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# Quantum dynamics of loop quantum gravity

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# QUANTUM DYNAMICS OF LOOP QUANTUM GRAVITY

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# Abstract

In the last 20 years, loop quantum gravity, a background independent approach to unify general relativity and quantum mechanics, has been widely investigated. The aim of loop quantum gravity is to construct a mathematically rigorous, background independent, nonperturbative quantum theory for the Lorentzian gravitational field on a four-dimensional manifold. In this approach, the principles of quantum mechanics are combined with those of general relativity naturally. Such a combination provides us a picture of ”quantum Riemannian geometry”, which is discrete at a fundamental scale. In the investigation of quantum dynamics, the classical expressions of constraints are quantized as operators. The quantum evolution is contained in the solutions of the quantum constraint equations. On the other hand, the semi-classical analysis has to be carried out in order to test the semiclassical limit of the quantum dynamics.

In this thesis, the structure of the dynamical theory in loop quantum gravity is presented pedagogically. The outline is as follows: first we review the classical formalism of general relativity as a dynamical theory of connections. Then the kinematical Ashtekar-Isham-Lewandowski representation is introduced as a foundation of loop quantum gravity. We discuss the construction of a Hamiltonian constraint operator and the master constraint programme, for both the cases of pure gravity and matter field coupling. Finally, some strategies are discussed concerning testing the semiclassical limit of the quantum dynamics.

# 1 Introduction

## 1.1 Motivation of Quantum Gravity

The current view of physics is that there exist four fundamental interactions: strong interaction, weak interaction, electromagnetic interaction and gravitational interaction. The description for the former three kinds of forces is quantized in the well-known standard model. The interactions are transmitted via the exchange of particles. However, the last kind of interaction, gravitational interaction, is described by Einstein's theory of general relativity, which is a classical theory which describes the gravitational field as a smooth metric tensor field on a manifold, i.e., a 4-dimensional spacetime geometry. There is no $\hbar$ and hence no quantum structure of spacetime. Thus there is a fundamental inconsistency in our current description of the whole physical world. Physicists widely accept the assumption that our world is quantized at fundamental level. So all interactions should be brought into the framework of quantum mechanics fundamentally. As a result, the gravitational field should also have "quantum structure".

Throughout the last century, our understanding of nature has considerably improved from macroscale to microscale, including the phenomena at molecule, atom, sub-atom, and elementary particle scale. The standard model of particle physics agrees with all present experimental tests in laboratory (see e.g. [158]). However, because unimaginably large amount of energy would be needed, no experimental tests exist for processes that happen near the Planck scale $\ell_p \equiv (G\hbar/c^3)^{1/2} \sim 10^{-33}cm$ and $t_p \equiv (G\hbar/c^5)^{1/2} \sim 10^{-43}s$, which are viewed as the most fundamental scales. The Planck scale arises naturally in attempts to formulate a quantum theory of gravity, since $\ell_p$ and $t_p$ are unique combinations of speed of light $c$, Planck constant $\hbar$, and gravitational constant $G$, which have the dimensions of length and time respectively. The dimensional arguments suggest that at Planck scale the smooth structure of spacetime should break down, and therefore the well-known quantum field theory is invalid since it depends on a fixed smooth background spacetime. Hence we believe that physicists should go beyond the successful standard model to explore the new physics near Planck scale, which is, perhaps, a quantum field theory without a background spacetime, and this quantum field theory should include the quantum theory of gravity. Moreover, current theoretical physics is thirsting for a quantum theory of gravity to solve at least the following fundamental difficulties.

- Classical Gravity - Quantum Matter Inconsistency

  The equation relating matter and the gravitational field is the famous Einstein field equation:
  $$R_{\alpha\beta}[g] - \frac{1}{2}R[g]g_{\alpha\beta} = \kappa T_{\alpha\beta}[g], \quad (1)$$
  where the left hand side of the equation concerns spacetime geometry which has classical smooth structure, while the right hand side concerns also matter field which is fundamentally quantum mechanical in standard model. In quantum field theory the energy-momentum tensor of matter field should be an operator-valued tensor $\hat{T}_{\alpha\beta}$. One possible way to keep classical geometry consistent with quantum matter is to replace $T_{\alpha\beta}[g]$ by the expectation value $< \hat{T}_{\alpha\beta}[g] >$ with respect to some quantum state of the matter on a fixed spacetime. However, in the solution of this equation the background $g_{\alpha\beta}$ has to be changed due to the non-vanishing of $< \hat{T}_{\alpha\beta}[g] >$. So one has to feed back the new metric

into the definition of the vacuum expectation value etc. The result of the iterations does not converge in general [70]. On the other hand, some other arguments show that such a semiclassical treatment may violate the principle of superposition in quantum mechanics [55]. This inconsistency motivates us to quantize the background geometry to arrive at an operator formula also on the left hand side of Eq.(1).

- Singularities in General Relativity

  Einstein's theory of General Relativity is considered as one of the most elegant theories in the 20th century. Many experimental tests confirm the theory in the classical domain [159]. However, Penrose and Hawking proved that singularities are inevitable in general spacetimes with matter satisfying certain conditions in, by now well known, singularity theorems (for a summary, see [91][156]). Thus general relativity as a classical theory breaks down in certain regions of spacetime in a generic way. One naturally expects that, in extra strong gravitational field domains near the singularities, the gravitational theory would probably be replaced by an unknown quantum theory of gravity.

- Infinities in Quantum Field Theory

  It is well known that there are infinity problems in quantum field theory in Minkowski spacetime. In curved spacetime, the problem of divergences is even more complicated, since the renormalization process in curved spacetime is ambiguous, the expectation value of stress tensor can be fixed up to some local curvature terms, and it also depends on a fundamental scale of spacetime. Although much progress on the renormalization have been made [92][157], a fundamentally satisfactory theory is still far from reaching. So it is expected that some quantum gravity theory, playing a fundamental role at Planck scale, could provide a natural cut-off to cure the infinities in quantum field theory. The situation of quantum field theory on a fixed spacetime looks just like that of quantum mechanics for particles in electromagnetic field before the establishing of quantum electrodynamics, where the particle mechanics (actress) is quantized but the background electromagnetic field (stage) is classical. The history suggests that such a semi-classical situation is only an approximation which should be replaced by a much more fundamental and satisfactory theory.

## 1.2 Purpose of Loop Quantum Gravity

The research on quantum gravity is quite active. Many quantization programmes for gravity are being carried out (for a summary see e.g. [146]). In these different kinds of approaches, Among these different kinds of approaches, the idea of loop quantum gravity finds its roots in researchers from the general relativity community. It follows closely the motivations of general relativity, and hence it is a quantum theory born with background independence. Roughly speaking, loop quantum gravity is an attempt to construct a mathematically rigorous, non-perturbative, background independent quantum theory of four-dimensional, Lorentzian general relativity plus all known matter in the continuum. The project of loop quantum gravity inherits the basic idea of Einstein that gravity is fundamentally spacetime geometry. Here one believes in that the theory of quantum gravity is a quantum theory of spacetime geometry with diffeomorphism invariance (this legacy is discussed comprehensively in Rovelli's book [122]). To carry out the quantization procedure, one first casts general relativity into the Hamiltonian formalism as a diffeomorphism invariant Yang-Mills gauge field theory with a compact internal gauge group. Thus the construction of loop quantum gravity can also be applied to all background independent gauge field theories. One can therefore claim that the theory can also be called as a background independent quantum gauge field theory.

All classical fields theories, other than the gravitational field, are defined on a fixed spacetime, which provides a foundation to the perturbative Fock space quantization. However general relativity is only defined on a manifold and hence is a background independent classical field theory, since gravity itself is the background. So the situation for gravity is much different from other fields by construction [122], namely gravity is not only the background stage, but also the dynamical actress. Such a double character for gravity leads to many difficulties in the understanding of general relativity and its quantization, since we cannot follow the strategy in ordinary quantum theory of matter fields. However, an amazing result in loop quantum gravity is that the background independent programme can even help us to avoid the difficulties in ordinary quantum field theory. In perturbative quantum field theory in curved spacetime, the definition of some basic physical quantities, such as the expectation value of energy-momentum, is ambiguous and it is difficult to calculate the back-reaction of quantum fields to the background spacetime [157]. One could speculate that the difficulty is related to the fact that the present formulation of quantum field theories is background dependent. For instance, the vacuum state of a quantum field is closely related to spacetime structure, which plays an essential role in the description of quantum field theory in curved spacetime and their renormalization procedures. However, if the quantization programme is by construction background independent and non-perturbative, it may be possible to solve the problems fundamentally. In loop quantum gravity there is no assumption of a priori background metric at all and the gravitational field and matter fields are coupled and fluctuating naturally with respect to each other on a common manifold.

In the following sections, we will review pedagogically the basic construction of a completely new, background independent quantum field theory, which is completely different from the known quantum field theory. For completeness and accuracy, we will use detailed mathematical terminology. However, for simplicity, we will skip the complicated proofs of many important statements. One may find the missing details in the references cited. Thus our review will not be comprehensive. We refer to Ref.[146] and [90] for a more detailed exploration, Refs. [20] and [148] for more advanced topics. It turns out that in the framework of loop quantum gravity all theoretical inconsistencies introduced in the previous section are likely to be cured. More precisely, one will see that there is no UV divergence in quantum fields of matter if they are coupled with gravity in the background independent approach. Also recent works show that the singularities in general relativity can be smeared out in symmetry-reduced models [43][101][48]. The crucial point is that gravity and matter are coupled and consistently quantized non-perturbatively so that the problems of classical gravity and quantum matter inconsistency disappear.

# 2 Classical Framework

## 2.1 Lagrangian Formalism

In order to canonically quantize classical gravity, a Hamiltonian analysis has to be performed to obtain a canonical formalism of the classical theory suitable to be represented on a Hilbert space. A well known canonical formalism of general relativity is the ADM formalism (geometrodynamics) derived from the Einstein–Hilbert action[156][97], which has been problematic to cast into a quantum theory rigorously. Another well-known action of general relativity is the Palatini formalism, where the tetrad and the connection are regarded as independent dynamical variables. However, the dynamics of the Palatini action has similar difficulties at the time of quantization as the dynamics derived from the Einstein–Hilbert action [4][87]. In 1986, Ashtekar presented a formalism of true connection dynamics for general relativity with a relatively simple Hamiltonian constraint, and thus opened the door to apply quantization techniques from gauge field theory [2][3][123]. However, a drawback of that formalism is that the canonical variables are complex, which need the implementation of complicated reality conditions if one is to represent real general relativity. Moreover, the quantization based on the complex connection could not be carried out rigorously, since the internal gauge group is noncompact. In 1995, Barbero modified the Ashtekar new variables to give a system of real canonical variables for dynamical theory of connections [34]. Then Holst constructed a generalized Palatini action to support Barbero's real connection dynamics [93]. Although there is a free parameter (Barbero-Immirzi parameter $\beta$) in the generalized Palatini action and the Hamiltonian constraint is more complicated than the Ashtekar one, the generalized Palatini Hamiltonian with the real connections is widely used by loop theorists for the quantization programme. All the following analysis is based on the generalized Palatini formalism.

Consider a 4-manifold, $M$, on which the basic dynamical variables in the generalized Palatini framework are a tetrad $e^\alpha_I$ and an $so(1,3)$-valued connection $\omega_\alpha^{\ IJ}$(not necessarily torsion-free), where the capital Latin indices $I,\ J, ...$ refer to the internal $SO(1,3)$ group and the Greek indices $\alpha,\ \beta, ...$ denote spacetime indices. A tensor with both spacetime indices and internal indices is named as a generalized tensor. The internal space is equipped with a Minkowskian metric $\eta_{IJ}$ (of signature $-,+,+,+$) fixed once for all, such that the spacetime metric reads:

$$g_{\alpha\beta} = \eta_{IJ} e^I_\alpha e^J_\beta.$$

The generalized Palatini action in which we are interested is given by [20]:

$$S_p[e^\beta_K, \omega_\alpha^{\ IJ}] = \frac{1}{2\kappa}\int_M d^4x (e) e^\alpha_I e^\beta_J (\Omega_{\alpha\beta}^{\ \ IJ} + \frac{1}{2\beta}\epsilon^{IJ}_{\ \ KL}\Omega_{\alpha\beta}^{\ \ KL}), \tag{2}$$

where $e$ is the square root of the determinant of the metric $g_{\alpha\beta}$, $\epsilon^{IJ}_{\ \ KL}$ is the internal Levi-Civita symbol, $\beta$ is the real Barbero-Immirzi parameter, and the $so(1,3)$-valued curvature 2-form $\Omega_{\alpha\beta}^{\ \ IJ}$ of the connection $\omega_\alpha^{\ IJ}$ reads:

$$\Omega_{\alpha\beta}^{\ \ IJ} := 2\mathcal{D}_{[\alpha}\omega_{\beta]}^{\ IJ} = \partial_\alpha\omega_\beta^{\ IJ} - \partial_\beta\omega_\alpha^{\ IJ} + \omega_\alpha^{\ IK} \wedge \omega_{\beta K}^{\ \ \ J},$$

here $\mathcal{D}_\alpha$ denote the $so(1,3)$ generalized covariant derivative with respect to $\omega_\alpha^{\ IJ}$ acting on both spacetime and internal indices. Note that the generalized Palatini action returns to the Palatini action when $\frac{1}{\beta} = 0$ and gives the (anti)self-dual Ashtekar formalism when one sets $\frac{1}{\beta} = \pm i$. Moreover, besides spacetime diffeomorphism transformations, the action is also invariant under internal $SO(1,3)$ rotations:

$$(e, \omega) \mapsto (e', \omega') = (b^{-1}e, b^{-1}\omega b + b^{-1}db),$$

for any $SO(1,3)$ valued function $b$ on $M$. The gravitational field equations are obtained by varying this action with respect to $e_I^\alpha$ and $\omega_\alpha{}^{IJ}$. We first study the variation with respect to the connection $\omega_\alpha{}^{IJ}$. One has

$$\delta\Omega_{\alpha\beta}{}^{IJ} = (d\,\delta\omega\,{}^{IJ})_{\alpha\beta} + \delta\omega_\alpha{}^{IK} \wedge \omega_{\beta K}{}^J + \omega_\alpha{}^{IK} \wedge \delta\omega_{\beta K}{}^J = 2\mathcal{D}_{[\alpha}\delta\omega_{\beta]}^{IJ}$$

by the definition of covariant generalized derivative $\mathcal{D}_\alpha$. Note that $\delta\omega_\alpha{}^{IJ}$ is a Lorentz covariant generalized tensor field since it is the difference between two Lorentz connections [107][104]. One thus obtains

$$\begin{aligned}
\delta S_p &= \frac{1}{2\kappa}\int_M d^4x(e)e_I^\alpha e_J^\beta(\delta\Omega_{\alpha\beta}{}^{IJ} + \frac{1}{2\beta}\epsilon^{IJ}{}_{KL}\delta\Omega_{\alpha\beta}{}^{KL}) \\
&= -\frac{1}{\kappa}\int_M (\delta\omega_\beta{}^{IJ} + \frac{1}{2\beta}\epsilon^{IJ}{}_{KL}\delta\omega_\beta{}^{KL})\mathcal{D}_\alpha[(e)e_I^\alpha e_J^\beta],
\end{aligned}$$

where we have used the fact that $\mathcal{D}_\alpha\widetilde{\lambda}^\alpha = \partial_\alpha\widetilde{\lambda}^\alpha$ for all vector density $\widetilde{\lambda}^\alpha$ of weight $+1$ and neglected the surface term. Then it gives the equation of motion:

$$\mathcal{D}_\alpha[(e)e_I^\alpha e_J^\beta] = -\frac{1}{4}\mathcal{D}_\alpha[\widetilde{\eta}^{\alpha\beta\gamma\delta}\epsilon_{IJKL}e_\gamma^K e_\delta^L] = 0,$$

where $\widetilde{\eta}^{\alpha\beta\gamma\delta}$ is the spacetime Levi-Civita symbol. This equation leads to the torsion-free Cartan's first equation:

$$\mathcal{D}_{[\alpha}e_{\beta]}^I = 0,$$

which means that the connection $\omega_\alpha{}^{IJ}$ is the unique torsion-free Levi-Civita spin connection compatible with the tetrad $e_I^\alpha$. As a result, the second term in the action (2) can be calculated as:

$$(e)e_I^\alpha e_J^\beta\epsilon^{IJKL}\Omega_{\alpha\beta KL} = \eta^{\alpha\beta\gamma\delta}R_{\alpha\beta\gamma\delta},$$

which is exactly vanishing, because of the symmetric properties of Riemann tensor. So the generalized Palatini action returns to the Palatini action, which will certainly give the Einstein field equation.

## 2.2 Hamiltonian Formalism

To carry out the Hamiltonian analysis of action (2), suppose the spacetime $M$ is topologically $\Sigma \times \mathbf{R}$ for some 3-dimensional compact manifold $\Sigma$ without boundary. We introduce a foliation parameterized by a smooth function $t$ and a time-evolution vector field $t^\alpha$ such that $t^\alpha(dt)_\alpha = 1$ in $M$, where $t^\alpha$ can be decomposed with respect to the unit normal vector $n^\alpha$ of $\Sigma$ as:

$$t^\alpha = Nn^\alpha + N^\alpha, \tag{3}$$

here $N$ is called the lapse function and $N^\alpha$ the shift vector [156][97]. The internal normal vector is defined as $n_I \equiv n_\alpha e^\alpha_I$. It is convenient to carry out a partial gauge fixing, i.e., fix a internal constant vector field $n^I$ with $\eta_{IJ}n^I n^J = -1$. Note that the gauge fixing puts no restriction on the real dynamics[1]. Then the internal vector space $V$ is 3+1 decomposed with a 3-dimensional subspace $W$ orthogonal to $n^I$, which will be the internal space on $\Sigma$. With respect to the internal normal $n^I$ and spacetime normal $n^\alpha$, the internal and spacetime projection maps are denoted by $q^I_i$ and $q^\alpha_a$ respectively, where we use $i, j, k, ...$ to denote the 3-dimensional internal space indices and $a, b, c, ...$ to denote the indices of space $\Sigma$. Then an internal reduced metric $\delta_{ij}$ and a reduced spatial metric on $\Sigma$, $q_{ab}$, are obtained by these two projection maps. The two metrics are related by:

$$q_{ab} = \delta_{ij} e^i_a e^j_b, \tag{4}$$

where the orthonormal co-triad on $\Sigma$ is defined by $e^i_a := e^I_\alpha q^i_I q^\alpha_a$. Now the internal gauge group $SO(1,3)$ is reduced to its subgroup $SO(3)$ which leaves $n^I$ invariant. Finally, two Levi-Civita symbols are obtained respectively as

$$\begin{aligned}\epsilon_{ijk} &:= q^I_i q^J_j q^K_k n^L \epsilon_{LIJK}, \\ \underset{\sim}{\eta}_{abc} &:= q^\alpha_a q^\beta_b q^\gamma_c t^\mu \underset{\sim}{\eta}_{\mu\alpha\beta\gamma},\end{aligned}$$

where the internal Levi-Civita symbol $\epsilon_{ijk}$ is an isomorphism of Lie algebra $so(3)$. Using the connection 1-form $\omega_\alpha{}^{IJ}$, one can defined two $so(3)$-valued 1-form on $\Sigma$:

$$\begin{aligned}\Gamma^i_a &:= \frac{1}{2} q^\alpha_a q^i_I \epsilon^{IJ}{}_{KL} n_J \omega_\alpha{}^{KL}, \\ K^i_a &:= q^i_I q^\alpha_a \omega_\alpha{}^{IJ} n_J,\end{aligned}$$

where $\Gamma$ is a spin connection on $\Sigma$ and $K$ will be related to the extrinsic curvature of $\Sigma$ on shell. After the 3+1 decomposition and the Legendre transformation, action (2) can be expressed as [93]:

$$S_p = \int_{\mathbf{R}} dt \int_\Sigma d^3x [\widetilde{P}^a_i \mathcal{L}_t A^i_a - \mathcal{H}_{tot}(A^i_a, \widetilde{P}^b_j, \Lambda^i, N, N^c)], \tag{5}$$

from which the symplectic structure on the classical phase space is obtained as

$$\{A^i_a(x), \widetilde{P}^b_j(y)\} := \delta^i_j \delta^a_b \delta^3(x, y), \tag{6}$$

where the configuration and conjugate momentum are defined respectively by:

$$\begin{aligned}A^i_a &:= \Gamma^i_a + \beta K^i_a, \\ \widetilde{P}^a_i &:= \frac{1}{2\kappa\beta} \widetilde{\eta}^{abc} \epsilon_{ijk} e^j_b e^k_c = \frac{1}{\kappa\beta} \sqrt{|\det q|} e^a_i,\end{aligned}$$

[1]However, there are some arguments that such a gauge fixing is a non-natural way to break the internal Lorentz symmetry (see e.g. [131]).

here $\det q$ is the determinant of the 3-metric $q_{ab}$ on $\Sigma$ and hence $\det q = (\kappa\beta)^3 \det P$. In the definition of the configuration variable $A^i_a$, we should emphasize that $\Gamma^i_a$ is restricted to be the unique torsion free $so(3)$-valued spin connection compatible with the triad $e^a_i$. This conclusion is obtained by solving a second class constraint in the Hamiltonian analysis [93]. In the Hamiltonian formalism, one starts with the fields $(A^i_a, \widetilde{P}^a_i)$. Then neither the basic dynamical variables nor their Poisson brackets depend on the Barbero-Immirzi parameter $\beta$. Hence, for the case of pure gravitational field, the dynamical theories with different $\beta$ are related by a canonical transformation. However, as we will see, the spectrum of geometric operators are modified by different value of $\beta$, and the non-perturbative calculation of black hole entropy is compatible with Bekenstein-Hawking's formula only for a specific value of $\beta$ [68]. In addition, it is argued that the Barbero-Immerzi parameter $\beta$ may lead to observable effects in principle when the gravitational field is coupled with Fermions [112]. In the decomposed action (5), the Hamiltonian density $\mathcal{H}_{tot}$ is a linear combination of constraints:

$$\mathcal{H}_{tot} = \Lambda^i G_i + N^a C_a + NC,$$

where $\Lambda^i \equiv -\frac{1}{2}\epsilon^i{}_{jk}\omega_t{}^{jk}$, $N^a$ and $N$ are Lagrange multipliers. The three kinds of constraints in the Hamiltonian are expressed as [20]:

$$\begin{aligned} G_i &= D_a\widetilde{P}^a_i := \partial_a\widetilde{P}^a_i + \epsilon_{ij}{}^k A^j_a\widetilde{P}^a_k, \\ C_a &= \widetilde{P}^b_i F^i_{ab} - \frac{1+\beta^2}{\beta}K^i_a G_i, \\ C &= \frac{\kappa\beta^2}{2\sqrt{|\det q|}}\widetilde{P}^a_i\widetilde{P}^b_j[\epsilon^{ij}{}_k F^k_{ab} - 2(1+\beta^2)K^i_{[a}K^j_{b]}] \\ &+ \kappa(1+\beta^2)\partial_a(\frac{\widetilde{P}^a_i}{\sqrt{|\det q|}})G^i, \end{aligned} \tag{7}$$

where the configuration variable $A^i_a$ performs as a $so(3)$-valued connection on $\Sigma$ and $F^i_{ab}$ is the $so(3)$-valued curvature 2-form of $A^i_a$ with the well-known expression:

$$F^i_{ab} := 2D_{[a}A^i_{b]} = \partial_a A^i_b - \partial_b A^i_a + \epsilon^i{}_{jk}A^j_a A^k_b.$$

In any dynamical system with constraints, the constraint analysis is essentially important because they reflect the gauge invariance of the system. From the above three kinds of constraints of general relativity, one can know the gauge invariance of the theory. The Gauss constraint $G_i = 0$ has crucial importance in formulating the general relativity into a dynamical theory of connections. The corresponding smeared constraint function, $\mathcal{G}(\Lambda) := \int_\Sigma d^3x\Lambda^i(x)G_i(x)$, generates a transformation on the phase space as:

$$\begin{aligned} \{A^i_a(x),\ \mathcal{G}(\Lambda)\} &= -D_a\Lambda^i(x) \\ \{\widetilde{P}^a_i(x),\ \mathcal{G}(\Lambda)\} &= \epsilon_{ij}{}^k\Lambda^j(x)\widetilde{P}^a_k(x), \end{aligned}$$

which are just the infinitesimal versions of the following gauge transformation for the $so(3)$-valued connection 1-form $\mathbf{A}$ and internal rotation for the $so(3)$-valued densitized vector field $\widetilde{\mathbf{P}}$ respectively:

$$(\mathbf{A}_a,\ \widetilde{\mathbf{P}}^b) \mapsto (g^{-1}\mathbf{A}_a g + g^{-1}(dg)_a,\ g^{-1}\widetilde{\mathbf{P}}^b g).$$

To display the meaning of the vector constraint $C_a = 0$, one may consider the smeared constraint function:

$$\mathcal{V}(\vec{N}) := \int_\Sigma d^3x(N^a\widetilde{P}_i^bF^i_{ab} - (N^aA^i_a)G_i).$$

It generates the infinitesimal spatial diffeomorphism by the vector field $N^a$ on $\Sigma$ as:

$$\{A^i_a(x),\ \mathcal{V}(\vec{N})\} = \mathcal{L}_{\vec{N}}A^i_a(x),$$
$$\{\widetilde{P}^a_i(x),\ \mathcal{V}(\vec{N})\} = \mathcal{L}_{\vec{N}}\widetilde{P}^a_i(x).$$

The smeared scalar constraint is weakly equivalent to the following function, which is re-expressed for quantization purpose as

$$\begin{aligned}\mathcal{S}(N) &:= \int_\Sigma d^3xN(x)\widetilde{C}(x)\\ &= \frac{\kappa\beta^2}{2}\int_\Sigma d^3xN\frac{\widetilde{P}^a_i\widetilde{P}^b_j}{\sqrt{|\det q|}}[\epsilon^{ij}{}_kF^k_{ab} - 2(1+\beta^2)K^i_{[a}K^j_{b]}].\end{aligned} \tag{8}$$

It generates the infinitesimal time evolution off $\Sigma$. The constraints algebra, i.e., the Poisson brackets between these constraints, play a crucial role in the quantization programme. It can be shown that the constraints algebra of (7) has the following form:

$$\begin{aligned}\{\mathcal{G}(\Lambda),\ \mathcal{G}(\Lambda')\} &= \mathcal{G}([\Lambda,\ \Lambda']),\\ \{\mathcal{G}(\Lambda),\ \mathcal{V}(\vec{N})\} &= -\mathcal{G}(\mathcal{L}_{\vec{N}}\Lambda),\\ \{\mathcal{G}(\Lambda),\ \mathcal{S}(N)\} &= 0,\\ \{\mathcal{V}(\vec{N}),\ \mathcal{V}(\vec{N}')\} &= \mathcal{V}([\vec{N},\ \vec{N}']),\\ \{\mathcal{V}(\vec{N}),\ \mathcal{S}(M)\} &= -\mathcal{S}(\mathcal{L}_{\vec{N}}M),\\ \{\mathcal{S}(N),\ \mathcal{S}(M)\} &= -\mathcal{V}((N\partial_bM - M\partial_bN)q^{ab})\\ &\quad -\mathcal{G}((N\partial_bM - M\partial_bN)q^{ab}A_a))\\ &\quad -(1+\beta^2)\mathcal{G}(\frac{[\widetilde{P}^a\partial_aN, \widetilde{P}^b\partial_bM]}{|\det q|}),\end{aligned} \tag{9}$$

where $|\det q|q^{ab} = \kappa^2\beta^2\widetilde{P}^a_i\widetilde{P}^b_j\delta^{ij}$. Hence the constraints algebra is closed under the Poisson brackets, i.e., the constraints are all first class. Note that the evolution of constraints is consistent since the Hamiltonian $H = \int_\Sigma d^3x\mathcal{H}_{tot}$ is a linear combination of the constraints functions. The evolution equations of the basic canonical pair read

$$\mathcal{L}_tA^i_a = \{A^i_a,\ H\}, \qquad \mathcal{L}_t\widetilde{P}^a_i = \{\widetilde{P}^a_i,\ H\}.$$

Together with the three constraint equations, they are completely equivalent to the Einstein field equations. Thus general relativity is cast as a dynamical theory of connections with a compact structure group. Before finishing the discussion of this section, several issues should be emphasized.

- Canonical Transformation Viewpoint

  The above construction can be reformulated in the language of canonical transformations, since the phase space of connection dynamics is the same as that of triad geometrodynamics. In the triad formalism the basic conjugate pair consists of densitized triad $\widetilde{E}^a_i = \beta\widetilde{P}^a_i$ and "extrinsic curvature" $K^i_a$. The Hamiltonian and constraints read

$$\begin{aligned}\mathcal{H}_{tot} &= \Lambda^i G'_i + N^a C_a + NC \\ G'_i &= \epsilon_{ij}{}^k K^j_a \widetilde{E}^a_k, &(10)\\ C_a &= \widetilde{E}^b_j \nabla_{[a} K^j_{b]}, &(11)\\ C &= \frac{1}{\sqrt{|\det q|}}[\frac{1}{2}|\det q| R + \widetilde{E}^{[a}_i \widetilde{E}^{b]}_j K^i_a K^j_b], &(12)\end{aligned}$$

  where $\nabla_a$ is the $SO(3)$ generalized derivative operator compatible with triad $e^a_i$ and $R$ is the scalar curvature with respect to it. Since $\widetilde{E}^a_i$ is a vector density of weight one, we have

$$\nabla_a \widetilde{E}^a_i = \partial_a \widetilde{E}^a_i + \epsilon_{ij}{}^k \Gamma^j_a \widetilde{E}^a_k = 0.$$

  One can construct the desired Gauss law by

$$\begin{aligned}G_i &:= \frac{1}{\beta}\nabla_a \widetilde{E}^a_i + G'_i, \\ &= \partial_a \widetilde{P}^a_i + \epsilon_{ij}{}^k (\Gamma^j_a + \beta K^j_a)\widetilde{P}^a_k,\end{aligned}$$

  which is weakly zero by construction. This motivates us to define the connection $A^a_i = \Gamma^i_a + \beta K^i_a$. Moreover, the transformation from the pair $(\widetilde{E}^a_i, K^j_b)$ to $(\widetilde{P}^a_i, A^j_b)$ can be proved to be a canonical transformation [34][146], i.e., the Poisson algebra of the basic dynamical variables is preserved under the transformation:

$$\begin{aligned}\widetilde{E}^a_i &\mapsto \widetilde{P}^a_i = \widetilde{E}^a_i/\beta \\ K^j_b &\mapsto A^j_b = \Gamma^j_b + \beta K^j_b,\end{aligned}$$

  as

$$\begin{aligned}\{\widetilde{P}^a_i(x),\ A^j_b(y)\} &= \{\widetilde{E}^a_i(x), K^j_b(y)\} = \delta^a_b \delta^j_i \delta(x,y), \\ \{A^i_a(x),\ A^j_b(y)\} &= \{K^i_a(x), K^j_b(y)\} = 0, \\ \{\widetilde{P}^a_i(x),\ \widetilde{P}^b_j(y)\} &= \{\widetilde{E}^a_i(x), \widetilde{E}^b_j(y)\} = 0.\end{aligned}$$

- The Preparation for Quantization

  The advantage of a dynamical theory of connections is that it is convenient to be quantized in a background independent fashion. In the following procedure of quantization, the quantum algebra of the elementary observables will be generated by *holonomy*, i.e., connection smeared on a curve, and *electric flux*, i.e., a densitized triad smeared on a 2-surface. So no information about a background geometry is needed to define the quantum algebra. In the remainder of the thesis, in order to incorporate also spinors, we will enlarge the internal gauge group to be $SU(2)$. This does not damage the prior constructions because the Lie algebra of $SU(2)$ is the same as that of $SO(3)$. Due to the well-known nice properties of compact Lie group $SU(2)$, such as the Haar measure and Peter-Weyl theorem, one can obtain the background independent representation of the quantum algebra and the spin-network decomposition of the kinematic Hilbert space.

- Analysis on Constraint Algebra

  The classical constraint algebra (9) is an infinite dimensional Poisson algebra. Unfortunately, it is not a Lie algebra since the Poisson bracket between two scalar constraints has structure function depending on dynamical variables. This causes problems when solving the constraints quantum mechanically. On the other hand, one can see from Eq.(9) that the algebra generated by Gauss constraints forms not only a subalgebra but also a 2-side ideal in the full constraint algebra. Thus one can first solve the Gauss constraints independently. It is convenient to find the quotient algebra with respect to the Gauss constraint subalgebra as

$$\begin{aligned}
\{\mathcal{V}(\vec{N}),\ \mathcal{V}(\vec{N}')\} &= \mathcal{V}([\vec{N},\vec{N}']), \\
\{\mathcal{V}(\vec{N}),\ \mathcal{S}(M)\} &= -\mathcal{S}(\mathcal{L}_{\vec{N}}M), \\
\{\mathcal{S}(N),\ \mathcal{S}(M)\} &= -\mathcal{V}((N\partial_b M - M\partial_b N)q^{ab}),
\end{aligned}$$

  which plays a crucial role in solving the constraints quantum mechanically. But the subalgebra generated by the diffeomorphism constraints can not form an ideal. Hence the procedures of solving the diffeomorphism constraints and solving Hamiltonian constraints are entangled with each other. This leads to certain ambiguity in the construction of a Hamiltonian constraint operator [134][149]. Fortunately, the **Master Constraint Project** addresses the above two problems as a whole by introducing a new classical constraint algebra [149]. The new algebra is a Lie algebra where the diffeomorphism constraints form a 2-side ideal. We will come back to this point in the discussion on quantum dynamics of loop quantum gravity.

# 3 Foundations of Loop Quantum Gravity

In this chapter, we will begin to quantize the above classical dynamics of connections as a background independent quantum field theory. The main purpose of the chapter is to construct a suitable kinematical Hilbert space $\mathcal{H}_{kin}$ for the representation of quantum observables. In the following discussion, we formulate the construction in the language of algebraic quantum field theory [85]. It should be emphasized that the following constructions can be generalized to all background independent non-perturbative gauge field theories with compact gauge groups.

## 3.1 General Programme for Algebraic Quantization

In the strategy of loop quantum gravity, a canonical programme is performed to quantize general relativity, which has been cast into a diffeomorphism invariant gauge field theory, or more generally, a dynamical system with constraints. The following is a summary for a general procedure to quantize a dynamical system with first class constraints [133][4].

- Algebra of Classical Elementary Observables

  One starts with the classical phase space $(\mathcal{M}, \{,\})$ and $R$ ($R$ can be countable infinity[2] ) first-class constraints $C_r(r = 1...R)$ such that $\{C_r, C_s\} = \Sigma_{t=1}^R {f_{rs}}^t C_t$, where ${f_{rs}}^t$ is generally a function on phase space, namely, the structure function of Poisson algebra. The algebra of classical elementary observables $\mathfrak{P}$ is defined as:

  **Definition 3.1.1**: *The algebra of classical elementary observables $\mathfrak{P}$ is a collection of functions $f(m), m \in \mathcal{M}$ on the phase space such that*
  (1) $f(m) \in \mathfrak{P}$ *should separate the points of $\mathcal{M}$, i.e., for any $m \neq m'$, there exists $f(m) \in \mathfrak{P}$, such that $f(m) \neq f(m')$;* (*analogy to the $p$ and $q$ in $\mathcal{M} = \mathrm{T}^*\mathbf{R}$.*)
  (2) $f(m), f'(m) \in \mathfrak{P} \Rightarrow \{f(m), f'(m)\} \in \mathfrak{P}$ (*closed under Poisson bracket*)*;*
  (3) $f(m) \in \mathfrak{P} \Rightarrow \bar{f}(m) \in \mathfrak{P}$ (*closed under complex conjugation*).

  So $\mathfrak{P}$ forms a sub $*$-Poisson algebra of $C^\infty(\mathcal{M})$. In the case of $\mathcal{M} = \mathrm{T}^*\mathbf{R}$, $\mathfrak{P}$ is generated by the conjugate pair $(q, p)$ with $\{q, p\} = 1$.

- Quantum Algebra of Elementary Observables

  Given the algebra of classical elementary observables $\mathfrak{P}$, a quantum algebra of elementary observables can be constructed as follows. Consider the formal finite sequences of classical observable $(f_1...f_n)$ with $f_k \in \mathfrak{P}$. Then the operations of multiplication and involution are defined as

$$\begin{aligned} (f_1, ..., f_n) \cdot (f'_1, ..., f'_m) &:= (f_1, ..., f_n, f'_1, ..., f'_m), \\ (f_1, .., f_n)^* &:= (\bar{f}_n, ..., \bar{f}_1). \end{aligned}$$

  One can define the formal sum of different sequences with different number of elements. Then the general element of the newly constructed free $*$-algebra $F(\mathfrak{P})$ of $\mathfrak{P}$, is formally

[2] This includes the case of field theory with infinite many degree of freedom, since one can introduce the expression $C_{n,\mu} = \int_\Sigma d^3x \phi_n(x) C_\mu(x)$, where $\{\phi_n(x)\}_{n=1}^\infty$ forms a system of basis in $L^2(\Sigma, d^3x)$.

expressed as $\sum_{k=1}^{N}(f_1^{(k)}, ...f_{n_k}^{(k)})$, where $f_{n_i}^{(i)} \in \mathfrak{P}$. Consider the elements of the form (sequences consisting of only one element)

$$(f + f') - (f) - (f'), \ \ (zf) - z(f), \ \ [(f), (f')] - i\hbar(\{f, f'\}),$$

where $z \in \mathbf{C}$ is a complex number, and the canonical commutation bracket is defined as

$$[(f), (f')] := (f) \cdot (f') - (f') \cdot (f).$$

A 2-side ideal $\mathfrak{I}$ of $F(\mathfrak{P})$ can be constructed from these element, and is preserved by the action of involution $*$. One thus obtains

**Definition 3.1.2**: *The quantum algebra $\mathfrak{A}$ of elementary observables is defined to be the quotient $*$-algebra $F(\mathfrak{P})/\mathfrak{I}$.*

Note that the motivation to construct a quantum algebra of elementary observables is to avoid the problem of operators ordering in quantum theory so that the quantum algebra $\mathfrak{A}$ can be represented on a Hilbert space without ordering ambiguities.

