the discrete phase space on  $\gamma$  is just the Cartesian product of the discrete phase space on each single edge of  $\gamma$ ; thus the twisted geometry parametrization of the discrete phase space on one copy of the edge can be generalized to that of the whole graph  $\gamma$  directly. One should note that the twisted geometry parameters  $(V_e, \tilde{V}_e, \xi_e, \eta_e)$  take the interpretation of the discrete geometry describing the dual lattice of  $\gamma$ , which can be explained explicitly as follows. First,  $\frac{1}{2}\eta_e V_e$  and  $\frac{1}{2}\eta_e \tilde{V}_e$  represent the area-weighted outward normal bivectors of the  $(D-1)$ -face dual to  $e$  in the perspective of source and target points of  $e$ , respectively, with  $\frac{1}{2}\eta_e$  being the dimensionless area of the  $(D-1)$ -face dual to  $e$ . Second, the holonomy  $h_e = u_e(V_e) e^{\tilde{z}^\mu \tilde{\tau}_\mu} e^{\xi_e \tau_o} \tilde{u}_e^{-1}(\tilde{V}_e)$  takes the interpretation that it rotates the inward normal  $-\frac{1}{2}\eta_e \tilde{V}_e$  of the  $(D-1)$ -face dual to  $e$  in the perspective of the target point of  $e$ , into the outward normal  $\frac{1}{2}\eta_e V_e$  of the  $(D-1)$ -face dual to  $e$  in the perspective of the source point of  $e$ , wherein  $u_e(V_e)$  and  $\tilde{u}_e(\tilde{V}_e)$  capture the contribution of intrinsic curvature, and  $e^{\xi_e \tau_o}$  captures the contribution of extrinsic curvature to this rotation. Moreover,  $\tilde{u}_e = e^{\tilde{z}^\mu \tilde{\tau}_\mu}$  are some redundant degrees of freedom for the reconstruction of the discrete geometry, and it also captures the gauge degrees of freedom with respect to edge-simplicity constraint. Now, beginning with the twisted geometry parameter space  $P_\gamma = \times_{e \in \gamma} P_e$ ,  $P_e := Q_{D-1}^e \times Q_{D-1}^e \times T_e^* S \times SO(D-1)_e$ , the gauge reduction with respect to the kinematic constraints—Gauss constraint and simplicity constraints—can proceed by following the guiding of the geometric interpretation of the twisted geometry parameters in the subset of  $P_\gamma$  with  $\eta_e \neq 0$ . Up to a double-covering symmetry, we first reduce the  $SO(D-1)_e$  fibers for each edge  $e$  to get the phase space  $\check{P}_\gamma := \times_{e \in \gamma} \check{P}_e$  with  $\check{P}_e := Q_{D-1}^e \times Q_{D-1}^e \times T_e^* S_e^1$ . Then, the discretized Gauss constraint (11) can be imposed to give the reduced phase space

$$\check{H}_\gamma := \check{P}_\gamma // SO(D+1)^{|V(\gamma)|} = (\times_{e \in \gamma} T_e^* S_e^1) \times (\times_{v \in \gamma} \mathfrak{P}_{\tilde{\eta}_v}) \quad (21)$$

with  $|V(\gamma)|$  being the number of the vertices in  $\gamma$  and

$$\mathfrak{P}_{\tilde{\eta}_v} := \{(V_{e_1}^{IJ}, \dots, V_{e_{n_v}}^{IJ}) \in \times_{e \in \{e_v\}} Q_{D-1}^e | G_v = 0\} / SO(D+1), \quad (22)$$

where we reoriented the edges linked to  $v$  to be outgoing at  $v$  without loss of generality,  $\{e_v\}$  represents the set of edges beginning at  $v$  with  $n_v$  being the number of elements in  $\{e_v\}$ , and  $G_v = \sum_{\{e_v\}} \eta_e V_{e_v}^{IJ}$  here. Further, we solve the vertex simplicity constraint equation (12) in the reduced phase space  $\check{H}_\gamma$  and get the final reduced twisted geometric space

$\check{H}_\gamma^s = (\times_{e \in \gamma} T_e^* S_e^1) \times (\times_{v \in \gamma} \mathfrak{P}_{\tilde{\eta}_v}^s)$  with  $\mathfrak{P}_{\tilde{\eta}_v}^s := \mathfrak{P}_{\tilde{\eta}_v} |_{S_v=0}$ . It has been shown that the generalized twisted geometry in the space  $\check{H}_\gamma^s$  is consistent with the Regge geometry on the spatial  $D$ -manifold  $\sigma$  if the shape match condition in the  $D$ -polytopes' gluing process is considered, which means the gauge reduction scheme in the parametrization space captures the correct physical degrees of freedom of all dimensional LQG in the kinematical level. Thus, based on this twisted geometry parametrization, one can conclude that, to get correct kinematical physical degrees of freedom, the anomalous vertex should be treated as a second class constraint while the Gauss constraint and edge simplicity constraint are treated as a first class constraint in discrete and quantum theory of all dimensional LQG. The reduction procedures can be roughly illustrated as follows [18];

$$\times_{e \in \gamma} T_e^* SO(D+1)_e \xrightarrow{(i)} \times_{e \in \gamma} \check{P}_e \xrightarrow{(ii)} \check{H}_\gamma \xrightarrow{(iii)} \check{H}_\gamma^s, \quad (23)$$

where the symplectic reductions with respect to edge simplicity constraint and Gaussian constraint are proceeded in step (i) and (ii), respectively, and in step (iii) the vertex simplicity constraint equation is solved.

The reduction of the holonomy-flux phase based on twisted geometry parametrization can be related to the reduction of the connection phase space by taking the continuum limit [18]. Observe that the choice for the Hopf sections is clearly nonunique, and the twisted geometric parametrization is given under one fixed choice of  $\{u_e, \tilde{u}_e\}$  for every edge  $e$ , under which the Levi-Civita holonomy  $h_e^\Gamma$  can be expressed in the form

$$h_e^\Gamma(V_{e'}, \tilde{V}_{e'}) \equiv u_e(e^{\tilde{z}^\mu \tilde{\tau}_\mu} e^{\xi_e \tau_o}) \tilde{u}_e^{-1}, \quad (24)$$

$$e' \in \{\{E(b(e))\}, \{E(t(e))\}\},$$

where  $\{E(b(e))\}$  and  $\{E(t(e))\}$  are the collections of edges linked to the beginning point  $b(e)$  of  $e$  and the target point  $t(e)$  of  $e$ , respectively,  $e^{\tilde{z}^\mu \tilde{\tau}_\mu}$  takes value in the subgroup  $SO(D-1) \subset SO(D+1)$  preserving both  $\delta_1^I$  and  $\delta_2^I$ . Note that the functions  $\zeta_e$  and  $\tilde{\zeta}_e^\mu$  are well-defined via the given  $h_e^\Gamma$  and the chosen Hopf sections. Then, let us take the continuum limit that makes the coordinate length of each edge of  $\gamma$  tends to 0, and we get

$$h_e = u_e e^{\xi_e \tau_o} e^{\tilde{z}^\mu \tilde{\tau}_\mu} \tilde{u}_e^{-1} \simeq \mathbb{I} + A_e, \quad (25)$$

$$X^{e'} \simeq \pi^{e'}, \quad (26)$$

and

$$h_e^\Gamma = u_e(e^{\tilde{z}^\mu \tilde{\tau}_\mu} e^{\xi_e \tau_o}) \tilde{u}_e^{-1} \simeq \mathbb{I} + \Gamma_e. \quad (27)$$

Furthermore, let us factor out  $h_e^\Gamma$  from  $h_e$  through the expressions

$$\begin{aligned} h_e &= h_e^\Gamma \left( e^{-\check{\xi}_e^\mu \tilde{u}_e \tilde{\tau}_\mu \tilde{u}_e^{-1}} e^{\check{\xi}_e^\mu \tilde{u}_e \tilde{\tau}_\mu \tilde{u}_e^{-1}} e^{-(\xi_e - \zeta_e) \tilde{V}_e} \right) \\ &= \left( e^{\check{\xi}_e^\mu u_e \tilde{\tau}_\mu u_e^{-1}} e^{-\check{\xi}_e^\mu u_e \tilde{\tau}_\mu u_e^{-1}} e^{(\xi_e - \zeta_e) V_e} \right) h_e^\Gamma. \end{aligned} \quad (28)$$

Recall the splitting

$$A_a^{IJ} = \Gamma_a^{IJ}(\pi) + \beta K_a^{IJ} \quad (29)$$

with  $\Gamma_a^{IJ}(\pi)$  being a function of  $\pi^{bKL}$  satisfying  $\Gamma_a^{IJ}(\pi) = \Gamma_a^{IJ}(e)$  on the simplicity constraint surface, and notice Eqs. (25) and (27), where we have the continuum limit

$$K_e \simeq \frac{1}{\beta} u_e (\xi_e^o \tau_o + \check{\xi}_e^\mu \tilde{\tau}_\mu) u_e^{-1}, \quad (30)$$

where  $\xi_e^o := \xi_e - \zeta_e$  and  $e^{\check{\xi}_e^\mu \tilde{\tau}_\mu} := e^{\check{\xi}_e^\mu \tilde{\tau}_\mu} e^{-\check{\xi}_e^\mu \tilde{\tau}_\mu}$ . Denote  $K_e^\perp := \frac{1}{\beta} u_e (\xi_e^o \tau_o) u_e^{-1}$  and  $K_e^{//} := \frac{1}{\beta} u_e (\check{\xi}_e^\mu \tilde{\tau}_\mu) u_e^{-1}$ , and we can clearly see that despite the anomaly in the vertex-simplicity constraints, our reduction procedure correctly removes the component  $K_e^{//}$ , while it preserves the component  $K_e^\perp$  that contributes to the extrinsic curvature as expressed in the same form as in the classical connection formulation. In other words, we have

$$\begin{aligned} \text{tr}(K_e \pi^{e'}) &\simeq \frac{1}{\beta} \text{tr}(u_e (\xi_e^o \tau_o + \check{\xi}_e^\mu \tilde{\tau}_\mu) u_e^{-1} X^{e'}) \\ &= \frac{1}{\beta} \text{tr}(u_e (\xi_e^o \tau_o) u_e^{-1} X^{e'}) = \text{tr}(K_e^\perp X^{e'}), \\ b(e) &= b(e') \end{aligned} \quad (31)$$

in the continuum limit. Indeed, on the constraint surface of both edge-simplicity and vertex-simplicity constraints, the component  $K_e^{//}$  has no projection on the bivector  $\pi^{e'} \simeq X^{e'} = \frac{1}{2} \eta_{e'} V_{e'}$  satisfying  $V_e^{[IJ} V_{e'}^{KL]} = 0$  with  $b(e) = b(e')$ , thus it provides no contribution to the extrinsic curvature as it showed in Eq. (31). Then, recall the pure gauge component  $\bar{K}_{aIJ}$  for nonanomalous simplicity constraint in continuum phase space, and one can conclude that the degrees of freedom of  $\check{\xi}_e^\mu$  are consistent with that of  $\bar{K}_{aIJ}$  in the continuum limit, so that the components  $\check{\xi}_e^\mu$  are regarded as the pure gauge (with respect to simplicity constraint) component in discrete phase space, which can be illustrated as [18]

$$\bar{K}_{aIJ} \xleftarrow[\text{in continuum limit}]{\text{correspondence of gauge degrees of freedom}} \check{\xi}_e^\mu. \quad (32)$$

### C. Classical gauge reduction with respect to simplicity constraint

To construct the gauge invariant variables with respect to the edge-simplicity constraint in the holonomy-flux phase space, one needs to reduce the holonomy and flux

variables, respectively. Let us focus on the constraint surface defined by the edge-simplicity constraint in the phase space  $T^*SO(D+1)$  associated with one single elementary edge  $e$  of  $\gamma$ . Based on the twisted geometry parametrization, the gauge transformation induced by the edge-simplicity constraint on the edge-simplicity constraint surface can be given by

$$\begin{aligned} \{X_e^{[IJ} X_e^{KL]}, h_e\} &= 2X_e^{[IJ} \{X_e^{KL]}, h_e\} \\ &\propto \eta_e V_e^{[IJ} (\tau^{KL]} u_e e^{\check{\xi}_e^\mu \tilde{\tau}_\mu} e^{\xi_e \tau_o} \tilde{u}_e^{-1}) \\ &= \eta_e (u_e (\check{\tau}_e^{IJKL} e^{\check{\xi}_e^\mu \tilde{\tau}_\mu}) e^{\xi_e \tau_o} \tilde{u}_e^{-1}) \end{aligned} \quad (33)$$

and

$$\{X_e^{[IJ} X_e^{KL]}, X_e^{MN}\} = 0, \quad (34)$$

where we defined  $\check{\tau}_e^{IJKL} := V_e^{[IJ} (u_e^{-1} \tau^{KL]} u_e) \in so(D-1)$ . It is easy to see that the edge simplicity constraint induces the transformation of the component  $e^{\check{\xi}_e^\mu \tilde{\tau}_\mu} \in SO(D-1)$  in the parametrization of  $h_e$ , and the flux is gauge invariant with respect to the edge-simplicity constraint on the constraint surface defined by the edge-simplicity constraint. Thus, we only need to focus on the reduction of holonomy. Let us introduce the averaging operation  $\mathbb{P}_S$  with respect to the gauge transformation induced by the edge-simplicity constraint in the discrete phase space, whose infinitely small transformation is generated by the edge-simplicity constraint as Eq. (33). Then, the action of  $\mathbb{P}_S$  on the constraint surface defined by the edge-simplicity constraint can be given as

$$\mathbb{P}_S \circ h_e := \int_{SO(D-1)} d\bar{g} (u_e e^{\xi_e \tau_o} (\bar{g} e^{\check{\xi}_e^\mu \tilde{\tau}_\mu} \tilde{u}_e^{-1}) = h_e^s, \quad (35)$$

$$\mathbb{P}_S \circ X_e = X_e, \quad (36)$$

where we used that  $h_e = u_e e^{\xi_e \tau_o} e^{\check{\xi}_e^\mu \tilde{\tau}_\mu} \tilde{u}_e^{-1}$ ,  $\bar{g} \in SO(D-1) \subset SO(D+1)$ , and  $h_e^s$  is the simplicity reduced holonomy defined by

$$h_e^s := u_e e^{\xi_e \tau_o} \mathbb{I}^s \tilde{u}_e^{-1}, \quad (37)$$

where  $(\mathbb{I}^s)_J^I := (\delta_1)^I (\delta_1)_J + (\delta_2)^I (\delta_2)_J$ . Now, the classical gauge invariant elementary variables with respect to the simplicity constraint are given by  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$ . Notice that they give a pair of gauge invariant functionals with respect to the simplicity constraint, instead of giving a point on the simplicity constraint surface. In details, the gauge transformation with respect to the simplicity constraint on the constraint surface is given by

$$h_e \rightarrow h'_e, X_e \rightarrow X_e,$$



wherein  $h_e = u_e e^{\xi_e \tau_o} (e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}) \tilde{u}_e^{-1}$  and  $h'_e = u_e e^{\xi_e \tau_o} (e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}) \tilde{u}_e^{-1}$ . It is easy to see that only the component  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  in  $h_e$  is changed along the gauge orbits with respect to the simplicity constraint. Since this component does not appear in the simplicity reduced holonomy  $h_e^s = u_e e^{\xi_e \tau_o} \mathbb{I}^s \tilde{u}_e^{-1}$ , one can conclude that  $(h_e^s, X_e)|_{X_e^{IJ} X_e^{KL}=0}$  are a pair of gauge invariant functionals with respect to simplicity constraint on the constraint surface. Now, by recalling the simplicity reduced connection  $A_{aIJ}^S := A_{aIJ} - \beta \bar{K}_{aIJ}$  constructed in connection phase space, we can establish the following correspondence  $A_{aIJ}^S$  and the simplicity reduced holonomy  $h_e^s$ ,

$$\begin{array}{ccc} (A_{aIJ}, \pi^{bKL}) & \xrightarrow{\text{regularization}} & (h_e, X_e) \\ \downarrow (1) & & \downarrow (2) \\ (A_{aIJ}^S, \pi^{bKL})|_{S^{abIJKL}=0} & \xrightarrow{\text{correspondence}} & (h_e^s, X_e)|_{S_e=0, S_o=0}, \end{array}$$

wherein the symplectic reductions with respect to simplicity constraint are proceeded in steps (1) and (2).

It has been pointed out that only the factor  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  in  $h_e$  is changed along the gauge orbits with respect to simplicity constraint, and thus the corresponding gauge degrees of freedom in the holonomy are contained entirely in this factor. However, it does not mean that the factor  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  is pure gauge. Notice that the edge simplicity constraint is a monomial of the flux and it is transformed by the Gaussian constraint in the adjoint transformation of  $so(D+1)$ . Thus, the pure gauge component with respect to simplicity constraint must also be transformed by the Gaussian constraint in the adjoint transformation of  $SO(D+1)$ . Nevertheless, it is not the case for the factor  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$ . Indeed, by recalling the Levi-Civita holonomy given by Eq. (27), one can factor out  $h_e^\Gamma$  from  $h_e$  through the expressions [18]

$$h_e = \left( u_e e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} e^{-\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} e^{(\xi_e - \zeta_e) \tau_o} u_e^{-1} \right) h_e^\Gamma = \left( u_e e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} e^{\xi_e \tau_o} u_e^{-1} \right) h_e^\Gamma \quad (38)$$

with  $\xi_e^o := \xi_e - \zeta_e$  and  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} := e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} e^{-\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$ . Notice  $h_e^\Gamma$  is purely determined by flux, thus it is invariant under the gauge transformation induced by edge simplicity constraint on the simplicity constraint surface. Then, it is easy to see that only the factor  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  in the decomposition (38) of  $h_e$  is changed along the gauge orbits with respect to the simplicity constraint, and it transforms by the Gaussian constraint in the adjoint transformation of some elements of  $SO(D+1)$  [18]. Hence, the pure gauge component in  $h_e$  is given by the factor  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$ . This result is consistency with that of Sec. II B which is achieved by considering the continuum limit. In the following part of this paper,  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  will be called the pure gauge component, and it is distinguished from the gauge component  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$ .

The simplicity reduced holonomy  $h_e^s$  corresponds to the simplicity reduced connection  $A_{aIJ}^S$  in the sense of gauge reduction, but  $h_e^s$  is not the holonomy defined by  $A_{aIJ}^S$ . This can be seen by considering the continuous limit of  $h_e^s$ , which reads

$$\begin{aligned} h_e^s &= u_e e^{\xi_e \tau_o} \mathbb{I}^s \tilde{u}_e^{-1} = u_e e^{\xi_e \tau_o} \mathbb{I}^s u_e^{-1} h_e^\Gamma \\ &\simeq (u_e \mathbb{I}^s u_e^{-1} + \beta K_e^\perp) (\mathbb{I} + \Gamma_e), \end{aligned}$$

where the appearance of  $\mathbb{I}^s$  leads that  $h_e^s$  is not the holonomy defined by  $A_{aIJ}^S$ . In fact, notice that the disappearance of  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  in  $h_e^s$  reduces not only the gauge degrees of freedom captured by  $\tilde{\zeta}_e^\mu$  but also the degrees of freedom of  $\tilde{\zeta}_e^\mu$  which corresponds to some components of  $\Gamma_{aIJ}$ . To retain  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  in the simplicity reduced holonomy, one may proceed with the gauge reduction of  $h_e$  with respect to the pure gauge component  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  by substituting  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} = e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  into Eq. (35). However, the result of this gauge reduction still gives  $h_e^s$ . More explicitly, similar to Eq. (35), one can take the averaging operation of  $h_e$  with respect to the gauge transformation induced by the simplicity constraint, which gives

$$\begin{aligned} &\int_{SO(D-1)} d\bar{g} (u_e e^{\xi_e \tau_o} (\bar{g} e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}) \tilde{u}_e^{-1}) \\ &= u_e e^{\xi_e \tau_o} (\mathbb{I}^s e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}) \tilde{u}_e^{-1} = u_e e^{\xi_e \tau_o} (\mathbb{I}^s) \tilde{u}_e^{-1}, \quad (39) \end{aligned}$$

where the gauge transformation only changes the pure gauge component  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  as  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} \rightarrow \bar{g} e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$ , and we use the fact that  $\mathbb{I}^s$  vanishes the factor  $e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu}$  by  $\mathbb{I}^s e^{\tilde{\zeta}_e^\mu \tilde{\tau}_\mu} = \mathbb{I}^s$  in the second “=” Hence, the gauge reduction procedure of  $h_e$  gives the simplicity reduced holonomy  $h_e^s$  unavoidably, which loses the structure of a holonomy, and it cannot catch the degrees of freedom of  $\tilde{\zeta}_e^\mu$ . Further, by using Eq. (39), one can check that  $h_\alpha^s$  constructed on a loop  $\alpha$  cannot capture the degrees of freedom of the intrinsic curvature, while it is able to capture the degrees of freedom of the extrinsic curvature properly; see more details in the Appendix. Thus, the variables constructed based on  $h_\alpha^s$  have different interpretations from that based on  $h_\alpha$ . Finally, we can conclude that the regularization of connection variables is not commutative to the gauge reduction with respect to the simplicity constraint in all dimensional LQG, and this point can be regarded as another aspect of the anomaly of the simplicity constraint.