- Representation of Quantum Algebra

  In order to obtain a quantum theory, we need to quantize the classical observables in the dynamical system. The, so called, quantization is nothing but a $*$-representation map[3] $\pi$ from the quantum algebra of elementary observable $\mathfrak{A}$ to the collection of linear operators $\mathcal{L}(\mathcal{H})$ on a Hilbert Space $\mathcal{H}$. At the level of quantum mechanics, the well-known Stone-Von Neumann Theorem concludes that in quantum mechanics, there is only one strongly continuous, irreducible, unitary representation of the Weyl algebra, up to unitary equivalence (see, for example, Ref.[113]). However, the conclusion of Stone-Von Neumann cannot be generalized to the quantum field theory because the latter has infinite many degrees of freedom (for detail, see, for example [157]). In quantum field theory, a representation can be constructed by GNS(Gel'fand-Naimark-Segal)-construction for a quantum algebra of elementary observable $\mathfrak{A}$, which is a unital $*$-algebra actually. The GNS-construction for the representation of quantum algebra $\mathfrak{A}$ is briefly summarized as follows.

  **Definition 3.1.3**: *Given a positive linear functional (a state) $\omega$ on $\mathfrak{A}$, the null space $\mathfrak{N}_\omega \in \mathfrak{A}$ with respect to $\omega$ is defined as $\mathfrak{N}_\omega := \{a \in \mathfrak{A} | \omega(a^* \cdot a) = 0\}$, which is a left ideal in $\mathfrak{A}$. Then a quotient map can be defined as $[.]$: $\mathfrak{A} \to \mathfrak{A}/\mathfrak{N}_\omega$; $a \mapsto [a] := \{a + b | b \in \mathfrak{N}_\omega\}$.*

[3] A map $\pi$: $\mathfrak{A} \to \mathcal{L}(\mathcal{H})$ is a *-representation if and only if (1) there exists a dense subspace $\mathcal{D}$ of $\mathcal{H}$ contained in $\cap_{a \in \mathfrak{A}}[D(\pi(a)) \cap D(\pi(a^*))]$ where $D(\pi(a))$ is the domain of the operator $\pi(a)$ and (2) for every $a, b \in \mathfrak{A}$ and $\lambda \in \mathbf{C}$ the following conditions are satisfied in $\mathcal{D}$,

$$\begin{aligned} \pi(a + b) = \pi(a) + \pi(b), \qquad & \pi(\lambda a) = \lambda \pi(a), \\ \pi(a \cdot b) = \pi(a)\pi(b), \qquad & \pi(a^*) = \pi(a)^\dagger. \end{aligned}$$

Note that $\mathcal{L}(\mathcal{H})$ fails to be an algebra because the domains of unbounded operators cannot be the whole Hilbert space. However, the collection of bounded operators on any Hilbert space is really a $*$-algebra.

*The GNS-representation for $\mathfrak{A}$ with respect to $\omega$ is a $*$-representation map: $\pi_\omega$: $\mathfrak{A} \to \mathcal{L}(\mathcal{H}_\omega)$, where $\mathcal{H}_\omega := \langle \mathfrak{A}/\mathfrak{N}_\omega \rangle$ and $\langle . \rangle$ denotes the completion with respect to the naturally equipped well-defined inner product*

$$< [a]|[b] >_{\mathcal{H}_\omega} := \omega(a^* \cdot b)$$

*on $\mathcal{H}_\omega$. This representation map is defined by*

$$\pi_\omega(a)[b] := [a \cdot b], \ \forall\, a \in \mathfrak{A} \text{ and } [b] \in \mathcal{H}_\omega,$$

*where $\pi_\omega(a)$ is an unbounded operator in general. Moreover, GNS-representation is a cyclic representation, i.e., $\exists\, \Omega_\omega \in \mathcal{H}_\omega$, such that $\langle \{\pi(a)\Omega_\omega | a \in \mathfrak{A}\} \rangle = \mathcal{H}_\omega$ and $\Omega_\omega$ is called a cyclic vector in the representation space. In fact $\Omega_\omega := [1]$ is a cyclic vector in $\mathcal{H}_\omega$ and $\langle \{\pi_\omega(a)\Omega_\omega | a \in \mathfrak{A}\} \rangle = \mathcal{H}_\omega$. As a result, the positive linear functional with which we begin can be expressed as*

$$\omega(a) = < \Omega_\omega | \pi_\omega(a) \Omega_\omega >_{\mathcal{H}_\omega} .$$

*Thus a positive linear functional on $\mathfrak{A}$ is equivalent to a cyclic representation of $\mathfrak{A}$, which is a triple $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$. Moreover, every non-degenerate representation is an orthogonal direct sum of cyclic representations (for proof, see [58]).*

So the kinematical Hilbert space $\mathcal{H}_{kin} = \mathcal{H}_\omega$ for the system with constrains can be obtained by GNS-construction. In the case that there are gauge symmetries in our dynamical system, supposing that there is a gauge group $G$ acting on $\mathfrak{A}$ by automorphisms $\alpha_g : \mathfrak{A} \to \mathfrak{A}$, $\forall\, g \in G$, it is preferred to construct a gauge invariant representation of $\mathfrak{A}$. So we require the positive linear functional $\omega$ on $\mathfrak{A}$ to be gauge invariant, i.e., $\omega \circ \alpha_g = \omega$. Then the group $G$ is represented on the Hilbert space $\mathcal{H}_\omega$ as:

$$U(g)\pi_\omega(a)\Omega_\omega = \pi_\omega(\alpha_g(a))\Omega_\omega,$$

and such a representation is a unitary representation of $G$. In loop quantum gravity, it is crucial to construct an internal gauge invariant and diffeomorphism invariant representation for the quantum algebra of elementary observables.

- Implementation of the Constraints

  In the Dirac quantization programme for a system with constraints, the constraints should be quantized as some operators in a kinematical Hilbert space $\mathcal{H}_{kin}$. One then solves them at quantum level to get a physical Hilbert space $\mathcal{H}_{phys}$, that is, to find a quantum analogy $\hat{C}_r$ of the classical constraint formula $C_r$ and to solve the general solution of the equation $\hat{C}_r\Psi = 0$. However, there are several problems in the construction of the constraint operator $\hat{C}_r$.

  (i) $C_r$ is in general not in $\mathfrak{P}$, so there is a factor ordering ambiguity in quantizing $C_r$ to be an operator $\hat{C}_r$.

  (ii) In quantum field theory, there are ultraviolet(UV) divergence problems in constructing operators. However, the UV divergence can be avoided in the background independent approach.

(iii) Sometimes, quantum anomalies may appear when there are structure functions in the Poisson algebra. Although classically we have $\{C_r, C_s\} = \Sigma_{t=1}^R f_{rs}{}^t C_t,\ r, s, t = 1, ..., R$, where $f_{rs}{}^t$ is a function on phase space, quantum mechanically it is possible that $[\hat{C}_r, \hat{C}_s] \neq i\hbar\Sigma_{t=1}^R \hat{f}_{rs}{}^t \hat{C}_t$ due to the ordering ambiguity between $\hat{f}_{rs}{}^t$ and $\hat{C}_t$. If one sets $[\hat{C}_r, \hat{C}_s] = \frac{i\hbar}{2}\Sigma_{t=1}^R(\hat{f}_{rs}{}^t\hat{C}_t + \hat{C}_t\hat{f}_{rs}{}^t)$, for $\Psi$ satisfying $\hat{C}_r\Psi = 0$, we have

$$[\hat{C}_r, \hat{C}_s]\Psi = \frac{i\hbar}{2}\sum_{t=1}^{R}\hat{C}_t\hat{f}_{rs}{}^t\Psi = \frac{i\hbar}{2}\sum_{t=1}^{R}[\hat{C}_t, \hat{f}_{rs}{}^t]\Psi. \tag{13}$$

However, $[\hat{C}_t, \hat{f}_{rs}{}^t]\Psi$ are not necessary to equal to zero for all $r, s, t = 1...R$. If not, the problem of quantum anomaly appears and the new quantum constraints $[\hat{C}_t, \hat{f}_{rs}{}^t]\Psi = 0$ have to be imposed on physical quantum states, since the classical Poisson brackets $\{C_r, C_s\}$ are weakly equal to zero on the constraint surface $\overline{\mathcal{M}} \subset \mathcal{M}$. Thus too many constraints are imposed and the physical Hilbert space $\mathcal{H}_{phys}$ would be too small. Therefore this is not a satisfactory solution and one needs to find a way to avoid the quantum anomalies.

- Solving the Constraints and Physical Hilbert Space

In general the original Dirac quantization approach can not be carried out directly, since there is usually no nontrivial $\Psi \in \mathcal{H}_{kin}$ such that $\hat{C}_r\Psi = 0$. This happens when the constraint operator $\hat{C}_r$ has "generalized eigenfunctions" rather than eigenfunctions. One then develops the so-called Refined Algebraic Quantization Programme, where the solutions of the quantum constraint can be found in the algebraic dual space of a dense subset in $\mathcal{H}_{kin}$ (see e.g. [84]). The quantum diffeomorphism constraint in loop quantum gravity is solved in this way. Another interesting way to solve the quantum constraints is the **Master Constraint Approach** proposed by Thiemann recently [149], which seems especially suited to deal with the particular feature of the constraint algebra of general relativity. A master constraint is defined as $\mathbf{M} := \frac{1}{2}\Sigma_{r,s=1}^R \mathbf{K}_{rs}C_s\bar{C}_r$ for some real positive matrix $\mathbf{K}_{rs}$. Classically one has $\mathbf{M} = 0$ if and only if $C_r = 0$ for all $r = 1...R$. So quantum mechanically one may consider solving the **Master Equation**: $\hat{\mathbf{M}}\Psi = 0$ to obtain the physical Hilbert space $\mathcal{H}_{phys}$ instead of solving $\hat{C}_r\Psi = 0,\ \forall\ r = 1...R$. Because the master constraint $\mathbf{M}$ is classically positive, one has opportunities to implement it as a self-adjoint operator on $\mathcal{H}_{kin}$. If it is indeed the case and $\mathcal{H}_{kin}$ is separable, one can use the direct integral representation of $\mathcal{H}_{kin}$ associated with the self-adjoint operator $\hat{\mathbf{M}}$ to obtain $\mathcal{H}_{phys}$:

$$\begin{aligned}\mathcal{H}_{kin} &\sim \int_{\mathbf{R}}^{\oplus} d\mu(\lambda)\mathcal{H}_\lambda^\oplus, \\ <\Phi|\Psi>_{kin} &= \int_{\mathbf{R}} d\mu(\lambda) <\Phi|\Psi>_{\mathcal{H}_\lambda^\oplus},\end{aligned} \tag{14}$$

where $\mu$ is a so-called spectral measure and $\mathcal{H}_\lambda^\oplus$ is the (generalized) eigenspace of $\hat{\mathbf{M}}$ with the eigenvalue $\lambda$. The physical Hilbert space is then formally obtained as $\mathcal{H}_{phys} = \mathcal{H}_{\lambda=0}^\oplus$ with the induced physical inner product $<\ |\ >_{\mathcal{H}_{\lambda=0}^\oplus}$ [4]. Now the issue of quantum anomaly

[4] One need to be careful for such a formal prescription, see the later discussion of master constraint or [63].

is represented in terms of the size of $\mathcal{H}_{phys}$ and the existence of sufficient numbers of semi-classical states.

- Physical Observables

  We denote $\mathcal{M}$ as the original unconstrained phase space, $\overline{\mathcal{M}}$ as the constraint surface, i.e., $\overline{\mathcal{M}} := \{m \in \mathcal{M} | C_r(m) = 0,\ \forall\ r = 1...R\}$, and $\hat{\mathcal{M}}$ as the reduced phase space, i.e. the space of orbits for gauge transformations generated by all $C_r$. The concept of Dirac observable is defined as the follows.

  **Definition 3.1.4**:
  (1) *A function $O$ on $\mathcal{M}$ is called a weak Dirac observable if and only if the function depends only on points of $\hat{\mathcal{M}}$, i.e., $\{O, C_r\}|_{\overline{\mathcal{M}}} = 0$ for all $r = 1...R$. For the quantum version, a self-adjoint operator $\hat{O}$ is a weak Dirac observable if and only if the operator can be well defined on the physical Hilbert space.*
  (2) *A function $O$ on $\mathcal{M}$ is called a strong Dirac observable if and only if $\{O, C_r\}|_{\mathcal{M}} = 0$ for all $r = 1...R$. For the quantum version, a self-adjoint operator $\hat{O}$ is a strong Dirac observable if and only if the operator can be defined on the kinematic Hilbert space $\mathcal{H}_{kin}$ and $[\hat{O}, \hat{C}_r] = 0$ in $\mathcal{H}_{kin}$ for all $r = 1...R$.*

  A physical observable is at least a weak Dirac observable. While Dirac observables have been found explicitly in symmetry reduced models, some even with an infinite number of degrees of freedom, it seems extremely difficult to find explicit expressions for them in full general relativity. Moreover the Hamiltonian is a linear combination of first-class constraints. So there is no dynamics in the reduced phase space, and the meaning of time evolution of the Dirac observables becomes subtle. However, using the concepts of partial and complete observables [121][115][122], a systematic method to get Dirac observables can be developed, and the problem of time in such system with a Hamiltonian $H = \Sigma_{r=1}^{R} \beta_r C_r$ may also be solved.

  Classically, let $f(m)$ and $\{T_r(m)\}_{r=1}^{R}$ be gauge non-invariant functions (partial observables) on phase space $\mathcal{M}$, such that $A_{sr} \equiv \{C_s, T_r\}$ is a non-degenerate matrix on $\mathcal{M}$. A system of classical weak Dirac observables (complete observables) $F^{\tau}_{f,T}$ labelled by a collection of real parameters $\tau \equiv \{\tau_r\}_{r=1}^{R}$ can be constructed as

  $$F^{\tau}_{f,T} := \sum_{\{n_1 \cdots n_R\}}^{\infty} \frac{(\tau_1 - T_1)^{n_1} \cdots (\tau_R - T_R)^{n_R}}{n_1! \cdots n_R!} \widetilde{X}_1^{n_1} \circ \cdots \circ \widetilde{X}_R^{n_R}(f),$$

  where $\widetilde{X}_r(f) := \{\Sigma_{s=1}^{R} A^{-1}_{rs} C_s,\ f\} \equiv \{\widetilde{C}_r,\ f\}$ . It can be verified that $[\widetilde{X}_r,\ \widetilde{X}_s]|_{\overline{\mathcal{M}}} = 0$ and $\{F^{\tau}_{f,T}, C_r\}|_{\overline{\mathcal{M}}} = 0$, for all $r = 1...R$ (for details see [61] and [62]).

  The partial observables $\{T_r(m)\}_{r=1}^{R}$ may be regarded as clock variables, and $\tau_r$ is the time parameter for $T_r$. The gauge is fixed by giving a system of functions $\{T_r(m)\}_{r=1}^{R}$ and corresponding parameters $\{\tau_r\}_{r=1}^{R}$, namely, a section in $\overline{\mathcal{M}}$ is selected by $T_r(m) = \tau_r$ for each $r$, and $F^{\tau}_{f,T}$ is the value of $f$ on the section. To solve the problem of dynamics, one assumes another set of canonical coordinates $(P_1, \cdots, P_{N-R}, \Pi_1, \cdots, \Pi_R; Q_1, \cdots, Q_{N-R}, T_1, \cdot\cdot$

$\cdot, T_R)$ by canonical transformations in the phase space $(\mathcal{M}, \{\ ,\ \})$, where $P_s$ and $\Pi_r$ are conjugate to $Q_s$ and $T_r$ respectively. After solving the complete system of constraints $\{C_r(P_i, Q_j, \Pi_s, T_t) = 0\}_{r=1}^{R}$, the Hamiltonian $H_r$ with respect to the time $T_r$ is obtained as $H_r := \Pi_r(P_i, Q_j, T_t)$. Given a system of constants $\{(\tau_0)_r\}_{r=1}^{R}$, for an observable $f(P_i, Q_j)$ depending only on $P_i$ and $Q_j$, the physical dynamics is given by [61][150]:

$$(\frac{\partial}{\partial \tau_r})_{\tau=\tau_0} F^{\tau}_{f,T}|_{\overline{\mathcal{M}}} = F^{\tau_0}_{\{H_r,f\},T}|_{\overline{\mathcal{M}}} = \{F^{\tau_0}_{H_r,T}, F^{\tau_0}_{f,T}\}|_{\overline{\mathcal{M}}},$$

where $F^{\tau_0}_{H_r,T}$ is the physical Hamiltonian function generating the evolution with respect to $\tau_r$. Thus one has addressed the problem of time and dynamics as a result.

- Semi-classical Analysis

  An important issue in the quantization is to check whether the quantum constraint operators have correct classical limits. This has to be done by using the kinematical semi-classical states in $\mathcal{H}_{kin}$. Moreover, the physical Hilbert space $\mathcal{H}_{phys}$ must contain enough semi-classical states to guarantee that the quantum theory one obtains can return to the classical theory when $\hbar \to 0$. The semi-classical states in a Hilbert space $\mathcal{H}$ should have the following properties.

  **Definition 3.1.5**: *Given a class of observables $\mathcal{S}$ which comprises a subalgebra in the space $\mathcal{L}(\mathcal{H})$ of linear operators on the Hilbert space, a family of (pure) states $\{\omega_m\}_{m\in\mathcal{M}}$ are said to be semi-classical with respect to $\mathcal{S}$ if and only if:*
  (1) *The observables in $\mathcal{S}$ should have correct semi-classical limit on semi-classical states and the fluctuations should be small, i.e.,*

$$\lim_{\hbar\to 0} |\frac{\omega_m(\hat{a}) - a(m)}{a(m)}| = 0,$$
$$\lim_{\hbar\to 0} |\frac{\omega_m(\hat{a}^2) - \omega_m(\hat{a})^2}{\omega_m(\hat{a})^2}| = 0,$$

  *for all $\hat{a} \in \mathcal{S}$.*
  (2) *The set of cyclic vectors $\Omega_m$ related to $\omega_m$ via the GNS-representation $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$ is dense in $\mathcal{H}$.*

  Seeking for semiclassical states are one of open issues of current research in loop quantum gravity. Recent original works focus on the construction of coherent states of loop quantum gravity in analogy with the coherent states for harmonic oscillator system [142][143] [144][145][19][15].

The above is the general programme to quantize a system with constraints. In the following subsection, we will apply the programme to the theory of general relativity and restrict our view to the representation with the properties of background independence and spatial diffeomorphism invariance.

## 3.2 Quantum Configuration Space

In quantum mechanics, the kinematical Hilbert space is $L^2(\mathbf{R}^3, d^3x)$, where the simple $\mathbf{R}^3$ is the classical configuration space of free particle which has finite degrees of freedom, and $d^3x$ is the Lebesgue measure on $\mathbf{R}^3$. In quantum field theory, it is expected that the kinematical Hilbert space is also the $L^2$ space on the configuration space of the field, which is infinite dimensional, with respect to some Borel measure naturally defined. However, it is often hard to define a concrete Borel measure on the classical configuration space, since the integral theory on infinite dimensional space is involved [57]. Thus the intuitive expectation should be modified, and the concept of quantum configuration space should be introduced as a suitable enlargement of the classical configuration space so that an infinite dimensional measure, often called cylindrical measure, can be well defined on it. The example of a scalar field can be found in the references [20][24]. For quantum gravity, it should be emphasized that the construction for quantum configuration space must be background independent. Fortunately, general relativity has been reformulated as a dynamical theory of $SU(2)$ connections, which would be great helpful for our further development.

The classical configuration space for gravitational field, which is denoted by $\mathcal{A}$, is a collection of the $su(2)$-valued connection 1-form field smoothly distributed on $\Sigma$. The idea of the construction for quantum configuration is due to the concept of holonomy.

**Definition 3.2.1**: *Given a smooth $SU(2)$ connection field $A_a^i$ and an analytic curve $c$ with the parameter $t \in [0, 1]$ supported on a compact subset (compact support ) of $\Sigma$, the corresponding holonomy is defined by the solution of the parallel transport equation [104]*

$$\frac{d}{dt}A(c,t) = -[A_a^i \dot{c}^a \tau_i]A(c,t), \tag{15}$$

*with the initial value $A(c, 0) = 1$, where $\dot{c}^a$ is the tangent vector of the curve and $\tau_i \in su(2)$ constitute an orthonormal basis with respect to the Killing-Cartan metric $\eta(\xi, \zeta) := -2\mathrm{Tr}(\xi\zeta)$, which satisfy $[\tau_i, \tau_j] = \epsilon^k_{\ ij}\tau_k$ and are fixed once for all. Thus the holonomy is an element in $SU(2)$, which can be expressed as*

$$A(c) = \mathcal{P}\exp\,(-\int_0^1 [A_a^i \dot{c}^a \tau_i]\, dt), \tag{16}$$

*where $A(c) \in SU(2)$ and $\mathcal{P}$ is a path-ordering operator along the curve $c$ (see the footnote at p382 in [104]).*

The definition can be well extended to the case of piecewise analytic curves via the relation:

$$A(c_1 \circ c_2) = A(c_1)A(c_2), \tag{17}$$

where $\circ$ stands for the composition of two curves. It is easy to see that a holonomy is invariant under the re-parametrization and is covariant under changing the orientation, i.e.,

$$A(c^{-1}) = A(c)^{-1}. \tag{18}$$

So one can formulate the properties of holonomy in terms of the concept of the equivalent classes of curves.

**Definition 3.2.2**: *Two analytic curves $c$ and $c'$ are said to be equivalent if and only if they have the same source $s(c)$ (beginning point ) and the same target $t(c)$ (end point ), and the holonomies of the two curves are equal to each other, i.e., $A(c) = A(c')$ $\forall A \in \mathcal{A}$. A equivalent class of analytic curves is defined to be an edge, and a piecewise analytic path is an composition of edges.*

To summarize, the holonomy is actually defined on the set $\mathcal{P}$ of piecewise analytic paths with compact supports. The two properties (17) and (18) mean that each connection in $\mathcal{A}$ is a homomorphism from $\mathcal{P}$, which is so-called a groupoid by definition [155], to our compact gauge group $SU(2)$. Note that the internal gauge transformation and spatial diffeomorphism act covariantly on a holonomy as

$$A(e) \mapsto g(t(e))^{-1}A(e)g(s(e)) \quad \text{and} \quad A(e) \mapsto A(\varphi \circ e), \tag{19}$$

for any $SU(2)$-valued function $g(x)$ on $\Sigma$ and spatial diffeomorphism $\varphi$. All above discussion is for classical smooth connections in $\mathcal{A}$. The quantum configuration space for loop quantum gravity can be constructed by extending the concept of holonomy, since its definition does not depend on an extra background. One thus obtains the quantum configuration space $\overline{\mathcal{A}}$ of loop quantum gravity as the following.

**Definition 3.2.3**: *The quantum configuration space $\overline{\mathcal{A}}$ is a collection of all quantum connections $A$, which are algebraic homomorphism maps without any continuity assumption from the collection of piecewise analytic paths with compact supports, $\mathcal{P}$, on $\Sigma$ to the gauge group $SU(2)$, i.e., $\overline{\mathcal{A}} := \mathrm{Hom}(\mathcal{P}, SU(2))$[5]. Thus for any $A \in \overline{\mathcal{A}}$ and edge $e$ in $\mathcal{P}$,*

$$A(e_1 \circ e_2) = A(e_1)A(e_2) \quad \text{and} \quad A(e^{-1}) = A(e)^{-1}.$$

*The transformations of quantum connections under internal gauge transformations and diffeomorphisms are defined by Eq.(19).*

The above discussion on the smooth connections shows that the classical configuration space $\mathcal{A}$ can be understood as a subset in the quantum configuration space $\overline{\mathcal{A}}$. Moreover, the Giles theorem [82] shows precisely that a smooth connection can be recovered from its holonomies by varying the length and location of the paths.

On the other hand, it was shown in [155][146] that the quantum configuration space $\overline{\mathcal{A}}$ can be constructed via a projective limit technique and admits a natural defined topology. To make the discussion precise, we begin with a few definitions:

**Definition 3.2.4**:

[5]It is easy to see that the definition of $\overline{\mathcal{A}}$ does not depend on the choice of local section in $SU(2)$-bundle, since the internal gauge transformations leave $\overline{\mathcal{A}}$ invariant.

1. *A finite set $\{e_1, ..., e_N\}$ of edges is said to be independent if the edges $e_i$ can only intersect each other at their sources $s(e_i)$ or targets $t(e_i)$.*

2. *A finite graph is a collection of a finite set $\{e_1, ..., e_N\}$ of independent edges and their vertices, i.e. their sources $s(e_i)$ and targets $t(e_i)$. We denote by $E(\gamma)$ and $V(\gamma)$ respectively as the sets of independent edges and vertices of a given finite graph $\gamma$. And $N_\gamma$ is the number of elements in $E(\gamma)$.*

3. *A subgroupoid $\alpha(\gamma) \subset \mathcal{P}$ can be generated from $\gamma$ by identifying $V(\gamma)$ as the set of objects and all $e \in E(\gamma)$ together with their inverses and finite compositions as the set of homomorphisms. This kind of subgoupoid in $\mathcal{P}$ is called tame subgroupoid. $\alpha(\gamma)$ is independent of the orientation of $\gamma$, so the graph $\gamma$ can be recovered from tame subgroupoid $\alpha$ up to the orientations on the edges. We will also denote by $N_\alpha$ the number of elements in $E(\gamma)$ where $\gamma$ is recovered by the tame subgroupoid $\alpha$.*

4. *$\mathcal{L}$ denotes the set of all tame subgroupoids in $\mathcal{P}$.*

One can equip a partial order relation $\prec$ on $\mathcal{L}$ [6], defined by $\alpha \prec \alpha'$ if and only if $\alpha$ is a subgroupoid in $\alpha'$. Obviously, for any two tame subgroupoids $\alpha \equiv \alpha(\gamma)$ and $\alpha' \equiv \alpha(\gamma')$ in $\mathcal{L}$, there exists $\alpha'' \equiv \alpha(\gamma'') \in \mathcal{L}$ such that $\alpha, \alpha' \prec \alpha''$, where $\gamma'' \equiv \gamma \cup \gamma'$. Define $X_\alpha \equiv Hom(\alpha, SU(2))$ as the set of all homomorphisms from the subgroupoid $\alpha(\gamma)$ to the group $SU(2)$. Note that an element $A_\alpha \in X_\alpha$ ($\alpha = \alpha(\gamma)$) is completely determined by the $SU(2)$ group elements $A(e)$ where $e \in E(\gamma)$, so that one has a bijection $\lambda : X_{\alpha(\gamma)} \to SU(2)^{N_\gamma}$, which induces a topology on $X_{\alpha(\gamma)}$ such that $\lambda$ is a topological homomorphism. For any pair $\alpha \prec \alpha'$, one can define a surjective projection map $P_{\alpha'\alpha}$ from $X_{\alpha'}$ to $X_\alpha$ by restricting the domain of the map $A_{\alpha'}$ from $\alpha'$ to the subgroupoid $\alpha$, and these projections satisfy the consistency condition $P_{\alpha'\alpha} \circ P_{\alpha''\alpha'} = P_{\alpha''\alpha}$. Thus a projective family $\{X_\alpha, P_{\alpha'\alpha}\}_{\alpha\prec\alpha'}$ is obtained by above constructions. Then the projective limit $\lim_\alpha(X_\alpha)$ is naturally obtained.

**Definition 3.2.5**: *The projective limit* $\lim_\alpha(X_\alpha)$ *of the projective family* $\{X_\alpha, P_{\alpha'\alpha}\}_{\alpha\prec\alpha'}$ *is a subset of the direct product space* $X_\infty := \prod_{\alpha\in\mathcal{L}} X_\alpha$ *defined by*

$$\lim_\alpha(X_\alpha) := \{\{A_\alpha\}_{\alpha\in\mathcal{L}} | P_{\alpha'\alpha}A_{\alpha'} = A_\alpha, \ \forall \ \alpha \prec \alpha'\}.$$

Note that the projection $P_{\alpha'\alpha}$ is surjective and continuous with respect to the topology of $X_\alpha$. One can equip the direct product space $X_\infty$ with the so-called Tychonov topology. Since any $X_\alpha$ is a compact Hausdorff space, by Tychonov theorem $X_\infty$ is also a compact Hausdorff space. One then can prove that the projective limit, $\lim_\alpha(X_\alpha)$, is a closed subset in $X_\infty$ and hence a compact Hausdorff space with respect to the topology induced from $X_\infty$. At last, one can find the relation between the projective limit and the prior constructed quantum configuration space $\overline{\mathcal{A}}$. As one might expect, there is a bijection $\Phi$ between $\overline{\mathcal{A}}$ and $\lim_\alpha(X_\alpha)$ [146]:

$$\begin{aligned} \Phi : \ \overline{\mathcal{A}} \ &\to \ \lim_\alpha(X_\alpha); \\ A \ &\mapsto \ \{A|_\alpha\}_{\alpha\in\mathcal{L}}, \end{aligned}$$

[6] A partial order on $\mathcal{L}$ is a relation, which is reflective ($\alpha \prec \alpha$), symmetric ($\alpha \prec \alpha', \ \alpha' \prec \alpha \Rightarrow \alpha' = \alpha$) and transitive ($\alpha \prec \alpha', \ \alpha' \prec \alpha'' \Rightarrow \alpha' \prec \alpha''$). Note that not all pairs in $\mathcal{L}$ need to have a relation.

where $A|_\alpha$ means the restriction of the domain of the map $A \in \overline{\mathcal{A}} = \mathrm{Hom}(\mathcal{P}, SU(2))$. As a result, the quantum configuration space is identified with the projective limit space and hence can be equipped with the topology. In conclusion, the quantum configuration space $\overline{\mathcal{A}}$ is constructed to be a compact Hausdorff topological space.

### 3.3 Cylindrical Functions on Quantum Configuration Space

Given the projective family $\{X_\alpha, P_{\alpha'\alpha}\}_{\alpha<\alpha'}$, the cylindrical function on its projective limit $\overline{\mathcal{A}}$ is well defined as follows.

**Definition 3.3.1**: *Let $C(X_\alpha)$ be the set of all continuous complex functions on $X_\alpha$, two functions $f_\alpha \in C(X_\alpha)$ and $f_{\alpha'} \in C(X_{\alpha'})$ are said to be equivalent or cylindrically consistent, denoted by $f_\alpha \sim f_{\alpha'}$, if and only if $P^*_{\alpha''\alpha} f_\alpha = P^*_{\alpha''\alpha'} f_{\alpha'}$, $\forall \alpha'' > \alpha, \alpha'$, where $P^*_{\alpha''\alpha}$ denotes the pullback map induced from $P_{\alpha''\alpha}$. Then the space $Cyl(\overline{\mathcal{A}})$ of cylindrical functions on the projective limit $\overline{\mathcal{A}}$ is defined to be the space of equivalent classes $[f]$, i.e.,*

$$Cyl(\overline{\mathcal{A}}) := [\cup_\alpha C(X_\alpha)]/\sim .$$

One then can easily prove the following proposition by definition.

**Proposition 3.3.1**:
*All continuous functions $f_\alpha$ on $X_\alpha$ are automatically cylindrical since each of them can generate a equivalent class $[f_\alpha]$ via the pullback map $P^*_{\alpha'\alpha}$ for all $\alpha' > \alpha$, and the dependence of $P^*_{\alpha'\alpha} f_\alpha$ on the groups associated to the edges in $\alpha'$ but not in $\alpha$ is trivial, i.e., by the definition of the pull back map,*

$$(P^*_{\alpha'\alpha} f_\alpha)(A(e_1), ..., A(e_{N_\alpha}), ..., A(e_{N_{\alpha'}})) = f_\alpha(A(e_1), ..., A(e_{N_\alpha})), \tag{20}$$

*where $N_\alpha$ denotes the number of independent edges in the graph recovered from the groupoid $\alpha$. On the other hand, by definition, given a cylindrical function $f \in Cyl(\overline{\mathcal{A}})$ there exists a suitable groupoid $\alpha$ such that $f = [f_\alpha]$, so one can identify $f$ with $f_\alpha$. Moreover, given two cylindrical functions $f,\ f' \in Cyl(\overline{\mathcal{A}})$, by definition of cylindrical functions and the property of projection map, there exists a common groupoid $\alpha$ and $f_\alpha,\ f'_\alpha \in C(X_\alpha)$ such that $f = [f_\alpha]$ and $f' = [f'_\alpha]$.*

Let $f, f' \in Cyl(\overline{\mathcal{A}})$, there exists graph $\alpha$ such that $f = [f_\alpha]$, and $f' = [f'_\alpha]$, then the following operations are well defined

$$f + f' := [f_\alpha + f'_\alpha],\ ff' := [f_\alpha f'_\alpha],\ zf := [zf_\alpha],\ \bar{f} := [\bar{f}_\alpha],$$

where $z \in \mathbf{C}$ and $\bar{f}$ denotes complex conjugate. So we construct $Cyl(\overline{\mathcal{A}})$ as an Abelian $*$-algebra. In addition, there is a unital element in the algebra because $Cyl(\overline{\mathcal{A}})$ contains constant functions. Moreover, we can well define the sup-norm for $f = [f_\alpha]$ by

$$\|f\| := \sup_{A_\alpha \in X_\alpha} |f_\alpha(A_\alpha)|, \tag{21}$$

which satisfies the $C^*$ property $\|f\bar{f}\| = \|f\|^2$. Then $\overline{Cyl(\overline{\mathcal{A}})}$ is a unital Abelian $C^*$-algebra, after the completion with respect to the norm.

From the theory of $C^*$-algebra, it is known that a unital Abelian $C^*$-algebra is identical to the space of continuous functions on its spectrum space via an isometric isomorphism, the so-called Gel'fand transformation (see e.g. [146]). So we have the following theorem [17][18], which finishes this section.

**Theorem 3.3.1**:
(1) *The space* $Cyl(\overline{\mathcal{A}})$ *has a structure of a unital Abelian* $C^*$*-algebra after completion with respect to the sup-norm.*

(2) *Quantum configuration space* $\overline{\mathcal{A}}$ *is the spectrum space of completed* $\overline{Cyl(\overline{\mathcal{A}})}$ *such that* $\overline{Cyl(\overline{\mathcal{A}})}$ *is identical to the space* $C(\overline{\mathcal{A}})$ *of continuous functions on* $\overline{\mathcal{A}}$*.*

## 3.4 Loop Quantum Kinematics

In analogy with the quantization procedure of section 3.1, in this subsection we would like to perform the background-independent construction of algebraic quantum field theory for general relativity. First we construct the algebra of classical observables. Taking account of the future quantum analogs, we define the algebra of classical observables $\mathfrak{P}$ as the Poission $*$-subalgebra generated by the functions of holonomies (cylindrical functions) and the fluxes of triad fields smeared on some 2-surface. Namely, one can define the classical algebra in analogy with geometric quantization in finite dimensional phase space case by the so-called classical Ashtekar-Corichi-Zapata holonomy-flux $*$-algebra as the following [96].

**Definition 3.4.1**
*The classical Ashtekar-Corichi-Zapata holonomy-flux $*$-algebra is defined to be a vector space* $\mathfrak{P}_{ACZ} := Cyl(\overline{\mathcal{A}}) \times \mathcal{V}^{\mathbf{C}}(\overline{\mathcal{A}})$, *where* $\mathcal{V}^{\mathbf{C}}(\overline{\mathcal{A}})$ *is the vector space of algebraic vector fields spanned by the vector fields* $\psi Y_f(S)$ $\psi \in Cyl(\overline{\mathcal{A}})$, *and their commutators, here the smeared flux vector field* $Y_f(S)$ *is defined by acting on any cylindrical function:*

$$Y_f(S)\psi := \{\int_S \underline{\eta}_{abc} \widetilde{P}^c_i f^i,\ \psi\},$$

*for any* $su(2)$*-valued function* $f^i$ *with compact supports on* $S$ *and* $\psi$ *are cylindrical functions on* $\overline{\mathcal{A}}$*. We equip* $\mathfrak{P}_{ACZ}$ *with the structure of an $*$-Lie algebra by:*
*(1) Lie bracket* $\{\ ,\ \}:\ \mathfrak{P}_{ACZ} \times \mathfrak{P}_{ACZ} \to\ \mathfrak{P}_{ACZ}$ *is defined by*

$$\{(\psi, Y),\ (\psi', Y')\} := (Y \circ \psi' - Y' \circ \psi, [Y, Y']),$$

*for all* $(\psi, Y),\ (\psi', Y') \in \mathfrak{P}_{ACZ}$ *with* $\psi, \psi' \in Cyl(\overline{\mathcal{A}})$ *and* $Y, Y' \in \mathcal{V}^{\mathbf{C}}(\overline{\mathcal{A}})$.

*(2) Involution:* $p \mapsto \bar{p}\ \forall\ p \in \mathfrak{P}_{ACZ}$ *is defined by complex conjugate of cylindrical functions and vector fields, i.e.,* $\bar{p} := (\overline{\psi}, \overline{Y})\ \forall\ p = (\psi, Y) \in \mathfrak{P}_{ACZ}$, *where* $\overline{Y}\psi := \overline{Y\overline{\psi}}$.