Since the constructions of kinds of operators in all dimensional LQG relies on the regularized formulation of the simplicity reduced connection  $A_{aIJ}^S$ , it is worthwhile to construct the holonomy corresponding to  $A_{aIJ}^S$ . Let us define

$$\begin{aligned} (h_e^S)^I_L &:= (h_e^S)^I_L + ((\mathbb{I})^I_J + V_e^{JK} V_{e,KJ})(h_e^\Gamma)^J_L \\ &= u_e e^{\xi_e \tau_o} e^{\tilde{\xi}_e \tau_\mu} \tilde{u}_e^{-1} \end{aligned} \quad (40)$$

on the gauge reduced holonomy-flux phase space with respect to the edge-simplicity constraint. One can check that

$$h_e^S = u_e e^{\xi_e \tau_o} u_e^{-1} h_e^\Gamma \simeq (\mathbb{I} + \beta K_e^\perp)(\mathbb{I} + \Gamma_e) \quad (41)$$

in the continuum limit. It is easy to see that  $h_e^S$  captures the physical degrees of freedom of both intrinsic and extrinsic curvature properly, and it can be regarded as the holonomy of  $A_{aIJ}^S$ . We conclude this point as

$$(A_{aIJ}^S, \pi^{bKL})|_{S_{abIJKL}=0} \xrightarrow{\text{regularization}} (h_e^S, X_e)|_{S_e=S_v=0}.$$

One should notice that the definition (40) of  $h_e^S$  only holds for the elementary edges  $e$  of  $\gamma$  whose dual lattice gives a  $D$ -polytope partition of  $\sigma$ . For a loop  $\alpha = e_1 \circ e_2 \circ \dots \circ e_n$  with  $e_1, e_2, \dots, e_n$  being elementary edges of  $\gamma$ , we have  $h_\alpha^S := h_{e_1}^S h_{e_2}^S \dots h_{e_n}^S$ . As we will see in Sec. IV, the properties of  $h_e^S$  and  $h_e^S$  will be the key ingredients in the construction of the scalar constraint operator.

### III. QUANTUM GAUGE REDUCTION WITH RESPECT TO SIMPLICITY CONSTRAINT

#### A. The solution space of quantum simplicity constraint

The Hilbert space  $\mathcal{H}$  of all dimensional LQG is given by the completion of the space of cylindrical functions on the quantum configuration space, which can be decomposed into the sectors—the Hilbert spaces associated with graphs. For a given graph  $\gamma$  with  $|E(\gamma)|$  edges, the related Hilbert space is given by  $\mathcal{H}_\gamma = L^2((SO(D+1))^{|E(\gamma)|}, d\mu_{\text{Haar}}^{|E(\gamma)|})$ . This Hilbert space associates with the classical phase space  $\times_{e \in \gamma} T^*SO(D+1)_e$  aforementioned. A basis of this space is given by the spin-network functions constructed on  $\gamma$  which are labeled by (1) an  $SO(D+1)$  representation  $\Lambda$  assigned to each edge of  $\gamma$ ; and (2) an intertwiner  $i_v$  assigned to each vertex  $v$  of  $\gamma$ . Then, each basis state  $\Psi_{\gamma, \vec{\Lambda}, \vec{i}}(\vec{h})$ , as a wave function on  $\times_{e \in \gamma} SO(D+1)_e$ , can be given by

$$\Psi_{\gamma, \vec{\Lambda}, \vec{i}}(\vec{h}(A)) \equiv \bigotimes_{v \in \gamma} i_v \triangleright \bigotimes_{e \in \gamma} \pi_{\Lambda_e}(h_e(A)), \quad (42)$$

where  $\vec{h}(A) := (\dots, h_e(A), \dots)$ ,  $\vec{\Lambda} := (\dots, \Lambda_e, \dots)$ ,  $e \in \gamma$ ,  $\vec{i} := (\dots, i_v, \dots)$ ,  $v \in \gamma$ ,  $\pi_{\Lambda_e}(h_e)$  denotes the matrix of holonomy  $h_e$  associated with edge  $e$  in the representation labeled by  $\Lambda_e$ , and  $\triangleright$  denotes the contraction of the representation matrixes of holonomies with the intertwiners. Hence, the wave function  $\Psi_{\gamma, \vec{\Lambda}, \vec{i}}(\vec{h}(A))$  is simply the product of the functions on  $SO(D+1)$ , which are given

by specified components of the holonomy matrices selected by the intertwiners at the vertices. The action of the elementary operators—holonomy operator and flux operator—on the spin-network functions can be given as

$$\begin{aligned} \hat{h}_e(A) \circ \Psi_{\gamma, \vec{\Lambda}, \vec{i}}(\vec{h}(A)) &= h_e(A) \Psi_{\gamma, \vec{\Lambda}, \vec{i}}(\vec{h}(A)), \\ \hat{F}_e^{IJ} \circ \Psi_{\gamma, \vec{\Lambda}, \vec{i}}(\vec{h}(A)) &= -i \hbar \kappa \beta R_e^{IJ} \Psi_{\gamma, \vec{\Lambda}, \vec{i}}(\vec{h}(A)), \end{aligned} \quad (43)$$

where the holonomy operator acts by multiplying,  $R_e^{IJ} := \text{tr}((\tau^{IJ} h_e)^T \frac{\partial}{\partial h_e})$  is the right invariant vector fields on  $SO(D+1)$  associated with the edge  $e$ , and  $T$  denoting the transposition of the matrix. Then, the other operators in all dimensional LQG, such as spatial geometric operators and scalar constraint operators, can be constructed based on these elementary operators [21–23].

Now one can proceed with the quantum gauge reduction procedures to obtain the kinematic physical Hilbert space. To achieve this goal, one needs to solve the kinematic constraints, including the Gaussian constraint, edge-simplicity constraint, and vertex-simplicity constraint in  $\mathcal{H}$ . Following the results given in Sec. II B, the Gaussian constraint and edge-simplicity constraint are imposed strongly and the corresponding solution space is spanned by the edge-simple and gauge invariant spin-network states, which are constructed by assigning simple representations of  $SO(D+1)$  to edges and gauge invariant intertwiners to vertices of the associated graphs. Besides, the anomalous vertex simplicity constraints are imposed weakly and the corresponding weak solutions are given by the spin-network states labeled by the simple coherent intertwiners at vertices [19]. Specifically, a typical spin-network state labeled by the gauge invariant simple coherent intertwiners at vertices is given by

$$\Psi_{\gamma, \vec{N}, \vec{\mathcal{I}}_{\text{s.c.}}}(\vec{h}(A)) = \text{tr}(\bigotimes_{e \in \gamma} \pi_{N_e}(h_e(A)) \bigotimes_{v \in \gamma} \mathcal{I}_v^{\text{s.c.}}), \quad (44)$$

where  $\pi_{N_e}(h_e(A))$  denotes the representation matrix of  $h_e(A)$  with  $N_e$  being a non-negative integer labeling a simple representation of  $SO(D+1)$ , and  $\vec{\mathcal{I}}_{\text{s.c.}}$  is defined by  $\vec{\mathcal{I}}_{\text{s.c.}} := (\dots, \mathcal{I}_v^{\text{s.c.}}, \dots)$  with  $\mathcal{I}_v^{\text{s.c.}}$  being the so-called gauge invariant simple coherent intertwiner labeling the vertex  $v \in \gamma$  [19]. More explicitly, the gauge invariant simple coherent intertwiner is defined as

$$\mathcal{I}_v^{\text{s.c.}} := \int_{SO(D+1)} dg \bigotimes_{e: b(e)=v} \langle N_e, V_e | g, \quad (45)$$

where all the edges linked to  $v$  are reoriented to be outgoing at  $v$  without loss of generality, the labels  $V_e$  satisfy the classical vertex-simplicity constraint as

$$V_e^{[IJ} V_{e'}^{KL]} = 0, \quad \forall b(e) = b(e') = v, \quad (46)$$

and  $|N_e, V_e\rangle$  is the Perelomov type coherent state in the simple representation space of  $SO(D+1)$  labeled by  $N_e$  [24], which satisfies

$$\langle N_e, V_e | \tau^{IJ} | N_e, V_e \rangle = \mathbf{i} N_e V_e^{IJ}, \quad (47)$$

where  $\tau^{IJ}$  is a basis element of  $so(D+1)$  and it acts on  $|N_e, V_e\rangle$  as an operator.

It is ready to relate the procedures of classical reduction with respect to simplicity constraint to the quantum case. Notice that the quantum theory is based on the holonomy-flux variables, so that we follow the reduction procedures introduced by the twisted geometry parametrization of holonomy-flux phase space. The key step in these procedures is the weak imposition of the quantum vertex-simplicity constraint. Such a treatment relies on the spin-network states labeled by the simple coherent intertwiners at vertices, which give the expectation value of the flux operator by their labels with minimal uncertainty [24]. Based on the fact that vertex simplicity constraint operators are purely composed by flux operators, we construct the simple coherent intertwiners labeled by the points on the constraint surface of both edge and vertex-simplicity constraints, which ensures that the spin-network states labeled by these simple coherent intertwiners at vertices weakly solve the quantum vertex simplicity constraints with minimal uncertainty [19]. With this key step being completed, we can realize the complete quantum reduction procedures and give the correspondence between the classical and quantum reductions, which can be illustrated as follows:

$$\begin{array}{ccc}
 \times_{e \in \gamma} T^* SO(D+1)_e & \xrightarrow{\text{quantization}} & \mathcal{H}_\gamma \\
 \downarrow & & \downarrow \text{(i)} \\
 \times_{e \in \gamma} \check{P}_e & \xrightarrow{\text{quantization}} & \mathcal{H}_\gamma^s \\
 \downarrow & & \downarrow \text{(ii)} \\
 \check{H}_\gamma & \xrightarrow{\text{quantization}} & \mathcal{H}_{\gamma, \text{inv.}}^s \\
 \downarrow & & \downarrow \text{(iii)} \\
 \check{H}_\gamma^s & \xrightarrow[\text{correspondence}]{\text{quantum}} & \mathcal{H}_{\gamma, \text{inv.}}^S
 \end{array} \quad (48)$$

where the procedures on the left-hand side repeat the classical reduction procedures of the holonomy-flux phase space given in the flow chart (23), and the procedures on the right-hand side are explained as follows. In step (i), the edge-simplicity constraint is imposed strongly, and we get the cylindrical function space  $\mathcal{H}_\gamma^s$  spanned by the spin-network functions whose edges are labeled by simple representations of  $SO(D+1)$ . Then in step (ii), we impose the quantum Gauss constraint that further restricts the state

space  $\mathcal{H}_\gamma^s$  to the gauge (with respect to the Gaussian constraint) invariant subspace  $\mathcal{H}_{\gamma, \text{inv.}}^s$ . In the key step (iii), we weakly impose the vertex-simplicity constraint based on the spin-network basis labeled by the coherent intertwiners, and it leads to the kinematical physical Hilbert space  $\mathcal{H}_{\gamma, \text{inv.}}^S$  of all dimensional LQG. The resulting space  $\mathcal{H}_{\gamma, \text{inv.}}^S$  is spanned by the spin-network states  $T_{\gamma, \vec{N}, \vec{I}_{s.c.}}(\vec{h}_e(A))$  defined by Eq. (44). Thus, the quantum reduction procedures of the state space on the right-hand side of (48) faithfully realize the quantum version of the classical reduction procedures of the holonomy-flux phase space, up to some quantum perturbations of the weakly vanishing vertex-simplicity constraint operators.

## B. Quantum gauge reduction of elementary operators with respect to simplicity constraint

To realize the quantum gauge reduction with respect to the simplicity constraint, let us introduce a new procedure to establish the gauge (with respect to the simplicity constraint) invariant holonomy and flux operators in this subsection, and they will be referred to as simplicity reduced holonomy and flux operators, respectively, in the following part of this paper. Since the gauge transformations with respect to simplicity constraint are generated by edge-simplicity constraint in holonomy-flux phase space, let us consider the construction of simplicity reduced holonomy and flux operators in the solution space  $\mathcal{H}_\gamma^s$  of quantum edge-simplicity constraint. It is easy to check that the flux operator  $\hat{X}_e$  satisfies

$$[\hat{X}_e^{MN}, \hat{X}_e^{[IJ} \hat{X}_e^{KL}]] \circ f_\gamma = 0, \quad \text{for } f_\gamma \in \mathcal{H}_\gamma^s \text{ and } e \in \gamma, \quad (49)$$

while the holonomy operator  $\hat{h}_e$  gives

$$[\hat{h}_e, \hat{X}_e^{[IJ} \hat{X}_e^{KL}]] \circ f_\gamma \neq 0, \quad \text{for } f_\gamma \in \mathcal{H}_\gamma^s \text{ and } e \in \gamma \quad (50)$$

generally, where  $\hat{X}_e^{[IJ} \hat{X}_e^{KL]}$  is the edge simplicity constraint operator which induces the gauge transformation with respect to the simplicity constraint in quantum theory. Thus, the flux operator  $\hat{X}_e$  is simplicity reduced in  $\mathcal{H}_\gamma^s$  while the holonomy operator  $\hat{h}_e$  is not. To find the simplicity reduced holonomy operator, let us define a projection operator  $\hat{\mathbb{P}}_S$  which projects an arbitrary quantum state in  $\mathcal{H}_\gamma$  into the solution space  $\mathcal{H}_\gamma^s$  of edge simplicity constraint. Then, one can check that

$$[\hat{\mathbb{P}}_S \hat{h}_e \hat{\mathbb{P}}_S, \hat{X}_e^{[IJ} \hat{X}_e^{KL}]] \circ f_\gamma = 0, \quad \text{for } f_\gamma \in \mathcal{H}_\gamma^s \text{ and } e \in \gamma. \quad (51)$$

Thus, the simplicity reduced holonomy operator  $\hat{h}_e^s$  can be defined as

$$\hat{h}_e^s := \hat{\mathbb{P}}_S \hat{h}_e \hat{\mathbb{P}}_S. \quad (52)$$

One should note that the action of  $\hat{\mathbb{P}}_S$  on the quantum state is distinguished with the action of  $\mathbb{P}_S$  on the classical variables  $(h_e, X_e)$ . To understand this point, notice that the quantum edge-simplicity constraint generates the infinitely small transformation of a cylindrical function  $f_\gamma(\dots, h_e, \dots)$  as

$$\begin{aligned} \hat{X}_e^{[IJ} \hat{X}_e^{KL]} \circ f_\gamma(\dots, h_e, \dots) &\propto \{X_e^{[IJ}, \{X_e^{KL]}, f_\gamma(\dots, h_e, \dots)\}\} \\ &\propto f_\gamma(\dots, \tau^{[IJ} \tau^{KL]} h_e, \dots), \end{aligned} \quad (53)$$

wherein the transformation of holonomy is not identical with the transformation of holonomy induced by the classical edge-simplicity constraint given in Eq. (15). Finally, we conclude the gauge reduction with respect to the simplicity constraint in both classical and quantum theory with Table I. Note that the quantum simplicity reduced variables  $(\hat{h}_e^s, \hat{X}_e)$  with domain  $\mathcal{H}_\gamma^s$  are constructed by projecting the action of holonomy and flux operators  $(\hat{h}_e, \hat{X}_e)$  into  $\mathcal{H}_\gamma^s$ , instead of quantizing the classical simplicity reduced variables  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$  directly. Thus, one may doubt whether  $(\hat{h}_e^s, \hat{X}_e)$  with domain  $\mathcal{H}_\gamma^s$  are the quantization of  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$ . In Sec. III D, we will confirm that  $(\hat{h}_e^s, \hat{X}_e)$  with domain  $\mathcal{H}_\gamma^s$  can be regarded as the quantization of  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$  by showing that  $(\hat{h}_e^s, \hat{X}_e)$  with domain  $\mathcal{H}_\gamma^s$  reproduce  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$  in the semiclassical limit.

However, as aforementioned in Sec. II C, since the simplicity reduced holonomy  $h_e^s$  is not able to capture the degrees of freedom of the intrinsic curvature properly, its quantum operator  $\hat{h}_e^s$  cannot be used to construct the scalar constraint operator that involves the intrinsic curvature. Thus, it is worthwhile to construct the operator  $\hat{h}_e^s$  which corresponds to the holonomy  $h_e^s$  of  $A_{alJ}^S$ . Recall

$$(h_e^s)^I_L := (h_e^s)^I_L + ((\mathbb{I})^I_J + V_e^{IK} V_{e,KJ})(h_e^\Gamma)^J_L \quad (54)$$

defined on the reduce holonomy-flux phase space with respect to the edge-simplicity constraint. It is easy to see that we still need to construct the operators corresponding to  $V_e$  and  $h_e^\Gamma$ . Notice that  $V^{IJ} = \frac{2X^{IJ}}{\sqrt{2X_{KL}X^{KL}}}$  holds on the edge-simplicity constraint surface, and thus we have

$$V_e^{IK} V_{e,KJ} = \frac{2X_e^{IK} X_{e,KJ}}{X_{e,MN} X_e^{MN}}, \quad (55)$$

and it can be quantized as a function of flux operator acting in the space  $\mathcal{H}_\gamma^s$ , which reads

$$\hat{V}_e^{IK} \hat{V}_{e,KJ} = 2\hat{X}_e^{IK} \hat{X}_{e,KJ} \left( \hat{X}_{e,MN} \hat{X}_e^{MN} \right)^{-1}, \quad (56)$$

where  $(\hat{X}_{e,MN} \hat{X}_e^{MN})^{-1}$  is the inverse operator of  $\hat{X}_{e,MN} \hat{X}_e^{MN}$ . It is easy to see that  $\hat{X}_{e,MN} \hat{X}_e^{MN}$  acts as the Casimir operator of  $SO(D+1)$ , and it has discrete eigenspectrum. Thus, the inverse operator of  $\hat{X}_{e,MN} \hat{X}_e^{MN}$  can be defined as

$$\left( \hat{X}_{e,MN} \hat{X}_e^{MN} \right)^{-1} := \sum E_k^{-1} |k\rangle \langle k|, \quad (57)$$

where  $|k\rangle$  represents the eigenstate of  $\hat{X}_{e,MN} \hat{X}_e^{MN}$  with  $E_k$  being the corresponding eigenvalue, and the summation takes over all of  $|k\rangle$  with  $E_k \neq 0$ . Then, the major obstacle to construct the operator corresponding to  $h_e^s$  is the quantization of  $h_e^\Gamma$ . Note that  $h_e^\Gamma$  is the holonomy of the spin connection  $\Gamma_{alJ}$  determined by  $\pi^{alJ}$ . Thus, it is reasonable to define the smeared spin connection operator  $\hat{\Gamma}_e := \Gamma_e(\hat{X})$  as a function of  $\hat{X}_e$ , and then the operator corresponding to  $h_e^\Gamma$  could be given by  $\hat{h}_e^\Gamma := \exp(\hat{\Gamma}_e)$ . However,  $\Gamma_{alJ}$  is a rather complicated function of  $\pi^{bKL}$  so that the construction of  $\hat{\Gamma}_e = \Gamma_e(\hat{X})$  is a knotty issue (see related research in Ref. [25]), and we will leave it to future study.

### C. Comparison between the gauge reductions with respect to simplicity and Gaussian constraints

It is interesting to compare the gauge reduction with respect to the simplicity constraint to that of the Gaussian constraint. In fact, the gauge reduction with respect to the Gauss constraint is quite different from that of the simplicity constraint, so that the gauge reduction procedure used in this article cannot be applied to the Gaussian constraint. Let us explain it explicitly as follows.

As shown in Eqs. (6) and (33), the key character of simplicity constraint is that the induced gauge transformations only transform some specific components of connection or holonomy, thus the gauge degrees of freedom can be eliminated by trimming these gauge components. More explicitly, in the discrete phase space, the simplicity

TABLE I. Gauge reduction with respect to the edge-simplicity constraint.

	Edge-simplicity constraint	Gauge invariant state	Simplicity reduced variables
Classical	$X_e^{[IJ} X_e^{KL]} \approx 0$	$(h_e^s, X_e) _{X_e^{[IJ} X_e^{KL]}=0}$	$(h_e^s, X_e) _{X_e^{[IJ} X_e^{KL]}=0}$
Quantum	$\hat{X}_e^{[IJ} \hat{X}_e^{KL]} \circ f_\gamma = 0$	$f_\gamma \in \mathcal{H}_\gamma^s$	$(\hat{h}_e^s, \hat{X}_e)$ with domain $\mathcal{H}_\gamma^s$



constraint induces such gauge transformations  $h_e \rightarrow h'_e$ , where  $h_e = u_e e^{\xi_e \tau_e} (e^{\bar{\xi}_e \bar{\tau}_e}) \tilde{u}_e^{-1}$  and  $h'_e = u_e e^{\xi_e \tau_e} (e^{\bar{\xi}_e \bar{\tau}_e}) \tilde{u}_e^{-1}$ . One can see that only the components  $e^{\bar{\xi}_e \bar{\tau}_e}$  in  $h_e$  are transformed by the simplicity constraint. Specifically, the gauge degrees of freedom with respect to the simplicity constraint in holonomy  $h_e$  are purely contained in the gauge component  $e^{\bar{\xi}_e \bar{\tau}_e}$  [see Eq. (33)]. The gauge reduction with respect to the simplicity constraint in discrete phase space proceeds by taking the average with respect to gauge transformation, which gives the simplicity reduced holonomy  $h_e^s$  on the edge-simplicity constraint surface defined by  $X_e^{[IJ} X_e^{KL]} = 0$  [see Eqs. (35) and (36), and Table II]. By recalling the twisted geometry interpretation of each component of the holonomy-flux variables introduced in Sec. II. 2, it is easy to see that the gauge components  $e^{\bar{\xi}_e \bar{\tau}_e}$  are trimmed in  $h_e^s$ , so that the gauge degrees of freedom in  $h_e$  are eliminated correctly and the resulting reduced variables  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$  capture the physical geometric degrees of freedom properly. Then, by introducing the projection operator  $\hat{\mathbb{P}}_S$  and defining the simplicity reduced holonomy operator  $\hat{h}_e^s$ , the gauge averaging projection with respect to the gauge transformation induced by the simplicity constraint is generalized to quantum theory, which leads to the simplicity reduced holonomy and flux operators  $(\hat{h}_e^s, \hat{X}_e)$  with domain  $\mathcal{H}_e^s$ .