*(3) $\mathfrak{P}_{ACZ}$ admits a natural action of $Cyl(\overline{\mathcal{A}})$ by*

$$\psi' \circ (\psi, Y) := (\psi'\psi, \psi' Y),$$

*which gives $\mathfrak{P}_{ACZ}$ a module structure.*

Note that the action of flux vector field $Y_f(S)$ on can be expressed explicitly on any cylindrical function $\psi_\gamma \in C^1(X_{\alpha(\gamma)})$ via a suitable regularization[146]:

$$\begin{aligned}
Y_f(S)\psi_\gamma &= \{\int_S \underline{\eta}_{abc}\widetilde{P}^c_i f^i,\ \psi_\gamma\}, \\
&= \sum_{e\in E(\gamma)} \{\int_S \underline{\eta}_{abc}\widetilde{P}^c_i f^i,\ A(e)_{mn}\}\frac{\partial}{\partial A(e)_{mn}}\psi_\gamma \\
&= \sum_{e\in E(\gamma)} \frac{\kappa(S,\ e)}{2} f^i(S\cap e)[\delta_{S\cap e, s(e)}(A(e)\tau_i)_{mn} - \delta_{S\cap e, t(e)}(\tau_i A(e))_{mn}]\frac{\partial}{\partial A(e)_{mn}}\psi_\gamma \\
&= \sum_{v\in V(\gamma)\cap S}\sum_{e\ at\ v} \frac{\kappa(S,\ e)}{2} f^i(v) X_i^{(e,v)}\psi_\gamma,
\end{aligned}$$

where $A(e)_{mn}$ is the $SU(2)$ matrix element of the holonomy along the edge $e$, $X_i^{(e,v)}$ is the left(right) invariant vector field $L^{(\tau_i)}(R^{(\tau_i)})$ of the group associated with the edge $e$ if $v$ is the source(target) of edge $e$ by definition:

$$\begin{aligned}
L^{(\tau_i)}\psi(A(e)) &:= \frac{d}{dt}|_{t=0}\psi(A(e)\exp(t\tau_i)), \\
R^{(\tau_i)}\psi(A(e)) &:= \frac{d}{dt}|_{t=0}\psi(\exp(-t\tau_i)A(e)),
\end{aligned}$$

and

$$\kappa(S,\ e) = \begin{cases} 0, & \text{if } e\cap S = \emptyset, \text{ or } e \text{ lies in } S; \\ 1, & \text{if } e \text{ lies above } S \text{ and } e\cap S = p; \\ -1, & \text{if } e \text{ lies below } S \text{ and } e\cap S = p. \end{cases}$$

Since the surface $S$ is oriented with normal $n_a$, "above" means $n_a\dot{e}^a|_p > 0$, and "below" means $n_a\dot{e}^a|_p < 0$, where $\dot{e}^a|_p$ is the tangent vector of $e$ at $p$. And one should consider $e\cap S$ contained in the set $V(\gamma)$ and some edges are written as the union of elementary edges which either lie in $S$, or intersect $S$ at their source or target. On the other hand, from the commutation relations for the left(right) invariant vector fields, one can see that the commutators between flux vector fields do not necessarily vanish when $S\cap S' \neq \emptyset$. This unusual property is the classical origin of the non-commutativity of quantum Riemannian structures [23].

The classical Ashtekar-Corichi-Zapata holonomy-flux $*$-algebra serves as a classical algebra of elementary observables in our dynamical system of gauge fields. Then one can construct the quantum algebra of elementary observables from $\mathfrak{P}_{ACZ}$ in analogy with Definition 3.1.2.

**Definition 3.4.2**[96]

*The abstract free algebra $F(\mathfrak{P}_{ACZ})$ of the classical $*$-algebra is defined by the formal direct sum of finite sequences of classical observables $(p_1, ..., p_n)$ with $p_k \in \mathfrak{P}_{ACZ}$, where the operations of multiplication and involution are defined as*

$$\begin{aligned}(p_1, ..., p_n) \cdot (p'_1, ..., p'_m) &:= (p_1, ..., p_n, p'_1, ..., p'_m),\\ (p_1, .., p_n)^* &:= (\bar{p}_n, ..., \bar{p}_1).\end{aligned}$$

*A 2-sided ideal $\mathfrak{I}$ can be generated by the following elements,*

$$\begin{gathered}(p + p') - (p) - (p'), \;\; (zp) - z(p),\\ [(p), (p')] - i\hbar(\{p, p'\}),\\ ((\psi, 0), p) - (\psi \circ p),\end{gathered}$$

*where the canonical commutation bracket is defined by*

$$[(p), (p')] := (p) \cdot (p') - (p') \cdot (p).$$

*Note that the ideal $\mathfrak{I}$ is preserved by the involution $*$, and the last set of generators in the ideal $\mathfrak{I}$ cancels the overcompleteness generated from the module structure of $\mathfrak{P}_{ACZ}$ [4].*
*The quantum holonomy-flux $*$-algebra is defined by the quotient $*$-algebra $\mathfrak{A} = F(\mathfrak{P}_{ACZ})/\mathfrak{I}$, which contains the unital element $1 := \widehat{((1, 0))}$. Note that a sup-norm has been defined by Eq.(21) for the Abelian sub-$*$-algebra $Cyl(\overline{\mathcal{A}})$ in $\mathfrak{A}$.*

For simplicity, we denote the one element sequences (equivalence classes) $(\widehat{(\psi, 0)})$ and $(\widehat{(0, Y)})$ $\forall\ \psi \in Cyl(\overline{\mathcal{A}}),\ Y \in \mathcal{V}^{\mathbf{C}}(\overline{\mathcal{A}})$ in $\mathfrak{A}$ by $\hat{\psi}$ and $\hat{Y}$ respectively, where the "hat" denotes the equivalence class with respect to the quotient. In particular, for all cylindrical functions $\hat{\psi}$ and flux vector fields $\hat{Y}_f(S)$,

$$\hat{\psi}^* = \hat{\bar{\psi}} \quad \text{and} \quad \hat{Y}_f(S)^* = \hat{Y}_f(S).$$

It can be seen that the free algebra $F(\mathfrak{P}_{ACZ})$ is simplified a great deal after the quotient, and every element of the quantum algebra $\mathfrak{A}$ can be written as a finite linear combination of elements of the form

$$\begin{aligned}&\hat{\psi},\\ &\hat{\psi}_1 \cdot \hat{Y}_{f_{11}}(S_{11}),\\ &\hat{\psi}_2 \cdot \hat{Y}_{f_{21}}(S_{21}) \cdot \hat{Y}_{f_{22}}(S_{22}),\\ &...\\ &\hat{\psi}_k \cdot \hat{Y}_{f_{k1}}(S_{k1}) \cdot \hat{Y}_{f_{k2}}(S_{k2}) \cdot ... \cdot \hat{Y}_{f_{kk}}(S_{kk}),\\ &...\end{aligned}$$

Moreover, given a cylindrical function $\psi$ and a flux vector field $Y_f(S)$, one has the relation from the commutation relation:

$$\hat{Y}_f(S) \cdot \hat{\psi} = i\hbar\widehat{Y_f(S)\psi} + \hat{\psi} \cdot \hat{Y}_f(S). \tag{22}$$

Then the kinematical Hilbert space $\mathcal{H}_{kin}$ can be obtained properly via the GNS-construction for unital $*$-algebra $\mathfrak{A}$ in the same way as in Definition 3.1.3. By the GNS-construction, a positive linear functional, i.e. a state $\omega_{kin}$, on $\mathfrak{A}$ defines a cyclic representation $(\mathcal{H}_{kin}, \pi_{kin}, \Omega_{kin})$ for $\mathfrak{A}$. In our case of quantum holonomy-flux $*$-algebra, the state with both Yang-Mills gauge invariance and diffeomorphism invariance is defined for any $\psi_\gamma \in Cyl(\overline{\mathcal{A}})$ and non-vanishing flux vector field $Y_f(S) \in \mathcal{V}^{\mathbf{C}}(\overline{\mathcal{A}})$ as [96]:

$$\omega_{kin}(\hat{\psi}_\gamma) := \int_{SU(2)^{N_\gamma}} \prod_{e\in E(\gamma)} d\mu_H(A(e))\psi_\gamma(\{A(e)\}_{e\in E(\gamma)}),$$
$$\omega_{kin}(\hat{a}\cdot\hat{Y}_f(S)) := 0, \quad \forall \hat{a} \in \mathfrak{A},$$

where $d\mu_H$ is the Haar measure on the compact group $SU(2)$ and $N_\gamma$ is the number of elements in $E(\gamma)$. This $\omega_{kin}$ is called Ashtekar-Isham-Lewandowski state. The null space $\mathfrak{N}_{kin} \in \mathfrak{A}$ with respect to $\omega_{kin}$ is defined as $\mathfrak{N}_{kin} := \{\hat{a} \in \mathfrak{A} | \omega_{kin}(\hat{a}^* \cdot \hat{a}) = 0\}$, which is a left ideal. Then a quotient map can be defined as:

$$\begin{array}{rccl} [.]: & \mathfrak{A} & \rightarrow & \mathfrak{A}/\mathfrak{N}_{kin}; \\ & \hat{a} & \mapsto & [\hat{a}] := \{\hat{a} + \hat{b} | \hat{b} \in \mathfrak{N}_{kin}\}. \end{array}$$

The GNS-representation for $\mathfrak{A}$ with respect to $\omega_{kin}$ is a representation map: $\pi_{kin}$: $\mathfrak{A} \rightarrow \mathcal{L}(\mathcal{H}_{kin})$ such that $\pi_{kin}(\hat{a}\cdot\hat{b}) = \pi_{kin}(\hat{a})\pi_{kin}(\hat{b})$, where $\mathcal{H}_{kin} := \langle \mathfrak{A}/\mathfrak{N}_{kin} \rangle = \langle Cyl(\overline{\mathcal{A}}) \rangle$ by straightforward verification and the $\langle \cdot \rangle$ denotes the completion with respect to the natural equipped inner product on $\mathcal{H}_{kin}$,

$$< [\hat{a}] | [\hat{b}] >_{kin} := \omega_{kin}(\hat{a}^* \cdot \hat{b}).$$

To show how this inner product works, given any two cylindrical functions $\psi = [\psi_\alpha], \psi' = [\psi'_{\alpha'}] \in Cyl(\overline{\mathcal{A}})$, the inner product between them is expressed as

$$< [\hat{\psi}] | [\hat{\psi}'] >_{kin} := \int_{X_{\alpha''}} (P^*_{\alpha''\alpha}\overline{\psi}_\alpha)(P^*_{\alpha''\alpha'}\psi'_{\alpha'}) d\mu_{\alpha''}, \tag{23}$$

for any groupoid $\alpha''$ containing both $\alpha$ and $\alpha'$. The measure $d\mu_\alpha$ on $X_\alpha$ is defined by the pull back of the product Haar measure $d\mu_H^{N_\alpha}$ on the product group $SU(2)^{N_\alpha}$ via the identification bijection between $X_\alpha$ and $SU(2)^{N_\alpha}$, where $N_\alpha$ is number of maximal analytic edges generating $\alpha$. In addition, a nice result shows that given such a family of measures $\{\mu_\alpha\}_{\alpha\in\mathcal{L}}$, a probability measure $\mu$ is uniquely well-defined on the quantum configuration space $\overline{\mathcal{A}}$ [17], such that the kinematical Hilbert space $\mathcal{H}_{kin}$ coincides with the collection of the square-integrable functions with respect to the measure $\mu$ on the quantum configuration space, i.e. $\mathcal{H}_{kin} = L^2(\overline{\mathcal{A}}, d\mu)$, just as we expected at the beginning of our construction.

The representation map $\pi_{kin}$ is defined by

$$\pi_{kin}(\hat{a})[\hat{b}] := [\hat{a}\cdot\hat{b}], \;\; \forall\, \hat{a} \in \mathfrak{A}, \text{ and } [\hat{b}] \in \mathcal{H}_{kin}.$$

Note that $\pi_{kin}(\hat{a})$ is an unbounded operator in general. It is easy to verify that

$$\pi_{kin}(\hat{Y}_f(S))[\hat{\psi}] = i\hbar[\widehat{Y_f(S)}\psi]$$

via Eq.(22), which gives the canonical momentum operator. In the following context, we denote the operator $\pi_{kin}(\hat{Y}_f(S))$ by $\hat{P}_f(S)$ on $\mathcal{H}_{kin}$, and just denote the elements $[\hat{\psi}]$ in $\mathcal{H}_{kin}$ by $\psi$ for simplicity.

Moreover, since $\Omega_{kin} := 1$ is a cyclic vector in $\mathcal{H}_{kin}$, the positive linear functional which we begin with can be expressed as

$$\omega_{kin}(\hat{a}) =< \Omega_{kin}|\pi_{kin}(\hat{a})\Omega_{kin} >_{kin} .$$

Thus the Ashtekar-Isham-Lewandowski state $\omega_{kin}$ on $\mathfrak{A}$ is equivalent to a cyclic representation $(\mathcal{H}_{kin}, \pi_{kin}, \Omega_{kin})$ for $\mathfrak{A}$, which is the Ashtekar-Isham-Lewandowski representation for quantum holonomy-flux $*$-algebra of background independent gauge field theory. One thus obtains the kinematical representation of loop quantum gravity via the construction of algebraic quantum field theory. It is important to note that the Ashtekar-Isham-Lewandowski state is the unique state on the quantum holonomy-flux $*$-algebra $\mathfrak{A}$ invariant under internal gauge transformations and spatial diffeomorphisms[7], which are both automorphisms $\alpha_g$ and $\alpha_\varphi$ on $\mathfrak{A}$ and can be verified that $\omega_{kin} \circ \alpha_g = \omega_{kin}$ and $\omega_{kin} \circ \alpha_\varphi = \omega_{kin}$. So these gauge transformations are represented as unitary transformations on $\mathcal{H}_{kin}$, while the cyclic vector $\Omega_{kin}$, representing "no geometry vacuum" state, is the unique state in $\mathcal{H}_{kin}$ invariant under internal gauge transformations and spatial diffeomorphisms. This is a very crucial uniqueness theorem for canonical quantization of gauge field theory [96]:

**Theorem 3.4.1**: *There exists exactly one Yang-Mills gauge invariant and spatial diffeomorphism invariant state (positive linear functional) on the quantum holonomy-flux $*$-algebra. In other words, there exists a unique Yang-Mills gauge invariant and spatial diffeomorphism invariant cyclic representation for the quantum holonomy-flux $*$-algebra, which is called Ashtekar-Isham-Lewandowski representation. Moreover, this representation is irreducible with respect to an exponential version of the quantum holonomy-flux algebra (defined in [130]), which is analogous to the Weyl algebra.*

Hence we have finished the construction of kinematical Hilbert space for background independent gauge field theory and represented the quantum holonomy-flux algebra on it. Then following the general programme presented in the last subsection, we should impose the constraints as operators on the kinematical Hilbert space since we are dealing with a gauge system.

## 3.5 Spin-network Decomposition of Kinematical Hilbert Space

The kinematical Hilbert space $\mathcal{H}_{kin}$ for loop quantum gravity has been well defined. In this subsection, it will be shown that $\mathcal{H}_{kin}$ can be decomposed into the orthogonal direct sum of 1-dimensional subspaces and find a basis, called spin-network basis, in the Hilbert space, which consists of uncountably infinite elements. So the kinematic Hilbert space is non-separable. In the following, we will show the decomposition in three steps.

- Spin-network Decomposition on a Single Edge

[7] The proof of this conclusion depends on the compact support property of the smear functions $f^i$ (see [96] for detail).

Given a graph consisting of only one edge $e$, which naturally associates with a group $SU(2) = X_{\alpha(e)}$, the elements of $X_{\alpha(e)}$ are the quantum connections only taking non-trivial values on $e$. Then we consider the decomposition of the Hilbert space $\mathcal{H}_{\alpha(e)} = L^2(X_{\alpha(e)}, d\mu_{\alpha(e)}) \simeq L^2(SU(2), d\mu_H)$, which is nothing but the space of square integrable functions on the compact group $SU(2)$ with the natural $L^2$ inner product. It is natural to define several operators on $\mathcal{H}_{\alpha(e)}$. First, the so-called configuration operator $\hat{f}(A(e))$ whose operation on any $\psi$ in a dense domain of $L^2(SU(2), d\mu_H)$ is nothing but multiplication by the function $f(A(e))$, i.e.,

$$\hat{f}(A(e))\psi(A(e)) := f(A(e))\psi(A(e)),$$

where $A(e) \in SU(2)$. Second, given any vector $\xi \in su(2)$, it generates left invariant vector field $L^{(\xi)}$ and right invariant vector field $R^{(\xi)}$ on $SU(2)$ by

$$L^{(\xi)}\psi(A(e)) := \frac{d}{dt}|_{t=0}\psi(A(e)\exp(t\xi)),$$
$$R^{(\xi)}\psi(A(e)) := \frac{d}{dt}|_{t=0}\psi(\exp(-t\xi)A(e)),$$

for any function $\psi \in C^1(SU(2))$. Then one can define the so-called momentum operators on the single edge by

$$\hat{J}_i^{(L)} = iL^{(\tau_i)} \quad \text{and} \quad \hat{J}_i^{(R)} = iR^{(\tau_i)},$$

where the generators $\tau_i \in su(2)$ constitute an orthonormal basis with respect to the Killing-Cartan metric. The momentum operators have the well-known commutation relation of the angular momentum operators in quantum mechanics:

$$[\hat{J}_i^{(L)}, \hat{J}_j^{(L)}] = i\epsilon^k_{\ ij}\hat{J}_k^{(L)}, \ [\hat{J}_i^{(R)}, \hat{J}_j^{(R)}] = i\epsilon^k_{\ ij}\hat{J}_k^{(R)}, \ [\hat{J}_i^{(L)}, \hat{J}_j^{(R)}] = 0.$$

Third, the Casimir operator on $\mathcal{H}_e$ can be expressed as

$$\hat{J}^2 := \delta^{ij}\hat{J}_i^{(L)}\hat{J}_j^{(L)} = \delta^{ij}\hat{J}_i^{(R)}\hat{J}_j^{(R)}. \tag{24}$$

The decomposition of $\mathcal{H}_e = L^2(SU(2), d\mu_H)$ is provided by the following Peter-Weyl Theorem.

**Theorem 3.5.1** [53]:
*Given a compact group $G$, the function space $L^2(G, d\mu_H)$ can be decomposed as an orthogonal direct sum of finite dimensional Hilbert spaces, and the matrix elements of the equivalence classes of finite dimensional irreducible representations of $G$ form an orthogonal basis in $L^2(G, d\mu_H)$.*

Note that a finite dimensional irreducible representation of $G$ can be regarded as a matrix-valued function on $G$, so the matrix elements are functions on $G$. Using this theorem, one can find the decomposition of the Hilbert space:

$$L^2(SU(2), d\mu_H) = \oplus_j[\mathcal{H}_j \otimes \mathcal{H}_j^*],$$

where $j$, labelling irreducible representations of $SU(2)$, are the half integers, $\mathcal{H}_j$ denotes the carrier space of the $j$-representation of dimension $2j+1$, and $\mathcal{H}_j^*$ is its dual space. The basis $\{\mathbf{e}_m^j \otimes \mathbf{e}_n^{j*}\}$ in $\mathcal{H}_j \otimes \mathcal{H}_j^*$ maps a group element $g \in SU(2)$ to a matrix $\{\pi_{mn}^j(g)\}$, where $m, n = -j, ..., j$. Thus the space $\mathcal{H}_j \otimes \mathcal{H}_j^*$ is spanned by the matrix element functions $\pi_{mn}^j$ of equivalent $j$-representations. Moreover, the spin-network basis can be defined.

**Proposition 3.5.1** [56]
*The system of spin-network functions on $\mathcal{H}_{\alpha(e)}$, consisting of matrix elements $\{\pi_{mn}^j\}$ in finite dimensional irreducible representations labelled by half-integers $\{j\}$, satisfies*

$$\hat{J}^2\pi_{mn}^j = j(j+1)\pi_{mn}^j, \;\; \hat{J}_3^{(L)}\pi_{mn}^j = m\pi_{mn}^j, \;\; \hat{J}_3^{(R)}\pi_{mn}^j = n\pi_{mn}^j,$$

*where $j$ is called angular momentum quantum number and $m, n = -j, ..., j$ magnetic quantum number. The normalized functions $\{\sqrt{2j+1}\pi_{mn}^j\}$ form an orthonormal basis in $\mathcal{H}_{\alpha(e)}$ by the above theorem and*

$$\int_{\overline{\mathcal{A}}_e} \overline{\pi_{m'n'}^{j'}}\pi_{mn}^j d\mu_e = \frac{1}{2j+1}\delta^{j'j}\delta_{m'm}\delta_{n'n},$$

*which is called the spin-network basis on $\mathcal{H}_{\alpha(e)}$. So the Hilbert space on a single edge has been decomposed into one dimensional subspaces.*

Note that the system of operators $\{\hat{J}^2, \hat{J}_3^{(R)}, \hat{J}_3^{(L)}\}$ forms a complete set of commutable operators in $\mathcal{H}_{\alpha(e)}$. There is a cyclic "vacuum state" in the Hilbert space, which is the $(j = 0)$-representation $\Omega_{\alpha(e)} = \pi^{j=0} = 1$, representing that there is no geometry on the edge.

- Spin-network Decomposition on Finite Graph

  Given a groupoid $\alpha$ generated by a graph $\gamma$ with $N$ oriented edges $e_i$ and $M$ vertices, one can define the configuration operators on the corresponding Hilbert space $\mathcal{H}_\alpha = L^2(X_\alpha, d\mu_\alpha) \simeq L^2(SU(2)^N, d\mu_H^N)$ by

$$\hat{f}(A(e_i))\psi(A(e_1), ..., A(e_N)) := f(A(e_i))\psi(A(e_1), ..., A(e_N)).$$

  The momentum operators $\hat{J}_i^{(e,v)}$ associated with a edge $e$ connecting a vertex $v$ are defined as

$$\hat{J}_i^{(e,v)} := (1 \otimes ... \otimes \hat{J}_i \otimes ... \otimes 1),$$

  where we set $\hat{J}_i = \hat{J}_i^{(L)}$ if $v = s(e)$ and $\hat{J}_i = \hat{J}_i^{(R)}$ if $v = t(e)$, so $\hat{J}_i^{(e,v)} = iX_i^{(e,v)}$. Note that $\hat{J}_i^{(e,v)}$ only acts nontrivially on the Hilbert space associated with the edge $e$. Then one can define a vertex operator associated with vertex $v$ in analogy with the total angular momentum operator via

$$[\hat{J}^v]^2 := \delta^{ij}\hat{J}_i^v\hat{J}_j^v,$$

where

$$\hat{J}_i^v := \sum_{e\ at\ v} \hat{J}_i^{(e,v)}.$$

Obviously, $\mathcal{H}_\alpha$ can be firstly decomposed by the representations on each edge $e$ of $\alpha$ as:

$$\begin{aligned}\mathcal{H}_\alpha &= \otimes_e \mathcal{H}_{\alpha(e)} = \otimes_e[\oplus_j(\mathcal{H}_j^e \otimes \mathcal{H}_j^{e*})] = \oplus_{\mathbf{j}}[\otimes_e(\mathcal{H}_j^e \otimes \mathcal{H}_j^{e*})] \\ &= \oplus_{\mathbf{j}}[\otimes_v(\mathcal{H}_{\mathbf{j}(s)}^{v=s(e)} \otimes \mathcal{H}_{\mathbf{j}(t)}^{v=t(e)})],\end{aligned}$$

where $\mathbf{j} := (j_1, ..., j_N)$ assigns to each edge an irreducible representation of $SU(2)$, in the fourth step the Hilbert spaces associated with the edges are allocated to the vertexes where these edges meet so that for each vertex $v$,

$$\mathcal{H}_{\mathbf{j}(s)}^{v=s(e)} \equiv \otimes_{s(e)=v}\mathcal{H}_j^e \quad \text{and} \quad \mathcal{H}_{\mathbf{j}(t)}^{v=t(e)} \equiv \otimes_{t(e)=v}\mathcal{H}_j^{e*}.$$

The group of gauge transformations $g(v) \in SU(2)$ at each vertex is reducibly represented on the Hilbert space $\mathcal{H}_{\mathbf{j}(s)}^{v=s(e)} \otimes \mathcal{H}_{\mathbf{j}(t)}^{v=t(e)}$ in a natural way. So this Hilbert space can be decomposed as a direct sum of irreducible representation spaces via Clebsch-Gordon decomposition:

$$\mathcal{H}_{\mathbf{j}(s)}^{v=s(e)} \otimes \mathcal{H}_{\mathbf{j}(t)}^{v=t(e)} = \oplus_l \mathcal{H}_{\mathbf{j}(v),l}^v .$$

As a result, $\mathcal{H}_\alpha$ can be further decomposed as:

$$\mathcal{H}_\alpha = \oplus_{\mathbf{j}}[\otimes_v(\oplus_l \mathcal{H}_{\mathbf{j}(v),l}^v)] = \oplus_{\mathbf{j}}[\oplus_{\mathbf{l}}(\otimes_v \mathcal{H}_{\mathbf{j}(v),l}^v)] \equiv \oplus_{\mathbf{j}}[\oplus_{\mathbf{l}}\mathcal{H}_{\alpha,\mathbf{j},\mathbf{l}}]. \tag{25}$$

It can also be viewed as the eigenvector space decomposition of the commuting operators $[\hat{J}^v]^2$ (with eigenvalues $l(l+1)$) and $[\hat{J}^e]^2 \equiv \delta^{ij}\hat{J}_i^e\hat{J}_j^e$. Note that $\mathbf{l} := (l_1, ..., l_M)$ assigns to each vertex(objective) of $\alpha$ an irreducible representation of $SU(2)$. One may also enlarge the set of commuting operators to further refine the decomposition of the Hilbert space. Note that the subspace of $\mathcal{H}_\alpha$ with $\mathbf{l} = 0$ is Yang-Mills gauge invariant, since the representation of gauge transformations is trivial.

- Spin-network Decomposition of $\mathcal{H}_{kin}$

  Since $\mathcal{H}_{kin}$ has the structure $\mathcal{H}_{kin} = \langle \cup_{\alpha\in\mathcal{L}}\mathcal{H}_\alpha \rangle$, one may consider to construct it as a direct sum of $\mathcal{H}_\alpha$ by canceling some overlapping components. The construction is precisely described as a theorem below.

  **Theorem 3.5.2**:
  *Consider assignments $\mathbf{j} = (j_1, ..., j_N)$ to the edges of any groupoid $\alpha \in \mathcal{L}$ and assignments $\mathbf{l} = (l_1, ..., l_M)$ to the vertices. The edge representation $j$ is non-trivial on each edge, and the vertex representation $l$ is non-trivial at each spurious[8] vertex, unless it is the base point of a close analytic loop. Let $\mathcal{H}'_\alpha$ be the Hilbert space composed by the*

[8]A vertex $v$ is spurious if it is bivalent and $e \circ e'$ is itself analytic edge with $e$, $e'$ meeting at $v$.

*subspaces $\mathcal{H}_{\alpha,\mathbf{j},\mathbf{l}}$ (assigned the above conditions) according to Eq.(25). Then $\mathcal{H}_{kin}$ can be decomposed as the direct sum of the Hilbert spaces $\mathcal{H}'_\alpha$, i.e.,*

$$\mathcal{H}_{kin} = \oplus_{\alpha\in\mathcal{L}}\mathcal{H}'_\alpha \oplus \mathbf{C}.$$

**Proof**:
Since the representation on each edge is non-trivial, by definition of the inner product, it is easy to see that $\mathcal{H}'_\alpha$ and $\mathcal{H}'_{\alpha'}$ are mutual orthogonal if one of the groupoids $\alpha$ and $\alpha'$ has at leat an edge $e$ more than the other due to

$$\int_{\overline{\mathcal{A}}_e} \pi^j_{mn} d\mu_e = \int_{\overline{\mathcal{A}}_e} 1\cdot\pi^j_{mn} d\mu_e = 0$$

for any $j \neq 0$. Now consider the case of the spurious vertex. An edge $e$ with $j$-representation in a graph is assigned the Hilbert space $\mathcal{H}^e_j \otimes \mathcal{H}^{e*}_j$. Inserting a vertex $v$ into the edge, one obtains two edges $e_1$ and $e_2$ split by $v$ both with $j$-representations, which belong to a different graph. By the decomposition of the corresponding Hilbert space,

$$\mathcal{H}^{e_1}_j \otimes \mathcal{H}^{e_1*}_j \otimes \mathcal{H}^{e_2}_j \otimes \mathcal{H}^{e_2*}_j = \mathcal{H}^{e_1}_j \otimes (\oplus_{l=0...2j}\mathcal{H}^v_l) \otimes \mathcal{H}^{e_2*}_j,$$

the subspace for all $l \neq 0$ are orthogonal to the space $\mathcal{H}^e_j \otimes \mathcal{H}^{e*}_j$, while the subspace for $l = 0$ coincides with $\mathcal{H}^e_j \otimes \mathcal{H}^{e*}_j$ since $\mathcal{H}^v_{l=0} = \mathbf{C}$ and $A(e) = A(e_1)A(e_2)$. This completes the proof.

Since there are uncountably many graphs on $\Sigma$, the kinematical Hilbert $\mathcal{H}_{kin}$ is non-separable. We denote the spin-network basis in $\mathcal{H}_{kin}$ by $\Pi_s$, $s = (\gamma(s), \mathbf{j}_s, \mathbf{m}_s, \mathbf{n}_s)$ and vacuum $\Omega_{kin} \equiv \Pi_0 = 1$, where

$$\Pi_s := \prod_{e\in E(\gamma(s))} \sqrt{2j_e+1}\pi^{j_e}_{m_e n_e} \qquad (j_e \neq 0),$$

which form a orthonormal basis with the relation $<\Pi_s|\Pi_{s'}>_{kin} = \delta_{ss'}$. And $Cyl_\gamma(\overline{\mathcal{A}}) \subset Cyl(\overline{\mathcal{A}})$ denotes the linear span of the spin network functions $\Pi_s$ for $\gamma(s) = \gamma$.

The spin-network basis can be used to construct the so-called spin network representation of loop quantum gravity.

**Definition 3.5.1**: *The spin-network representation is a vector space $\widetilde{\mathcal{H}}$ of complex valued functions*

$$\widetilde{\Psi}: S \to \mathbf{C};\ s \mapsto \widetilde{\Psi}(s),$$

*where $S$ is the set of the labels $s$ for the spin network states. $\widetilde{\mathcal{H}}$ is equipped with the scalar product*

$$<\widetilde{\Psi}, \widetilde{\Psi}'> := \sum_{s\in S} \overline{\widetilde{\Psi}(s)}\widetilde{\Psi}(s)'$$

*between square summable functions.*

The relation between the Hilbert spaces $\widetilde{\mathcal{H}}$ and $\mathcal{H}_{kin}$ is clarified by the following proposition [146].

**Proposition 3.5.2:**
*The spin-network transformation*

$$T:\ \mathcal{H}_{kin}\ \to\ \widetilde{\mathcal{H}};\ \ \Psi\ \mapsto\ \widetilde{\Psi}(s) :=< \Pi_s,\ \Psi >_{kin}$$

*is a unitary transformation with inverse*

$$T^{-1}\Psi = \sum_{s\in S}\widetilde{\Psi}(s)\Pi_s.$$

Thus the connection representation and the spin-network representation are "Fourier transforms" of each other, where the role of the kernel of the integral is played by the spin-network basis. Note that, in the gauge invariant Hilbert space of loop quantum gravity which we will define later, the Fourier transform with respect to the gauge invariant spin-network basis is the so-called loop transform, which leads to the unitary equivalent loop representation of the theory [118][73][122].

To conclude this subsection, we show the explicit representation of elementary observables on the kinematical Hilbert space $\mathcal{H}_{kin}$. The action of canonical momentum operator $\hat{P}_f(S)$ on differentiable cylindrical functions $\psi_\gamma \in Cyl_\gamma(\overline{\mathcal{A}})$ can be expressed as

$$\begin{aligned}
\hat{P}_f(S)\psi_\gamma(\{A(e)\}_{e\in E(\gamma)}) &= \frac{\hbar}{2}\sum_{v\in V(\gamma)\cap S} f^i(v)[\sum_{e\ at\ v}\kappa(S,\ e)\hat{J}_i^{(e,v)}]\psi_\gamma(\{A(e)\}_{e\in E(\gamma)}) \\
&= \frac{\hbar}{2}\sum_{v\in V(\gamma)\cap S} f^i(v)[\hat{J}_{i(u)}^{(S,v)} - \hat{J}_{i(d)}^{(S,v)}]\psi_\gamma(\{A(e)\}_{e\in E(\gamma)}),
\end{aligned} \tag{26}$$

where

$$\begin{aligned}
\hat{J}_{i(u)}^{(S,v)} &\equiv \hat{J}_i^{(e_1,v)} + ... + \hat{J}_i^{(e_u,v)}, \\
\hat{J}_{i(d)}^{(S,v)} &\equiv \hat{J}_i^{(e_{u+1},v)} + ... + \hat{J}_i^{(e_{u+d},v)},
\end{aligned} \tag{27}$$

for the edges $e_1,...,e_u$ lying above $S$ and $e_{u+1},...,e_{u+d}$ lying below $S$. And it was proved that the operator $\hat{P}_f(S)$ is essentially self-adjoint on $\mathcal{H}_{kin}$ [146]. On the other hand, it is obvious to construct configuration operators by spin-network functions:

$$\hat{\Pi}_s\psi_\gamma(\{A(e)\}_{e\in E(\gamma)}) := \Pi_s(\{A(e)\}_{e\in E(\gamma(s))})\psi_\gamma(\{A(e)\}_{e\in E(\gamma)}).$$

Note that $\hat{\Pi}_s$ may change the graph, i.e., $\hat{\Pi}_s$: $Cyl_\gamma(\overline{\mathcal{A}}) \to Cyl_{\gamma\cup\gamma(s)}(\overline{\mathcal{A}})$. So far, the elementary operators of quantum kinematics have been well defined on $\mathcal{H}_{kin}$.

## 3.6 Quantum Riemannian Geometry

The well-established quantum kinematics of loop quantum gravity is now in the same status as Riemannian geometry before the appearance of general relativity and Einstein's equation, giving general relativity mathematical foundation and offering living place to the Einstein equation. Instead of classical geometric quantities, such as length, area, volume etc., the quantities in quantum geometry are operators on the kinematical Hilbert space $\mathcal{H}_{kin}$, and their spectrum serve as the possible values of the quantities in measurements. So far, the kinematical quantum geometric operators constructed properly in loop quantum gravity include length operator [141], area operator [125][21], two different volume operators [18][125][22], $\hat{Q}$ operator [100], etc.. Recently, a consistency check was proposed for the different regularizations of the volume operator [77][78]. We thus will only introduce the volume operator defined by Ashtekar and Lewandowski [22], which is shown to be correct in the consistency check.

First, we define the area operator with respect to a 2-surface $S$ by the elementary operators. Given a closed 2-surface or a surface $S$ with boundary, we can divide it into a large number $N$ of small area cells $S_I$. Taking account of the classical expression of an area, we set the area of the 2-surface to be the limit of the Riemannian sum

$$A_S := \lim_{N\to\infty}[A_S]_N = \lim_{N\to\infty}\kappa\beta\sum_{I=1}^{N}\sqrt{P_i(S_I)P_j(S_I)\delta^{ij}}.$$

Then one can unambiguously obtain a quantum area operator from the canonical momentum operators $\hat{P}_i(S)$ smeared by constant functions. Given a cylindrical function $\psi_\gamma \in Cyl_\gamma(\overline{\mathcal{A}})$ which has second order derivatives, the action of the area operator on $\psi_\gamma$ is defined in the limit by requiring that each area cell contains at most only one intersecting point $v$ of the graph $\gamma$ and $S$ as

$$\hat{A}_S\psi_\gamma := \lim_{N\to\infty}[\hat{A}_S]_N\psi_\gamma = \lim_{N\to\infty}\kappa\beta\sum_{I=1}^{N}\sqrt{\hat{P}_i(S_I)\hat{P}_j(S_I)\delta^{ij}}\,\psi_\gamma.$$

The regulator $N$ is easy to remove, since the result of the operation of the operator $\hat{P}_i(S_I)$ does not change when $S_I$ shrinks to a point. Since the refinement of the partition does not affect the result of action of $[\hat{A}_S]_N$ on $\psi_\gamma$, the limit area operator $\hat{A}_S$, which is shown to be self-adjoint [21], is well defined on $\mathcal{H}_{kin}$ and takes the explicit expression as:

$$\hat{A}_S\psi_\gamma = 4\pi\beta\ell_p^2\sum_{v\in V(\gamma\cap S)}\sqrt{(\hat{J}^{(S,v)}_{i(u)}-\hat{J}^{(S,v)}_{i(d)})(\hat{J}^{(S,v)}_{j(u)}-\hat{J}^{(S,v)}_{j(d)})\delta^{ij}}\,\psi_\gamma,$$

where $\hat{J}^{(S,v)}_{i(u)}$ and $\hat{J}^{(S,v)}_{i(d)}$ have been defined in Eq.(27). It turns out that the finite linear combinations of spin-network basis in $\mathcal{H}_{kin}$ diagonalizes $\hat{A}_S$ with eigenvalues given by finite sums,

$$a_S = 4\pi\beta\ell_p^2\sum_{v}\sqrt{2j_v^{(u)}(j_v^{(u)}+1)+2j_v^{(d)}(j_v^{(d)}+1)-j_v^{(u+d)}(j_v^{(u+d)}+1)}, \tag{28}$$

where $j^{(u)}$, $j^{(d)}$ and $j^{(u+d)}$ are arbitrary half-integers subject to the standard condition

$$j^{(u+d)} \in \{|j^{(u)}-j^{(d)}|, |j^{(u)}-j^{(d)}|+1, ..., j^{(u)}+j^{(d)}\}. \tag{29}$$

Hence the spectrum of the area operator is fundamentally pure discrete, while its continuum approximation becomes excellent exponentially rapidly for large eigenvalues. However, in fundamental level, the area is discrete and so is the quantum geometry. One can see that the eigenvalue of $\hat{A}_S$ does not vanish even in the case where only one edge intersects the surface at a single point, whence the quantum geometry is distributional.