The situation of the gauge reduction with respect to the Gaussian constraint is quite different from that of the simplicity constraint. Usually, the Gaussian constraint induces the gauge transformations  $h_e \rightarrow g_{s(e)} h_e g_{t(e)}^{-1}$ ,  $X_e \rightarrow g_{s(e)} X_e g_{t(e)}^{-1}$ . Compared with that of the simplicity constraint, there is no guarantee that one can specify some gauge components of holonomy-flux variables transformed by the Gaussian constraint, with the physical degrees of freedom being contained in the remaining components. Thus, it is not valid to eliminate the gauge degrees of freedom with respect to the Gaussian constraint by trimming the gauge components. This result is concluded in Table II.

#### D. Realization of quantum gauge reduction based on twisted geometry coherent state

To show the semiclassical property of the simplicity reduced operators with respect to the twisted geometry coherent state, let us consider the phase space and the Hilbert space associated with a single edge  $e$  in all

dimensional LQG. Then, we have the simplicity reduced operators  $(\hat{h}_e^s, \hat{X}_e)$  with domain  $\mathcal{H}_e^s$  and the twisted geometry coherent state  $\check{\Psi}_{\mathbb{H}_e^o} \in \mathcal{H}_e^s$  labeled by the twisted geometry parameters  $\mathbb{H}_e^o := (\eta_e, \xi_e, V_e, \tilde{V}_e)$  on the edge  $e$ , where the semiclassicality parameter  $t$  is defined by  $t := \frac{\kappa \hbar}{a^{D-1}}$ . Denoted by  $\phi_{\mathbb{H}_e^o}^t := \frac{\check{\Psi}_{\mathbb{H}_e^o}}{\|\check{\Psi}_{\mathbb{H}_e^o}\|}$  the normalized twisted geometry coherent state and then the semiclassical property of  $\hat{h}_e^s$  and  $\hat{X}_e$  can be shown by evaluating their expectation values and matrix elements in the twisted geometry coherent state basis. These calculations have been done in Refs. [26–28], and it has been shown that the expectation values and matrix elements of  $\hat{h}_e^s$  and  $\hat{X}_e$  are well-estimated by their classical correspondence  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$ . More explicitly, one notices that

$$\langle \phi_{\mathbb{H}_e^o}^t | \hat{h}_e^s | \phi_{\mathbb{H}_e^o}^t \rangle = \langle \phi_{\mathbb{H}_e^o}^t | \hat{\mathbb{P}}_S \hat{h}_e \hat{\mathbb{P}}_S | \phi_{\mathbb{H}_e^o}^t \rangle = \langle \phi_{\mathbb{H}_e^o}^t | \hat{h}_e | \phi_{\mathbb{H}_e^o}^t \rangle, \quad (58)$$

and then the expectation values of  $\hat{h}_e^s$  and  $\hat{X}_e$  are evaluated by

$$\langle \phi_{\mathbb{H}_e^o}^t | \hat{X}_e^{IJ} | \phi_{\mathbb{H}_e^o}^t \rangle \stackrel{\text{large } \eta_e}{=} \frac{\eta_e}{2} V^{IJ} (1 + \mathcal{O}(t)) \quad (59)$$

and

$$\langle \phi_{\mathbb{H}_e^o}^t | u_e^{-1} \hat{h}_e \tilde{u}_e | \phi_{\mathbb{H}_e^o}^t \rangle \stackrel{\text{large } \eta_e}{=} u_e^{-1} h_e^s \tilde{u}_e (1 + \mathcal{O}(t)), \quad (60)$$

respectively. Moreover, the matrix elements of  $\hat{h}_e^s$  and  $\hat{X}_e$  are evaluated by

$$\left| \langle \phi_{\mathbb{H}_e^o}^t | \hat{X}_e^{IJ} | \phi_{\mathbb{H}'_e^o}^t \rangle - \frac{\eta'_e}{2} V'^{IJ} \langle \phi_{\mathbb{H}_e^o}^t | \phi_{\mathbb{H}'_e^o}^t \rangle \right| \stackrel{\text{large } \eta_e}{\lesssim} t |f_X(\mathbb{H}_e^o, \mathbb{H}'_e^o)| \cdot |\langle \phi_{\mathbb{H}_e^o}^t | \phi_{\mathbb{H}'_e^o}^t \rangle| \quad (61)$$

and

$$\left| \langle \phi_{\mathbb{H}_e^o}^t | u_e^{-1} \hat{h}_e \tilde{u}'_e | \phi_{\mathbb{H}'_e^o}^t \rangle - u_e^{-1} h_e^s \tilde{u}'_e \langle \phi_{\mathbb{H}_e^o}^t | \phi_{\mathbb{H}'_e^o}^t \rangle \right| \stackrel{\text{large } \eta_e}{\lesssim} t |f_h(\mathbb{H}_e^o, \mathbb{H}'_e^o)| \cdot |\langle \phi_{\mathbb{H}_e^o}^t | \phi_{\mathbb{H}'_e^o}^t \rangle|, \quad (62)$$

respectively, where  $f_X(\mathbb{H}_e^o, \mathbb{H}'_e^o)$  and  $f_h(\mathbb{H}_e^o, \mathbb{H}'_e^o)$  are functions that are always suppressed by the exponentially decayed factor  $|\langle \phi_{\mathbb{H}_e^o}^t | \phi_{\mathbb{H}'_e^o}^t \rangle|$  for  $\mathbb{H}_e^o \neq \mathbb{H}'_e^o$ , and  $u'_e, \tilde{u}'_e$  in

TABLE II. Comparison between the gauge reductions with respect to simplicity and Gaussian constraints.

	Gauge transformation	Gauge components	Reduced variables
Simplicity constraint	$(h_e \rightarrow h'_e, X_e \rightarrow X_e) _{X_e^{[IJ} X_e^{KL]}=0}$	$\exp(\bar{\xi}_e \bar{\tau}_e)$	$(h_e^s, X_e) _{X_e^{[IJ} X_e^{KL]}=0}$
Gaussian constraint	$h_e \rightarrow g_{s(e)} h_e g_{t(e)}^{-1}, X_e \rightarrow g_{s(e)} X_e g_{t(e)}^{-1}$	N/A	N/A

the holonomy operator  $u_e^{-1} \widehat{h}_e \tilde{u}'_e$  act on the basis vectors that select a specific matrix element of the holonomy in the definition representation of  $SO(D+1)$ . As one can see, the simplicity reduced operators  $(\widehat{h}_e^s, \widehat{X}_e)$  with domain  $\mathcal{H}_e^s$  reproduce the classical simplicity reduced variables  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$  in the semiclassical limit, thus it is reasonable to regard  $(\widehat{h}_e^s, \widehat{X}_e)$  with domain  $\mathcal{H}_e^s$  as the quantization of  $(h_e^s, X_e)|_{X_e^{[IJ} X_e^{KL]}=0}$ . This confirms our argument proposed in Sec. III B.

It is worthwhile to clarify the reason why the standard holonomy operator  $\hat{h}_e$ , as a gauge variant (with respect to both of the Gaussian and simplicity constraints) variable, has a nonvanishing expectation value in the gauge (with respect to the simplicity constraint) invariant state, while it only has a vanishing expectation value in the gauge (with respect to the Gaussian constraint) invariant state. Indeed, the reason can be seen from the following two facts, which read

$$\mathbb{P}_G \hat{h}_e \mathbb{P}_G |\phi_\gamma\rangle = 0, \quad \forall |\phi_\gamma\rangle \in \mathcal{H}_\gamma, \quad (63)$$

and

$$\hat{\mathbb{P}}_S \hat{h}_e \hat{\mathbb{P}}_S |\phi_\gamma\rangle \neq 0, \quad \exists |\phi_\gamma\rangle \in \mathcal{H}_\gamma, \quad (64)$$

where  $\mathbb{P}_G$  is the projection operator which project a state in  $\mathcal{H}_\gamma$  to the gauge invariant (with respect to the Gauss constraint) state space. This result also reflects the difference between the simplicity constraint and the Gaussian constraint in another perspective.

#### IV. ON THE CONSTRUCTION OF QUANTUM SCALAR CONSTRAINT IN ALL DIMENSIONAL LQG

The simplicity reduced holonomy  $h_e^s$  takes a different geometric interpretation from the original holonomy  $h_e$ . Hence, the operators whose constructions involve holonomies should be considered carefully, to ensure that they take the correct geometric interpretations. In this section, we will consider the construction of the scalar constraint operator. As we will see, since the appearance of the simplicity reduced holonomy  $h_e^s$ , the standard strategy fails to give a correct scalar constraint operator in all dimensional LQG. To overcome this problem, we will propose three new strategies to construct the scalar constraint operator, which point out the directions of further research on the dynamics of all dimensional LQG. Notice that our discussions focus only on the factors involving holonomies in the scalar constraint; thus the analyses of the factors composed by fluxes are omitted in our study, and one can find the related research in Refs. [15,23].

#### A. The problematic standard strategy

Recall that we have introduced the scalar constraint  $C[A, \pi]$  in the connection phase space by substituting  $q_{cd}[\pi]$  and  $P^{ef}[A, \pi]$  into the scalar constraint  $C(q_{cd}, P^{ef})$  in the ADM phase space in Sec. II. To simplify our further analysis, we will consider an equivalent formulation of the scalar constraint in the connection phase space in this section. Similar to the analog in the  $SU(2)$  connection formulation of  $(1+3)$ -dimensional GR, one can establish the scalar constraint in  $SO(D+1)$  connection formulation of  $(1+D)$ -dimensional GR with two terms—the so-called Euclidean term  $C_E$  and Lorentzian term  $C_L$  [15]. The Euclidean term  $C_E$  reads

$$C_E := \frac{1}{\sqrt{\det(q)}} F_{abIJ} \pi^{aIK} \pi_K^{bJ} \quad (65)$$

with  $F_{abIJ} := \partial_a A_{bIJ} - \partial_b A_{aIJ} + \delta^{KL} A_{aIK} A_{bLJ} - \delta^{KL} A_{aJK} A_{bLI}$ . Define

$$C_E[1] := \int_\sigma d^D y C_E(y), \quad (66)$$

and then the Lorentzian term  $C_L$  reads

$$\begin{aligned} C_L &:= -\frac{8(1+\beta^2)}{\sqrt{\det(q)}} K_{[a|I|} K_{b]J} E^{aI} E^{bJ} \\ &= \frac{4(1+\beta^2)}{\sqrt{\det(q)}} [K_b^a K_a^b - K^2], \end{aligned} \quad (67)$$

where  $K(x) := K_{aI}(x) E^{aI}(x)$  and  $K_b^a := K_{bI} E^{aI}$  are given by

$$K(x) = -\frac{1}{4\kappa\beta^2} \{C_E(x), V(x, \epsilon)\} \quad (68)$$

and

$$K_{aI}(x) E^{bI}(x) = -\frac{1}{8\kappa^2\beta^3} \pi^{bKL}(x) \{A_{aKL}(x), \{C_E[1], V(x, \epsilon)\}\} \quad (69)$$

on the constraint surface of both Gaussian and simplicity constraints, with  $R(x, \epsilon) \ni x$  being a  $D$ -dimensional hypercube with coordinate scale  $\epsilon$  and  $V(x, \epsilon)$  being the volume of  $R(x, \epsilon)$ . One can check that  $C_E$  contains the pure gauge component  $\bar{K}_{aIJ}$  through the identity

$$\begin{aligned} C_E &:= \frac{1}{\sqrt{\det(q)}} F_{abIJ} \pi^{aIK} \pi_K^{bJ} \\ &= -\sqrt{\det(q)} R - \frac{\beta^2}{\sqrt{\det(q)}} (4[K_b^a K_a^b - K^2] \\ &\quad + (\bar{K}_{bIK} E^{aI})(\bar{K}_{aJ}^K E^{bJ})), \end{aligned} \quad (70)$$

which holds on the constraint surface of both Gaussian and simplicity constraints, where  $R$  is the scalar curvature of  $\Gamma_{aIJ}$  defined by

$$R := -\frac{1}{\det(q)} R_{abIJ} \pi^{aIK} \pi_K^{bJ} \quad (71)$$

with  $R_{abIJ} := \partial_a \Gamma_{bIJ} - \partial_b \Gamma_{aIJ} + \delta^{KL} \Gamma_{aIK} \Gamma_{bLJ} - \delta^{KL} \Gamma_{aJK} \Gamma_{bLI}$ . Thus, to get the correct gauge invariant ADM scalar constraint on the constraint surface of both Gaussian and simplicity constraints, the scalar constraint in the  $SO(D+1)$  connection formulation of  $(1+D)$ -dimensional GR must contain an additional term  $\frac{\beta^2}{\sqrt{\det(q)}} (\bar{K}_{bIK} E^{aI}) (\bar{K}_{aJ}^K E^{bJ})$  to cancel the gauge variant term in  $C_E$ , and the final scalar constraint reads

$$C = C_E + C_L + \frac{\beta^2}{\sqrt{\det(q)}} (\bar{K}_{bIK} E^{aI}) (\bar{K}_{aJ}^K E^{bJ}). \quad (72)$$

Comparing with the  $SU(2)$  loop quantum gravity in  $(1+3)$ -dimension, the additional term  $\frac{\beta^2}{\sqrt{\det(q)}} (\bar{K}_{bIK} E^{aI}) (\bar{K}_{aJ}^K E^{bJ})$  introduces a huge obstacle to regularize and quantize the scalar constraint in all dimensional LQG. By projecting the covariant derivation of  $\pi^{aIJ}$  properly, the term  $\frac{\beta^2}{\sqrt{\det(q)}} (\bar{K}_{bIK} E^{aI}) (\bar{K}_{aJ}^K E^{bJ})$  can be reformulated as a term that is composed by the connection variables [13].

However, this term is a rather complicated function of  $A_{aIJ}$  and  $\pi^{bIJ}$  so that its regularization and quantization are full of ambiguities [15]. Indeed, the key issue already appears when one considers the quantization of the Euclidean term in the scalar constraint. As we will see, the operator  $\hat{C}_E$  corresponding to the Euclidean term loses its original geometric interpretation if one considers its matrix elements in the space  $\bigoplus_{\gamma} \mathcal{H}_{\gamma}^s$ , since the simplicity reduced holonomy which will appear in the matrix elements of  $\hat{C}_E$  cannot give the curvatures correctly. Let us explain this point explicitly as follows.

Following the regularization and quantization procedures introduced in [15], the Euclidean term  $C_E$  and Lorentzian term  $C_L$  can be quantized directly, which leads to

$$\hat{C}_E[N] = \lim_{\epsilon \rightarrow 0} \sum_{\square \in \mathfrak{P}} \hat{C}_E^{\square}[N], \quad \hat{C}_L[N] = \lim_{\epsilon \rightarrow 0} \sum_{\square \in \mathfrak{P}} \hat{C}_L^{\square}[N] \quad (73)$$

with

$$\hat{C}_E^{\square}[N] := N(v_{\square}) \cdot \epsilon \left( \frac{\widehat{\pi^{[aIK]} \pi_K^{b]J}}}{\sqrt{\det(q)}} \right)_{v_{\square}} \cdot (\hat{h}_{\alpha_{s_a s_b}})_{[IJ]} \quad (74)$$

and

$$\begin{aligned} \hat{C}_L^{\square}[N] := & \frac{2(1+\beta^2)}{(8\kappa^2 \hbar^2 \beta^3)^2} N(v_{\square}) \cdot \epsilon \left( \frac{\widehat{\pi^{[aIK]}}}{\sqrt{\det(q)}} \right)_{v_{\square}} \cdot (\widehat{h_{s_a}})_I \left[ (\widehat{h_{s_a}^{-1}})_{MK}, [\hat{C}_E[1], \hat{V}(v_{\square}, \epsilon)] \right] \\ & \cdot \epsilon \left( \frac{\widehat{\pi^{b]JL}}}{\sqrt{\det(q)}} \right)_{v_{\square}} \cdot (\widehat{h_{s_b}})_J \left[ (\widehat{h_{s_b}^{-1}})_{NK}, [\hat{C}_E[1], \hat{V}(v_{\square}, \epsilon)] \right], \end{aligned} \quad (75)$$

where  $N(x)$  is the lapse function,  $\square$  denotes an elementary cell of the hypercubic partition  $\mathfrak{P}$  of  $\sigma$ ,  $\epsilon$  represents the scale of  $\square$ ,  $v_{\square}$  is a vertex of  $\square$ ,  $s_a$  represents the edges of  $\square$  based at  $v_{\square}$ ,  $\alpha_{s_a s_b}$  represents the oriented loop based at  $v_{\square}$

and  $s_a, s_b$ . Besides, the operators  $\epsilon \left( \frac{\widehat{\pi^{[aIK]} \pi_K^{b]J}}}{\sqrt{\det(q)}} \right)_{v_{\square}}$  and

$\epsilon \left( \frac{\widehat{\pi^{aIK}}}{\sqrt{\det(q)}} \right)_{v_{\square}}$  are constructed by regularizing and quantizing

the factors  $\frac{\pi^{aIK} \pi_K^{bJ}}{\sqrt{\det(q)}}$  and  $\frac{\pi^{aIK}}{\sqrt{\det(q)}}$ , respectively, with the regularization being compatible with the partition  $\mathfrak{P}$  at  $v_{\square}$  (see more details in Ref. [15]). Notice that the operator

$\epsilon \left( \frac{\widehat{\pi^{[aIK]} \pi_K^{b]J}}}{\sqrt{\det(q)}} \right)_{v_{\square}}$  is a polynomial of  $(\hat{V}(v_{\square}, \epsilon))^{1+x}$  and

$\hat{h}_{s_a} (\hat{V}(v_{\square}, \epsilon))^{1+x} \hat{h}_{s_a}^{-1}$  with  $x > -1$ ; thus it is commutative

with  $\hat{\mathbb{P}}_S$ .

Now, let us show that the simplicity reduced holonomy will appear in the matrix elements of  $\hat{C}_E$  in  $\bigoplus_{\gamma} \mathcal{H}_{\gamma}^s$  inevitably. Consider a state  $|\phi\rangle \in \bigoplus_{\gamma} \mathcal{H}_{\gamma}^s$  which satisfies

$$\hat{\mathbb{P}}_S |\phi\rangle = |\phi\rangle, \quad (76)$$

and we have

$$\langle \phi | \hat{C}_E[N] | \phi' \rangle = \langle \phi | \hat{\mathbb{P}}_S \hat{C}_E[N] \hat{\mathbb{P}}_S | \phi' \rangle = \langle \phi | \hat{C}_E^s[N] | \phi' \rangle, \quad (77)$$

where we defined

$$\hat{C}_E^s[N] := \lim_{\epsilon \rightarrow 0} \sum_{\square \in \mathfrak{P}} \hat{C}_E^{s,\square}[N] \quad (78)$$

with

$$\hat{C}_E^{\text{s},\square}[N] := N(v_\square) \cdot e^{\left(\frac{\pi^{[a|IK]}\pi_K^{b]J}}{\sqrt{\det(q)}}\right)_{v_\square}} \cdot (\hat{h}^s_{\alpha_{sa},\alpha_{sb}})_{[IJ]}, \quad (79)$$

which is given by replacing the holonomy operator  $\hat{h}_{\alpha_{sa},\alpha_{sb}}$  in  $\hat{C}_E[N]$  by the simplicity reduced one  $\hat{h}^s_{\alpha_{sa},\alpha_{sb}}$ . By this we can conclude that the matrix elements of  $\hat{C}_E[N]$  are identical to that of  $\hat{C}_E^s[N]$  in the space  $\bigoplus_\gamma \mathcal{H}_\gamma^s$ . The key point of this result is that, if one considers the matrix element of  $\hat{C}_E[N]$  in the space  $\bigoplus_\gamma \mathcal{H}_\gamma^s$ , the holonomy operator  $\hat{h}_{\alpha_{sa},\alpha_{sb}}$  is reduced to the simplicity holonomy operator  $\hat{h}^s_{\alpha_{sa},\alpha_{sb}}$  and  $\hat{C}_E[N]$  is reduced to  $\hat{C}_E^s[N]$ . Note that the physical interpretation of this scalar constraint operator relies on the geometric meaning of the standard holonomy  $h_{\alpha_{sa},\alpha_{sb}}$ , while the geometric interpretation of the simplicity reduced holonomy  $h^s_{\alpha_{sa},\alpha_{sb}}$  is different from that of  $h_{\alpha_{sa},\alpha_{sb}}$ . Thus, the action of  $\hat{C}_E[N]$  in  $\bigoplus_\gamma \mathcal{H}_\gamma^s$  cannot reveal the physical meaning of the classical scalar constraint  $C_E$  at quantum level. Besides, Eq. (75) is also not the operator corresponding to  $C_L$ , since its definition relies on the operator  $\hat{C}_E[1]$ .