The form of Ashtekar and Lewandowski's volume operator was introduced for the first time in [18], and its detailed properties are discussed in [22]. Given a region $R$ with a fixed coordinate system $\{x^a\}_{a=1,2,3}$ in it, one can introduce a partition of $R$ in the following way. Divide $R$ into small volume cells $C$ such that, each cell $C$ is a cube with coordinate volume less than $\epsilon$ and two different cells only share the points on their boundaries. In each cell $C$, we introduce three 2-surfaces $s = (S^1, S^2, S^3)$ such that $x^a$ is constant on the surface $S^a$. We denote this partition $(C, s)$ as $\mathcal{P}_\epsilon$. Then the volume of the region $R$ can be expressed classically as

$$V_R^s = \lim_{\epsilon\to 0} \sum_C \sqrt{|q_{C,s}|},$$

where

$$q_{C,s} = \frac{(\kappa\beta)^3}{3!}\epsilon^{ijk}\underline{\eta}_{abc} P_i(S^a)P_j(S^b)P_k(S^c).$$

This motivates us to define the volume operator by naively changing $P_i(S^a)$ to $\hat{P}_i(S^a)$:

$$\begin{aligned}
\hat{V}_R^s &= \lim_{\epsilon\to 0} \sum_C \sqrt{|\hat{q}_{C,s}|}, \\
\hat{q}_{C,s} &= \frac{(\kappa\beta)^3}{3!}\epsilon^{ijk}\underline{\eta}_{abc} \hat{P}_i(S^a)\hat{P}_j(S^b)\hat{P}_k(S^c).
\end{aligned}$$

Note that, given any cylindrical function $\psi_\gamma \in Cyl_\gamma(\overline{\mathcal{A}})$, we require the vertexes of the graph $\gamma$ to be at the intersecting points of the triples of 2-surfaces $s = (S^1, S^2, S^3)$ in corresponding cells. Thus the limit operator will trivially exist due to the same reason in the case of the area operator. However, the volume operator defined here depends on the choice of orientations for the triples of surfaces $s = (S^1, S^2, S^3)$, or essentially, the choice of coordinate systems. So it is not uniquely defined. Since, for all choice of $s = (S^1, S^2, S^3)$, the resulting operators have correct semi-classical limit, one settles up the problem by averaging different operators labelled by different $s$ [22]. The process of averaging removes the freedom in defining the volume operator up to an overall constant $\kappa_0$. The resulting self-adjoint operator acts on any cylindrical function $\psi_\gamma \in Cyl_\gamma(\overline{\mathcal{A}})$ as

$$\hat{V}_R\,\psi_\gamma = \kappa_0 \sum_{v\in V(\alpha)} \sqrt{|\hat{q}_{v,\gamma}|}\,\psi_\gamma,$$

where

$$\hat{q}_{v,\gamma} = (8\pi\beta\ell_p^2)^3 \frac{1}{48} \sum_{e,e',e''\ at\ v} \epsilon^{ijk}\epsilon(e,e',e'')\hat{J}_i^{(e,v)}\hat{J}_j^{(e',v)}\hat{J}_k^{(e'',v)},$$

here $\epsilon(e, e', e'') \equiv \mathrm{sgn}(\epsilon_{abc}\dot{e}^a\dot{e}'^b\dot{e}''^c)|_v$ with $\dot{e}^a$ as the tangent vector of edge $e$ and $\epsilon_{abc}$ as the orientation of $\Sigma$. The only unsatisfactory point in the present volume operator is the choice ambiguity of $\kappa_0$. However, fortunately, the most recent discussion shows that the overall undetermined constant $\kappa_0$ can be fixed to be $\sqrt{6}$ by the consistency check between the volume operator and the triad operator [77][78].

# 4 Implementation of Quantum Constraints

After constructing the kinematical Hilbert space $\mathcal{H}_{kin}$ of loop quantum gravity, one should implement the constraints on it to obtain the physical Hilbert space which encodes the complete information of quantum dynamics of general relativity, since the Hamiltonian of general relativity is a linear combination of the constraints. Recalling the constraints (7) in the Hamiltonian formalism and the Poission algebra (9) among them, the subalgebra generated by the Gauss constraints $\mathcal{G}(\Lambda)$ forms a Lie algebra and a 2-sided ideal in the constraints algebra. So in this section, we first solve the Gaussian constraints independently of the other two kinds of constraints and find the solution space $\mathcal{H}^G$, which is constituted by internal gauge invariant quantum states. Then, although the subalgebra generated by the diffeomorphism constraints is not an ideal in the constraint algebra, we still would like to solve them independently of the scalar constraints for technical convenience. After that, the quantum operator corresponding to the Hamiltonian constraint(scalar constraint) is defined on the kinematical Hilbert space, and we will also discuss an alterative for the implementation of the scalar constraint, which is called the master constraint programme by modifying the classical constraint algebra.

## 4.1 Solutions of Quantum Gaussian Constraint

Recall that the classical expression of Gauss constraints reads

$$\mathcal{G}(\Lambda) = \int_\Sigma d^3x \Lambda^i D_a \widetilde{P}^a_i = -\int_\Sigma d^3x \widetilde{P}^a_i D_a \Lambda^i \equiv -P(D\Lambda),$$

where $D_a\Lambda^i = \partial_a \Lambda^i + \epsilon^i{}_{jk} A^j_a \Lambda^k$. As the situation of triad flux, the Gauss constraints can be defined as cylindrically consistent vector fields $Y_{D\Lambda}$ on $\overline{\mathcal{A}}$, which act on any cylindrical function $f_\gamma \in Cyl_\gamma(\overline{\mathcal{A}})$ by

$$Y_{D\Lambda} \circ f_\gamma(\{A(e)\}_{e\in E(\gamma)}) := \{-P(D\Lambda), f_\gamma(\{A(e)\}_{e\in E(\gamma)})\}.$$

Then the Gauss constraint operator can be defined in analogy with the momentum operator, which acts on $f_\gamma$ as:

$$\begin{aligned}\hat{\mathcal{G}}(\Lambda) f_\gamma(\{A(e)\}_{e\in E(\gamma)}) &:= i\hbar Y_{D\Lambda} f_\gamma(\{A(e)\}_{e\in E(\gamma)}) \\ &= \hbar \sum_{v\in V(\gamma)} [\Lambda^i(v) \hat{J}^v_i] f(\{A(e)\}_{e\in E(\gamma)}),\end{aligned}$$

which is the generator of internal gauge transformations on $Cyl_\gamma(\overline{\mathcal{A}})$. The kernel of the operator is easily obtained in terms of the spin-network decomposition, which is the internal gauge invariant Hilbert space:

$$\mathcal{H}^G = \oplus_{\alpha,\mathbf{j}} \mathcal{H}'_{\alpha,\mathbf{j},\mathbf{l}=0} \oplus \mathbf{C}.$$

One then naturally gets the gauge invariant spin-network basis $T_s$, $s = (\gamma(s), \mathbf{j}_s, \mathbf{i}_s)$ in $\mathcal{H}^G$ via a group averaging technique at each vertex[126][25][32](we will call $T_s$ spin-network state in the following context):

$$T_{s=(\gamma,\mathbf{j},\mathbf{i})} = \bigotimes_{v\in V(\gamma)} i_v \bigotimes_{e\in E(\gamma)} \pi^{j_e}(A(e)), \quad (j_e \neq 0)$$

assigning a non-trivial spin representation $j$ on each edge and a invariant tensor $i$ (intertwiner) on each vertex. We denote the vector space of finite linear combinations of vacuum state and gauge invariant spin-network states $Cyl(\overline{\mathcal{A}/\mathcal{G}})$, which is dense in $\mathcal{H}^G$. And $Cyl_\gamma(\overline{\mathcal{A}/\mathcal{G}}) \subset Cyl(\overline{\mathcal{A}/\mathcal{G}})$ denotes the linear span of the gauge invariant spin network functions $T_s$ for $\gamma(s) = \gamma$. All Yang-Mills gauge invariant operators are well defined on $\mathcal{H}^G$. However, the condition of acting on gauge invariant states often changes the structure of the spectrum of quantum geometric operators. For the area operator, the spectrum depends on certain global properties of the surface $S$ (see [20][21] for details). For the volume operators, a non-zero spectrum arises from at least 4-valent vertices.

## 4.2 Solutions of Quantum Diffeomorphism Constraint

Unlike the strategy in solving Gaussian constraint, one cannot define an operator for the quantum diffeomorphism constraint as the infinitesimal generator of finite diffeomorphism transformations (unitary operators since the measure is diffeomorphism invariant) represented on $\mathcal{H}_{kin}$. The representation of finite diffeomorphisms is a family of unitary operators $\hat{U}_\varphi$ acting on cylindrical functions $\psi_\gamma$ by

$$\hat{U}_\varphi \psi_\gamma := \psi_{\varphi\circ\gamma}, \tag{30}$$

for any spatial diffeomorphism $\varphi$ on $\Sigma$. An 1-parameter subgroup $\varphi_t$ in the group of spatial diffeomorphisms is then represented as an 1-parameter unitary group $\hat{U}_{\varphi_t}$ on $\mathcal{H}_{kin}$. However, $\hat{U}_{\varphi_t}$ is not weakly continuous, since the subspaces $\mathcal{H}'_{\alpha(\gamma)}$ and $\mathcal{H}'_{\alpha(\varphi_t\circ\gamma)}$ are orthogonal to each other no matter how small the parameter $t$ is. So one always has

$$| <\psi_\gamma|\hat{U}_{\varphi_t}|\psi_\gamma>_{kin} - <\psi_\gamma|\psi_\gamma>_{kin} | = <\psi_\gamma|\psi_\gamma>_{kin} \neq 0, \tag{31}$$

even in the limit when $t$ goes to zero. Therefore, the infinitesimal generator of $\hat{U}_{\varphi_t}$ does not exist. In the strategy to solve the diffeomorphism constraint, due to the Lie algebra structure of diffeomorphism constraints subalgebra, the so-called group averaging technique is employed. We now outline the procedure. First, given a colored graph (a graph $\gamma$ and a cylindrical function living on it), one can define the group of graph symmetries $GS_\gamma$ by

$$GS_\gamma := Diff_\gamma / TDiff_\gamma,$$

where $Diff_\gamma$ is the group of all diffeomorphisms preserving the colored $\gamma$, and $TDiff_\gamma$ is the group of diffeomorphisms which trivially acts on $\gamma$. We define a projection map by averaging with respect to $GS_\gamma$ to obtain the subspace in $Cyl_\gamma$ which is invariant under the transformation of $GS_\gamma$:

$$\hat{P}_{Diff,\gamma}\psi_\gamma := \frac{1}{n_\gamma}\sum_{\varphi\in GS_\gamma}\hat{U}_\varphi\psi_\gamma,$$

for all cylindrical functions $\psi_\gamma \in \mathcal{H}'_{\alpha(\gamma)}$, where $n_\gamma$ is the number of the finite elements of $GS_\gamma$. Second, we average with respect to all remaining diffeomorphisms which move the graph $\gamma$. For each cylindrical function $\psi_\gamma \in Cyl_\gamma(\overline{\mathcal{A}/\mathcal{G}})$, there is an element $\eta(\psi_\gamma)$ associated to it in the algebraic dual space $Cyl^\star$ of $Cyl(\overline{\mathcal{A}/\mathcal{G}})$, which acts on any cylindrical function $\phi_{\gamma'} \in Cyl_\gamma(\overline{\mathcal{A}/\mathcal{G}})$ as:

$$\eta(\psi_\gamma)[\phi_{\gamma'}] := \sum_{\varphi \in Diff(\Sigma)/Diff_\gamma} < \hat{U}_\varphi \hat{P}_{Diff,\gamma} \psi_\gamma | \phi_{\gamma'} >_{kin} .$$

It is well defined since, for any given graph $\gamma'$, only finite terms are non-zero in the summation. It is easy to verify that $\eta(\psi_\gamma)$ is invariant under the group action of $Diff(\Sigma)$, since

$$\eta(\psi_\gamma)[\hat{U}_\varphi \phi_{\gamma'}] = \eta(\psi_\gamma)[\phi_{\gamma'}].$$

Thus we have defined a rigging map $\eta : \ Cyl(\overline{\mathcal{A}/\mathcal{G}}) \to Cyl^\star_{Diff}$, which maps every cylindrical function to a diffeomorphism invariant one, where $Cyl^\star_{Diff}$ is spanned by vacuum state $T_0 = 1$ and rigged spin-network functions $T_{[s]} \equiv \{\eta(T_s)\}$, $[s] = ([\gamma], \mathbf{j}, \mathbf{i})$ associated with diffeomorphism classes $[\gamma]$ of graphs $\gamma$. Moreover a Hermitian inner product can be defined on $Cyl^\star_{Diff}$ by the natural action of the algebraic functional:

$$< \eta(\psi_\gamma) | \eta(\phi_{\gamma'}) >_{Diff} := \eta(\psi_\gamma)[\phi_{\gamma'}].$$

The diffeomorphism invariant Hilbert space $\mathcal{H}_{Diff}$ is defined by the completion of $Cyl^\star_{Diff}$ with respect to the above inner product $< \ | \ >_{Diff}$. The diffeomorphism invariant spin-network functions $T_{[s]}$ form an orthonormal basis in $\mathcal{H}_{Diff}$. Finally, we have obtained the general solutions invariant under both Yang-Mills gauge transformations and spatial diffeomorphisms.

In general relativity, the problem of observables is a subtle issue due to the diffeomorphism invariance [116][119][120]. Now we discuss the operators as diffeomorphism invariant observables on $\mathcal{H}_{Diff}$. We call an operator $\hat{O} \in \mathcal{L}(\mathcal{H}_{kin})$ a strong observable if and only if $\hat{U}_\varphi^{-1} \hat{O} \hat{U}_\varphi = \hat{O}$, $\forall \ \varphi \in Diff(\Sigma)$. We call it a weak observable if and only if $\hat{O}$ leaves $\mathcal{H}_{Diff}$ invariant. Then it is easy to see that a strong observable $\hat{O}$ must be a weak one. One notices that a strong observable $\hat{O}$ can first be defined on $\mathcal{H}_{Diff}$ by its dual operator $\hat{O}^\star$ as

$$(\hat{O}^\star \Phi_{Diff})[\psi] := \Phi_{Diff}[\hat{O}\psi],$$

then one gets

$$(\hat{O}^\star \Phi_{Diff})[\hat{U}_\varphi \psi] = \Phi_{Diff}[\hat{O}\hat{U}_\varphi \psi] = \Phi_{Diff}[\hat{U}_\varphi^{-1} \hat{O} \hat{U}_\varphi \psi] = (\hat{O}^\star \Phi_{Diff})[\psi],$$

for any $\Phi_{Diff} \in \mathcal{H}_{Diff}$ and $\psi \in \mathcal{H}_{kin}$. Hence $\hat{O}^\star \Phi_{Diff}$ is also diffeomorphism invariant. In addition, a strong observable also has the property of $\hat{O}^\star \eta(\psi_\gamma) = \eta(\hat{O}^\dagger \psi_\gamma)$ since, $\forall \ \phi_{\gamma'}, \psi_\gamma \in \mathcal{H}_{kin}$,

$$\begin{aligned}
& < \hat{O}^\star \eta(\psi_\gamma) | \eta(\phi_{\gamma'}) >_{Diff} = (\hat{O}^\star \eta(\psi_\gamma))[\phi_{\gamma'}] = \eta(\psi_\gamma)[\hat{O}\phi_{\gamma'}] \\
= & \sum_{\varphi \in Diff(\Sigma)/Diff_\gamma} < \hat{U}_\varphi \hat{P}_{Diff,\gamma} \psi_\gamma | \hat{O} \phi_{\gamma'} >_{kin} \\
= & \frac{1}{n_\gamma} \sum_{\varphi \in Diff(\Sigma)/Diff_\gamma} \sum_{\varphi' \in GS_\gamma} < \hat{U}_\varphi \hat{U}_{\varphi'} \psi_\gamma | \hat{O} \phi_{\gamma'} >_{kin} \\
= & \frac{1}{n_\gamma} \sum_{\varphi \in Diff(\Sigma)/Diff_\gamma} \sum_{\varphi' \in GS_\gamma} < \hat{U}_\varphi \hat{U}_{\varphi'} \hat{O}^\dagger \psi_\gamma | \phi_{\gamma'} >_{kin} \\
= & < \eta(\hat{O}^\dagger \psi_\gamma) | \eta(\phi_{\gamma'}) >_{Diff} .
\end{aligned}$$

Note that the Hilbert space $\mathcal{H}_{Diff}$ is still non-separable if one considers the $C^n$ diffeomorphisms with $n > 0$. However, if one extends the diffeomorphisms to be semi-analytic diffeomotphisms, i.e. homomorphisms that are analytic diffeomorphisms up to finite isolated points (which can be viewed as an extension of the classical concept to the quantum case), the Hilbert space $\mathcal{H}_{Diff}$ would be separable [69][20].

## 4.3 Hamiltonian Constraint Operator

In the following, we consider the issue of scalar constraint in loop quantum gravity. One may first construct a Hamiltonian constraint (scalar constraint) operator in $\mathcal{H}_{kin}$ or $\mathcal{H}_{Diff}$, then attempt to find the physical Hilbert space $\mathcal{H}_{phys}$ by solving the quantum Hamiltonian constraint. However, difficulties arise here due to the special role played by the scalar constraints in the constraint algebra (9). First, the scalar constraints do not form a Lie subalgebra. Hence the strategy of group averaging cannot be used directly on $\mathcal{H}_{kin}$ for them. Second, modulo the Gaussian constraint, there is still a structure function in the Poisson bracket between two scalar constraints:

$$\{\mathcal{S}(N), \mathcal{S}(M)\} = -\mathcal{V}((N\partial_b M - M\partial_b N)q^{ab}), \tag{32}$$

which raises the danger of quantum anomalyies in quantization. Moreover, the diffeomorphism constraints do not form an ideal in the quotient constraint algebra modulo the Gaussian constraints. This fact results in that the scalar constraint operator cannot be well defined on $\mathcal{H}_{Diff}$, as it does not commute with the diffeomorphism transformations $\hat{U}_\varphi$. Thus the previous construction of $\mathcal{H}_{Diff}$ does not appear very useful for the final construction of $\mathcal{H}_{phys}$, which is our final goal. However, one may still first try to construct a Hamiltonian constraint operator in $\mathcal{H}_{kin}$ for technical convenience.

We recall the classical expression of Hamiltonian constraint:

$$\begin{aligned}
\mathcal{S}(N) &:= \frac{\kappa\beta^2}{2}\int_\Sigma d^3x N \frac{\widetilde{P}^a_i \widetilde{P}^b_j}{\sqrt{|\det q|}}[\epsilon^{ij}{}_k F^k_{ab} - 2(1+\beta^2)K^i_{[a}K^j_{b]}] \\
&= \mathcal{S}_E(N) - 2(1+\beta^2)\mathcal{T}(N).
\end{aligned} \tag{33}$$

The main idea of the construction is to first express $\mathcal{S}(N)$ in terms of the combination of Poisson brackets between the variables which have been represented as operators on $\mathcal{H}_{kin}$, then replace the Poisson brackets by canonical commutators between the operators. We will use the volume functional for a region $R \subset \Sigma$ and the extrinsic curvature functional defined by:

$$K := \kappa\beta \int_\Sigma d^3x \widetilde{P}^a_i K^i_a.$$

A key trick here is to consider the following classical identity of the co-triad $e^i_a(x)$ [134]:

$$e^i_a(x) = \frac{(\kappa\beta)^2}{2}\underset{\sim}{\eta}_{abc}\epsilon^{ijk}\frac{\widetilde{P}^b_j \widetilde{P}^c_k}{\sqrt{\det q}}(x) = \frac{2}{\kappa\beta}\{A^i_a(x), V_R\},$$

where $V_R$ is the volume functional for a neighborhood $R$ containing $x$. And the expression of the extrinsic curvature 1-form $K^i_a(x)$:

$$K^i_a(x) = \frac{1}{\kappa\beta}\{A^i_a(x), K\}.$$

Note that $K$ can be expressed by a Poisson bracket between the constant-smeared Euclidean Hamiltonian constraint and the total volume of the space $\Sigma$:

$$K = \beta^{-2}\{\mathcal{S}_E(1), V_\Sigma\}. \tag{34}$$

Thus one can obtain the equivalent classical expressions of $\mathcal{S}_E(N)$ and $\mathcal{T}(N)$ as:

$$\begin{aligned}
\mathcal{S}_E(N) &= \frac{\kappa\beta^2}{2}\int_\Sigma d^3xN\frac{\widetilde{P}^a_i\widetilde{P}^b_j}{\sqrt{|\det q|}}\epsilon^{ij}{}_kF^k_{ab} \\
&= -\frac{2}{\kappa^2\beta}\int_\Sigma d^3xN(x)\widetilde{\eta}^{abc}\mathrm{Tr}(\mathbf{F}_{ab}(x)\{\mathbf{A}_c(x), V_{R_x}\}), \\
\mathcal{T}(N) &= \frac{\kappa\beta^2}{2}\int_\Sigma d^3xN\frac{\widetilde{P}^a_i\widetilde{P}^b_j}{\sqrt{|\det q|}}K^i_{[a}K^j_{b]} \\
&= -\frac{2}{\kappa^4\beta^3}\int_\Sigma d^3xN(x)\widetilde{\eta}^{abc}\mathrm{Tr}(\{\mathbf{A}_a(x), K\}\{\mathbf{A}_b(x), K\}\{\mathbf{A}_c(x), V_{R_x}\}),
\end{aligned}$$

where $\mathbf{A}_a = A^i_a\tau_i$, $\mathbf{F}_{ab} = F^i_{ab}\tau_i$, Tr represents the trace of the Lie algebra matrix, and $R_x \subset \Sigma$ denotes an arbitrary neighborhood of $x \in \Sigma$. In order to quantize the Hamiltonian constraint as a well-defined operator on $\mathcal{H}_{kin}$, one has to express the classical formula of $\mathcal{S}(N)$ in terms of holonomies $A(e)$ and other variables with clear quantum analogs. As a first attempt [134], this can be realized by introducing a triangulation $T(\epsilon)$, where the parameter $\epsilon$ describes how fine the triangulation is, and the triangulation will fill out the spatial manifold $\Sigma$ when $\epsilon \to 0$. Given a tetrahedron $\Delta \in T(\epsilon)$, we use $\{s_i(\Delta)\}_{i=1,2,3}$ to denote the three outgoing oriented segments in $\Delta$ with a common beginning point $v(\Delta) = s(s_i(\Delta))$, and use $a_{ij}(\Delta)$ to denote the arc connecting the end points of $s_i(\Delta)$ and $s_j(\Delta)$. Then several loops $\alpha_{ij}(\Delta)$ are formed by $\alpha_{ij}(\Delta) := s_i(\Delta) \circ a_{ij}(\Delta) \circ s_j(\Delta)^{-1}$. Thus we have the identities:

$$\begin{aligned}
\{\int_{s_i(\Delta)}\mathbf{A}_a\dot{s}^a_i(\Delta), V_{R_{v(\Delta)}}\} &= -A(s_i(\Delta))^{-1}\{A(s_i(\Delta)), V_{R_{v(\Delta)}}\} + o(\epsilon), \\
\{\int_{s_i(\Delta)}\mathbf{A}_a\dot{s}^a_i(\Delta), K\} &= -A(s_i(\Delta))^{-1}\{A(s_i(\Delta)), K\} + o(\epsilon), \\
\int_{P_{ij}}\mathbf{F}_{ab}(x) &= \frac{1}{2}A(\alpha_{ij}(\Delta))^{-1} - \frac{1}{2}A(\alpha_{ij}(\Delta)) + o(\epsilon^2),
\end{aligned}$$

where $P_{ij}$ is the plane with boundary $\alpha_{ij}$. Note that the above identities are constructed by taking account of internal gauge invariance of the final formula of Hamiltonian constraint operator. So we have the regularized expression of $\mathcal{S}(N)$ by the Riemannian sum [134]:

$$\mathcal{S}^\epsilon_E(N) = \frac{2}{3\kappa^2\beta}\sum_{\Delta\in T(\epsilon)}N(v(\Delta))\epsilon^{ijk}\times$$

$$
\begin{aligned}
& \quad \mathrm{Tr}(A(\alpha_{ij}(\Delta))^{-1}A(s_k(\Delta))^{-1}\{A(s_k(\Delta)), V_{R_{v(\Delta)}}\}), \\
\mathcal{T}^\epsilon(N) &= \frac{\sqrt{2}}{6\kappa^4\beta^3}\sum_{\Delta\in T(\epsilon)} N(v(\Delta))\epsilon^{ijk}\times \\
& \quad \mathrm{Tr}(A(s_i(\Delta))^{-1}\{A(s_i(\Delta)), K\}A(s_j(\Delta))^{-1}\{A(s_j(\Delta)), K\}\times \\
& \quad A(s_k(\Delta))^{-1}\{A(s_k(\Delta)), V_{R_{v(\Delta)}}\}), \\
\mathcal{S}^\epsilon(N) &= \mathcal{S}^\epsilon_E(N) - 2(1+\beta^2)\mathcal{T}^\epsilon(N),
\end{aligned} \tag{35}
$$

such that $\lim_{\epsilon\to 0}\mathcal{S}^\epsilon(N) = \mathcal{S}(N)$. It is clear that the above regulated formula of $\mathcal{S}(N)$ is invariant under internal gauge transformations. Since all constituents in the expression have clear quantum analogs, one can quantize the regulated Hamiltonian constraint as an operator on $\mathcal{H}_{kin}$ (or $\mathcal{H}^G$) by replacing them by the corresponding operators and Poisson brackets by canonical commutators, i.e.,

$$
\begin{aligned}
& A(e)\mapsto \hat{A}(e), \quad V_R\mapsto \hat{V}_R, \quad \{\,,\,\}\mapsto \frac{[\,,\,]}{i\hbar}, \\
\text{and} \qquad & K\mapsto \hat{K}^\epsilon = \frac{\gamma^{-2}}{i\hbar}[\hat{\mathcal{S}}^\epsilon_E(1), \hat{V}_\Sigma].
\end{aligned}
$$

Removing the regulator by $\epsilon\to 0$, it turns out that one can obtain a well-defined limit operator on $\mathcal{H}_{kin}$ (or $\mathcal{H}^G$) with respect to a natural operator topology.

Now we begin to construct the Hamiltonian constraint operator in analogy with the classical expression (57). All we should do is define the corresponding regulated operators on different $\mathcal{H}'_\alpha$ separately, then remove the regulator $\epsilon$ so that the limit operator is defined on $\mathcal{H}_{kin}$ (or $\mathcal{H}^G$) cylindrically consistently. In the following, given a vertex and three edges intersecting at the vertex in a graph $\gamma$ of $\psi_\gamma\in Cyl_\gamma(\overline{\mathcal{A}/\mathcal{G}})$, we construct one triangulation of the neighborhood of the vertex adapted to the three edges. Then we average with respect to the triples of edges meeting at the given vertex. Precisely speaking, one can make the triangulations $T(\epsilon)$ with the following properties [134][146].

- The chosen triple of edges in the graph $\gamma$ is embedded in a $T(\epsilon)$ for all $\epsilon$, so that the vertex $v$ of $\gamma$ where the three edges meet coincides with a vertex $v(\Delta)$ in $T(\epsilon)$.
- For every triple of segments $(e_1,\ e_2,\ e_3)$ of $\gamma$ such that $v = s(e_1) = s(e_2) = s(e_3)$, there is a tetrahedra $\Delta\in T(\epsilon)$ such that $v = v(\Delta) = s(s_i(\Delta))$, and $s_i(\Delta)\subset e_i,\ \forall\, i = 1,2,3$. We denote such a tetrahedra as $\Delta^0_{e_1,e_2,e_3}$.
- For each tetrahedra $\Delta^0_{e_1,e_2,e_3}$ one can construct seven additional tetrahedron $\Delta^{\wp}_{e_1,e_2,e_3},\ \wp = 1,...,7$, by backward analytic extensions of $s_i(\Delta)$ so that $U_{e_1,e_2,e_3} := \cup^7_{\wp=0}\Delta^{\wp}_{e_1,e_2,e_3}$ is a neighborhood of $v$.
- The triangulation must be fine enough so that the neighborhoods $U(v) := \cup_{e_1,e_2,e_3}U_{e_1,e_2,e_3}(v)$ are disjoint for different vertices $v$ and $v'$ of $\gamma$. Thus for any open neighborhood $U_\gamma$ of the graph $\gamma$, there exists a triangulation $T(\epsilon)$ such that $\cup_{v\in V(\gamma)}U(v)\subseteq U_\gamma$.
- The distance between a vertex $v(\Delta)$ and the corresponding arcs $a_{ij}(\Delta)$ is described by the parameter $\epsilon$. For any two different $\epsilon$ and $\epsilon'$, the arcs $a_{ij}(\Delta^\epsilon)$ and $a_{ij}(\Delta^{\epsilon'})$ with respect to one vertex $v(\Delta)$ are semi-analytically diffeomorphic with each other.

- With the triangulations $T(\epsilon)$, the integral over $\Sigma$ is replaced by the Riemanian sum:

$$\begin{array}{rcl}\int_{\Sigma} & = & \int_{U_\alpha} + \int_{\Sigma - U_\alpha} , \\ \int_{U_\alpha} & = & \sum_{v\in V(\alpha)} \int_{U(v)} + \int_{U_\alpha - \cup_v U(v)} , \\ \int_{U(v)} & = & \frac{1}{E(v)} \sum_{e_1,e_2,e_3} [\int_{U_{e_1,e_2,e_3}(v)} + \int_{U(v) - U_{e_1,e_2,e_3},(v)} ],\end{array}$$

where $n(v)$ is the valence of the vertex $v = s(e_1) = s(e_2) = s(e_3)$, and $E(v) \equiv \begin{pmatrix} n(v) \\ 3 \end{pmatrix}$ denotes the binomial coefficient which comes from the averaging with respect to the triples of edges meeting at given vertex $v$. One then observes that

$$\int_{U_{e_1,e_2,e_3}(v)} = 8 \int_{\Delta^0_{e_1,e_2,e_3}(v)}$$

in the limit $\epsilon \to 0$.

- The triangulations for the regions

$$\begin{array}{l} U(v) - U_{e_1,e_2,e_3}(v), \\ U_\alpha - \cup_{v\in V(\alpha)} U(v), \\ \Sigma - U_\alpha, \end{array} \tag{36}$$

are arbitrary. These regions do not contribute to the construction of the operator, since the commutator term $[A(s_i(\Delta)), V_{R_{v(\Delta)}}]\psi_\alpha$ vanishes for all tetrahedron $\Delta$ in the regions (36).

Thus we find the regulated expression of Hamiltonian constraint operator with respect to the triangulations $T(\epsilon)$ as [134]

$$\begin{array}{rcl}\hat{\mathcal{S}}^\epsilon_{E,\gamma}(N) & = & \frac{16}{3i\hbar\kappa^2\beta} \sum_{v\in V(\gamma)} \frac{N(v)}{E(v)} \sum_{v(\Delta)=v} \epsilon^{ijk} \times \\ & & \mathrm{Tr}(\hat{A}(\alpha_{ij}(\Delta))^{-1} \hat{A}(s_k(\Delta))^{-1} [\hat{A}(s_k(\Delta)), \hat{V}_{U^\epsilon_v}]), \\ \hat{\mathcal{T}}^\epsilon_\gamma(N) & = & -\frac{4\sqrt{2}}{3i\hbar^3\kappa^4\beta^3} \sum_{v\in V(\gamma)} \frac{N(v)}{E(v)} \sum_{v(\Delta)=v} \epsilon^{ijk} \times \\ & & \mathrm{Tr}(\hat{A}(s_i(\Delta))^{-1}[\hat{A}(s_i(\Delta)), \hat{K}^\epsilon] \hat{A}(s_j(\Delta))^{-1}[\hat{A}(s_j(\Delta)), \hat{K}^\epsilon] \times \\ & & \hat{A}(s_k(\Delta))^{-1}[\hat{A}(s_k(\Delta)), \hat{V}_{U^\epsilon_v}]), \\ \hat{\mathcal{S}}^\epsilon(N)\psi_\gamma & = & [\hat{\mathcal{S}}^\epsilon_{E,\gamma}(N) - 2(1+\beta^2)\hat{\mathcal{T}}^\epsilon_\gamma(N)]\psi_\gamma = \sum_{v\in V(\gamma)} N(v) \hat{\mathcal{S}}^\epsilon_v \psi_\gamma,\end{array}$$

for any cylindrical function $\psi_\gamma \in Cyl_\gamma(\overline{\mathcal{A}/\mathcal{G}})$ is a finite linear combination of spin-network states $T_s$ with $\gamma(s) = \gamma$.

By construction, the operation of $\hat{S}^\epsilon(N)$ on any $\psi_\gamma \in Cyl_\gamma(\overline{\mathcal{A}/\mathcal{G}})$ is reduced to a finite combination of that of $\hat{S}^\epsilon_v$ with respect to different vertices of $\gamma$. Hence, for each $\epsilon > 0$, $\hat{S}^\epsilon(N)$ is a well-defined internal gauge invariant and diffeomorphism covariant operator on $Cyl(\overline{\mathcal{A}/\mathcal{G}})$.

The last step is to remove the regulator by taking the limit $\epsilon \to 0$. However, the action of the Hamiltonian constraint operator on $\psi_\gamma$ adds arcs $a_{ij}(\Delta)$ with a $\frac{1}{2}$-representation with respect to each $v(\Delta)$ of $\gamma$[9], i.e. the action of $\hat{S}^\epsilon(N)$ on cylindrical functions is graph-changing. Hence the operator does not converge with respect to the weak operator topology in $\mathcal{H}_{kin}$ when $\epsilon \to 0$, since different $\mathcal{H}'_{\alpha(\gamma)}$ with different graphs $\gamma$ are mutually orthogonal. Thus one has to define a weaker operator topology to make the operator limit meaningful. By physical motivation and the naturally available Hilbert space $\mathcal{H}_{Diff}$, the convergence of $\hat{S}^\epsilon(N)$ holds with respect to the so-called Uniform Rovelli-Smolin Topology [124], where one defines $\hat{S}^\epsilon(N)$ to converge if and only if $\Psi_{Diff}[\hat{S}^\epsilon(N)\phi]$ converge for all $\Psi_{Diff} \in Cyl^\star_{Diff}$ and $\phi \in Cyl(\overline{\mathcal{A}/\mathcal{G}})$. Since the value of $\Psi_{Diff}[\hat{S}^\epsilon(N)\phi]$ is actually independent of $\epsilon$ by the fifth property of the triangulations, the sequence converges to a nontrivial result $\Psi_{Diff}[\hat{S}^{\epsilon_0}(N)\phi]$ with arbitrary fixed $\epsilon_0 > 0$. Thus we have defined a diffeomorphism covariant, densely defined, closed but non-symmetric operator, $\hat{S}(N) = \lim_{\epsilon\to 0}\hat{S}^\epsilon(N) = \hat{S}^{\epsilon_0}(N)$, on $\mathcal{H}_{kin}$ (or $\mathcal{H}^G$) representing the Hamiltonian constraint. Moreover, a dual Hamiltonian constraint operator $\hat{S}'^\epsilon(N)$ is also defined on $Cyl^\star$ depending on a specific value of $\epsilon$

$$(\hat{S}'^\epsilon(N)\Psi)[\phi] := \Psi[\hat{S}^\epsilon(N)\phi],$$

for all $\Psi \in Cyl^\star$ and $\phi \in Cyl(\overline{\mathcal{A}/\mathcal{G}})$. For $\Psi_{Diff} \in Cyl^\star_{Diff} \subset Cyl^\star$, one gets

$$(\hat{S}'(N)\Psi_{Diff})[\phi] = \Psi_{Diff}[\hat{S}^\epsilon(N)\phi].$$

which is independent of the value of $\epsilon$.

Several remarks on the Hamiltonian constraint operator are listed in the following.

- Finiteness of $\hat{S}(N)$ on $\mathcal{H}_{kin}$

  In ordinary quantum field theory, the continuous quantum field is only recovered when one lets lattice spacing to approach zero, i.e., takes the continuous cut-off parameter to its continuous limit. However, this will produce the well-known infinities in quantum field theory and make the Hamiltonian operator ill-defined on the Fock space. So it seems surprising that our operator $\hat{S}(N)$ is still well defined, when one takes the limit $\epsilon \to 0$ with respect to the Uniform Rovelli-Smolin Topology so that the triangulation goes to the continuum. The reason behind it is that the cut-off parameter is essentially noneffective due to the diffeomorphism invariance of our quantum field theory. This is why there is no UV divergence in the background independent quantum gauge field theory with diffeomorphism invariance. On the other hand, from a convenient viewpoint, one may think the Hamiltonian constraint operator as an operator dually defined on a dense domain in $\mathcal{H}_{Diff}$. However, we will see that the dual Hamiltonian constraint operator cannot leave $\mathcal{H}_{Diff}$ invariant.

[9]The Hamiltonian constraint operator depends indeed on the choice of the representation $j$ on the arcs $a_{ij}(\Delta)$, which is known as one of the regularization ambiguities in the construction of quantum dynamics. For the simplicity of the theory, one often choose the lowest label of representation $j = \frac{1}{2}$.

- Implementation of Dual Quantum Constraint Algebra

  One important task is to check whether the commutator algebra (quantum constraint algebra) among the corresponding quantum operators of constraints both physically and mathematically coincides with the classical constraint algebra by substituting quantum constraint operators to classical constraint functionals and commutators to Poisson brackets. Here the quantum anomaly has to be avoided in the construction of constraint operators (see the discussion for Eq.(13)). First, the subalgebra of the quantum diffeomorphism constraint algebra is free of anomaly by construction:

$$\hat{U}_{\varphi}\hat{U}_{\varphi'}\hat{U}_{\varphi}^{-1}\hat{U}_{\varphi'}^{-1} = \hat{U}_{\varphi\circ\varphi'\circ\varphi^{-1}\circ\varphi'^{-1}},$$

  which coincides with the exponentiated version of the Poisson bracket between two diffeomorphism constraints generating the transformations $\varphi, \varphi' \in Diff(\Sigma)$.