The issue of the scalar constraint operator given above can also be considered in another perspective. It is reasonable to argue that the expectation value of the scalar constraint operator for a coherent state in  $\bigoplus_\gamma \mathcal{H}_\gamma^s$  would fail to produce the correct semiclassical limit. Let us explain this point explicitly as follows. Recalling the results of Refs. [26–28] which have been briefly reviewed in Sec. III D, it has been shown that the matrix elements of the standard holonomy operator in the twisted geometry coherent basis of  $\mathcal{H}_\gamma^s$  are well evaluated by the simplicity reduced holonomy given by the twisted geometry parameters. Thus, the expectation value of the standard holonomy operator in the coherent state in  $\mathcal{H}_\gamma^s$  fails to reproduce the degrees of freedom that should be contained in the holonomy. Besides, the Ehrenfest property of the twisted geometry coherent state proven in Ref. [27] ensures that the expectation value of a function of the elementary operators reproduce, to zeroth order in  $\hbar$ , the value of the corresponding classical function at the twisted geometry space point where the coherent state is peaked. More specifically, by using the Ehrenfest property of the twisted geometry coherent state, the expectation value of  $\hat{C}_E[N]$  in the twisted geometry coherent state  $\phi_{\gamma,\mathbb{H}^o}^t \in \mathcal{H}_\gamma^s$  can be evaluated by

$$\begin{aligned} \langle \phi_{\gamma,\mathbb{H}^o}^t | \hat{C}_E[N] | \phi_{\gamma,\mathbb{H}^o}^t \rangle &= \langle \phi_{\gamma,\mathbb{H}^o}^t | C_E[N](\hat{h}_e, \hat{X}_e) | \phi_{\gamma,\mathbb{H}^o}^t \rangle \\ &= C_E[N](h_e^s, X_e) \end{aligned} \quad (80)$$

at zeroth order of  $\hbar$ , where  $h_e^s$  and  $X_e$  are determined by the twisted geometry parameters  $\mathbb{H}_e^o = (\eta_e, \xi_e, V_e, \tilde{V}_e)$  on each

edge  $e$ , and we considered the hypercubic graph  $\gamma$  and the nongraph changing scheme of the action of  $\hat{C}_E[N]$ . Notice that we use the gauge (with respect to the Gaussian constraint) variant coherent state in Eq. (80), and it is reasonable to argue that the result of Eq. (80) still holds for the gauge (with respect to the Gaussian constraint) invariant coherent state in  $\mathcal{H}_\gamma^s$  based on the peakedness property of twisted geometry coherent state [26]. Now, one can conclude that the expectation value of the Euclidean term  $\hat{C}_E[N]$  of the scalar constraint operator in the twisted geometry coherent state fails to produce the correct semiclassical limit.

In fact, the twisted geometry coherent states are constructed in the space  $\mathcal{H}_\gamma^s$ ; thus their wave functions are constants instead of peaks along a gauge orbit of the simplicity constraint. In other words, the wave function of a twisted geometry coherent state in  $\mathcal{H}_\gamma^s$  does not peak at a point but peaks at a gauge orbit of simplicity constraint. This is the reason why the twisted geometry coherent state in  $\mathcal{H}_\gamma^s$  cannot produce the correct semiclassical limit of the scalar constraint operator. Indeed, to eliminate the gauge degrees of freedom with respect to the simplicity constraint, one must impose the edge simplicity constraint strongly, and it leads the solution space  $\mathcal{H}_\gamma^s$  inevitably. More specifically, the wave function of a state in  $\mathcal{H}_\gamma^s$  must be a constant along each of the gauge orbits of the simplicity constraint. Hence, essentially, it is caused by the treatment of strong imposition of the edge simplicity constraint that the twisted geometry coherent state in  $\mathcal{H}_\gamma^s$  can not produce the correct semiclassical limit of scalar constraint operator.

One may consider two schemes to deal with the issue that the expectation value of the scalar constraint operator given above in the coherent state in  $\mathcal{H}_\gamma^s$  fails to produce the correct semiclassical limit. In the first scheme, one can construct the coherent states in the Hilbert space  $\mathcal{H}_\gamma$ , by requiring that the wave function of each of the coherent states is peaked at a point instead of a gauge orbit. Nevertheless, such a kind of coherent states must involve the nonsimple representation of  $SO(D+1)$ , and thus the edge simplicity constraint cannot be solved strongly. In the second scheme, one can consider redefining the scalar constraint operator to ensure that it has a correct geometric meaning and semiclassical limit. We would like to discuss the second scheme in the following part of this article, and the first scheme will be left to future research.

## B. New strategies

The failure of the previous construction of the scalar constraint operator arises from what the simplicity reduced holonomies cannot reveal about the geometric meanings of the connections. Nevertheless, by analyzing the explicit structure of the simplicity reduced holonomies, the quantum gauge reduction with respect to the simplicity



constraint introduced in the sections above provides us new strategies to construct the scalar constraint operator in all dimensional LQG. To simplify the discussions, we first claim that the scalar constraint operators constructed in the following subsections are defined in the space  $\mathcal{H}^s := \bigoplus_{\gamma} \mathcal{H}_{\gamma}^s$  which vanishes the edge-simplicity constraint operator.

### 1. The first strategy

In the first strategy, let us recall the simplicity reduced connection

$$A_{aIJ}^S \equiv A_{aIJ} - \beta \bar{K}_{aIJ}, \quad (81)$$

and its curvature is defined by

$$F_{abIJ}^S := \partial_a A_{bIJ}^S - \partial_b A_{aIJ}^S + \delta^{KL} A_{aIK}^S A_{bLJ}^S - \delta^{KL} A_{aJK}^S A_{bLI}^S. \quad (82)$$

It is easy to check

$$\begin{aligned} C_E^S &:= \frac{1}{\sqrt{\det(q)}} F_{abIJ}^S \pi^{aIK} \pi_K^{bJ} \\ &= -\sqrt{\det(q)} R - \frac{4\beta^2}{\sqrt{\det(q)}} [K_{ab} K^{ab} - K^2] \end{aligned} \quad (83)$$

and

$$K_{aI}(x) E^{bI}(x) = -\frac{1}{8\kappa^2 \beta^3} \pi^{bKL}(x) \{A_{aKL}(x), \{C_E^S[1], V(x, \epsilon)\}\} \quad (84)$$

hold on the constraint surface of both Gaussian and simplicity constraints. Then, the scalar constraint can be expressed as

$$C = C_E^S + C_L. \quad (85)$$

Now, let us consider the regularization and quantization of  $C_E^S$ . Notice that  $C_E^S$  takes the same formulation as  $C_E$  except that the connection  $A_{aIJ}$  in  $C_E$  is replaced by  $A_{aIJ}^S$  in  $C_E^S$ . Moreover, recall that the smearing version of  $A_{aIJ}^S$  is given by  $h_e^S$ . Thus, following a similar regularization and quantization procedures as that of  $C_E$ , we can give the operator corresponding to  $C_E^S$  as

$$\hat{C}_E^S[N] = \lim_{\epsilon \rightarrow 0} \sum_{\square \in \mathfrak{P}} \hat{C}_E^{S, \square}[N] \quad (86)$$

with

$$\hat{C}_E^{S, \square}[N] := N(v_{\square}) \cdot \epsilon \left( \frac{\pi^{[a|IK|} \pi_K^{b]J}}{\sqrt{\det(q)}} \right)_{v_{\square}} \cdot (\widehat{h}_{\alpha_{sa}, \beta_b}^S)_{[IJ]}, \quad (87)$$

which is given by replacing the holonomy operator  $\hat{h}_{\alpha_{sa}, \beta_b}$  in  $\hat{C}_E[N]$  by another holonomy operator  $\widehat{h}_{\alpha_{sa}, \beta_b}^S$  corresponding to the classical holonomy  $h_e^S$  of  $A_{aIJ}^S$ . Accordingly, the operator corresponding to  $C_L$  is given by

$$\hat{C}_L[N] = \lim_{\epsilon \rightarrow 0} \sum_{\square \in \mathfrak{P}} \hat{C}_L^{\square}[N] \quad (88)$$

with

$$\begin{aligned} \hat{C}_L^{\square}[N] &:= \frac{2(1+\beta^2)}{(8\kappa^2 \hbar^2 \beta^3)^2} N(v_{\square}) \cdot \epsilon \left( \frac{\pi^{[a|IK|}}{\sqrt{\det(q)}} \right)_{v_{\square}} \cdot (\widehat{h}_{s_a}^M) \left[ (\widehat{h}_{s_a}^{-1})_{MK}, [\hat{C}_E^S[1], \hat{V}(v_{\square}, \epsilon)] \right] \\ &\quad \cdot \epsilon \left( \frac{\pi^{b]JL}}{\sqrt{\det(q)}} \right)_{v_{\square}} \cdot (\widehat{h}_{s_b}^N) \left[ (\widehat{h}_{s_b}^{-1})_{NK}, [\hat{C}_E^S[1], \hat{V}(v_{\square}, \epsilon)] \right]. \end{aligned} \quad (89)$$

Finally, one can conclude that the scalar constraint operator in all dimensional LQG can be given as

$$\hat{C}[N] = \hat{C}_E^S[N] + \hat{C}_L[N], \quad (90)$$

where  $\hat{C}_E^S[N]$  and  $\hat{C}_L[N]$  are defined in Eqs. (86) and (88), respectively.

### 2. The second strategy

In this strategy, we still consider the expression (85) of the scalar constraint and keep the regularization and

quantization scheme for  $C_E^S$  in (85). Then, let us consider a new scheme of the regularization and quantization of  $C_L$  in (85). By using Eq. (A8) in the Appendix, one can regularize  $C_L$  by defining

$$C_{L, \text{alt}}^{\square}[N] := \frac{8(1+\beta^2)}{\beta^2} N(v_{\square}) \cdot \epsilon \left( \frac{\pi^{[a|IK|} \pi_K^{b]J}}{\sqrt{\det(q)}} \right)_{v_{\square}} \cdot (h_{\alpha_{sa}, \beta_b}^S)_{[IJ]}, \quad (91)$$

and one can verify that

$$C_L[N] = \lim_{\epsilon \rightarrow 0} \sum_{\square \in \mathfrak{P}} C_{L,\text{alt}}^\square[N] \quad (92)$$

holds on the constraint surface defined by both Gaussian and simplicity constraints. Then, the operator corresponding to  $C_L[N]$  can be given by

$$\hat{C}_L[N] = \lim_{\epsilon \rightarrow 0} \sum_{\square \in \mathfrak{P}} \hat{C}_{L,\text{alt}}^\square[N] \quad (93)$$

with

$$\hat{C}_{L,\text{alt}}^\square[N] := \frac{8(1+\beta^2)}{\beta^2} N(v_\square) \cdot \epsilon \left( \frac{\pi^{[a|IK]}\pi^{b]J}}{\sqrt{\det(q)}} \right)_{v_\square} \cdot (\hat{h}^s_{\alpha_{sa, sb}})_{[IJ]}. \quad (94)$$

Here one should notice that  $\hat{h}^s_{\alpha_{sa, sb}}$  can be substituted by  $\hat{h}_{\alpha_{sa, sb}}$  when one consider the matrix elements of  $\hat{C}_L[N]$  in  $\mathcal{H}^s$ , since the matrix elements of  $\hat{h}^s_{\alpha_{sa, sb}}$  and  $\hat{h}_{\alpha_{sa, sb}}$  in  $\mathcal{H}^s$  are identical. Finally, in this strategy, the scalar constraint operator in all dimensional LQG is given by Eq. (90) with  $\hat{C}_E^S[N]$  and  $\hat{C}_L[N]$  being defined in Eqs. (86) and (93) respectively.