  Second, the quantum constraint algebra between the dual Hamiltonian constraint operator $\mathcal{S}'(N)$ and the finite diffeomorphism transformation $\hat{U}_{\varphi}$ on diffeomorphism-invariant states coincides with the classical Poisson algebra between $\mathcal{V}(\vec{N})$ and $\mathcal{S}(M)$. Given a cylindrical function $\phi_{\gamma}$ associated with a graph $\gamma$ and the triangulations $T(\epsilon)$ adapted to the graph $\alpha$, the triangulations $T(\varphi\circ\epsilon) \equiv \varphi\circ T(\epsilon)$ are compatible with the graph $\varphi\circ\gamma$. Then we have by definition:

$$\begin{aligned}
&(-([\hat{\mathcal{S}}(N), \hat{U}_{\varphi}])'\Psi_{Diff})[\phi_{\gamma}] \\
= \ & ([\hat{\mathcal{S}}'(N), \hat{U}'_{\varphi}]\Psi_{Diff})[\phi_{\gamma}] \\
= \ & \Psi_{Diff}[\hat{\mathcal{S}}^{\epsilon}(N)\phi_{\gamma} - \hat{\mathcal{S}}^{\epsilon}(N)\phi_{\varphi\circ\gamma}] \\
= \ & \sum_{v\in V(\gamma)}\{N(v)\Psi_{Diff}[\hat{\mathcal{S}}^{\epsilon}_{v}\phi_{\gamma}] - N(\varphi\circ v)\Psi_{Diff}[\hat{\mathcal{S}}^{\varphi\circ\epsilon}_{\varphi\circ v}\phi_{\varphi\circ\gamma}]\} \\
= \ & \sum_{v\in V(\gamma)}[N(v) - N(\varphi\circ v)]\Psi_{Diff}[\hat{\mathcal{S}}^{\epsilon}_{v}\phi_{\gamma}] \\
= \ & (\hat{\mathcal{S}}'(N - \varphi^{*}N)\Psi_{Diff})[\phi_{\gamma}]. \qquad (37)
\end{aligned}$$

  Thus there is no anomaly. However, Eq.(37) also explains why the Hamiltonian constraint operator $\hat{\mathcal{S}}(N)$ cannot leave $\mathcal{H}_{Diff}$ invariant.

  Third, we compute the commutator between two Hamiltonian constraint operators. Notice that

$$\begin{aligned}
&[\hat{\mathcal{S}}(N), \hat{\mathcal{S}}(M)]\phi_{\gamma} \\
= \ & \sum_{v\in V(\gamma)}[M(v)\hat{\mathcal{S}}(N) - N(v)\hat{\mathcal{S}}(M)]\hat{\mathcal{S}}^{\epsilon}_{v}\phi_{\gamma} \\
= \ & \sum_{v\in V(\gamma)}\sum_{v'\in V(\gamma')}[M(v)N(v') - N(v)M(v')]\hat{\mathcal{S}}^{\epsilon'}_{v'}\hat{\mathcal{S}}^{\epsilon}_{v}\phi_{\gamma},
\end{aligned}$$

  where $\gamma'$ is the graph changed from $\gamma$ by the action of $\hat{\mathcal{S}}(N)$ or $\hat{\mathcal{S}}(M)$, which adds the arcs $a_{ij}(\Delta)$ on $\gamma$, $T(\epsilon)$ is the triangulation adapted to $\gamma$ and $T(\epsilon')$ adapted to $\gamma'$. Since the newly added vertices by $\hat{\mathcal{S}}^{\epsilon}_v$ is planar, they will never contributes the final result. So one has

$$
\begin{aligned}
& [\hat{\mathcal{S}}(N), \hat{\mathcal{S}}(M)]\phi_\gamma \\
= & \sum_{v,v' \in V(\gamma), v \neq v'} [M(v)N(v') - N(v)M(v')]\hat{\mathcal{S}}^{\epsilon'}_{v'}\hat{\mathcal{S}}^{\epsilon}_{v}\phi_\gamma \\
= & \frac{1}{2} \sum_{v,v' \in V(\gamma), v \neq v'} [M(v)N(v') - N(v)M(v')][\hat{\mathcal{S}}^{\epsilon'}_{v'}\hat{\mathcal{S}}^{\epsilon}_{v} - \hat{\mathcal{S}}^{\epsilon'}_{v}\hat{\mathcal{S}}^{\epsilon}_{v'}]\phi_\gamma \\
= & \frac{1}{2} \sum_{v,v' \in V(\gamma), v \neq v'} [M(v)N(v') - N(v)M(v')][(\hat{U}_{\varphi_{v',v}} - \hat{U}_{\varphi_{v,v'}})\hat{\mathcal{S}}^{\epsilon}_{v'}\hat{\mathcal{S}}^{\epsilon}_{v}]\phi_\gamma,
\end{aligned}
\tag{38}
$$

where we have used the facts that $[\hat{\mathcal{S}}^{\epsilon}_v, \hat{\mathcal{S}}^{\epsilon'}_{v'}] = 0$ for $v \neq v'$and there exists a diffeomorphism $\varphi_{v,v'}$ such that $\hat{\mathcal{S}}^{\epsilon'}_{v'}\hat{\mathcal{S}}^{\epsilon}_{v} = \hat{U}_{\varphi_{v',v}}\hat{\mathcal{S}}^{\epsilon}_{v'}\hat{\mathcal{S}}^{\epsilon}_{v}$. Obviously, we have in the Uniform Rovelli-Smolin Topology

$$([\hat{\mathcal{S}}(N), \hat{\mathcal{S}}(M)])'\Psi_{Diff} = 0$$

for all $\Psi_{Diff} \in Cyl^{\star}_{Diff}$. As we have seen in classical expression Eq.(32), the Poisson bracket of any two Hamiltonian constraints is given by a generator of the diffeomrophism transformations. Therefore it is mathematically consistent with the classical expression that two Hamiltonian constraint operators commute on diffeomorphism invariant states, as it is presented above. However, as it has been discussed in [72][95], the domain of dual Hamiltonian constraint operator can be extended to a slightly larger space (habitat) in $Cyl^{\star}$, whose elements are not necessary diffeomorphism invariant. And it turns out that the commutator between two Hamiltonian constraint operators continues to vanish on the habitat, which seems to be problematic. Fortunately, the quantum operator corresponding to the right hand side of classical Poisson bracket (32) also annihilates every state in the habitat [72], so the quantum constraint algebra is consistent at this level. But it is not clear that whether the quantum constraint algebra, especially the commutator between two Hamiltonian constraint is consistent with the classical one (32) on some larger space in $Cyl^{\star}$ containing more diffeomorphism variant states[10]. On the other hand, more works on the semi-classical analysis are also needed to test the classical limit of Eq.(38) and commutation relation (32). The way to do it is looking for some proper semi-classical states for calculating the classical limit of the operators. But due to the graph-changing property of the Hamiltonian constraint operator, the semi-classical analysis for the Hamiltonian constraint operator and the quantum constraint algebra is still an open issue so far.

- General Regularization Scheme of the Hamiltonian Constraint

  In [20], a general scheme of regulation is introduced for the quantization of the Hamiltonian constraint, and includes Thiemann's regularization we introduced above as a specific choice. Such a general regularization can be summarized as follows: first, we assign a

[10]However, some scholars disagree with such an argument involving the habitat and consider the habitat to be unphysical and completely irrelevant (see, e.g. Ref.[151]).

partition of $\Sigma$ into cells $\square$ of arbitrary shape. In every cell of the partition we define edges $s_J$, $J = 1, ..., n_s$ and loops $\beta_i$, $i = 1, ..., n_\beta$, where $n_s$, $n_\beta$ may be different for different cells. We use $\epsilon$ to represent the scale of the cell $\square$ Then fix an arbitrary chosen representation $\rho$ of $SU(2)$. This structure is called a *permissible classical regulator* if the regulated Hamiltonian constraint expression with respect to this partition has correct limit when $\epsilon \to 0$.

Second, we assign the diffeomorphism covariant property and let the partition adapted to the choice of the graph. That is, given a cylindrical function $\psi_\gamma \in Cyl^3_\gamma(\overline{\mathcal{A}/\mathcal{G}})$, we make the partition sufficiently refined that every vertex $v \in V(\gamma)$ is contained in exact one cell of the partition. And if $(\gamma,\ v)$ is diffeomorphic to $(\gamma',\ v')$ then, for every $\epsilon$ and $\epsilon'$, the quintuple $(\gamma,\ v,\ \square,\ (s_J),\ (\beta_i))$ is diffeomorphic to the quintuple $(\gamma',\ v',\ \square',\ (s'_J),\ (\beta'_i))$, where $\square$ and $\square'$ are the cells in the partitions with respect to $\gamma$ and $\gamma'$ respectively, containing $v$ and $v'$ respectively.

As a result, the Hamiltonian constraint operator in this general regularization scheme is expressed as:

$$\begin{aligned}
\hat{\mathcal{S}}^\epsilon_{E,\gamma}(N) &= \sum_{v\in V(\gamma)} \frac{N(v)}{i\hbar\kappa^2\beta} \sum_{i,J} C^{iJ}\mathrm{Tr}((\rho[A(\beta_i)] - \rho[A(\beta_i^{-1})])\rho[A(s_J^{-1})][\rho[A(s_J)],\ \hat{V}_{U^\epsilon_v}]), \\
\hat{\mathcal{T}}^\epsilon_\gamma(N) &= \sum_{v\in V(\gamma)} \frac{iN(v)}{\hbar^3\kappa^4\beta^3} \sum_{I,J,K} T^{IJK}\mathrm{Tr}(\rho[A(s_I^{-1})][\rho[A(s_I)],\ \hat{K}]\rho[A(s_J^{-1})][\rho[A(s_J)],\ \hat{K}] \\
&\times\ \rho[A(s_K^{-1})][\rho[A(s_K)],\ \hat{V}_{U^\epsilon_v}]), \\
\hat{\mathcal{S}}^\epsilon(N)\psi_\gamma &= [\hat{\mathcal{S}}^\epsilon_{E,\gamma}(N) - 2(1+\beta^2)\hat{\mathcal{T}}^\epsilon_\gamma(N)]\psi_\gamma,
\end{aligned}$$

where $C^{iJ}$ and $T^{IJK}$ are fixed constants independent of the value of $\epsilon$, the values of them are determined such that the above expressions have correct classical limits. After removing the regulator $\epsilon$ via diffeomorphism invariance the same as we did above, we obtain a well-defined diffeomorphism covariant operator on $\mathcal{H}_{kin}$ (or $\mathcal{H}^G$) in the sense of the Uniform Rovelli-Smolin Topology, or dual-define the operator on some suitable domain in $Cyl^\star$. Note that such a general scheme of construction exhibits that there is a great deal of freedom in choosing the regulators, so that there are considerable ambiguities in our quantization for seeking a proper quantum dynamics for gravity, which is also an open issue today.

## 4.4 Master Constraint Programme

Although the Hamiltonian constraint operator introduced above is densely defined on $\mathcal{H}_{kin}$ and diffeomorphism covariant, there are still several unsettled problems which are listed below.

- It is unclear whether the commutator between two Hamiltonian constraint operators reproduces the classical Poisson bracket between two Hamiltonian constraints. Hence it is unclear if the quantum Hamiltonian constraint produces the correct quantum dynamics with correct classical limit [72][95].

- The dual Hamiltonian constraint operator does not leave the Hilbert space $\mathcal{H}_{Diff}$ invariant. Thus the inner product structure of $\mathcal{H}_{Diff}$ cannot be employed in the construction of physical inner product.
- Classically the collection of Hamiltonian constraints does not form a Lie algebra. So one cannot employ group averaging strategy in solving the Hamiltonian constraint quantum mechanically, since the strategy depends crucially on group structure.

One may see that all above issues come from the properties of the constraint algebra at classical level. However, if one could construct an alternative classical constraint algebra, giving the same constraint phase space, which is a Lie algebra (no structure functions), where the subalgebra of diffeomorphism constraints forms an ideal, then the programme of solving the constraints would be in a much better position. Such a constraint Lie algebra was first introduced by Thiemann in [149]. The central idea is to introduce the master constraint:

$$\mathbf{M} := \frac{1}{2}\int_\Sigma d^3x \frac{|\widetilde{C}(x)|^2}{\sqrt{|\det q(x)|}}, \tag{39}$$

where $\widetilde{C}(x)$ is the scalar constraint in Eq.(8). One then gets the master constraint algebra:

$$\begin{aligned} \{\mathcal{V}(\vec{N}),\ \mathcal{V}(\vec{N}')\} &= \mathcal{V}([\vec{N},\vec{N}']), \\ \{\mathcal{V}(\vec{N}),\ \mathbf{M}\} &= 0, \\ \{\mathbf{M},\ \mathbf{M}\} &= 0. \end{aligned}$$

The master constraint programme has been well tested in various examples [63][64][65] [66][67]. In the following, we extend the diffeomorphism transformations such that the Hilbert space $\mathcal{H}_{Diff}$ is separable. This separability of $\mathcal{H}_{Diff}$ and the positivity and the diffeomorphism invariance of $\mathbf{M}$ will be working together properly and provide us with powerful functional analytic tools in the programme to solve the constraint algebra quantum mechanically. The regularized version of the master constraint can be expressed as

$$\mathbf{M}^\epsilon := \frac{1}{2}\int_\Sigma d^3y \int_\Sigma d^3x \chi_\epsilon(x-y)\frac{\widetilde{C}(y)}{\sqrt{V_{U_y^\epsilon}}}\frac{\widetilde{C}(x)}{\sqrt{V_{U_x^\epsilon}}}.$$

Introducing a partition $\mathcal{P}$ of the 3-manifold $\Sigma$ into cells $C$, we have an operator $\hat{H}^\epsilon_C$ acting on any cylindrical function $f_\gamma \in Cyl_\gamma(\overline{\mathcal{A}/\mathcal{G}})$ in $\mathcal{H}^G$ as

$$\hat{H}^\epsilon_C\, f_\gamma = \sum_{v\in V(\gamma)} \frac{\chi_C(v)}{E(v)} \sum_{v(\Delta)=v} \hat{h}^{\epsilon,\Delta}_v f_\gamma, \tag{40}$$

via a family of state-dependent triangulations $T(\epsilon)$ on $\Sigma$ as we did in the last section, where $\chi_C(v)$ is the characteristic function of the cell $C(v)$ containing a vertex $v$ of the graph $\gamma$, and the expression of $\hat{h}^{\epsilon,\Delta}_v$ reads

$$\begin{aligned} \hat{h}^{\epsilon,\Delta}_v &= \frac{16}{3i\hbar\kappa^2\beta}\epsilon^{ijk}\mathrm{Tr}(\hat{A}(\alpha_{ij}(\Delta))^{-1}\hat{A}(s_k(\Delta))^{-1}[\hat{A}(s_k(\Delta)),\ \sqrt{\hat{V}_{U_v^\epsilon}}]) \\ &\quad +2(1+\beta^2)\frac{4\sqrt{2}}{3i\hbar^3\kappa^4\beta^3}\epsilon^{ijk}\mathrm{Tr}(\hat{A}(s_i(\Delta))^{-1}[\hat{A}(s_i(\Delta)),\hat{K}^\epsilon] \\ &\quad \hat{A}(s_j(\Delta))^{-1}[\hat{A}(s_j(\Delta)),\ \sqrt{\hat{V}_{U_v^\epsilon}}]\hat{A}(s_k(\Delta))^{-1}[\hat{A}(s_k(\Delta)),\hat{K}^\epsilon]). \end{aligned} \tag{41}$$

Note that $\hat{h}_v^{\epsilon,\Delta}$ is similar to that involved in the regulated Hamiltonian constraint operator in the last section, while the only difference is that now the volume operator is replaced by its quare-root in Eq.(41). Hence the action of $\hat{H}_C^{\epsilon}$ on $f_\gamma$ adds arcs $a_{ij}(\Delta)$ with 1/2-representation with respect to each $v(\Delta)$ of $\gamma$. Thus, for each $\epsilon > 0$, $\hat{H}_C^{\epsilon}$ is a Yang-Mills gauge invariant and diffeomorphism covariant operator defined on $Cyl(\overline{\mathcal{A}/\mathcal{G}})$. The family of such operators can give a limit operator $\hat{H}_C$ densely defined on $\mathcal{H}^G$ by the uniform Rovelli-Smollin topology. Then a master constraint operator, $\hat{\mathbf{M}}$, acting on any $\Psi_{Diff} \in Cyl^\star_{Diff}$ can be defined as [88]

$$(\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma] := \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \Psi_{Diff}[\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_C^{\epsilon}(\hat{H}_C^{\epsilon'})^\dagger f_\gamma], \tag{42}$$

for any $f_\gamma$ is a finite linear combination of spin-network function. Note that $\hat{H}_C^{\epsilon}(\hat{H}_C^{\epsilon'})^\dagger f_\gamma$ is also a finite linear combination of spin-network functions on an extended graph with the same skeleton of $\gamma$, hence the value of $(\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma]$ is finite for any given $\Psi_{Diff}$. Thus $\hat{\mathbf{M}}\Psi_{Diff}$ lies in the algebraic dual of the space of cylindrical functions. Furthermore, we can show that $\hat{\mathbf{M}}$ leaves the diffeomorphism invariant distributions invariant. For any diffeomorphism transformation $\varphi$ on $\Sigma$,

$$\begin{aligned}
(\hat{U}'_\varphi\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma] &= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \Psi_{Diff}[\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_C^{\epsilon}(\hat{H}_C^{\epsilon'})^\dagger \hat{U}_\varphi f_\gamma] \\
&= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \Psi_{Diff}[\hat{U}_\varphi \sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_{\varphi^{-1}(C)}^{\varphi^{-1}(\epsilon)}(\hat{H}_{\varphi^{-1}(C)}^{\varphi^{-1}(\epsilon')})^\dagger f_\gamma] \\
&= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \Psi_{Diff}[\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_C^{\epsilon}(\hat{H}_C^{\epsilon'})^\dagger f_\gamma],
\end{aligned} \tag{43}$$

where in the last step, we used the fact that the diffeomorphism transformation $\varphi$ leaves the partition invariant in the limit $\mathcal{P} \to \sigma$ and relabel $\varphi(C)$ to be $C$. So we have the result

$$(\hat{U}'_\varphi\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma] = (\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma]. \tag{44}$$

So given a diffeomorphism invariant spin-network state $T_{[s]}$, the result state $\hat{\mathbf{M}}T_{[s]}$ must be a diffeomorphism invariant element in the algebraic dual of $Cyl(\overline{\mathcal{A}/\mathcal{G}})$, which means that

$$\hat{\mathbf{M}}T_{[s]} = \sum_{[s_1]} c_{[s_1]}T_{[s_1]},$$

then

$$\lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} T_{[s]}[\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_C^{\epsilon}(\hat{H}_C^{\epsilon'})^\dagger T_{s_2}] = \sum_{[s_1]} c_{[s_1]}T_{[s_1]}[T_{s_2}],$$

where the cylindrical function $\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_C^{\epsilon'}(\hat{H}_C^{\epsilon})^\dagger T_{s_2}$ is a finite linear combination of spin-network functions on some graphs $\gamma\,'$ with the same skeleton of $\gamma(s_2)$ up to finite number of arcs. Hence fixing the diffeomorphism equivalence class $[s]$, only for spin-networks $s_2$ lies in finite number of diffeomorphism equivalence class the left hand side of the last equation is non-zero. So there are also only finite number of classes $[s_1]$ in the right hand side such that $c_{[s_1]}$ is non-zero. As a result, $\hat{\mathbf{M}}T_{[s]}$ is a finite linear combination of diffeomorphism invariant spin-network states and lies in the Hilbert space of diffeomorphism invariant states $\mathcal{H}_{Diff}$ for any $[s]$. And $\hat{\mathbf{M}}$ is densely defined on $\mathcal{H}_{Diff}$.

Given two diffeomorphism invariant spin-network functions $T_{[s_1]}$ and $T_{[s_2]}$, one can give the matrix elements of $\hat{\mathbf{M}}$ as [88][89]

$$\begin{aligned}
& \overline{< T_{[s_1]}|\hat{\mathbf{M}}|T_{[s_2]} >_{Diff}} \\
= & \ (\hat{\mathbf{M}}T_{[s_2]})[T_{s_1\in[s_1]}] \\
= & \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \sum_{C\in\mathcal{P}} \frac{1}{2}\overline{T_{[s_2]}[\hat{H}^{\epsilon}_C(\hat{H}^{\epsilon'}_C)^\dagger T_{s_1\in[s_1]}]} \\
= & \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \sum_{C\in\mathcal{P}} \frac{1}{2}\frac{1}{n_{\gamma(s_2)}} \sum_{\varphi\in Diff(\Sigma)/Diff_{\gamma(s_2)}} \sum_{\varphi'\in GS_{\gamma(s_2)}} \\
\times & \ \overline{< \hat{U}_\varphi \hat{U}_{\varphi'} T_{s_2\in[s_2]}|\hat{H}^{\epsilon}_C(\hat{H}^{\epsilon'}_C)^\dagger T_{s_1\in[s_1]} >_{Kin}} \\
= & \sum_s \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \sum_{C\in\mathcal{P}} \frac{1}{2}\frac{1}{n_{\gamma(s_2)}} \sum_{\varphi\in Diff(\Sigma)/Diff_{\gamma(s_2)}} \sum_{\varphi'\in GS_{\gamma(s_2)}} \\
\times & \ \overline{< \hat{U}_\varphi \hat{U}_{\varphi'} T_{s_2\in[s_2]}|\hat{H}^{\epsilon}_C T_s >_{Kin} < T_s|(\hat{H}^{\epsilon'}_C)^\dagger T_{s_1\in[s_1]} >_{Kin}} \\
= & \sum_{[s]} \sum_{v\in V(\gamma(s\in[s]))} \frac{1}{2} \lim_{\epsilon,\epsilon'\to 0} \\
\times & \ \overline{T_{[s_2]}[\hat{H}^{\epsilon}_v T_{s,c\in[s,c]}] \sum_{s,c\in[s,c]} < T_s|(\hat{H}^{\epsilon'}_v)^\dagger T_{s_1\in[s_1]} >_{Kin}}, \qquad (45)
\end{aligned}$$

where $Diff_\gamma$ is the set of diffeomorphisms leaving the colored graph $\gamma$ invariant, $GS_\gamma$ denotes the graph symmetry quotient group $Diff_\gamma/TDiff_\gamma$ where $TDiff_\gamma$ is the diffeomorphism which is trivial on the graph $\gamma$, and $n_\gamma$ is the number of elements in $GS_\gamma$. Note that we have used the resolution of identity trick in the fourth step. Since only a finite number of terms in the sum over spin-networks $s$, cells $C \in \mathcal{P}$, and diffeomorphism transformations $\varphi$ are non-zero respectively, we can interchange the sums and the limit. In the fifth step, we take the limit $C \to v$ and split the sum $\sum_s$ into $\sum_{[s]}\sum_{s\in[s]}$, where $[s, c]$ denotes the diffeomorphism equivalent class associated with $s$. Here we also use the fact that, given $\gamma(s)$ and $\gamma(s')$ which are different up to a diffeomorphism transformation, there is always a diffeomorphism $\varphi$ transforming the graph associated with $\hat{H}^{\epsilon}_v T_s$ ($v \in \gamma(s)$) to that of $\hat{H}^{\epsilon}_{v'} T_{s'}$ ($v' \in \gamma(s')$) with $\varphi(v) = v'$, hence $T_{[s_2]}[\hat{H}^{\epsilon}_v T_{s\in[s]}]$ is constant for different $s \in [s]$.

Since the term $\sum_{s\in[s]} < T_s|(\hat{H}^{\epsilon'}_v)^\dagger T_{s_1\in[s_1]} >_{Kin}$ is independent of the parameter $\epsilon'$, one can see that by fixing a arbitrary family of state-dependent triangulations $T(\epsilon')$,

$$\begin{aligned}
& \sum_{s\in[s]} < T_s|(\hat{H}^{\epsilon'}_v)^\dagger T_{s_1\in[s_1]} >_{Kin} \\
= & \sum_{\varphi} < U_\varphi T_s|(\hat{H}^{\epsilon'}_v)^\dagger T_{s_1\in[s_1]} >_{Kin} \\
= & \sum_{\varphi} < \hat{H}^{\epsilon'}_v U_\varphi T_s|T_{s_1\in[s_1]} >_{Kin}
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{\varphi} < U_{\varphi}\hat{H}^{\varphi^{-1}(\epsilon')}_{\varphi^{-1}(v)} T_s | T_{s_1\in[s_1]} >_{Kin} \\
&= \overline{T_{[s_1]}[\hat{H}^{\varphi^{-1}(\epsilon')}_{v\in V(\gamma(s))} T_s]}, \qquad (46)
\end{aligned}
$$

where $\varphi$ are the diffeomorphism transformations spanning the diffeomorphism equivalent class $[s]$. Note that the kinematical inner product in above sum is non-vanishing if and only if $\varphi(\gamma(s)))$ coincides with the graph obtained from certain skeleton $\gamma(s_1)$ by the action of $(\hat{H}^{\epsilon'}_v)^\dagger$ and $v \in V(\varphi(\gamma(s)))$, i.e., the scale $\varphi^{-1}(\epsilon')$ of the diffeomorphism images of the tetrahedrons added by the action coincides with the scale of certain tetrahedrons in $\gamma(s)$ and $\varphi^{-1}(v)$ is a vertex in $\gamma(s)$. Then we can express the matrix elements (83) as:

$$
\begin{aligned}
& < T_{[s_1]}|\hat{\mathbf{M}}|T_{[s_2]} >_{Diff} \\
&= \sum_{[s]} \sum_{v\in V(\gamma(s\in[s]))} \frac{1}{2} \lim_{\epsilon,\epsilon'\to 0} \overline{T_{[s_2]}[\hat{H}^{\epsilon}_v T_{s\in[s]}]} T_{[s_1]}[\hat{H}^{\epsilon'}_v T_{s\in[s]}] \\
&= \sum_{[s]} \sum_{v\in V(\gamma(s\in[s]))} \frac{1}{2} \overline{(\hat{H}'_v T_{[s_2]})[T_{s\in[s]}]} (\hat{H}'_v T_{[s_1]})[T_{s\in[s]}]. \qquad (47)
\end{aligned}
$$

From Eq.(85) and the fact that the master constraint operator $\hat{\mathbf{M}}$ is densely defined on $\mathcal{H}_{Diff}$, it is obvious that $\hat{\mathbf{M}}$ is a positive and symmetric operator in $\mathcal{H}_{Diff}$. Therefore, the quadratic form $Q_{\mathbf{M}}$ associated with $\hat{\mathbf{M}}$ is closable [114]. The closure of $Q_{\mathbf{M}}$ is the quadratic form of a unique self-adjoint operator $\hat{\overline{\mathbf{M}}}$, called the Friedrichs extension of $\hat{\mathbf{M}}$. We relabel $\hat{\overline{\mathbf{M}}}$ to be $\hat{\mathbf{M}}$ for simplicity. From the construction of $\hat{\mathbf{M}}$, the qualitative description of the kernel of the Hamiltonian constraint operator in Ref.[136] can be transcribed to describe the solutions to the equation: $\hat{\mathbf{M}}\Psi_{Diff} = 0$. In particular, the diffeomorphism invariant cylindrical functions based on at most 2-valent graphs are obviously normalizable solutions. In conclusion, there exists a positive and self-adjoint operator $\hat{\mathbf{M}}$ on $\mathcal{H}_{Diff}$ corresponding to the master constraint (75), and zero is in the point spectrum of $\hat{\mathbf{M}}$.

Note that the quantum constraint algebra can be easily checked to be anomaly free. i.e.,

$$
[\hat{\mathbf{M}}, \hat{U}'_{\varphi}] = 0, \quad [\hat{\mathbf{M}}, \hat{\mathbf{M}}] = 0.
$$

which is consistent with the classical master constraint algebra in this sense. As a result, the difficulty of the original Hamiltonian constraint algebra can be avoided by introducing the master constraint algebra, due to the Lie algebra structure of the latter. Since zero is in the spectrum of $\hat{\mathbf{M}}$ [140], the further task is to obtain the physical Hilbert space $\mathcal{H}_{phys}$ which is the kernel of the master constraint operator with some suitable physical inner product, and the issue of quantum anomaly is represented in terms of the size of $\mathcal{H}_{phys}$ and the existence of semi-classical states. Note that we will see in the next section that the master constraint programme can be straightforwardly generalized to include matter fields [89]. We list some open problems in the master constraint programme for further research.

- Kernel of Master Constraint Operator

  Since the master constraint operator $\hat{\mathbf{M}}$ is self-adjoint, it is a practical problem to define DID of $\mathcal{H}_{Diff}$:

$$
\mathcal{H}_{Diff} \sim \int^{\oplus} d\mu(\lambda) \mathcal{H}^{\oplus}_{\lambda},
$$

$$< \Phi|\Psi >_{Diff} \;=\; \int_{\mathbf{R}} d\mu(\lambda) < \Phi|\Psi >_{\mathcal{H}^{\oplus}_{\lambda}},$$

where $\mu(\lambda)$ is the spectral measure with respect to the master constraint operator $\hat{\mathbf{M}}$. It is expected that we can identify $\mathcal{H}^{\oplus}_{\lambda=0}$ with the physical Hilbert space. However, such a prescription is ambiguous in the case that zero is only in the continuous spectrum, loses physical information in the case that zero is an embedded eigenvalue and unambiguous only if zero is an isolated eigenvalue in which case however the whole machinery of the DID is not needed at all because $\mathcal{H}^{\oplus}_{\lambda=0} \subset \mathcal{H}_{Diff}$ and the physical inner product coincide with the kinematical (differomorphism invariant) one [63]. There are some improved prescriptions also presented in [63] by decomposing the measure with respect to the spectrum types before direct integral decomposition, some ambiguities can be canceled by some physical criterion, e.g., a complete subalgebra of bounded Dirac observables should be represented irreducibly as self-adjoint operators on the physical Hilbert space, and the resulting physical Hilbert space should admits a sufficient number of semiclassical states. Nonetheless, due to the complicated structure of the master constraint operator, it is difficult anyhow to manage the spectrum analysis and direct integral decomposition. On the other hand, for the self-adjointness of the master constraint operator and the Lie-algebra structure of the constraint algebra, a formal group averaging strategy was introduced in [149] as a more concrete way to get the physical Hilbert space. It is realized by a formal rigged map $\eta_{phys}$:

$$\begin{aligned} \eta_{phys}: \quad & Cyl^{\star}_{Diff} \rightarrow \Phi_{phys} \\ & f \mapsto \eta_{phys}(f) := \int_{\mathbf{R}} \frac{dt}{2\pi} < e^{i\hat{\mathbf{M}}t} f| \,.\, >_{Diff}, \end{aligned}$$

where $e^{i\hat{\mathbf{M}}t}$ is a one parameter continuous unitary group on $\mathcal{H}_{Diff}$ by the self-adjointness of $\hat{\mathbf{M}}$, and $\Phi_{phys}$ is a subset of the algebraic dual of $Cyl^{\star}_{Diff}$. It is trivial to see that $\eta_{phys}(f)$ is invariant under the (dual) transformation of $e^{i\hat{\mathbf{M}}t}$. Thus a inner product can be formally defined between two algebraic functionals $\eta_{phys}(f)$ and $\eta_{phys}(f')$ in $\Phi_{phys}$ via:

$$\begin{aligned} < \eta_{phys}(f)|\eta_{phys}(f') >_{phys} \;&:=\; \eta_{phys}(f)[f'], \\ &=\; \int_{\mathbf{R}} \frac{dt}{2\pi} < e^{i\hat{\mathbf{M}}t} f|f' >_{Diff} \\ &=\; \int_{\mathbf{R}} \frac{dt}{2\pi} \int_{\mathbf{R}} d\mu(\lambda) e^{i\lambda t} < f(\lambda)|f'(\lambda) >_{\mathcal{H}^{\oplus}_{\lambda}} \\ &=\; \int_{\mathbf{R}} d\mu(\lambda)\delta(\lambda) < f(\lambda)|f'(\lambda) >_{\mathcal{H}^{\oplus}_{\lambda}} \\ &=\; [\int_{\mathbf{R}} d\mu(\lambda)\delta(\lambda)] < f(0)|f'(0) >_{\mathcal{H}^{\oplus}_{\lambda=0}}, \end{aligned}$$

where we have used the spectrum decomposition with respect to the self-adjoint operator $\hat{\mathbf{M}}$, the operator $e^{i\hat{\mathbf{M}}t}$ is represented by multiplication by a number $e^{i\lambda t}$ on each $\mathcal{H}^{\oplus}_{\lambda}$, and the vector valued function $f(\lambda)$ is the spectrum decomposition representation of state $f \in \mathcal{H}_{Diff}$. Although we can see from the above argument that the physical inner product is proportional to the inner product in the fiber Hilbert space $\mathcal{H}^{\oplus}_{\lambda=0}$, unfortunately, the factor $\int_{\mathbf{R}} d\mu(\lambda)\delta(\lambda)$ is divergent when $\mu$ has pure point part, e.g. zero is in the discrete spectrum of $\hat{\mathbf{M}}$. That is one reason why we claim that the above argument is formal.

On the other hand, the group averaging strategy and the formal physical inner product we just defined has potential relationships with path-integral formulation and spin foam models due to the positivity of the master constraint operator $\hat{\mathbf{M}}$ [149], and hopefully, we may obtain the physical transition amplitude from this physical inner product in the future. However, the whole technique of group averaging for solving the master constraint is still formal so far, and the rigorous calculations for it has not done yet as far as we know.

- Dirac Observables

  Classically, one can prove that a function $O \in C^{\infty}(\mathcal{M})$ is a weak observable with respect to the scalar constraint if and only if

$$\{O, \{O, \mathbf{M}\}\}|_{\overline{\mathcal{M}}} = 0.$$

  We define $O$ to be a strong observable with respect to the scalar constraint if and only if

$$\{O, \mathbf{M}\}|_{\mathcal{M}} = 0,$$

  and to be a ultra-strong observable if and only if

$$\{O, \mathcal{S}(N)\}|_{\mathcal{M}} = 0.$$

  In quantum version, an observable $\hat{O}$ is a weak Dirac observable if and only if $\hat{O}$ leaves $\mathcal{H}_{phys}$ invariant, while $\hat{O}$ is now called a strong Dirac observable if and only if $\hat{O}$ commutes with the master constraint operator $\hat{\mathbf{M}}$. Given a bounded self-adjoint operator $\hat{O}$ defined on $\mathcal{H}_{Diff}$, for instance, a spectral projection of some observables leaving $\mathcal{H}_{Diff}$ invariant, if the uniform limit exists, the bounded self-adjoint operator defined by group averaging

$$\widehat{[O]} := \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} dt\ \hat{U}(t)^{-1}\hat{O}\hat{U}(t)$$

  commutes with $\hat{\mathbf{M}}$ and hence becomes a strong Dirac observable on the physical Hilbert space.

- Testing the Classical Limit of the Master Constraint Operator

  One needs to construct spatial diffeomorphism invariant semiclassical states to calculate the expectation value and fluctuation of the master constraint operator. If the results coincide with the classical values up to $\hbar$ corrections, one can go ahead to finish our quantization programme with confidence.

# 5 Quantum Matter Field on a Quantum Background

In ordinary quantum field theory, the quantum field is defined on a smooth background spacetime. However, it is expected that the smooth structure of a spacetime may break down at Planck scale, so the present treatment of quantum field theory is valid only in a semiclassical sense. Thus we would like to modify the formulation of present quantum field theory to make it compatible with the quantum theory of gravity(spacetime) which we already established in previous sections so as to explore the behavior of the quantum matter field under Planck scale and at extremely strong gravitational fields, e.g. inside the black hole or at the early age of the universe.

In the following, an alternative quantization of scalar field will be introduced, the advantage of such a quantization scheme is that the quantum scalar field doesn't depend on the background. We will also see that the quantization technique for the previous Hamiltonian constraint can be generalized to quantize the Hamiltonian of matter fields coupled to gravity. Then it is shown that an operator corresponding to the Hamiltonian of the scalar field can be well defined on the coupled diffeomorphism invariant Hilbert space. It is even positive and self-adjoint without any divergence. Thus quantum gravity acts exactly as a natural regulator for the quantum scalar field in the polymer representation. Moreover, to study the whole dynamical system of the scalar field coupled to gravity, a Hamiltonian constraint operator is defined in the coupled kinematical Hilbert space. The contribution of the scalar field to the Hamiltonian constraint can be promoted to a positive self-adjoint operator. To avoid possible quantum anomalies and find the physical Hilbert space, we will also introduce the master constraint programme for the coupled system. A self-adjoint master constraint operator is obtained in the diffeomorphism invariant Hilbert space, which assures the feasibility of the programme.

## 5.1 Polymer-like Representation of a Scalar Field

We begin with the total Hamiltonian of the gravity coupled with a massless real scalar field which is a linear combination of constraints:

$$\mathcal{H}_{tot} = \Lambda^i G_i + N^a C_a + NC,$$

where $\Lambda^i$, $N^a$ and $N$ are Lagrange multipliers, and the three constraints in the Hamiltonian are expressed as [30][87]:

$$\begin{aligned}
G_i &= D_a\widetilde{P}^a_i := \partial_a\widetilde{P}^a_i + \epsilon_{ij}{}^k A^i_a \widetilde{P}^a_k, &(48)\\
C_a &= \widetilde{P}^b_i F^i_{ab} - A^i_a G_i + \widetilde{\pi}\partial_a\phi, &(49)\\
C &= \frac{\kappa\beta^2}{2\sqrt{|\det q|}}\widetilde{P}^a_i\widetilde{P}^b_j[\epsilon^{ij}{}_k F^k_{ab} - 2(1+\beta^2)K^i_{[a}K^j_{b]}]\\
&+ \frac{1}{\sqrt{|\det q|}}[\frac{\kappa^2\beta^2\alpha_M}{2}\delta^{ij}\widetilde{P}^a_i\widetilde{P}^b_j(\partial_a\phi)\partial_b\phi + \frac{1}{2\alpha_M}\widetilde{\pi}^2], &(50)
\end{aligned}$$

here the real number $\alpha_M$ is the coupling constant, and $\widetilde{\pi}$ denotes the momentum conjugate to $\phi$:

$$\widetilde{\pi} := \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \frac{\alpha_M}{N}\sqrt{|\det q|}(\dot{\phi} - N^a\partial_a\phi).$$

Thus one has the elementary Poisson brackets

$$\begin{aligned}\{A_a^i(x), \widetilde{P}_j^b(y)\} &= \delta_b^a \delta_j^i \delta(x, y), \\ \{\phi(x), \widetilde{\pi}(y)\} &= \delta(x, y).\end{aligned}$$

Note that the second term of the Hamiltonian constraint (50) is just the Hamiltonian of the real scalar field.

Then we look for the background independent representation for the real scalar field coupled to gravity, following the polymer representation of the scalar field [27]. The classical configuration space, $\mathcal{U}$, consists of all real-valued smooth functions $\phi$ on $\Sigma$. Given a set of a finite number of points $X = \{x_1, ..., x_N\}$ in $\Sigma$, a equivalence relation can be defined by: given two scalar field $\phi_1, \phi_2 \in \mathcal{U}$, $\phi_1 \sim \phi_2$ if and only if $\exp[i\lambda_i\phi_1(x_i)] = \exp[i\lambda_j\phi_2(x_j)]$ for all $x_i \in X$ and all real number $\lambda_j$. Hence we obtain a bijection between $\mathcal{U}/\sim$ and $\overline{\mathbf{R}}_X$, which is $N$ copies of the Bohr compactification of $\mathbf{R}$ [132]. Since one can define a projective family with respect to the set of point (graph for scalar field), thus a projective limit $\overline{\mathcal{U}}$, which is a compact topological space, is obtained as the quantum configuration space of scalar field. Next, we denote by $Cyl_X(\overline{\mathcal{U}})$ the vector space generated by finite linear combinations of the following functions of $\phi$:

$$T_{X,\lambda}(\phi) := \prod_{x_j \in X} \exp[i\lambda_j\phi(x_j)],$$

where $\lambda \equiv (\lambda_1, \lambda_2, \cdots, \lambda_N)$ are arbitrary non-zero real numbers assigned at each point. It is obvious that $Cyl_X(\overline{\mathcal{U}})$ has the structure of a $*$-algebra. The vector space $Cyl(\overline{\mathcal{U}})$ of all cylindrical functions on $\mathcal{U}$ is defined by the linear span of the linear span of $T_0 = 1$ and $T_{X,\lambda}$. Completing $Cyl(\overline{\mathcal{U}})$ with respect to the sup norm, one obtains a unital Abelian $C^*$-algebra $\overline{Cyl(\overline{\mathcal{U}})}$. Thus one can use the GNS structure to construct its cyclic representations. A preferred positive linear functional $\omega_0$ on $\overline{Cyl(\overline{\mathcal{U}})}$ is defined by

$$\omega_0(T_{X,\lambda}) = \begin{cases} 1 & \text{if } \lambda_j = 0\ \forall j \\ 0 & \text{otherwise,} \end{cases}$$

which defines a diffeomorphism-invariant faithful Borel measure $\mu$ on $\overline{\mathcal{U}}$ as

$$\int_{\overline{\mathcal{U}}} d\mu(T_{X,\lambda}) = \begin{cases} 1 & \text{if } \lambda_j = 0\ \forall j \\ 0 & \text{otherwise.} \end{cases} \tag{51}$$

Thus one obtains the Hilbert space, $\mathcal{H}_{kin}^{KG}$ which is defined by $L^2(\overline{\mathcal{U}}, d\mu)$, of square integrable functions on a compact topological measure space $\overline{\mathcal{U}}$ with respect to $\mu$. The inner product can be expressed explicitly as:

$$< T_c|T_{c'} >_{kin}^{KG} = \delta_{cc'}, \tag{52}$$

where the label $c := (X, \lambda)$ are called scalar-network.

As one might expect, the quantum configuration space $\overline{\mathcal{U}}$ is just the Gel'fand spectrum of $\overline{Cyl(\overline{\mathcal{U}})}$. More concretely, for a single point set $X_0 \equiv \{x_0\}$, $Cyl_{X_0}(\overline{\mathcal{U}})$ is the space of all almost periodic functions on a real line $\mathbf{R}$. The Gel'fand spectrum of the corresponding $C^*$-algebra

$\overline{Cyl_{X_0}(\overline{\mathcal{U}})}$ is the Bohr completion $\overline{\mathbf{R}}_{x_0}$ of $\mathbf{R}$ [27], which is a compact topological space such that $\overline{Cyl_{X_0}(\overline{\mathcal{U}})}$ is the $C^*$-algebra of all continuous functions on $\overline{\mathbf{R}}_{x_0}$. Since $\mathbf{R}$ is densely embedded in $\overline{\mathbf{R}}_{x_0}$, $\overline{\mathbf{R}}_{x_0}$ can be regarded as a completion of $\mathbf{R}$.

It is clear from Eq.(51) that an orthonomal basis in $\mathcal{H}_{kin}^{KG}$ is given by the scalar vacuum $T_0 = 1$ and so-called scalar-network functions $T_c(\phi)$, where $c = (X, \lambda)$ and $\lambda \equiv (\lambda_1, \lambda_2, \cdots, \lambda_N)$ are non-zero real numbers. So the total kinematical Hilbert space $\mathcal{H}_{kin}$ is the direct product of the kinematical Hilbert space $\mathcal{H}_{kin}^{GR}$ for gravity and the kinematical Hilbert space for real scalar field, i.e., $\mathcal{H}_{kin} := \mathcal{H}_{kin}^{GR} \otimes \mathcal{H}_{kin}^{KG}$. Then the spin-scalar-network state $T_{s,c} \equiv T_s(A) \otimes T_c(\phi) \in Cyl_{\gamma(s)}(\overline{\mathcal{A}/\mathcal{G}}) \otimes Cyl_{X(c)}(\overline{\mathcal{U}}) \equiv Cyl_{\gamma(s,c)}$ is a gravity-scalar cylindrical function on graph $\gamma(s, c) \equiv \gamma(s) \cup X(c)$. Note that generally $X(c)$ may not coincide with the vertices of the graph $\gamma(s)$. It is straightforward to see that all of these functions constitutes an orthonormal basis in $\mathcal{H}_{kin}$ as

$$< T_{s'}(A) \otimes T_{c'}(\phi) | T_s(A) \otimes T_c(\phi) >_{kin} = \delta_{s's}\delta_{c'c} \, .$$

Note that none of $\mathcal{H}_{kin}$, $\mathcal{H}_{kin}^{GR}$ and $\mathcal{H}_{kin}^{KG}$ is a separable Hilbert space.

Given a pair $(x_0, \lambda_0)$, there is an elementary configuration for the scalar field, the so-called point holonomy,

$$U(x_0, \lambda_0) := \exp[i\lambda_0\phi(x_0)].$$

It corresponds to a configuration operator $\hat{U}(x_0, \lambda_0)$, which acts on any cylindrical function $\psi(\phi) \in Cyl_{X(c)}(\overline{\mathcal{U}})$ by

$$\hat{U}(x_0, \lambda_0)\psi(\phi) = U(x_0, \lambda_0)\psi(\phi). \tag{53}$$

All these operators are unitary. But since the family of operators $\hat{U}(x_0, \lambda)$ fails to be weakly continuous in $\lambda$, there is no field operator $\hat{\phi}(x)$ on $\mathcal{H}_{kin}^{KG}$. The momentum functional smeared on a 3-dimensional region $R \subset \Sigma$ is expressed by

$$\pi(R) := \int_R d^3x \widetilde{\pi}(x).$$

The Poisson bracket between the momentum functional and a point holonomy can be easily calculated to be

$$\{\pi(R), U(x, \lambda)\} = -i\lambda\chi_R(x)U(x, \lambda),$$

where $\chi_R(x)$ is the characteristic function for the region $R$. So the momentum operator is defined by the action on scalar network functions $T_{c=(X,\lambda)}$ as

$$\hat{\pi}(R)T_c(\phi) := i\hbar\{\pi(R), T_c(\phi)\} = \hbar[\sum_{x_j \in X} \lambda_j\chi(x_j)]T_c(\phi).$$

Now we can impose the quantum constraints on $\mathcal{H}_{kin}$ and consider the quantum dynamics. First, the Gauss constraint can be solved independently of $\mathcal{H}_{kin}^{KG}$, since it only involves the gravitational field. It is also expected that the diffeomorphism constraint can be implemented by the group averaging strategy in the similar way as in the case of pure gravity. Given a spatial diffeomorphism transformation $\varphi$, a unitary transformation $\hat{U}_\varphi$ was induced by $\varphi$ in the Hilbert space $\mathcal{H}_{kin}$, which is expressed as

$$\hat{U}_\varphi T_{s=(\gamma(s),\mathbf{j},\mathbf{i}),c=(X(c),\lambda)} = T_{\varphi\circ s=(\varphi(\gamma(s)),\mathbf{j},\mathbf{i}),\varphi\circ c=(\varphi(X(c)),\lambda)}.$$

Then the differomorphism invariant spin-scalar-network functions are defined by group averaging as

$$T_{[s,c]} := \frac{1}{n_{\gamma(s,c)}} \sum_{\varphi\in Diff(\Sigma)/Diff_{\gamma(s,c)}} \sum_{\varphi'\in GS_{\gamma(s,c)}} \hat{U}_\varphi \hat{U}_{\varphi'} T_{s,c}, \tag{54}$$

where $Diff_\gamma$ is the set of diffeomorphisms leaving the colored graph $\gamma$ invariant, $GS_\gamma$ denotes the graph symmetry quotient group $Diff_\gamma/TDiff_\gamma$ where $TDiff_\gamma$ is the set of the diffeomorphisms which is trivial on the graph $\gamma$, and $n_\gamma$ is the number of elements in $GS_\gamma$. Following the standard strategy in quantization of pure gravity, an inner product can be defined on the vector space spanned by the diffeomorphism invariant spin-scalar-network functions (and the vacuum states for gravity, scalar and both respectively) such that they form an orthonormal basis as:

$$< T_{[s,c]}|T_{[s',c']} >_{Diff} := T_{[s,c]}[T_{s',c'\in[s',c']}] = \delta_{[s,c],[s',c']}. \tag{55}$$

After the completion procedure, we obtain the expected Hilbert space of diffeomorphism invariant states for the scalar field coupled to gravity, which is denoted by $\mathcal{H}_{Diff}$.

## 5.2 Diffeomorphism Invariant Hamiltonian of a Scalar Field

In the following discussion, we consider the quantum scalar field on a fluctuating background. A similar idea was considered in Ref.[139], where a Hamiltonian operator with respect to a U(1) group representation of the scalar field is defined on a kinematical Hilbert space $\mathcal{H}_{kin'}$ of matter coupled to gravity. Then an effective Hamiltonian operator of the scalar field can be constructed as a quadratic form via

$$\begin{aligned} & < \psi_{matter},\ \hat{H}^{eff}_{matter}(m)\ \psi'_{matter} >^{KG}_{kin'} \\ := \ & < \psi_{grav}(m)\otimes\psi_{matter},\ \hat{H}_{matter}\ \psi_{grav}(m)\otimes\psi'_{matter} >_{kin'}, \end{aligned} \tag{56}$$

where $\psi_{grav}(m) \in \mathcal{H}^{GR}_{kin}$ presents a semiclassical state of gravity approximating some classical spacetime background $m$ where the quantum scalar field lives. Thus the effective Hamiltonian operator $\hat{H}^{eff}_{matter}(m)$ of scalar field contains also the information of the fluctuating background *metric*. In the light of this idea, we will construct a Hamiltonian operator $\hat{\mathcal{S}}_{KG}$ for scalar field in the polymer-like representation. It turns out that this Hamiltonian operator can be defined in the Hilbert space $\mathcal{H}_{Diff}$ of diffeomorphism invariant states for scalar field coupled to gravity without UV-divergence. So the quantum dynamics of the scalar field is obtained in a diffeomorphism invariant way, which is expected in the programme of loop quantum gravity. Thus, here an effective Hamiltonian operator of the scalar field could be extracted in $\mathcal{H}_{Diff}$ by defining $< \Psi_{[m]}(A,\phi),\ \hat{\mathcal{S}}_{KG}\ \Psi_{[m]}(A,\phi) >_{Diff}$ to be its expectation value on diffeomorphism invariant states $\Psi(\phi)$ of the scalar field, where the diffeomorphism invariant semiclassical state $\Psi_{[m]}(A)$ represents certain fluctuating geometry with spatial diffeomorphism invariance, and the label

$[m]$ denotes the classical geometry approximated by $\Psi_{[m]}(A)$. Moreover, the quadratic properties of the scalar field Hamiltonian will provide powerful functional analytic tools in the quantization procedure, such that the self-adjointness of the Hamiltonian operator can be proved by a theorem in functional analysis.

Then the crucial point is to define an operator corresponding to the Hamiltonian functional $\mathcal{S}_{KG}$ of the scalar field, which can be decomposed into two parts

$$\mathcal{S}_{KG} = \mathcal{S}_{KG,\phi} + \mathcal{S}_{KG,Kin},$$

where

$$\begin{aligned}
\mathcal{S}_{KG,\phi} &= \frac{\kappa^2\beta^2\alpha_M}{2}\int_\Sigma d^3x \frac{1}{\sqrt{|\det q|}}\delta^{ij}\widetilde{P}^a_i\widetilde{P}^b_j(\partial_a\phi)\partial_b\phi, \\
\mathcal{S}_{KG,Kin} &= \frac{1}{2\alpha_M}\int_\Sigma d^3x \frac{1}{\sqrt{|\det q|}}\widetilde{\pi}^2.
\end{aligned}$$

We will employ the following identities:

$$\widetilde{P}^a_i = \frac{1}{2\kappa\beta}\widetilde{\eta}^{abc}\epsilon_{ijk}e^j_b e^k_c \quad \text{and} \quad e^i_a(x) = \frac{2}{\kappa\beta}\{A^i_a(x), V_{U_x}\},$$

where $\widetilde{\eta}^{abc}$ denotes the Levi-Civita tensor tensity and $V_{U_x}$ is the volume of an arbitrary neighborhood $U_x$ containing the point $x$. By using the point-splitting strategy, the regulated version of the Hamiltonian is obtained as:

$$\begin{aligned}
\mathcal{S}_{KG,\phi} &= \frac{\kappa^2\beta^2\alpha_M}{2}\int_\Sigma d^3y\int_\Sigma d^3x\chi_\epsilon(x-y)\delta^{ij}\times \\
&\quad \frac{1}{\sqrt{V_{U^\epsilon_x}}}\widetilde{P}^a_i(x)(\partial_a\phi(x))\frac{1}{\sqrt{V_{U^\epsilon_y}}}\widetilde{P}^b_j(y)\partial_b\phi(y) \\
&= \frac{32\alpha_M}{\kappa^4\beta^4}\int_\Sigma d^3y\int_\Sigma d^3x\chi_\epsilon(x-y)\delta^{ij}\times \\
&\quad \widetilde{\eta}^{aec}(\partial_a\phi(x))\mathrm{Tr}(\tau_i\{\mathbf{A}_e(x), V^{3/4}_{U^\epsilon_x}\}\{\mathbf{A}_c(x), V^{3/4}_{U^\epsilon_x}\})\times \\
&\quad \widetilde{\eta}^{bfd}(\partial_b\phi(y))\mathrm{Tr}(\tau_j\{\mathbf{A}_f(y), V^{3/4}_{U^\epsilon_y}\}\{\mathbf{A}_d(y), V^{3/4}_{U^\epsilon_y}\}), \\
\mathcal{S}_{KG,Kin} &= \frac{1}{2\alpha_M}\int_\Sigma d^3x\widetilde{\pi}(x)\int_\Sigma d^3y\widetilde{\pi}(y)\times \\
&\quad \int_\Sigma d^3u\frac{\det(e^i_a(u))}{(V_{U^\epsilon_u})^{3/2}}\int_\Sigma d^3w\frac{\det(e^i_a(w))}{(V_{U^\epsilon_w})^{3/2}}\chi_\epsilon(x-y)\chi_\epsilon(u-x)\chi_\epsilon(w-y) \\
&= \frac{1}{2\alpha_M}\frac{2^8}{9(\kappa\beta)^6}\int_\Sigma d^3x\widetilde{\pi}(x)\int_\Sigma d^3y\widetilde{\pi}(y)\times \\
&\quad \int_\Sigma d^3u\,\widetilde{\eta}^{abc}\mathrm{Tr}(\{\mathbf{A}_a(u), \sqrt{V_{U^\epsilon_u}}\}\{\mathbf{A}_b(u), \sqrt{V_{U^\epsilon_u}}\}\{\mathbf{A}_c(u), \sqrt{V_{U^\epsilon_u}}\})\times \\
&\quad \int_\Sigma d^3w\,\widetilde{\eta}^{def}\mathrm{Tr}(\{\mathbf{A}_d(w), \sqrt{V_{U^\epsilon_w}}\}\{\mathbf{A}_e(w), \sqrt{V_{U^\epsilon_w}}\}\{\mathbf{A}_f(w), \sqrt{V_{U^\epsilon_w}}\})\times \\
&\quad \chi_\epsilon(x-y)\chi_\epsilon(u-x)\chi_\epsilon(w-y),
\end{aligned}$$

where we denote by $\mathbf{A}_a \equiv A^i_a\tau_i$, $\chi_\epsilon(x-y)$ the characteristic function of a box containing $x$ with scale $\epsilon$ such that $\lim_{\epsilon\to 0}\chi_\epsilon(x-y)/\epsilon^3 = \delta(x-y)$, and $V_{U^\epsilon_x}$ is the volume of the box. In order to quantize the Hamiltonian $\mathcal{S}_{KG}$ as a well-defined operator in the polymer-like representation, we have to express the classical formula of the Hamiltonian in terms of elementary variables with clear quantum analogs by introducing a triangulation $T(\epsilon)$ of $\Sigma$, where the parameter $\epsilon$ describes how fine the triangulation is. The quantity regulated on the triangulation is required to have correct limit when $\epsilon \to 0$. Given a tetrahedron $\Delta \in T(\epsilon)$, we use $\{s_i(\Delta)\}_{i=1,2,3}$ to denote the three outgoing oriented segments in $\Delta$ with a common beginning point $v(\Delta) = s(s_i(\Delta))$ and use $a_{ij}(\Delta)$ to denote the arcs connecting the end points of $s_i(\Delta)$ and $s_j(\Delta)$. Then several loops $\alpha_{ij}(\Delta)$ are formed by $\alpha_{ij}(\Delta) := s_i(\Delta) \circ a_{ij}(\Delta) \circ s_j(\Delta)^{-1}$. Thus we have the identities:

$$\{\int_{s(\Delta)} dt\, \mathbf{A}_a \dot{s}^a(t), V^{3/4}_{U^\epsilon_{s(s(\Delta))}}\} \;=\; -A(s(\Delta))^{-1}\{A(s(\Delta)), V^{3/4}_{U^\epsilon_{s(s(\Delta))}}\} + o(\epsilon),$$

and

$$\int_{s(\Delta)} dt\, \partial_a\phi \dot{s}^a(t) \;=\; \frac{1}{i\lambda} U(s(s(\Delta)),\lambda)^{-1}[U(t(s(\Delta)),\lambda) - U(s(s(\Delta)),\lambda)] + o(\epsilon)$$

for nonzero $\lambda$, where $s(s(\Delta))$ and $t(s(\Delta))$ denote respectively the beginning and end points of segment $s(\Delta)$ with scale $\epsilon$ associated with a tetrahedron $\Delta$. Regulated on the triangulation, the scalar field Hamiltonian reads

$$\begin{aligned}
\mathcal{S}^\epsilon_{KG,\phi} \;=\;& -\frac{4\alpha_M}{9\kappa^4\beta^4} \sum_{\Delta'\in T(\epsilon)} \sum_{\Delta\in T(\epsilon)} \chi_\epsilon(v(\Delta)-v(\Delta'))\delta^{ij} \times \\
& \epsilon^{lmn}\frac{1}{\lambda} U(v(\Delta),\lambda)^{-1}[U(t(s_l(\Delta)),\lambda) - U(v(\Delta),\lambda)] \times \\
& \mathrm{Tr}(\tau_i A(s_m(\Delta))^{-1}\{A(s_m(\Delta)), V^{3/4}_{U^\epsilon_{v(\Delta)}}\} A(s_n(\Delta))^{-1}\{A(s_n(\Delta)), V^{3/4}_{U^\epsilon_{v(\Delta)}}\}) \times \\
& \epsilon^{kpq}\frac{1}{\lambda} U(v(\Delta'),\lambda)^{-1}[U(t(s_k(\Delta')),\lambda) - U(v(\Delta'),\lambda)] \times \\
& \mathrm{Tr}(\tau_j A(s_p(\Delta'))^{-1}\{A(s_p(\Delta')), V^{3/4}_{U^\epsilon_{v(\Delta')}}\} A(s_q(\Delta'))^{-1}\{A(s_q(\Delta')), V^{3/4}_{U^\epsilon_{v(\Delta')}}\}), \\
\mathcal{S}^\epsilon_{KG,Kin} \;=\;& \frac{16}{81\alpha_M(\kappa\beta)^6} \sum_{\Delta\in T(\epsilon)} \sum_{\Delta'\in T(\epsilon)} \pi(\Delta)\pi(\Delta') \times \\
& \sum_{\Delta''\in T(\epsilon)} \epsilon^{imn}\mathrm{Tr}(A(s_i(\Delta''))^{-1}\{A(s_i(\Delta'')), \sqrt{V_{U^\epsilon_{v(\Delta'')}}}\} \times \\
& A(s_m(\Delta''))^{-1}\{A(s_m(\Delta'')), \sqrt{V_{U^\epsilon_{v(\Delta'')}}}\} \times \\
& A(s_n(\Delta''))^{-1}\{A(s_n(\Delta'')), \sqrt{V_{U^\epsilon_{v(\Delta'')}}}\}) \times \\
& \sum_{\Delta'''\in T(\epsilon)} \epsilon^{jkl}\mathrm{Tr}(A(s_j(\Delta'''))^{-1}\{A(s_j(\Delta''')), \sqrt{V_{U^\epsilon_{v(\Delta''')}}}\} \times \\
& A(s_k(\Delta'''))^{-1}\{A(s_k(\Delta''')), \sqrt{V_{U^\epsilon_{v(\Delta''')}}}\} \times \\
& A(s_l(\Delta'''))^{-1}\{A(s_l(\Delta''')), \sqrt{V_{U^\epsilon_{v(\Delta''')}}}\}) \times \\
& \chi_\epsilon(v(\Delta)-v(\Delta'))\chi_\epsilon(v(\Delta'')-v(\Delta))\chi_\epsilon(v(\Delta''')-v(\Delta')).
\end{aligned} \tag{57}$$

Note that the above regularization is explicitly dependent on the parameter $\lambda$, which will lead to a kind of quantization ambiguity of the real scalar field dynamics in polymer-like representation. Introducing a partition $\mathcal{P}$ of the 3-manifold $\Sigma$ into cells $C$, we can smear the essential "square roots" of $\mathcal{S}^{\epsilon}_{KG,\phi}$ and $\mathcal{S}^{\epsilon}_{KG,Kin}$ in one cell $C$ respectively and promote them as regulated operators in $\mathcal{H}_{kin}$ with respect to triangulations $T(\epsilon)$ depending on spin-scalar-network state $T_{s,c}$ as

$$
\begin{aligned}
\hat{W}^{\epsilon,C}_{\phi,i}T_{s,c} &= \sum_{v\in V(\gamma(s,c))}\frac{\chi_C(v)}{E(v)}\sum_{v(\Delta)=v}\hat{h}^{\epsilon,\Delta}_{\phi,v,i}T_{s,c}, \\
\hat{W}^{\epsilon,C}_{Kin}T_{s,c} &= \sum_{v\in V(\gamma(s,c))}\frac{\chi_C(v)}{E(v)}\sum_{v(\Delta)=v}\hat{h}^{\epsilon,\Delta}_{Kin,v}T_{s,c},
\end{aligned} \tag{58}
$$

where $\chi_C(v)$ is the characteristic function of the cell $C$, and

$$
\begin{aligned}
\hat{h}^{\epsilon,\Delta}_{\phi,v,i} &:= \frac{i}{\hbar^2}\epsilon^{lmn}\frac{1}{\lambda(v)}\hat{U}(v,\lambda(v))^{-1}[\hat{U}(t(s_l(\Delta)),\lambda(v))-\hat{U}(v,\lambda(v))]\times \\
&\quad \mathrm{Tr}(\tau_i\hat{A}(s_m(\Delta))^{-1}[\hat{A}(s_m(\Delta)),\hat{V}^{3/4}_{U^\epsilon_v}]\hat{A}(s_n(\Delta))^{-1}[\hat{A}(s_n(\Delta)),\hat{V}^{3/4}_{U^\epsilon_v}]), \\
\hat{h}^{\epsilon,\Delta}_{Kin,v} &:= \frac{1}{(i\hbar)^3}\hat{\pi}(v)\epsilon^{lmn}\mathrm{Tr}(\hat{A}(s_l(\Delta))^{-1}[\hat{A}(s_l(\Delta)),\sqrt{\hat{V}_{U^\epsilon_v}}]\times \\
&\quad \hat{A}(s_m(\Delta))^{-1}[\hat{A}(s_m(\Delta)),\sqrt{\hat{V}_{U^\epsilon_v}}]\times \\
&\quad \hat{A}(s_n(\Delta))^{-1}[\hat{A}(s_n(\Delta)),\sqrt{\hat{V}_{U^\epsilon_v}}]).
\end{aligned} \tag{59}
$$

Both operators in (58) and their adjoint operators are densely defined on $\mathcal{H}_{kin}$. We now give several remarks on their properties.

- Removal of regulator $\epsilon$

  It is not difficult to see that the action of the operator $\hat{W}^{\epsilon,C}_{\phi,i}$ on a spin-scalar-network function $T_{s,c}$ is graph-changing. It adds finite number of vertices with representation $\lambda(v)$ at $t(s_i(\Delta))$ with distance $\epsilon$ from the vertex $v$. Recall that the action of the gravitational Hamiltonian constraint operator on a spin network function is also graph-changing. As a result, the family of operators $\hat{W}^{\epsilon,C}_{\phi,i}$ also fails to be weakly converged when $\epsilon\to 0$. However, due to the diffeomorphism covariant properties of the triangulation, the limit operator can be well-defined via the uniform Rovelli-Smolin topology, or equivalently, the operator can be dually defined on diffeomorphism invariant states. But the dual operator cannot leave $\mathcal{H}_{Diff}$ invariant.

- Quantization ambiguity

  As a main difference of the dynamics in polymer-like representation from that in U(1) group representation [138], a continuous label $\lambda$ appears explicitly in the expression of (58). Hence there is an one-parameter quantization ambiguity due to the real scalar field. Recall that the construction of gravitational Hamiltonian constraint operator also has a similar ambiguity due to the choice of the representations $j$ of the edges added by its action. A related quantization ambiguity also appears in the dynamics of loop quantum cosmology [50].

Since our quantum field theory is expected to be diffeomorphism invariant, we would like to define the Hamiltonian operator of polymer scalar field in the diffeomorphism invariant Hilbert space $\mathcal{H}_{Diff}$. For this purpose we fix the parameter $\lambda$ to be a non-zero constant at every point. Then what we will do is to employ the new quantization strategy developed in Refs. [149] and [140]. We first construct a quadratic form in the light of a new inner product defined in Ref.[140] on the algebraic dual $\mathcal{D}^\star$ of the space of cylindrical functions which is spanned by spin-scalar-networks $T_{s,c}$ (where the family of labels $s, c$ includes the vacuum states for gravity, scalar and both). Then we prove that the quadratic form is closed. Note that, although the calculation employing this inner product is formal, it can lead to a well-defined expression of the desired quadratic form Eq.(65). Since an arbitrary element of $\mathcal{D}^\star$ is of the form $\Psi = \sum_{s,c} c_{s,c} < T_{s,c}| \cdot >_{kin}$, one can formally define an inner product $< \cdot |\cdot >_\star$ on $\mathcal{D}^\star$ via

$$\begin{aligned} <\Psi, \Psi'>_\star &:= <\sum_{s,c} c_{s,c} < T_{s,c}| \cdot >_{kin} | \sum_{s',c'} c'_{s',c'} < T_{s',c'}| \cdot >_{kin}>_\star \\ &:= \sum_{s,c;s',c'} c_{s,c}\overline{c'_{s',c'}} < T_{s,c}|T_{s',c'} >_{kin} \frac{1}{\sqrt{\aleph([s,c])\aleph([s',c'])}} \\ &= \sum_{s,c} c_{s,c}\overline{c'_{s,c}}\frac{1}{\aleph([s,c])}, \end{aligned} \tag{60}$$

where the Cantor aleph $\aleph$ denotes the cardinal of the set $[s, c]$. Note that we exchange the coefficients on which the complex conjugate was taken in Ref.[140], so that the inner product $< \Psi_{Diff}|\Psi'_{Diff} >_\star$ reduces to $< \Psi_{Diff}|\Psi'_{Diff} >_{Diff}$ for any $\Psi_{Diff}, \Psi'_{Diff} \in \mathcal{H}_{Diff}$. Completing the quotient with respect to the null vectors by this inner product, one gets a Hilbert space $\mathcal{H}_\star$. Our purpose is to construct a quadratic form associated to some positive and symmetric operator in analogy with the classical expression of (57). So the quadratic form should first be given in a positive and symmetric version. It is then natural to define two quadratic forms on a dense subset of $\mathcal{H}_{Diff} \subset \mathcal{H}_\star$ as:

$$\begin{aligned} Q_{KG,\phi}(\Psi_{Diff}, \Psi'_{Diff}) &:= \lim_{\mathcal{P}\to\Sigma} \sum_{C\in\mathcal{P}} 64 \times \frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij} < \hat{W}'^C_{\phi,i}\Psi_{Diff}|\hat{W}'^C_{\phi,j}\Psi'_{Diff} >_\star, \\ Q_{KG,Kin}(\Psi_{Diff}, \Psi'_{Diff}) &:= \lim_{\mathcal{P}\to\Sigma} \sum_{C\in\mathcal{P}} 8^4 \times \frac{16}{81\alpha_M(\kappa\beta)^6} < \hat{W}'^C_{Kin}\Psi_{Diff}|\hat{W}'^C_{Kin}\Psi'_{Diff} >_\star, \end{aligned} \tag{61}$$

for any two states $\Psi_{Diff}$ and $\Psi'_{Diff}$ which are finite linear combinations of $T_{[s,c]}$, where the dual limit operator $\hat{W}'^C$ of either family of $\hat{W}^{\epsilon,C}_{\phi,i}$ or $\hat{W}^{\epsilon,C}_{Kin}$ in (58) is naturally defined on diffeomorphism invariant states as

$$\hat{W}'^C\Psi_{Diff}[T_{s,c}] = \lim_{\epsilon\to 0} \Psi_{Diff}[\hat{W}^{\epsilon,C}T_{s,c}]. \tag{62}$$

To show that the quadratic forms are well defined, we write

$$\begin{aligned} \hat{W}'^C_{\phi,i}\Psi_{Diff} = \sum_{s,c} w^\Psi_{\phi,i,s,c}(C) < T_{s,c}| \cdot >_\star \ &\Rightarrow\ w^\Psi_{\phi,i,s,c}(C) = (\hat{W}'^C_{\phi,i}\Psi_{Diff})[T_{s,c}], \\ \hat{W}'^C_{Kin}\Psi_{Diff} = \sum_{s,c} w^\Psi_{Kin,s,c}(C) < T_{s,c}| \cdot >_\star \ &\Rightarrow\ w^\Psi_{Kin,s,c}(C) = (\hat{W}'^C_{Kin}\Psi_{Diff})[T_{s,c}]. \end{aligned}$$

Then, by using the inner product (60) the quadratic forms in (61) become

$$
\begin{aligned}
& Q_{KG,\phi}(\Psi_{Diff},\Psi'_{Diff}) \\
:= & \lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}} 64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}\sum_{s,c} w^{\Psi}_{\phi,i,s,c}(C)\overline{w^{\Psi'}_{\phi,j,s,c}(C)}\frac{1}{\aleph([s,c])} \\
= & \lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}} 64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}\sum_{[s,c]}\frac{1}{\aleph([s,c])}\sum_{s,c\in[s,c]} w^{\Psi}_{\phi,i,s,c}(C)\overline{w^{\Psi'}_{\phi,j,s,c}(C)}, \\
& \overline{Q_{KG,Kin}(\Psi_{Diff},\Psi'_{Diff})} \\
:= & \lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}} 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}\sum_{s,c} w^{\Psi}_{Kin,s,c}(C)\overline{w^{\Psi'}_{Kin,s,c}(C)}\frac{1}{\aleph([s,c])} \\
= & \lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}} 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}\sum_{[s,c]}\frac{1}{\aleph([s,c])}\sum_{s,c\in[s,c]} w^{\Psi}_{Kin,s,c}(C)\overline{w^{\Psi'}_{Kin,s,c}(C)}.
\end{aligned}
\tag{63}
$$

Note that, since $\Psi_{Diff}$ is a finite linear combination of the diffeomorphism invariant spin-scalar-network basis, taking account of the operational property of $\hat{W}'^C$ there are only a finite number of terms in the summation $\sum_{[s,c]}$ contributing to (63). Hence we can interchange $\sum_{[s,c]}$ and $\lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}}$ in above calculation. Moreover, for a sufficiently fine partition such that each cell contains at most one vertex, the sum over cells therefore reduces to finite terms with respect to the vertices of $\gamma(s,c)$. So we can interchange $\sum_{s,c\in[s,c]}$ and $\lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}}$ to obtain:

$$
\begin{aligned}
& Q_{KG,\phi}(\Psi_{Diff},\Psi'_{Diff}) \\
= & 64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}\sum_{[s,c]}\frac{1}{\aleph([s,c])}\sum_{s,c\in[s,c]}\lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}} w^{\Psi}_{\phi,i,s,c}(C)\overline{w^{\Psi'}_{\phi,j,s,c}(C)} \\
= & 64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}\sum_{[s,c]}\frac{1}{\aleph([s,c])}\sum_{s,c\in[s,c]}\sum_{v\in V(\gamma(s,c))}(\hat{W}'^v_{\phi,i}\Psi_{Diff})[T_{s,c}]\overline{(\hat{W}'^v_{\phi,j}\Psi'_{Diff})[T_{s,c}]}, \\
& Q_{KG,Kin}(\Psi_{Diff},\Psi'_{Diff}) \\
= & 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}\sum_{[s,c]}\frac{1}{\aleph([s,c])}\sum_{s,c\in[s,c]}\lim_{\mathcal{P}\to\Sigma}\sum_{C\in\mathcal{P}} w^{\Psi}_{Kin,s,c}(C)\overline{w^{\Psi'}_{Kin,s,c}(C)} \\
= & 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}\sum_{[s,c]}\frac{1}{\aleph([s,c])}\sum_{s,c\in[s,c]}\sum_{v\in V(\gamma(s,c))}(\hat{W}'^v_{Kin}\Psi_{Diff})[T_{s,c}]\overline{(\hat{W}'^v_{Kin}\Psi'_{Diff})[T_{s,c}]},
\end{aligned}
\tag{64}
$$

where the limit $\mathcal{P}\to\Sigma$ has been taken so that $C\to v$. Since given $\gamma(s,c)$ and $\gamma(s',c')$ which are different up to a diffeomorphism transformation, there is always a diffeomorphism $\varphi$ transforming the graph associated with $\hat{W}^{\epsilon,v}T_{s,c}$ ($v\in\gamma(s,c)$) to that of $\hat{W}^{\epsilon,v'}T_{s',c'}$ ($v'\in\gamma(s',c')$) with $\varphi(v)=v'$, $(\hat{W}'^v\Psi_{Diff})[T_{s,c\in[s,c]}]$ is constant for different $(s,c)\in[s,c]$, i.e., all the $\aleph([s,c])$ terms in the sum over $(s,c)\in[s,c]$ are identical. Hence the final expressions of the two quadratic forms can be written as:

$$
Q_{KG,\phi}(\Psi_{Diff},\Psi'_{Diff})
$$

$$
\begin{aligned}
&= 64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}\sum_{[s,c]}\sum_{v\in V(\gamma(s,c))}(\hat{W}'^{v}_{\phi,i}\Psi_{Diff})[T_{s,c\in[s,c]}]\overline{(\hat{W}'^{v}_{\phi,j}\Psi'_{Diff})[T_{s,c\in[s,c]}]},\\
&Q_{KG,Kin}(\Psi_{Diff},\Psi'_{Diff})\\
&= 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}\sum_{[s,c]}\sum_{v\in V(\gamma(s,c))}(\hat{W}'^{v}_{Kin}\Psi_{Diff})[T_{s,c\in[s,c]}]\overline{(\hat{W}'^{v}_{Kin}\Psi'_{Diff})[T_{s,c\in[s,c]}]}.
\end{aligned}
\tag{65}
$$

Note that both quadratic forms in (65) have finite results and hence their form domains are dense in $\mathcal{H}_{Diff}$. Moreover, both of them are obviously positive, and the following theorem will demonstrate their closedness.