### 3. The third strategy

Notice that the operator  $\hat{C}_E^S[N]$  which is involved in the first and second strategies depends on the operator  $\hat{h}_e^S$  corresponding to the holonomy  $h_e^S$  of  $A_{alJ}^S$ . However, the explicit expression of  $\hat{h}_e^S$  involves another operator  $\hat{h}_e^I$  whose construction is still a difficult issue. In the third strategy, we consider a new expression of scalar constraint to avoid the difficulty of the operator  $\hat{C}_E^S[N]$ . One can reexpress the scalar constraint as

$$C = \frac{1}{(1+\beta^2)} C_L - \sqrt{\det(q)} R. \quad (95)$$

By regularizing and quantizing Eq. (95), we could get a new scalar constraint operator

$$\hat{C}[N] = \frac{1}{(1+\beta^2)} \hat{C}_L[N] - \hat{R}[N], \quad (96)$$

where  $\hat{C}_L[N]$  is given by Eq. (93) and  $\hat{R}[N]$  is the operator corresponding to

$$\tilde{R}[N] := \int_\sigma d^D y N(y) \sqrt{\det(q)} R(y). \quad (97)$$

Notice that the operator  $\hat{R}[N]$  has not been constructed yet in all dimensional LQG. Nevertheless, its analog in  $SU(2)$

LQG has been constructed and studied in various methods [25,29–31]. It is expected to extend these methods to all dimensional LQG to give the explicit expression of  $\hat{R}[N]$ . We leave this task to further researches.

## V. CONCLUSION

The gauge reduction with respect to the simplicity constraint has been discussed in both classical and quantum theory of all dimensional loop quantum gravity. In the classical connection phase space, the symplectic reduction with respect to simplicity and Gaussian constraints can proceed without anomaly, which leads to the ADM phase space correctly. Different with the continuum connection theory, the simplicity constraints in the discrete holonomy-flux phase space become anomalous. It has been shown that, in order to gives the discrete twisted geometry correctly, one should proceed with the gauge reduction with respect to the edge simplicity constraint and then impose the vertex simplicity constraint weakly, i.e., solving the vertex simplicity constraint equations. However, once we consider the gauge reduction with respect to the edge simplicity constraint in holonomy-flux phase space, we find that the simplicity reduced holonomy  $h_e^s$  cannot capture the degrees of freedom of intrinsic curvature, since its continuum limit does not reproduce the simplicity reduced connection  $A_{alJ}^S$ . Besides, the matrix elements of holonomy operator  $\hat{h}_e$  are identical with that of the simplicity reduced holonomy operator  $\hat{h}_e^s := \hat{\mathbb{P}}_S \hat{h}_e \hat{\mathbb{P}}_S$  in the space  $\mathcal{H}^s$  spanned by the states vanishing edge simplicity constraint, which means that the classical correspondence of  $\hat{h}_e$  acting in  $\mathcal{H}^s$  is given by  $h_e^s$  instead of  $h_e$ .

This result leads that the standard strategy fails to give a correct scalar constraint operator in all dimensional LQG. Our analysis shows that, in the twisted geometry coherent state in  $\mathcal{H}_\gamma^s$ , the expectation value of the scalar constraint operator given by the standard strategy fails to produce the correct semiclassical limit. Indeed, this issue is caused by the fact that the wave function of a coherent state in  $\mathcal{H}_\gamma^s$  does not peak at a point but peak at a gauge orbit of simplicity constraint. We have mentioned that two schemes can be considered to deal with this issue. In the first scheme, one can construct the coherent states in the Hilbert space  $\mathcal{H}_\gamma$ , by requiring that the wave function of each of the coherent states is peaked at a point instead of a gauge orbit. Nevertheless, such a kind of coherent states must involve the nonsimple representation of  $SO(D+1)$ , and thus the edge simplicity constraint cannot be solved strongly. In the second scheme, one can consider redefining the scalar constraint operator to ensure that it has correct geometric meaning and semiclassical limit. We have discussed the second scheme in this article, and the first scheme remains for future research.

Following the second scheme, we have proposed three new strategies to construct the scalar constraint operator in

Sec. IV B. In the first strategy, we establish the holonomy  $h_e^S$  of the simplicity reduced connection  $A_{aIJ}^S$ , which captures degrees of freedom of the intrinsic and extrinsic curvature correctly, and then the operator  $\widehat{h}_e^S$  is used to substitute  $\widehat{h}_e$  to construct the scalar constraint operator. In the second strategy, we consider an alternative of the Lorentzian part of the scalar constraint operator based on the simplicity reduced holonomy operator  $\widehat{h}_e^S$ . In the third strategy, a new method is considered to treat the spatial scalar curvature term in the scalar constraint. Generally, the issues introduced by the gauge reduction with respect to the simplicity constraint are discussed in this paper, and several strategies are proposed to deal with them. Nevertheless, these strategies still need further studies. As we mentioned before,  $\widehat{h}_e^S$  involved in first and second strategies contains the operator that corresponds to the holonomy of Levi-Civita connection, and this operator has not been constructed yet in all dimensional LQG. Besides, though the spatial scalar curvature operator involved in the third strategy has been established in  $SU(2)$  LQG, we still need to generalize it to all dimensional theory. We leave these tasks for future research.

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### APPENDIX: THE INHERENT CURVATURE IN $h_\alpha^S$

To clarify the inherent curvature in the simplicity resolved holonomy  $h_e^S$ , let us consider its behavior in a continuum limit. Give a hypercubic graph  $\gamma$  embedded in  $\sigma$  with the coordinate length of the elementary edges of  $\gamma$  being  $\epsilon$ . Then, we have the holonomy-flux phase space  $\times_{e \in E(\gamma)} T^*SO(D+1)_e$  associated with  $\gamma$ . One can proceed with the gauge reduction with respect to the edge-simplicity constraint in this phase space, which leads to the reduced space composed by the elements  $(h_e^S, X_e)_{e \in E(\gamma)}$ , which are parametrized by twisted geometry parameters as

$$h_e^S = u_e e^{\xi \epsilon \tau_o} \mathbb{I}^S \tilde{u}_e^{-1}, \quad X_e = \frac{1}{2} \eta_e V_e, \quad (\text{A1})$$

where  $(\mathbb{I}^S)^I_J := \delta_1^I \delta_1^J + \delta_2^I \delta_2^J$  is a  $(D+1) \times (D+1)$  matrix. We can further solve the vertex simplicity constraint

equation, and our following analysis is restricted on the constraint surface defined by the vertex simplicity constraint in reduced space composed by  $(h_e^S, X_e)_{e \in E(\gamma)}$ . Notice that  $h_e^S$  is a gauge (with respect to Gaussian constraint) covariant holonomy. To simplify our analysis, we can always proceed with a gauge transformation to ensure

$$V_e^{IJ} = 2\delta_1^I v_e^J, \quad \tilde{V}_e^{IJ} = 2\delta_1^I \tilde{v}_e^J, \quad \forall e \in E(\gamma). \quad (\text{A2})$$

Then, we have  $(h_e^\Gamma)^I_J \delta_1^J = \delta_1^I$  and

$$(\Gamma_e)^I_J \delta_1^J = (\mathcal{O}(\epsilon^2))^I \quad (\text{A3})$$

with  $\epsilon$  being small enough. To analyze the curvature captured by  $h_e^S$ , let us choose arbitrary minimal square loop  $\alpha \subset \gamma$  composed by  $\alpha = e_1 \circ e_2 \circ e_3 \circ e_4$  and consider  $h_\alpha^S = h_{e_1}^S h_{e_2}^S h_{e_3}^S h_{e_4}^S$ . With the gauge conditions (A2) being satisfied, we can further fix a gauge that ensures

$$v_{e_1}^I = -v_{e_3}^I, \quad v_{e_2}^I = -v_{e_4}^I \quad \text{and} \quad v_{e_1}^I v_{e_2}^J \delta_{IJ} = 0. \quad (\text{A4})$$

By these conditions one has

$$\begin{aligned} (u_{e_1} \mathbb{I}^S u_{e_1}^{-1} u_{e_2} \mathbb{I}^S u_{e_2}^{-1})^I_J &= (u_{e_2} \mathbb{I}^S u_{e_2}^{-1} u_{e_3} \mathbb{I}^S u_{e_3}^{-1})^I_J \\ &= (u_{e_3} \mathbb{I}^S u_{e_3}^{-1} u_{e_4} \mathbb{I}^S u_{e_4}^{-1})^I_J = \delta_1^I \delta_1^J. \end{aligned} \quad (\text{A5})$$

Then, recall

$$\begin{aligned} h_e^S &= u_e e^{\xi \epsilon \tau_o} \mathbb{I}^S \tilde{u}_e^{-1} \\ &\simeq (u_e \mathbb{I}^S u_e^{-1} + \beta K_e^\perp + \mathcal{O}(\epsilon^2)) (\mathbb{I} + \Gamma_e + \mathcal{O}(\epsilon^2)), \end{aligned} \quad (\text{A6})$$

one can expand  $h_\alpha^S$  as

$$\begin{aligned} (h_\alpha^S)_{[KL]} \bar{\eta}_I^K \bar{\eta}_J^L &= (h_{e_1}^S h_{e_2}^S h_{e_3}^S h_{e_4}^S)_{[KL]} \bar{\eta}_I^K \bar{\eta}_J^L \\ &= \beta^2 (K_{e_1}^\perp K_{e_4}^\perp)_{[IJ]} + \mathcal{O}(\epsilon^3). \end{aligned} \quad (\text{A7})$$

In the continuum limit, it reads

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} \frac{(h_\alpha^S)_{[KL]} \bar{\eta}_I^K \bar{\eta}_J^L}{\epsilon^2} &= \beta^2 \check{K}_{a[lK]} \check{K}_{bJ]}^K \dot{e}_1^a(v) \dot{e}_4^b(v) \\ &= -\beta^2 K_{a[l} K_{bJ]} \dot{e}_1^a(v) \dot{e}_4^b(v), \end{aligned} \quad (\text{A8})$$

where  $\check{K}_{aIJ} := K_{aIJ} - K_{aIJ} \bar{\eta}_I^K \bar{\eta}_J^L = 2\delta_{[I}^1 K_{aJ]}$  with  $\bar{\eta}_I^K := \delta_I^K - \delta_1^I \delta_1^K$ ,  $v$  is the source point of  $e_1$  and the target point of  $e_4$ , and  $\dot{e}_1^a(v)$  and  $\dot{e}_4^b(v)$  are the tangent vectors of  $e_1$  and  $e_4$  at  $v$ , respectively. Thus, we conclude that  $(h_\alpha^S)_{[KL]} \bar{\eta}_I^K \bar{\eta}_J^L$  capture the degrees of freedom of extrinsic curvature properly.

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