**Theorem 5.2.1**: *Both $Q_{KG,\phi}$ and $Q_{KG,Kin}$ are densely defined, positive and closed quadratic forms on $\mathcal{H}_{Diff}$, which are associated uniquely with two positive self-adjoint operators respectively on $\mathcal{H}_{Diff}$ such that*

$$
\begin{aligned}
Q_{KG,\phi}(\Psi_{Diff},\Psi'_{Diff}) &= <\Psi_{Diff}|\hat{\mathcal{S}}_{KG,\phi}|\Psi'_{Diff}>_{Diff}\\
Q_{KG,Kin}(\Psi_{Diff},\Psi'_{Diff}) &= <\Psi_{Diff}|\hat{\mathcal{S}}_{KG,Kin}|\Psi'_{Diff}>_{Diff}\ .
\end{aligned}
$$

*Therefore the Hamiltonian operator*

$$
\hat{\mathcal{S}}_{KG}:=\hat{\mathcal{S}}_{KG,\phi}+\hat{\mathcal{S}}_{KG,Kin} \tag{66}
$$

*is positive and also have a unique self-adjoint extension.*

**Proof**: We follow the strategy developed in Refs.[140] and [88] to prove that both $Q_{KG,\phi}$ and $Q_{KG,Kin}$ are closeable and uniquely induce two positive self-adjoint operators $\hat{\mathcal{S}}_{KG,\phi}$ and $\hat{\mathcal{S}}_{KG,Kin}$. One can formally define $\hat{\mathcal{S}}_{KG,\phi}$ and $\hat{\mathcal{S}}_{KG,Kin}$ acting on diffeomorphism invariant spin-scalar network functions via:

$$
\hat{\mathcal{S}}_{KG,\phi}\ T_{[s_1,c_1]} := \sum_{[s_2,c_2]}Q_{KG,\phi}(T_{[s_2,c_2]},T_{[s_1,c_1]})T_{[s_2,c_2]}, \tag{67}
$$

$$
\hat{\mathcal{S}}_{KG,Kin}\ T_{[s_1,c_1]} := \sum_{[s_2,c_2]}Q_{KG,Kin}(T_{[s_2,c_2]},T_{[s_1,c_1]})T_{[s_2,c_2]}. \tag{68}
$$

Then we need to show that both of the above operators are densely defined on the Hilbert space $\mathcal{H}_{Diff}$. Given a diffeomorphism invariant spin-scalar network function $T_{[s_1,c_1]}$, there are only a finite number of terms $T_{[s_1,c_1]}[\hat{W}^{\epsilon,v}T_{s,c\in[s,c]}]$ which are nonzero in the sum over equivalent classes $[s,c]$ in (65). On the other hand, given one spin-scalar-network function $T_{s,c\in[s,c]}$, there are also only a finite number of possible $T_{[s_2,c_2]}$ such that the terms $\overline{T_{[s_2,c_2]}[\hat{W}^{\epsilon,v}T_{s,c\in[s,c]}]}$ are nonzero. As a result, only a finite number of terms survive in both sums over $[s_2,c_2]$ in Eqs. (67) and (68). Hence both $\hat{\mathcal{S}}_{KG,\phi}$ and $\hat{\mathcal{S}}_{KG,Kin}$ are well defined on spin-scalar-network basis. Then it follows from Eqs. (65), (67) and (68) that they are positive and symmetric operators densely defined in $\mathcal{H}_{Diff}$, whose quadratic forms coincide with $Q_{KG,\phi}$ and $Q_{KG,Kin}$ on their form domains. Hence both $Q_{KG,\phi}$ and $Q_{KG,Kin}$ have positive closures and uniquely induce self-adjoint

(Friedrichs) extensions of $\hat{\mathcal{S}}_{KG,\phi}$ and $\hat{\mathcal{S}}_{KG,Kin}$ respectively [114], which we denote by $\hat{\mathcal{S}}_{KG,\phi}$ and $\hat{\mathcal{S}}_{KG,Kin}$ as well. As a result, the Hamiltonian operator $\hat{\mathcal{S}}_{KG}$ defined by Eq.(66) is also positive and symmetric. Hence it has a unique self-adjoint (Friedrichs) extension.

□

We notice that, from a different perspective, one can construct the same Hamiltonian operator $\hat{\mathcal{H}}_{KG}$ without introducing an inner product on $\mathcal{D}^\star$. The construction is sketched as follows. Using the two well-defined operators $\hat{W}^{\epsilon,C}_{\phi,i}$ and $\hat{W}^{\epsilon,C}_{Kin}$ as in (58), as well as their adjoint operators $(\hat{W}^{\epsilon,C}_{\phi,i})^\dagger$ and $(\hat{W}^{\epsilon,C}_{Kin})^\dagger$, one may define two operators on $\mathcal{H}_{Diff}$ corresponding to the two terms in (57) by

$$
\begin{aligned}
(\hat{\mathcal{S}}_{KG,\phi}\Psi_{Diff})[T_{s,c}] &= \lim_{\epsilon,\epsilon'\to 0,\mathcal{P}\to\Sigma}\Psi_{Diff}[\sum_{C\in\mathcal{P}} 64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}\hat{W}^{\epsilon,C}_{\phi,i}(\hat{W}^{\epsilon',C}_{\phi,j})^\dagger T_{s,c}] \\
(\hat{\mathcal{S}}_{KG,Kin}\Psi_{Diff})[T_{s,c}] &= \lim_{\epsilon,\epsilon'\to 0,\mathcal{P}\to\Sigma}\Psi_{Diff}[\sum_{C\in\mathcal{P}} 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}\hat{W}^{\epsilon,C}_{Kin}(\hat{W}^{\epsilon',C}_{Kin})^\dagger T_{s,c}],
\end{aligned}
\tag{69}
$$

for any spin-scalar-network $T_{s,c}$. In analogy with the discussion about the master constraint operator and Ref.[88], it can be shown that both above operators leave $\mathcal{H}_{Diff}$ invariant and are densely defined on $\mathcal{H}_{Diff}$. Moreover, the quadratic forms associated with them coincide with the quadratic forms in (65). Thus the Hamiltonian operator $\hat{\mathcal{S}}_{KG} := \hat{\mathcal{S}}_{KG,\phi} + \hat{\mathcal{S}}_{KG,Kin}$ coincides with the one constructed in the quadratic form approach.

In summary, we have constructed a positive self-adjoint Hamiltonian operator on $\mathcal{H}_{Diff}$ for the polymer-like scalar field, depending on a chosen parameter $\lambda$. Thus there is an 1-parameter ambiguity in the construction. However, there is no UV divergence in this quantum Hamiltonian without renormalization, since quantum gravity plays the role of a natural regulator for the polymer-like scalar field.

## 5.3 Hamiltonian Constraint Equation for the Coupled System

In this section we consider the whole dynamical system of scalar field coupled to gravity. Recall that in perturbative quantum field theory in curved spacetime, the definition of some basic physical quantities, such as the expectation value of the energy-momentum, is ambiguous and it is challenging difficult to calculate the back-reaction of quantum fields on the background spacetime [157]. This is reflected by the fact that the semi-classical Einstein equation,

$$
R_{\alpha\beta}[g]-\frac{1}{2}R[g]g_{\alpha\beta}=\kappa<\hat{T}_{\alpha\beta}[g]>, \tag{70}
$$

are known to be inconsistent and ambiguous [70][146]. One could speculate that the difficulty is related to the fact that the usual formulation of quantum field theories are background dependent. Following this line of thought, if the quantization programme is by construction non-perturbative and background independent, it may be possible to solve the problems fundamentally. In loop quantum gravity, there is no assumption of a priori background metric at all. The quantum geometry and quantum matter fields are coupled and fluctuating naturally with respect to each other on a common manifold. On the other hand, there exists the "time problem" in quantum theory of pure gravity, since all the physical states have to satisfy certain version of quantum Wheeler-DeWitt constraint equation. However, the situation could improve when matter field is coupled to gravity [54][122]. In the following construction, we impose the quantum Hamiltonian constraint on $\mathcal{H}_{kin}$, and thus define a quantum Wheeler-DeWitt constraint equation for the scalar field coupled to gravity. Then one can gain an insight into the problem of time from the coupled equation, and the back-reaction of the quantum scalar field is included in the framework of loop quantum gravity.

We now define an operator in $\mathcal{H}_{kin}$ corresponding to the scalar field part $\mathcal{S}_{KG}(N)$ of the total Hamiltonian constraint functional, which can be read out from Eqs. (35) and (50) as

$$\mathcal{S}_{KG}(N) \;=\; \mathcal{S}_{KG,\phi}(N) + \mathcal{S}_{KG,Kin}(N),$$

where

$$\begin{aligned}\mathcal{S}_{KG,\phi}(N) &= \frac{\kappa^2\beta^2\alpha_M}{2}\int_\Sigma d^3x N \frac{1}{\sqrt{|\det q|}}\delta^{ij}\widetilde{P}^a_i\widetilde{P}^b_j(\partial_a\phi)\partial_b\phi,\\ \mathcal{S}_{KG,Kin}(N) &= \frac{1}{2\alpha_M}\int_\Sigma d^3x N\frac{1}{\sqrt{|\det q|}}\widetilde{\pi}^2.\end{aligned}$$

In analogy with the regularization and quantization in the previous section, the regulated version of quantum Hamiltonian constraint $\hat{\mathcal{S}}^\epsilon_{KG}(N)$ of scalar field is expressed by taking the limit $C \to v$:

$$\begin{aligned}\hat{\mathcal{S}}^\epsilon_{KG}(N)T_{s,c} \;:=\; &\sum_{v\in V(\gamma(s,c))} N(v)[64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}(\hat{W}^{\epsilon,v}_{\phi,i})^\dagger\hat{W}^{\epsilon,v}_{\phi,j}\\ &+\; 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}(\hat{W}^{\epsilon,v}_{Kin})^\dagger\hat{W}^{\epsilon,v}_{Kin}]T_{s,c},\end{aligned} \tag{71}$$

where for any $v\in V(\gamma(s,c))$, the operators

$$\begin{aligned}\hat{W}^{\epsilon,v}_{\phi,i}T_{s,c} &= \frac{1}{E(v)}\sum_{v(\Delta)=v}\hat{h}^{\epsilon,\Delta}_{\phi,v,i}T_{s,c},\\ \hat{W}^{\epsilon,v}_{Kin}T_{s,c} &= \frac{1}{E(v)}\sum_{v(\Delta)=v}\hat{h}^{\epsilon,\Delta}_{Kin,v}T_{s,c},\end{aligned}$$

and their adjoints are all densely defined in $\mathcal{H}_{kin}$. Hence the family of Hamiltonian constraint operators (71) is also densely defined, and the regulator $\epsilon$ can be removed via the Uniform Rovelli-Smollin topology, or equivalently the limit operator dually acts on diffeomorphism invariant states as

$$(\hat{\mathcal{S}}'_{KG}(N)\Psi_{Diff})[f] = \lim_{\epsilon\to 0}\Psi_{Diff}[\hat{\mathcal{S}}^\epsilon_{KG}(N)f], \tag{72}$$

for any $f\in Cyl(\overline{\mathcal{A}/\mathcal{G}})\otimes Cyl(\overline{\mathcal{U}})$. Similar to the dual of $\hat{S}_{GR}(N)$, the operator $\hat{\mathcal{S}}'_{KG}(N)$ fails to commute with the dual of finite diffeomorphism transformation operators, unless the smearing function $N(x)$ is a constant function over $\Sigma$. In fact, the dual Hamiltonian constraint operator smeared by $N = 1$ is just the diffeomorphism invariant Hamiltonian we just defined in the last subsection. From Eq.(71), it is not difficult to prove that for positive $N(x)$ the Hamiltonian constraint operator $\hat{\mathcal{S}}_{KG}(N)$ of a scalar field is positive and symmetric in $\mathcal{H}_{kin}$ and hence has a unique self-adjoint extension [89]. Our construction of $\hat{\mathcal{S}}_{KG}(N)$ is similar to that of the Higgs field Hamiltonian constraint in Ref.[138]. However, like the case of $\hat{\mathcal{S}}_{KG}$, there is a one-parameter ambiguity in our construction of $\hat{\mathcal{S}}_{KG}(N)$ due to the real scalar field, which is manifested as the continuous parameter $\lambda$ in the expression of $\hat{h}^{\epsilon,\Delta}_{\phi,v,i}$ in (59). Note that now $\lambda$ is not required to be a constant, i.e., its value can be changed from one point to another. Thus the total Hamiltonian constraint operator of scalar field coupled to gravity has been obtained as

$$\hat{\mathcal{S}}(N) = \hat{\mathcal{S}}_{GR}(N) + \hat{\mathcal{S}}_{KG}(N). \tag{73}$$

Again, there is no UV divergence in this quantum Hamiltonian constraint. Recall that, in standard quantum field theory the UV divergence can only be cured by a renormalization procedure, in which one has to multiply the Hamiltonian by a suitable power of the regulating parameter $\epsilon$. However, now $\epsilon$ has naturally disappeared from the expression of (73). So renormalization is not needed for the polymer-like scalar field coupled to gravity, since quantum gravity has played the role of a natural regulator. This result heightens our confidence that the issue of divergences in quantum field theory can be cured in the framework of loop quantum gravity.

Now we have obtained the desired matter-coupled quantum Hamiltonian constraint equation

$$-(\hat{\mathcal{S}}'_{KG}(N)\Psi_{Diff})[f] = (\hat{\mathcal{S}}'_{GR}(N)\Psi_{Diff})[f]. \tag{74}$$

Comparing it with the well-known Schördinger equation for a particle,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H(\hat{x}, \widehat{-i\hbar\frac{\partial}{\partial x}})\psi(x,t),$$

where $\psi(x,t) \in L^2(\mathbf{R}, dx)$ and $t$ is a parameter labeling time evolution, one may take the viewpoint that the matter field constraint operator $\hat{\mathcal{S}}'_{KG}(N)$ plays the role of $i\hbar\frac{\partial}{\partial t}$. Then $\phi$ appears as the parameter labeling the evolution of the gravitational field state. In the reverse viewpoint, the gravitational field would become the parameter labeling the evolution of the quantum matter field. Note that such an idea has been successfully applied in a loop quantum cosmology model to help us to understand the quantum nature of big bang in the deep Planck regime [28][29].

## 5.4 Master Constraint for the Coupled System

Recall that in order to avoid possible quantum anomalies and find the physical Hilbert space of quantum gravity, the master constraint programme was first introduced in the last section. The central idea is to construct an alternative classical constraint algebra, giving the same constraint phase space, which is a Lie algebra (no structure functions) and where the subalgebra of diffeomorphism constraints forms an ideal. A self-adjoint master constraint operator for loop quantum gravity is then proposed on $\mathcal{H}_{Diff}$. The master constraint programme can be generalized to matter fields coupled to gravity in a straightforward way. We now take the massless real scalar field to demonstrate the construction of a master constraint operator according to the same strategy as we did in the last section. By this approach one not only avoids possible quantum anomalies which might appear in the conventional canonical quantization method, but also might give a qualitative description of the physical Hilbert space for the coupled system. We introduce the master constraint for the scalar field coupled to gravity as

$$\mathbf{M} := \frac{1}{2}\int_\Sigma d^3x \frac{|C(x)|^2}{\sqrt{|\det q(x)|}}, \tag{75}$$

where $C(x)$ is the Hamiltonian constraint in (50). After solving the Gaussian constraint, one gets the master constraint algebra as a Lie algebra:

$$\begin{aligned} \{\mathcal{V}(\vec{N}),\ \mathcal{V}(\vec{N}')\} &= \mathcal{V}([\vec{N},\vec{N}']), \\ \{\mathcal{V}(\vec{N}),\ \mathbf{M}\} &= 0, \\ \{\mathbf{M},\ \mathbf{M}\} &= 0, \end{aligned} \tag{76}$$

where the subalgebra of diffeomorphism constraints forms an ideal. So it is possible to define a corresponding master constraint operator on $\mathcal{H}_{Diff}$. In the following, the positivity and the diffeomorphism invariance of $\mathbf{M}$ will be working together properly and provide us with powerful functional analytic tools in the quantization procedure.

The regulated version of the master constraint can be expressed via a point-splitting strategy as:

$$\mathbf{M}^\epsilon := \frac{1}{2}\int_\Sigma d^3y \int_\Sigma d^3x \chi_\epsilon(x-y)\frac{C(y)}{\sqrt{V_{U^\epsilon_y}}}\frac{C(x)}{\sqrt{V_{U^\epsilon_x}}}. \tag{77}$$

Introducing a partition $\mathcal{P}$ of the 3-manifold $\Sigma$ into cells $C$, we have an operator $\hat{H}^\epsilon_C$ acting on any spin-scalar-network state $T_{s,c}$ via a family of state-dependent triangulation $T(\epsilon)$,

$$\begin{aligned} \hat{H}^\epsilon_C T_{s,c} &= \sum_{v\in V(\gamma(s,c))}\frac{\chi_C(v)}{E(v)}\sum_{v(\Delta)=v}\hat{h}^{\epsilon,\Delta}_{GR,v}T_{s,c} \\ &+ \sum_{v\in V(\gamma(s,c))}\frac{\chi_C(v)}{E(v)}[64\times\frac{4\alpha_M}{9\kappa^4\beta^4}\delta^{ij}(\hat{w}^{\epsilon,v}_{\phi,i})^\dagger\hat{w}^{\epsilon,v}_{\phi,j} \\ &+ 8^4\times\frac{16}{81\alpha_M(\kappa\beta)^6}(\hat{w}^{\epsilon,v}_{Kin})^\dagger\hat{w}^{\epsilon,v}_{Kin}]T_{s,c}, \end{aligned} \tag{78}$$

where

$$\begin{aligned} \hat{h}^{\epsilon,\Delta}_{GR,v} &= \frac{16}{3i\hbar\kappa^2\beta}\epsilon^{ijk}\mathrm{Tr}(\hat{A}(\alpha_{ij}(\Delta))^{-1}\hat{A}(s_k(\Delta))^{-1}[\hat{A}(s_k(\Delta)),\ \sqrt{\hat{V}_{U^\epsilon_v}}]) \\ &+ (1+\beta^2)\frac{8\sqrt{2}}{3i\hbar^3\kappa^4\beta^3}\epsilon^{ijk}\mathrm{Tr}(\hat{A}(s_i(\Delta))^{-1}[\hat{A}(s_i(\Delta)),\hat{K}^\epsilon] \\ &\times \hat{A}(s_j(\Delta))^{-1}[\hat{A}(s_j(\Delta)),\hat{K}^\epsilon]\hat{A}(s_k(\Delta))^{-1}[\hat{A}(s_k(\Delta)),\ \sqrt{\hat{V}_{U^\epsilon_v}}]), \\ \hat{w}^{\epsilon,v}_{\phi,i} &= \frac{i}{\hbar^2}\sum_{v(\Delta)=v}\epsilon^{lmn}\frac{1}{\lambda}\hat{U}(v,\lambda)^{-1}[\hat{U}(t(s_l(\Delta)),\lambda)-\hat{U}(v,\lambda)] \\ &\times \mathrm{Tr}(\tau_i\hat{A}(s_m(\Delta))^{-1}[\hat{A}(s_m(\Delta)),\hat{V}^{5/8}_{U^\epsilon_v}]\hat{A}(s_n(\Delta))^{-1}[\hat{A}(s_n(\Delta)),\hat{V}^{5/8}_{U^\epsilon_v}]), \end{aligned}$$

$$\begin{aligned}\hat{w}^{\epsilon,v}_{Kin} &= \frac{1}{(i\hbar)^3}\sum_{v(\Delta)=v}\hat{\pi}(v)\epsilon^{lmn}\\ &\times\ \mathrm{Tr}(\hat{A}(s_l(\Delta))^{-1}[\hat{A}(s_l(\Delta)),\hat{V}^{5/12}_{U^\epsilon_v}]\hat{A}(s_m(\Delta))^{-1}[\hat{A}(s_m(\Delta)),\hat{V}^{5/12}_{U^\epsilon_v}]\\ &\times\ \hat{A}(s_n(\Delta))^{-1}[\hat{A}(s_n(\Delta)),\hat{V}^{5/12}_{U^\epsilon_v}]). \end{aligned} \tag{79}$$

Hence the action of $\hat{H}^\epsilon_C$ on a cylindrical function $f_\gamma$ adds analytical arcs $a_{ij}(\Delta)$ with $\frac{1}{2}$-representation and points at $t(s_i(\Delta))$ with representation constant $\lambda$ with respect to each vertex $v(\Delta)$ of $\gamma$. Thus, for each $\epsilon > 0$, $\hat{H}^\epsilon_C$ is a $SU(2)$ gauge invariant and diffeomorphism covariant operator defined on $Cyl(\overline{\mathcal{A}/\mathcal{G}}) \otimes Cyl(\overline{\mathcal{U}})$. The limit operator $\hat{H}_C$ is densely defined on $\mathcal{H}_{Kin}$ by the uniform Rovelli-Smolin topology. And the same result holds for the adjoint operator $(\hat{H}^\epsilon_C)^\dagger$

Then a master constraint operator, $\hat{\mathbf{M}}$, on $\mathcal{H}_{Diff}$ can be defined by:

$$(\hat{\mathbf{M}}\Psi_{Diff})[T_{s,c}] := \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}\Psi_{Diff}[\sum_{C\in\mathcal{P}}\frac{1}{2}\hat{H}^\epsilon_C(\hat{H}^{\epsilon'}_C)^\dagger T_{s,c}]. \tag{80}$$

Since $\hat{H}^\epsilon_C(\hat{H}^{\epsilon'}_C)^\dagger T_{s,c}$ is a finite linear combination of spin-scalar-network functions on an graph with skeleton $\gamma$, the value of $(\hat{\mathbf{M}}\Psi_{Diff})[T_{s,c}]$ is finite for a given $\Psi_{Diff}$ that is a finite linear combination of $T_{[s,c]}$. So $\hat{\mathbf{M}}\Psi_{Diff}$ is in the algebraic dual of the space of cylindrical functions. Moreover, we can show that it is diffeomorphism invariant. For any diffeomorphism transformation $\varphi$,

$$\begin{aligned}(\hat{U}'_\varphi\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma] &= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}\Psi_{Diff}[\sum_{C\in\mathcal{P}}\frac{1}{2}\hat{H}^\epsilon_C(\hat{H}^{\epsilon'}_C)^\dagger\hat{U}_\varphi f_\gamma]\\ &= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}\Psi_{Diff}[\hat{U}_\varphi\sum_{C\in\mathcal{P}}\frac{1}{2}\hat{H}^{\varphi^{-1}(\epsilon)}_{\varphi^{-1}(C)}(\hat{H}^{\varphi^{-1}(\epsilon')}_{\varphi^{-1}(C)})^\dagger f_\gamma]\\ &= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}\Psi_{Diff}[\sum_{C\in\mathcal{P}}\frac{1}{2}\hat{H}^\epsilon_C(\hat{H}^{\epsilon'}_C)^\dagger f_\gamma],\end{aligned} \tag{81}$$

for any cylindrical function $f_\gamma$, where in the last step, we used the fact that the diffeomorphism transformation $\varphi$ leaves the partition invariant in the limit $\mathcal{P}\to\Sigma$ and relabel $\varphi(C)$ to be $C$. So we have the result

$$(\hat{U}'_\varphi\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma] = (\hat{\mathbf{M}}\Psi_{Diff})[f_\gamma]. \tag{82}$$

So given a diffeomorphism invariant spin-scalar-network state $T_{[s,c]}$, the result state $\hat{\mathbf{M}}T_{[s,c]}$ must be a diffeomorphism invariant element in the algebraic dual of $Cyl(\overline{\mathcal{A}/\mathcal{G}})\otimes Cyl(\overline{\mathcal{U}})$, which means that

$$\hat{\mathbf{M}}T_{[s,c]} = \sum_{[s_1,c_1]} c_{[s_1,c_1]}T_{[s_1,c_1]},$$

then

$$\lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}T_{[s,c]}[\sum_{C\in\mathcal{P}}\frac{1}{2}\hat{H}^\epsilon_C(\hat{H}^{\epsilon'}_C)^\dagger T_{s_2,c_2}] = \sum_{[s_1,c_1]}c_{[s_1,c_1]}T_{[s_1,c_1]}[T_{s_2,c_2}],$$

where the cylindrical function $\sum_{C\in\mathcal{P}}\frac{1}{2}\hat{H}^{\epsilon'}_C(\hat{H}^{\epsilon}_C)^\dagger T_{s_2,c_2}$ is a finite linear combination of spin-scalar-network functions on some graphs $\gamma'$ with the same skeleton of $\gamma(s_2,c_2)$ up to finite number of arcs and vertices. Hence fixing the diffeomorphism equivalence class $[s,c]$, only for spin-scalar-networks $s_2,c_2$ lying in a finite number of diffeomorphism equivalence class on the left hand side of the last equation is non-zero. So there are also only finite number of classes $[s_1,c_1]$ in the right hand side such that $c_{[s_1,c_1]}$ is non-zero. As a result, $\hat{\mathbf{M}}T_{[s,c]}$ is a finite linear combination of diffeomorphism invariant spin-network states so lies in the Hilbert space of diffeomorphism invariant states $\mathcal{H}_{Diff}$ for any $[s,c]$. And $\hat{\mathbf{M}}$ is densely defined on $\mathcal{H}_{Diff}$.

We now compute the matrix elements of $\hat{\mathbf{M}}$. Given two diffeomorphism invariant spin-scalar-network functions $T_{[s_1,c_1]}$ and $T_{[s_2,c_2]}$, the matrix element of $\hat{\mathbf{M}}$ is calculated as

$$
\begin{aligned}
& \overline{< T_{[s_1,c_1]}|\hat{\mathbf{M}}|T_{[s_2,c_2]} >_{Diff}} \\
= & \ (\hat{\mathbf{M}}T_{[s_2,c_2]})[T_{s_1,c_1\in[s_1,c_1]}] \\
= & \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}\sum_{C\in\mathcal{P}}\frac{1}{2}\overline{T_{[s_2,c_2]}[\hat{H}^{\epsilon}_C(\hat{H}^{\epsilon'}_C)^\dagger T_{s_1,c_1\in[s_1,c_1]}]} \\
= & \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}\sum_{C\in\mathcal{P}}\frac{1}{2}\frac{1}{n_{\gamma(s_2,c_2)}}\sum_{\varphi\in Diff/Diff_{\gamma(s_2,c_2)}}\sum_{\varphi'\in GS_{\gamma(s_2,c_2)}} \\
\times & \ \overline{< \hat{U}_\varphi\hat{U}_{\varphi'}T_{s_2,c_2\in[s_2,c_2]}|\hat{H}^{\epsilon}_C(\hat{H}^{\epsilon'}_C)^\dagger T_{s_1,c_2\in[s_1,c_1]} >_{Kin}} \\
= & \sum_{s,c}\lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0}\sum_{C\in\mathcal{P}}\frac{1}{2}\frac{1}{n_{\gamma(s_2,c_2)}}\sum_{\varphi\in Diff/Diff_{\gamma(s_2,c_2)}}\sum_{\varphi'\in GS_{\gamma(s_2,c_2)}} \\
\times & \ \overline{< \hat{U}_\varphi\hat{U}_{\varphi'}T_{s_2,c_2\in[s_2,c_2]}|\hat{H}^{\epsilon}_C T_{s,c} >_{Kin}< \Pi_{s,c}|(\hat{H}^{\epsilon'}_C)^\dagger T_{s_1,c_1\in[s_1,c_1]} >_{Kin}} \\
= & \sum_{[s,c]}\sum_{v\in V(\gamma(s,c\in[s,c]))}\frac{1}{2}\lim_{\epsilon,\epsilon'\to 0} \\
\times & \ \overline{T_{[s_2,c_2]}[\hat{H}^{\epsilon}_v T_{s,c\in[s,c]}]\sum_{s,c\in[s,c]} < T_{s,c}|(\hat{H}^{\epsilon'}_v)^\dagger T_{s_1,c_1\in[s_1,c_1]} >_{Kin}},
\end{aligned}
\tag{83}
$$

where $Diff_\gamma$ is the set of diffeomorphisms leaving the colored graph $\gamma$ invariant, $GS_\gamma$ denotes the graph symmetry quotient group $Diff_\gamma/TDiff_\gamma$ where $TDiff_\gamma$ is the diffeomorphisms which is trivial on the graph $\gamma$, and $n_\gamma$ is the number of elements in $GS_\gamma$. Note that we have used the resolution of identity trick in the fourth step. Since only a finite number of terms in the sum over spin-scalar-networks $(s,c)$, cells $C\in\mathcal{P}$, and diffeomorphism transformations $\varphi$ are non-zero respectively, we can interchange the sums and the limit. In the fifth step, we take the limit $C\to v$ and split the sum $\sum_{s,c}$ into $\sum_{[s,c]}\sum_{s,c\in[s,c]}$, where $[s,c]$ denotes the diffeomorphism equivalence class associated with $(s,c)$. Here we also use the fact that, given $\gamma(s,c)$ and $\gamma(s',c')$ which are different up to a diffeomorphism transformation, there is always a diffeomorphism $\varphi$ transforming the graph associated with $\hat{H}^{\epsilon}_{v,\gamma(s,c)}T_{s,c}$ $(v\in\gamma(s,c))$ to that of $\hat{H}^{\epsilon}_{v'\gamma(s',c')}T_{s',c'}$ $(v'\in\gamma(s',c'))$ with $\varphi(v)=v'$, hence $T_{[s_2,c_2]}[\hat{H}^{\epsilon}_{v,\gamma(s,c)}T_{s,c\in[s,c]}]$ is constant for different $(s,c)\in[s,c]$.

Since the term $\sum_{s,c\in[s,c]} < T_{s,c}|(\hat{H}^{\epsilon'}_v)^\dagger T_{s_1,c_1\in[s_1,c_1]} >_{Kin}$ is independent of the parameter $\epsilon'$, one can see that by fixing a family of arbitrary state-dependent triangulations $T(\epsilon')$,

$$\sum_{s,c\in[s,c]} < T_{s,c}|(\hat{H}^{\epsilon'}_v)^\dagger T_{s_1,c_1\in[s_1,c_1]} >_{Kin}$$

$$
\begin{aligned}
&= \sum_{\varphi} < U_\varphi T_{s,c} | (\hat{H}_v^{\epsilon'})^\dagger T_{s_1,c_1 \in [s_1,c_1]} >_{Kin} \\
&= \sum_{\varphi} < \hat{H}_v^{\epsilon'} U_\varphi T_{s,c} | T_{s_1,c_1 \in [s_1,c_1]} >_{Kin} \\
&= \sum_{\varphi} < U_\varphi \hat{H}^{\varphi^{-1}(\epsilon')}_{\varphi^{-1}(v)} T_{s,c} | T_{s_1,c_1 \in [s_1,c_1]} >_{Kin} \\
&= \overline{T_{[s_1,c_1]}[\hat{H}^{\varphi^{-1}(\epsilon')}_{v \in V(\gamma(s,c))} T_{s,c}]},
\end{aligned} \tag{84}
$$

where $\varphi$ are the diffeomorphism transformations spanning the diffeomorphism equivalence class $[s, c]$. Note that the kinematical inner product in the above sum is non-vanishing if and only if $\varphi(\gamma(s, c)))$ coincides with the extended graph obtained from certain skeleton $\gamma(s_1, c_1)$ by the action of $(\hat{H}_v^{\epsilon'})^\dagger$ and $v \in V(\varphi(\gamma(s, c)))$, i.e., the scale $\varphi^{-1}(\epsilon')$ of the diffeomorphism images of the tetrahedrons added by the action coincides with the scale of certain tetrahedrons in $\gamma(s, c)$ and $\varphi^{-1}(v)$ is a vertex in $\gamma(s, c)$. Then we can express the matrix elements (83) as:

$$
\begin{aligned}
& < T_{[s_1,c_1]} | \hat{\mathbf{M}} | T_{[s_2,c_2]} >_{Diff} \\
&= \sum_{[s,c]} \sum_{v \in V(\gamma(s,c \in [s,c]))} \frac{1}{2} \lim_{\epsilon,\epsilon' \to 0} \overline{T_{[s_2,c_2]}[\hat{H}_v^{\epsilon} T_{s,c \in [s,c]}]} T_{[s_1,c_1]}[\hat{H}_v^{\epsilon'} T_{s,c \in [s,c]}] \\
&= \sum_{[s,c]} \sum_{v \in V(\gamma(s,c \in [s,c]))} \frac{1}{2} \overline{(\hat{H}_v' T_{[s_2,c_2]})[T_{s,c \in [s,c]}]} (\hat{H}_v' T_{[s_1,c_1]})[T_{s,c \in [s,c]}].
\end{aligned} \tag{85}
$$

From Eq.(85) and the result that the master constraint operator $\hat{\mathbf{M}}$ is densely defined on $\mathcal{H}_{Diff}$, it is obvious that $\hat{\mathbf{M}}$ is a positive and symmetric operator on $\mathcal{H}_{Diff}$. Hence, it is associated with a unique self-adjoint operator $\hat{\overline{\mathbf{M}}}$, called the Friedrichs extension of $\hat{\mathbf{M}}$. We relabel $\hat{\overline{\mathbf{M}}}$ to be $\hat{\mathbf{M}}$ for simplicity. In conclusion, there exists a positive and self-adjoint operator $\hat{\mathbf{M}}$ on $\mathcal{H}_{Diff}$ corresponding to the master constraint (75). It is then possible to obtain the physical Hilbert space of the coupled system by the direct integral decomposition of $\mathcal{H}_{Diff}$ with respect to $\hat{\mathbf{M}}$.

Note that the quantum constraint algebra can be easily checked to be anomaly free. Eq.(82) assures that the master constraint operator commutes with finite diffeomorphism transformations, i.e.,

$$
[\hat{\mathbf{M}}, \hat{U}'_\varphi] = 0. \tag{86}
$$

Also it is obvious that the master constraint operator commutes with itself,

$$
[\hat{\mathbf{M}}, \hat{\mathbf{M}}] = 0. \tag{87}
$$

So the quantum constraint algebra is precisely consistent with the classical constraint algebra (76) in this sense. As a result, the difficulty of the original Hamiltonian constraint algebra can be avoided by introducing the master constraint algebra, due to the Lie algebra structure of the latter.

# 6 The Semiclassical Limit of Quantum Dynamics

As shown in previous chapters, both the Hamiltonian constraint operator $\hat{\mathcal{S}}(N)$ and the master constraint operator $\hat{\mathbf{M}}$ can be well defined in the framework of loop quantum gravity. However, since the Hilbert spaces $\mathcal{H}_{kin}$ and $\mathcal{H}_{Diff}$, the operators $\hat{\mathcal{S}}(N)$ and $\hat{\mathbf{M}}$ are constructed in such ways that are drastically different from usual quantum field theory, one has to check whether the constraint operators and the corresponding algebras have correct semiclassical limits with respect to suitable semiclassical states.

## 6.1 The Construction of Coherent States

In order to find the proper semiclassical states and check the classical limit of the theory, the idea of a non-normalizable coherent state defined by a generalized Laplace operator and its heat kernel was introduced for the first time in [26]. Recently, kinematical coherent states were constructed in two different approaches. One leads to the so-called complexifier coherent states proposed by Thiemann et al [142][143][144][145]. The other was proposed by Varadarajan [152][153][154] and further developed by Ashtekar et al [19][15].

The complexifier approach is motivated by the coherent state construction for compact Lie groups [86]. One begins with a positive function $C$ (complexifier) on the classical phase space and arrives at a "coherent state" $\psi_m$, which more possibly belongs to the dual space $Cyl^\star$ rather than $\mathcal{H}_{kin}$. However, one may consider the so-called "cut-off state" of $\psi_m$ with respect to a finite graph as a graph-dependent coherent state in $\mathcal{H}_{kin}$ [146]. By construction, the coherent state $\psi_m$ is an eigenstate of an annihilation operator coming also from the complexifier $C$ and hence has the desired semiclassical properties [143][144]. We now sketch the basic idea of its construction. Given the Hilbert space $\mathcal{H}$ for a dynamical system with constraints and a subalgerba of observables $\mathcal{S}$ in the space $\mathcal{L}(\mathcal{H})$ of linear operators on $\mathcal{H}$, the semiclassical states with respect to $\mathcal{S}$ are defined in Definition 3.1.5. Kinematical coherent states $\{\Psi_m\}_{m\in\mathcal{M}}$ are semiclassical states which in addition satisfy the annihilation operator property [142][146], namely there exists a certain non-self-adjoint operator $\hat{z} = \hat{a} + i\lambda\hat{b}$ with $\hat{a},\ \hat{b} \in \mathcal{S}$ and a certain squeezing parameter $\lambda$, such that

$$\hat{z}\,\Psi_m = z(m)\Psi_m. \tag{88}$$

Note that Eq.(88) implies that the minimal uncertainty relation is saturated for the pair of elements $(\hat{a},\ \hat{b})$, i.e.,

$$\Psi_m([\hat{a} - \Psi_m(\hat{a})]^2) = \Psi_m([\hat{b} - \Psi_m(\hat{b})]^2) = \frac{1}{2}|\Psi_m([\hat{a}, \hat{b}])|. \tag{89}$$

Note also that coherent states are usually required to satisfy the additional peakedness property, namely for any $m \in \mathcal{M}$ the overlap function $| < \Psi_m, \Psi_{m'} > |$ is concentrated in a phase volume $\frac{1}{2}|\Psi_m([\hat{q}, \hat{p}])|$, where $\hat{q}$ is a configuration operator and $\hat{p}$ a momentum operator. So the central element in the construction is to define a suitable "annihilation operator" $\hat{z}$ in analogy with the simplest case of harmonic oscillator. A powerful tool named as "complexifier" is introduced in Ref.[142] to define a meaningful $\hat{z}$ operator which can give rise to kinematical coherent states for a general quantum system.

**Definition 6.1.1**: *Given a phase space $\mathcal{M} = \mathrm{T}^*C$ for some dynamical system with configuration coordinates $q$ and momentum coordinates $p$, a complexifier, $C$, is a positive smooth function on $\mathcal{M}$, such that*
(1) *$C/\hbar$ is dimensionless;*
(2) $\lim_{\|p\|\to\infty} \frac{|C(m)|}{\|p\|} = \infty$ *for some suitable norm on the space of the momentum;*
(3) *Certain complex coordinates $(z(m), \bar{z}(m))$ of $\mathcal{M}$ can be constructed from $C$.*

Given a well-defined complexifier $C$ on phase space $\mathcal{M}$, the programme for constructing coherent states associated with $C$ can be carried out as the following.

- Complex polarization

  The condition (3) in Definition 7.3.1 implies that the complex coordinate $z(m)$ of $\mathcal{M}$ can be constructed via

$$z(m) := \sum_{n=0}^{\infty} \frac{i^n}{n!}\{q, C\}_{(n)}(m), \tag{90}$$

  where the multiple Poisson bracket is inductively defined by $\{q, C\}_{(0)} = q$, $\{q, C\}_{(n)} = \{\{q, C\}_{(n-1)}, C\}$. One will see that $z(m)$ can be regarded as the classical version of an annihilation operator.

- Defining the annihilation operator

  After the quantization procedure, a Hilbert space $\mathcal{H} = L^2(C, d\mu)$ with a suitable measure $d\mu$ on a suitable configuration space $C$ can be constructed. It is reasonable to assume that $C$ can be defined as a positive self-adjoint operator $\hat{C}$ on $\mathcal{H}$. Then a corresponding operator $\hat{z}$ can be defined by transforming the Poisson brackets in Eq.(90) into commutators, i.e.,

$$\hat{z} := \sum_{n=0}^{\infty} \frac{i^n}{n!}\frac{1}{(i\hbar)^n}[\hat{q}, \hat{C}]_{(n)} = e^{-\hat{C}/\hbar}\hat{q}e^{\hat{C}/\hbar}, \tag{91}$$

  which is called as an annihilation operator.

- Constructing coherent states

  Let $\delta_{q'}(q)$ be the $\delta$-distribution on $C$ with respect to the measure $d\mu$. Since $\hat{C}$ is assumed to be positive and self-adjoint, the conditions (1) and (2) in Definition 7.3.1 imply that $e^{-\hat{C}/\hbar}$ is a well-defined "smoothening operator". So it is quite possible that the heat kernel evolution of the $\delta$-distribution, $e^{-\hat{C}/\hbar}\delta_{q'}(q)$, is a square integrable function in $\mathcal{H}$, which is even analytic. Then one may analytically extend the variable $q'$ in $e^{-\hat{C}/\hbar}\delta_{q'}(q)$ to complex values $z(m)$ and obtain a class of states $\psi'_m$ as

$$\psi'_m(q) := [e^{-\hat{C}/\hbar}\delta_{q'}(q)]_{q'\to z(m)}, \tag{92}$$

  such that one has

$$\hat{z}\,\psi'_m(q) := [e^{-\hat{C}/\hbar}\hat{q}\delta_{q'}(q)]_{q'\to z(m)} = [q' e^{-\hat{C}/\hbar}\delta_{q'}(q)]_{q'\to z(m)} = z(m)\,\psi'_m(q). \tag{93}$$

Hence $\psi'_m$ is automatically an eigenstate of the annihilation operator $\hat{z}$. So it is natural to define coherent states $\psi_m(q)$ by normalizing $\psi'_m(q)$.

One may check that all the coherent state properties usually required are likely to be satisfied by the above complexifier coherent states $\psi_m(q)$ [146]. As a simple example, in the case of one-dimensional harmonic oscillator with Hamiltonian $H = \frac{1}{2}(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2)$, one may choose the complexifier $C = p^2/(2m\omega)$. It is straightforward to check that the coherent state constructed by the above procedure coincides with the usual harmonic oscillator coherent state up to a phase [146]. So the complexifier coherent state can be considered as a suitable generalization of the concept of usual harmonic oscillator coherent state.

The complexifer approach can be used to construct kinematical coherent states in loop quantum gravity. Given a suitable complexifier $C$, for each analytic path $e \subset \Sigma$ one can define

$$A^{\mathbf{C}}(e) := \sum_{n=0}^{\infty} \frac{i^n}{n!}\{A(e), C\}_{(n)}, \tag{94}$$

where $A(e) \in SU(2)$ is assigned to $e$. As the complexifier $C$ is assumed to give rise to a positive self-adjoint operator $\hat{C}$ on the kinematical Hilbert space $\mathcal{H}_{kin}$, one further supposes that $\hat{C}/\hbar T_s = \tau\lambda_s T_s$, where $\tau$ is a so-called classicality parameter, $\{T_s(A)\}_s$ form a basis in $\mathcal{H}_{kin}$ and are analytic in $A \in \overline{\mathcal{A}}$. Moreover the $\delta$-distribution on the quantum configuration space $\overline{\mathcal{A}}$ can be formally expressed as $\delta_{A'}(A) = \sum_s T_s(A')\overline{T_s(A)}$. Thus by applying Eq.(92) one obtains coherent states

$$\psi'_{A^{\mathbf{C}}}(A) = (e^{-\hat{C}/\hbar})\delta_{A'}(A)|_{A' \to A^{\mathbf{C}}} = \sum_s e^{-\tau\lambda_s} T_s(A^{\mathbf{C}})\overline{T_s(A)}. \tag{95}$$

However, since there are an uncountably infinite number of terms in the expression (95), the norm of $\psi'_{A^{\mathbf{C}}}(A)$ would in general be divergent. So $\psi'_{A^{\mathbf{C}}}(A)$ is generally not an element of $\mathcal{H}_{kin}$ but rather a distribution on a dense subset of $\mathcal{H}_{kin}$. In order to test the semiclassical limit of quantum geometric operators on $\mathcal{H}_{kin}$, one may further consider the "cut-off state" of $\psi'_{A^{\mathbf{C}}}(A)$ with respect to a finite graph $\gamma$ as a graph-dependent coherent state in $\mathcal{H}_{kin}$ [146]. So the key input in the construction is to choose a suitable complexifer. There are vast possibilities of choice. For example, a candidate complexifier $C$ is considered in Ref.[148] such that the corresponding operator acts on cylindrical functions $f_\gamma$ by

$$(\hat{C}/\hbar)f_\gamma = \frac{1}{2}(\sum_{e \in E(\gamma)} l(e)\hat{J}_e^2)f_\gamma, \tag{96}$$

where $\hat{J}_e^2$ is the Casimir operator defined by Eq.(24) associated to the edge $e$, the positive numbers $l(e)$ satisfying $l(e \circ e') = l(e) + l(e')$ and $l(e^{-1}) = l(e)$ serves as a classicalization parameter. Then it can be shown from Eq.(94) that $A^{\mathbf{C}}(e)$ is an element of $SL(2, \mathbf{C})$. So the classical interpretation of the annihilation operators is simply the generalized complex $SU(2)$ connections. It has been shown in Refs. [143] and [144] that the "cut-off state" of the corresponding coherent state,

$$\psi_{A^{\mathbf{C}},\gamma}(A) = \psi'_{A^{\mathbf{C}},\gamma}(A)/||\psi'_{A^{\mathbf{C}},\gamma}(A)||, \tag{97}$$

with

$$\psi'_{A^{\mathbf{C}},\gamma}(A) := \sum_{s,\gamma(s)=\gamma} e^{-\frac{1}{2}\sum_{e\in E(\gamma(s))} l(e)j_e(j_e+1)} T_s(A^{\mathbf{C}})\overline{T_s(A)}. \tag{98}$$

has desired semiclassical properties in testing the kinematical operators (e.g. holonomy and flux). But unfortunately, these cut-off coherent states cannot be directly used to test the semi-classical limit of the Hamiltonian constraint operator $\hat{\mathcal{S}}(N)$, since $\hat{\mathcal{S}}(N)$ is graph-changing so that its expectation values with respect to these cut-off states are always zero! So further work in this approach is expected in order to overcome the difficulty. Anyway, the complexifier approach provides a clean construction mechanism and manageable calculation method for semiclassical analysis in loop quantum gravity.

We now turn to the second approach. As we have seen, loop quantum gravity is based on quantum geometry, where the fundamental excitations are one-dimensional polymer-like. On the other hand, low energy physics is based on quantum field theories which are constructed in a flat spacetime continuum. The fundamental excitations of these fields are 3-dimensional, typically representing wavy undulations on the background Minkowskian geometry. The core strategy in this approach is then to relate the polymer excitations of quantum geometry to Fock states used in low energy physics and to locate Minkowski Fock states in the background independent framework. Since the quantum Maxwell field can be constructed in both Fock representation and polymer-like representation, one first gains insights from the comparison between the two representations, then generalizes the method to quantum geometry. A "Laplacian operator" can be defined on $\mathcal{H}_{kin}$ [26][19], from which one may define a candidate coherent state $\Phi_0$, also in $Cyl^\star$, corresponding to the Minkowski spacetime. To calculate the expectation values of kinematical operators, one considers the so-called "shadow state" of $\Phi_0$, which is the restriction of $\Phi_0$ to a given finite graph. However, the construction of shadow states is subtly different from that of cut-off states.

We will only describe the simple case of the Maxwell field to illustrate the ideas of the construction [152][153][20]. Following the quantum geometry strategy discussed in Sec.4, the quantum configuration space $\overline{\mathbf{A}}$ for the polymer representation of the $U(1)$ gauge theory can be similarly constructed. A generalized connection $\mathbf{A} \in \overline{\mathbf{A}}$ assigns each oriented analytic edge in $\Sigma$ an element of $U(1)$. The space $\overline{\mathbf{A}}$ carries a diffeomorphism and gauge invariant measure $\mu_0$ induced by the Haar measure on $U(1)$, which gives rise to the Hilbert space, $\mathcal{H}_0 := L^2(\overline{\mathbf{A}}, d\mu_0)$, of polymer states. The basic operators are holonomy operators $\hat{\mathbf{A}}(e)$ labeled by one-dimensional edges $e$, which act on cylindrical functions by multiplication, and smeared electric field operators $\hat{E}(g)$ for suitable test one-forms $g$ on $\Sigma$, which are self-adjoint. Note that, since the gauge group $U(1)$ is Abelian, it is more convenient to smear the electric fields in 3 dimensions [20]. The eigenstates of $\hat{E}(g)$, so-called flux network states $\mathcal{N}_{\alpha,\vec{n}}$, provide an orthonormal basis in $\mathcal{H}_0$, which are defined for any finite graph $\alpha$ with $N$ edges as:

$$\mathcal{N}_{\alpha,\vec{n}}(\mathbf{A}) := [\mathbf{A}(e_1)]^{n_1}[\mathbf{A}(e_2)]^{n_2}\cdots[\mathbf{A}(e_N)]^{n_N}, \tag{99}$$

where $\vec{n} \equiv (n_1,\cdots,n_N)$ assigns an integer $n_I$ to each edge $e_I$. The action of $\hat{E}(g)$ on the flux network states reads

$$\hat{E}(g)\,\mathcal{N}_{\alpha,\vec{n}} = -\hbar(\sum_I n_I \int_{e_I} g)\mathcal{N}_{\alpha,\vec{n}}. \tag{100}$$

In this polymer-like representation, cylindrical functions are the finite linear combinations of flux network states and span a dense subspace of $\mathcal{H}_0$. Denote by **Cyl** the set of cylindrical functions and by $\mathbf{Cyl}^\star$ its algebraic dual. One then has a triplet $\mathbf{Cyl} \subset \mathcal{H}_0 \subset \mathbf{Cyl}^\star$ in analogy with the case of loop quantum gravity.

The Schrödinger or Fock representation of the Maxwell field, on the other hand, depends on the Minkowski background metric. Here the Hilbert space is given by $\mathcal{H}_F = L^2(\mathcal{S}', d\mu_F)$, where $\mathcal{S}'$ is the appropriate space of tempered distributions on $\Sigma$ and $\mu_F$ is the Gaussian measure. The basic operators are connections $\hat{\mathbf{A}}(f)$ smeared in 3 dimensions with suitable vector densities $f$ and smeared electric fields $\hat{E}(g)$. But $\hat{\mathbf{A}}(e)$ fail to be well defined. To resolve this tension between the two representations, one proceeds as follows. Let $\vec{x}$ be the Cartesian coordinates of a point in $\Sigma = \mathbf{R}^3$. Introduce a test function by using the Euclidean background metric on $\mathbf{R}^3$,

$$f_r(\vec{x}) = \frac{1}{(2\pi)^{3/2} r^3} \exp(-|\vec{x}|^2/2r^2), \tag{101}$$

which approximates the Dirac delta function for small $r$. The Gaussian smeared form factor for an edge $e$ is defined as

$$X^a_{(e,r)}(\vec{x}) := \int_e ds\, f_r(\vec{e}(s) - \vec{x})\dot{e}^a. \tag{102}$$

Then one can define a smeared holonomy for $e$ by

$$\mathbf{A}_{(r)}(e) := \exp[-i \int_{\mathbf{R}^3} X^a_{(e,r)}(\vec{x}) A_a(\vec{x})], \tag{103}$$

where $A_a(\vec{x})$ is the $U(1)$ connection one-form of the Maxwell field on $\Sigma$. Similarly one can define Gaussian smeared electric fields by

$$E_{(r)}(g) := \int_{\mathbf{R}^3} g_a(\vec{x}) \int_{\mathbf{R}^3} f_r(\vec{y} - \vec{x}) E^a(\vec{y}). \tag{104}$$

In this way one obtains two Poission bracket algebras. One is formed by smeared holonomies and electric fields with

$$\begin{aligned} \{\mathbf{A}_{(r)}(e), \mathbf{A}_{(r)}(e')\} &= 0 = \{E(g), E(g')\} \\ \{\mathbf{A}_{(r)}(e), E(g)\} &= -i(\int_{\mathbf{R}^3} X^a_{(e,r)} g_a)\, \mathbf{A}_{(r)}(e). \end{aligned} \tag{105}$$

The other is formed by unsmeared holonomies and Gaussian smeared electric fields with

$$\begin{aligned} \{\mathbf{A}(e), \mathbf{A}(e')\} &= 0 = \{E_{(r)}(g), E_{(r)}(g')\} \\ \{\mathbf{A}(e), E_{(r)}(g)\} &= -i(\int_{\mathbf{R}^3} X^a_{(e,r)} g_a)\, \mathbf{A}(e). \end{aligned} \tag{106}$$

Obviously, there is an isomorphism between them,

$$I_r :\ (\mathbf{A}_{(r)}(e), E(g)) \mapsto (\mathbf{A}(e), E_{(r)}(g)). \tag{107}$$

Using the isomorphism $I_r$, one can pass back and forth between the polymer and the Fock representations. Specifically, the image of the Fock vacuum can be shown to be the following element of $\mathbf{Cyl}^{\star}$ [152][153],

$$(V| \ = \ \sum_{\alpha,\vec{n}} \exp[-\frac{\hbar}{2}\sum_{IJ} G_{IJ} n_I n_J]\,(\mathcal{N}_{\alpha,\vec{n}}|, \tag{108}$$

where $(\mathcal{N}_{\alpha,\vec{n}}| \in \mathbf{Cyl}^{\star}$ maps the flux network function $|\mathcal{N}_{\alpha,\vec{n}}\rangle$ to one and every other flux network functions to zero. While the states $(\mathcal{N}_{\alpha,\vec{n}}|$ do not have any knowledge of the underlying Minkowskian geometry, this information is coded in the matrix $G_{IJ}$ associated with the edges of the graph $\alpha$, given by [20]

$$G_{IJ} \ = \int_{e_I} dt\dot{e}^a_I(t) \int_{e_J} dt'\dot{e}_J{}^b(t') \int d^3x\,\delta_{ab}(\vec{x})\,[f_r(\vec{x}-\vec{e}_I(t))\,|\Delta|^{-\frac{1}{2}}\,f(\vec{x},\vec{e}_J(t'))], \tag{109}$$

where $\delta_{ab}$ is the flat Euclidean metric and $\Delta$ its Laplacian. Therefore, one can single out the Fock vacuum state directly in the polymer representation by invoking Poincaré invariance without any reference to the Fock space. Similarly, one can directly locate in $\mathbf{Cyl}^{\star}$ all coherent states as the eigenstates of the exponentiated annihilation operators. Since $\mathbf{Cyl}^{\star}$ does not have an inner product, one uses the notion of shadow states to do semiclassical analysis in the polymer representation. From Eq.(108), the action of the Fock vacuum $(V|$ on $\mathcal{N}_{\alpha,\vec{n}}$ reads

$$(V|\mathcal{N}_{\alpha,\vec{n}}\rangle \ = \int_{\overline{\mathbf{A}}_\alpha} d\mu^0_\alpha\,\overline{V}_\alpha \mathcal{N}_{\alpha,\vec{n}}, \tag{110}$$

where the state $V_\alpha$ is in the Hilbert space $\mathcal{H}_\alpha$ for the graph $\alpha$ and given by

$$V_\alpha(\mathbf{A}) \ = \ \sum_{\vec{n}} \exp[-\frac{\hbar}{2}\sum_{IJ} G_{IJ} n_I n_J]\,\mathcal{N}_{\alpha,\vec{n}}(\mathbf{A}). \tag{111}$$

Thus for any cylindrical functions $\varphi_\alpha$ associated with $\alpha$,

$$(V|\varphi_\alpha\rangle \ = \langle V_\alpha|\varphi_\alpha\rangle, \tag{112}$$

where the inner product in the right hand side is taken in $\mathcal{H}_\alpha$. Hence $V_\alpha(\mathbf{A})$ are referred to as "shadows" of $(V|$ on the graphs $\alpha$. The set of all shadows captures the full information in $(V|$. By analyzing shadows on sufficiently refined graphs, one can introduce criteria to test if a given element of $\mathbf{Cyl}^{\star}$ represents a semi-classical state [20]. It turns out that the state $(V|$ does satisfy this criterion and hence can be regarded as semi-classical in the polymer representation.

The mathematical and conceptual tools gained from simple models like the Maxwell fields are currently being used to construct semiclassical states of quantum geometry. A candidate kinematical coherent state corresponding to the Minkowski spacetime has been proposed by Ashtekar and Lewandowki in the light of a "Laplacian operator" [19][20]. However, the detailed structure of this coherent state is yet to be analyzed and there is no a priori guarantee that it is indeed a semiclassical state.

One may find comparisons of the two approaches from both sides [147][20]. It turns out that Varadarajan's Laplacian coherent state for the polymer Maxwell field can also be derived from

Thiemann's complexifier method. However, one cannot find a complexifier to get the coherent state proposed by Ashtekar et al. for loop quantum gravity. Both approaches have their own virtues and need further developments. The complexifier approach provides a clear construction mechanism and manageable calculation method, while the Laplacian operator approach is related closely with the well-known Fock vacuum state. One may also expect that a judicious combination of the two approaches may lead to significant progress in the semiclassical analysis of loop quantum gravity.

## 6.2 Algebraic Quantum Gravity Approach

As we have shown in the last subsection, although Thiemann's complexifier coherent state has a clear calculable mechanism and correct semi-classical properties in testing kinematical operators, it fails to be a qualified semi-classical state for the quantum dynamics since the semiclassical limit of the Hamiltonian constraint operator $\hat{S}(N)$ or master constraint operator $\hat{\mathbf{M}}$ is clearly not correct, both $\hat{S}(N)$ and $\hat{\mathbf{M}}$ are graph-changing so that their expectation values with respect to these cut-off coherent states are always zero. So a possible way to avoid such a problem is to define a non-graph-changing version of Hamiltonian constraint operator or similarly, a master constraint operator. However, such a modification is hard to make in the framework of loop quantum gravity since the action of Hamiltonian constraint operator always adds several arcs on certain graphs. But if the framework of loop quantum gravity is suitably modified then it turns out that a version of non-graph-changing Hamiltonian constraint operator can be proposed and the semi-classical analysis for the quantum dynamics can be carried out with the complexifier coherent states defined previously. Such a modification is recently made by Thiemann in [79][80][81] and is called algebraic quantum gravity (AQG) approach. We describe it briefly in what follows.

Algebraic quantum gravity is a new approach to canonical quantum gravity suggested by loop quantum gravity. But in contrast to loop quantum gravity, the quantum kinematics of algebraic quantum gravity is determined by an abstract $*$-algebra generated by a countable set of elementary operators labeled by a single algebraic graph with countably infinite number of edges, while in loop quantum gravity the elementary operators are labeled by a collection of embedded graphs with finite number of edges. Thus one can expect that in algebraic quantum gravity, we lose the information of the topological and differential structure of the manifold in all the quantization procedure before we do semi-classical analysis. Hence the quantum theory will be of course independent of the topology and differential structure of the manifold but based only on an algebraic graph, which only contains the information of the number of vertices and their oriented valence.

**Definition 6.2.1**: *An oriented algebraic graph is an abstract graph specified by its adjacency matrix $\alpha$, which is an $N \times N$ matrix. One of its entries $\alpha_{IJ}$ stand for the number of edges that start at vertex $I$ and end at vertex $J$. The valence of the vertex $I$ is given by $v_I = \sum_J(\alpha_{IJ} + \alpha_{JI})$. We also use $V(\alpha)$ and $E(\alpha)$ to denote the sets of vertices and edges respectively.*

In our quantization procedure, we fix a specific cubic algebraic graph with a countably infinite number of edges $N = \aleph$ and the valence of each vertex $v_I = 2 \times \dim(\Sigma)$. Such a specific choice, although it detracts from the generality of the theory, is practically sufficient for our use in the semiclassical analysis.

Given the algebraic graph $\alpha$, we define a quantum $*$-algebra by associating with each edge $e$ an element $A(e)$ of a compact, connected, semisimple Lie group $G$ and an element $E_j(e)$ take value in its Lie algebra $\mathfrak{g}$. These elements are subject to the commutation relations

$$\begin{aligned}
&[\hat{A}(e), \hat{A}(e')] = 0,\\
&[\hat{E}_j(e), \hat{A}(e')] = i\hbar Q^2 \delta_{e,e'} \tau_j/2\hat{A}(e),\\
&[\hat{E}_j(e), \hat{A}(e')] = -i\hbar Q^2 \delta_{e,e'} f_{jkl} \hat{E}_l(e'),
\end{aligned}$$

and $*$-relations

$$\hat{A}(e)^* = [\hat{A}(e)^{-1}]^T, \quad \hat{E}_j(e)^* = \hat{E}_j(e),$$

where $Q$ stands for the coupling constant, $\tau_j$ is the generators in the Lie algebra $\mathfrak{g}$ and $f_{jkl}$ is the structure constant of $\mathfrak{g}$. We denote the abstract quantum $*$-algebra generated by above elements and relations by $\mathfrak{A}$.

A natural representation of $\mathfrak{A}$ is the infinite tensor product Hilbert space $\mathcal{H}^{\otimes} = \otimes_e \mathcal{H}_e$ where $\mathcal{H}_e = L^2(G, d\mu_H)$[145], whose element is denoted by $\otimes_f \equiv \otimes_e f_e$. Two elements $\otimes_f$ and $\otimes_{f'}$ in $\mathcal{H}^{\otimes}$ are said to be strongly equivalent if $\sum_e | < f_e, f'_e >_{\mathcal{H}_e} -1|$ converges. We denote by $[f]$ the strongly equivalence class containing $\otimes_f$. It turns out that two elements in $\mathcal{H}^{\otimes}$ are orthogonal if they lie in different strongly equivalence classes. Hence the infinite tensor Hilbert space $\mathcal{H}^{\otimes}$ can be decomposed as a direct sum of the Hilbert subspaces (sectors) $\mathcal{H}^{\otimes}_{[f]}$ which are the closure of strongly equivalence classes $[f]$. Furthermore, although each sector $\mathcal{H}^{\otimes}_{[f]}$ is separable and has a natural Fock space structure, the whole Hilbert space $\mathcal{H}^{\otimes}$ is non-separable since there are uncountably infinite number of strongly equivalence classes in it. Our basic elements in the quantum algebra are represented on $\mathcal{H}^{\otimes}$ in an obvious way

$$\begin{aligned}
\hat{A}(e)\otimes_f &:= [A(e) f_e] \otimes [\otimes_{e' \neq e} f_{e'}],\\
\hat{E}_j(e)\otimes_f &:= [i\hbar Q^2 X^e_j f_e] \otimes [\otimes_{e' \neq e} f_{e'}].
\end{aligned}$$

As one might have expected, all these operators are densely defined and $E_j(e)$ is essentially self-adjoint. Given a vertex $v \in V(\alpha)$, the volume operator can be constructed by using the operators we just defined

$$\hat{V}_v := \ell_p^3 \sqrt{|\frac{1}{48} \sum_{e_1 \cap e_2 \cap e_3 = v} \epsilon_v(e_1, e_2, e_3) \epsilon^{ijk} \hat{E}_i(e_1) \hat{E}_j(e_2) \hat{E}_k(e_3)|},$$

where the values of $\epsilon_v(e_1, e_2, e_3)$ should be assigned once for all for each vertex. When we embed the algebraic graph into some manifold, the embedding should be consistent with the assigned values of $\epsilon_v(e_1, e_2, e_3)$.

Then we discuss the quantum dynamics. By the regularization methods frequently used in the last two sections, the half densitized constraints can be quantized to be composite operators as we list below.

- Gauss constraint

$$\hat{G}_j(v) := \hat{Q}_v^{(1/2)} \sum_{e \; at \; v} \hat{E}_j(e);$$

- Spatial diffeomorphism constraint

$$\begin{aligned}\hat{D}_j(v) \;&:=\; \frac{1}{E(v)} \sum_{e_1 \cap e_2 \cap e_3 = v} \frac{\epsilon_v(e_1, e_2, e_3)}{|L(v, e_1, e_2)|} \\ &\times \sum_{\beta \in L(v, e_1, e_2)} \mathrm{Tr}(\tau_j [\hat{A}(\beta) - \hat{A}(\beta)^{-1}] \hat{A}(e_3)[\hat{A}(e_3)^{-1}, \sqrt{\hat{V}_v}]);\end{aligned}$$

- Euclidean Hamiltonian constraint (up to an overall factor)

$$\begin{aligned}\hat{H}_E^{(r)}(v) \;&:=\; \frac{1}{E(v)} \sum_{e_1 \cap e_2 \cap e_3 = v} \frac{\epsilon_v(e_1, e_2, e_3)}{|L(v, e_1, e_2)|} \\ &\times \sum_{\beta \in L(v, e_1, e_2)} \mathrm{Tr}([\hat{A}(\beta) - \hat{A}(\beta)^{-1}] \hat{A}(e_3)[\hat{A}(e_3)^{-1}, \hat{V}_v^{(r)}]);\end{aligned}$$

- Lorentzian Hamiltonian constraint (up to an overall factor)

$$\begin{aligned}\hat{T}(v) \;&:=\; \frac{1}{E(v)} \sum_{e_1 \cap e_2 \cap e_3 = v} \epsilon_v(e_1, e_2, e_3) \\ &\times \mathrm{Tr}(\hat{A}(e_1)[\hat{A}(e_1)^{-1}, [\hat{H}_E^{(1)}, \hat{V}]] \hat{A}(e_2)[\hat{A}(e_2)^{-1}, [\hat{A}(e_3)^{-1}, [\hat{H}_E^{(1)}, \hat{V}]] \\ &\times \hat{A}(e_3)[\hat{A}(e_3)^{-1}, \sqrt{\hat{V}_v}]), \\ \hat{H}(v) \;&=\; \hat{H}_E^{(1/2)}(v) + \hat{T}(v); \end{aligned} \tag{113}$$

where $\hat{V} := \sum_v \hat{V}_v$, $\hat{H}_E^{(1)} := \sum_v \hat{H}_E^{(1)}(v)$ and

$$\begin{aligned}\hat{Q}_v^{(r)} \;&:=\; \frac{1}{E(v)} \sum_{e_1 \cap e_2 \cap e_3 = v} \epsilon_v(e_1, e_2, e_3) \\ &\times \mathrm{Tr}(\hat{A}(e_1)[\hat{A}(e_1)^{-1}, \hat{V}_v^{(r)}] \hat{A}(e_2)[\hat{A}(e_2)^{-1}, \hat{V}_v^{(r)}] \hat{A}(e_3)[\hat{A}(e_3)^{-1}, \hat{V}_v^{(r)}]).\end{aligned}$$

$L(v, e_1, e_2)$ denotes the set of minimal loops starting at $v$ along $e_1$ and ending at $v$ along $e_2^{-1}$. And a loop $\beta \in L(v, e_1, e_2)$ is said to be minimal provided that there is no other loop within $\alpha$ satisfying the same restrictions with fewer edges traversed. Note that since we only have a single cubic algebraic graph, the diffeomorphism constraint can only be implemented by defining the operators corresponding to diffeomorphism generators because a finite diffeomorphism transformation is not meaningful in our algebraic treatment unless the algebraic graph is embedded in a manifold. As a result, the (extended) master constraint can be expressed as a quadratic combination:

$$\hat{\mathbf{M}} := \sum_{v \in V(\alpha)} [\hat{G}_j(v)^\dagger \hat{G}_j(v) + \hat{D}_j(v)^\dagger \hat{D}_j(v) + \hat{H}(v)^\dagger \hat{H}(v)].$$

It is trivial to see that all the above operators are non-graph-changing and embedding independent because we have only worked on a single algebraic graph so far. However, when we test the semiclassical limit of these operators, especially the master constraint operators, we should specify an embedding map $X$ which map a algebraic graph to be an embedded one. With this specific embedding, we can see the correspondence between the classical algebra of elementary observables and the quantum $*$-algebra. We define the holonomy and suitably modified flux by

$$\begin{aligned} A(e) &:= A(X(e)) := \mathcal{P}\exp(\int_{X(e)} A), \\ E_j(e) &:= -2\mathrm{Tr}[\tau_j \int_{S_e} \epsilon_{abc}\mathrm{d}x^a \wedge \mathrm{d}x^b A(\rho_e(x))E^c(x)A(\rho_e(x))^{-1}], \end{aligned}$$

where $S_e$ is a face which intersects the edge $X(e)$ only at an interior point $p_e$ of both $S_e$ and $X(e)$. We choose a system of paths $\{\rho_e(x)\}_x$ for all $x \in S_e$, such that $\rho_e(x)$ starts at $s(X(e))$ along $X(e)$ until $p_e$ and then runs within $S_e$ until $x$. As one might expect, the quantum $*$-algebra we defined previously is just consistent with the classical Poisson algebra generated by these holonomis and fluxes:

$$\begin{aligned} &\{A(e), A(e')\} = 0, \\ &\{E_j(e), A(e')\} = Q^2\delta_{e,e'}\tau_j/2A(e), \\ &\{E_j(e), A(e')\} = -Q^2\delta_{e,e'}f_{jkl}E_l(e'). \end{aligned}$$

Then we consider the coherent states. By employing the Laplacian complexifier on each edge

$$C_e := -\frac{1}{2Q^2a_e^2}E_j(e)E_j(e),$$

the coherent state is obtained as it was in the last section:

$$\Psi^{t_e}_{e;(A,E)}(A) \equiv \Psi^{t_e}_{e;g(A,E)}(A(e)) = \sum_\pi \dim(\pi)e^{-t\lambda_\pi}\chi_\pi(g(A,E)A(e)),$$

where $\lambda_\pi$ denotes the eigenvalue of the Laplacian on $G$ and $t = \ell_p^2/a_e^2$ represents the classicalization parameter. The coherent state peaks at the complexified classical phase space point

$$g(A,E) := \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\{C_e, A(e)\}_n = \exp(iE(e)/a_e^2)A(e),$$

note that the parameter $a_e$ is specified such that $E(e)/a_e^2$ is dimensionless. Hence the coherent state on the whole graph is represented by an infinite tensor product state:

$$\Psi^t_{A,E}(A) := \bigotimes_{e\in E(\alpha)} \frac{\Psi^{t_e}_{e;(A,E)}(A)}{||\Psi^{t_e}_{e;(A,E)}(A)||}.$$

The peakness, fluctuation and other semiclassical properties of these states have been checked in [143][144] in which the most important part is that

$$< \Psi_{A,E}|\hat{A}(e)|\Psi_{A,E} >= A(e) \qquad < \Psi_{A,E}|\hat{E}(e)|\Psi_{A,E} >= E(e)$$

up to terms which vanish faster than any power of $t_e$ as $t_e \to 0$. And the fluctuations are small.

With the semiclassical state we just constructed, the expectation value of the above (extended) master constraint operator can be calculated and its semiclassical limit can be tested. In the following, we summarize the result of the calculation. In [80], a semiclassical calculation for the master constraint operator is carried out based on a cubic algebraic graph. The calculation makes use of a simplifying assumption: we substitute the gauge group for gravity $SU(2)$ by $U(1)^3$. And the result of the calculation shows that in $U(1)^3$ case the (extended) master constraint operator has correct semiclassical limit

$$\lim_{t\to 0} < \Psi^t_m|\hat{\mathbf{M}}|\Psi^t_m >= \mathbf{M}^{\mathrm{cubic}}[m] \to \mathbf{M}[m] \ \ (\epsilon \to 0)$$

where $m$ represents a phase space point and $\epsilon$ is the lattice parameter such that the lattice become continuum as $\epsilon \to 0$. In addition, it is shown that the next-to-leading order terms which contribute to the fluctuation of $\hat{\mathbf{M}}$ are finite.

Moreover, the calculation in [81] shows that the result of the exact non-Abelian calculation matches precisely the results of the Abelian approximation, provided that we replace the classical $U(1)^3$ terms $\{h^j_e, p^e_j\}_{j=1,2,3}$ by $\{\mathrm{Tr}(\tau_j A(e)), \mathrm{Tr}(\tau_j E(e))\}_{j=1,2,3}$, which means that the theory of algebraic quantum gravity admits a semiclassical limit whose infinitesimal gauge symmetry agrees with that of general relativity.

# 7 Conclusion and Discussion

As it was shown in the previous sections, loop quantum gravity offers a conceptually clear and mathematically rigorous approach to quantize general relativity. In this approach, we are seeking new physics deeply below the Planck scale. In the kinematical framework, a quantum Riemannian geometry is established and some geometrical operators, e.g. area, volume, are well-defined, and their spectrum are shown to be discrete, which means that the structure of the space may be discrete below the Planck scale. Such a new phenomena sheds light on quantum field theory, lattice gauge theory and their renormalization. Moreover, the program in the quantum dynamics of loop quantum gravity represents significant progress in the research area of quantum gravity. Before loop quantum gravity, the quantum Wheeler-DeWitt equation was only a formal equation and from concrete calculations. However, in the framework of loop quantum gravity, we already have a well-defined quantum Hamiltonian constraint operator which has an explicit action on kinematical states, so that the quantum Wheeler-DeWitt equation is well-defined in loop quantum gravity. On the other hand, the matter field can also be quantized in this framework and we show that the matter Hamiltonian is free of UV-divergence and don't need a renormalization process. Furthermore, with the coupled matter field, a matter coupled Hamiltonian constraint operator is obtained so that the problem of time may be solved and, such an idea is being translated into a new understanding of the early universe in the context of loop quantum cosmology.

Although great progress has been made, as an unfinished framework, loop quantum gravity still has many issues to be solved in the future research. To conclude this thesis, we list some of those in the following:

- First of all, we don't have the complete solutions for either Hamiltonian constraint equation or master constraint equation. Thus one cannot explicitly construct the physical Hilbert space for loop quantum gravity. So the quantum dynamics of gravity is essentially unknown so far.

- To make contact with experimental results, one should know the observables in the quantum theory which have to be invariant under gauge transformation. However, some of the Dirac observables that have been constructed involve an infinite number of derivatives and extremely hard to manage [150][61][62].

- The semiclassical limit of loop quantum gravity is unknown so far, although a great deal of progress has been made in the context of algebraic quantum gravity. And in algebraic quantum gravity, further research work is needed to show the fluctuation of master constraint operator should be small.

- As it was shown at the end of section 4.3, the regularization process for the Hamiltonian constraint operator is ambiguous and there is a list of free parameters. Thus it is also a research project to remove as many ambiguities as possible. And some work has been recently done in this direction [110].

- The Immirzi parameter is another free parameter in the framework of loop quantum gravity, which comes in with the classical formulation. In the classical theory, different values of the Immirzi parameter label equivalent classical theories since they are connected by canonical transformations. However, in quantum theory, it is problematic because the representation with different Immirzi parameter are not unitarily equivalent.

- The construction of loop quantum gravity crucially depends on the compactness of its gauge group $SU(2)$, which comes from an internal partial gauge fixing. And it is argued that the internal Lorentz symmetry is broken in a non-natural way [131]. So it seems to be better to switch back to the complex Ashtekar variables which are free of the internal gauge fixing and preserve the internal Lorentz symmetry and, will also greatly simplify the Hamiltonian constraint. However, the price is that we should work on non-compact gauge group $SL(2, \mathbf{C})$, and there is no satisfactory quantization programme for the $SL(2, \mathbf{C})$-gravity so far, although some work has been done in this direction [71][105][106].

- As it was shown in section 6.2, algebraic quantum gravity provides a clear way to make many calculations accessible and the semiclassical analysis can be carried out in this framework. And it seems that the construction of algebraic quantum gravity admits the non-compact internal gauge group (or non-compact reduced configuration space) since there is only one graph in quantization process. However, in this framework, the restriction of the possible representation is so loose that there even exists a possible representation in which the spectrum of geometrical operators are continuous.

- The transition amplitude calculation for loop quantum gravity is accessible in the so-called spin foam model and depends on a unclear conjecture of GFT/spinfoam duality. On the other hand, it is still not clear how to build a path-integral formulation and connect with spin foam models from the canonical approach, and such a connection may give the needed support for GFT/spinfoam duality.

- We have constructed the dynamics of matter quantum field theory on a quantum background in section 5. However, it is not clear how we can make the connection with the ordinary quantum field theory on curved spacetime. Moreover, it is still an problem how to find the non-perturbative correspondence of Hadamard states in perturbative quantum field theory in curved spacetime, although some hints of a connection may come out in spin foam calculations [127][42].

# References


[1] M. Arnsdorf and S. Gupta, Loop quantum gravity on non-compact spaces, Nucl. Phys. B **577**, 529 (2000).

[2] A. Ashtekar, New variables for classical and quantum gravity, Phys. Rev. Lett. **57**, 2244 (1986).

[3] A. Ashtekar, New Hamitonian formulation of general relativity, Phys. Rev. D **36**, 1587 (1987).

[4] A. Ashtekar, Lectures on Non-perturbative Canonical Gravity, (World Scientific, Singapore, 1991).

[5] A. Ashtekar, J. C. Baez, and K. Krasnov, Quantum geometry of isolated horizon and black hole entropy, Adv. Theor. Math. Phys. **4**, 1 (2000).

[6] A. Ashtekar, C. Beetle, and J. Lewandowski, Mechanics of rotating isoloted horizons, Phys. Rev. D **64**, 044016 (2001).

[7] A. Ashtekar, C. Beetle, and J. Lewandowski, Geometry of generic isolated horizons, Class. Quantum Grav. **19**, 1195 (2002).

[8] A. Ashtekar and M. Bojowald, Black hole evaporation: A paradigm, Class. Quantum Grav. **22**, 3349 (2005).

[9] A. Ashtekar and M. Bojowald, Quantum geometry and the Schwarzschild singularity, Class. Quantum Grav. **23**, 391 (2006).

[10] A. Ashtekar, M. Bojowald, and J. Lewandowski, Mathematical structure of loop quantum cosmology, Adv. Theor. Math. Phys. **7**, 233 (2003).

[11] A. Ashtekar, L. Bombelli, and A. Corichi, Semiclassical states for constrained systems, Phys. Rev. D **72**, 025008 (2005).

[12] A. Ashtekar, J. Engle, and C. van der Broeck, Quantum horizons and black hole entropy: Inclusion of distortion and rotation, Class. Quantum Grav. **22**, L27 (2005).

[13] A. Ashtekar, J. Engle, T. Powlowski, and C. van der Broeck, Mutipole moments of isolated horizons, Class. Quantum Grav. **21**, 2549 (2004).

[14] A. Ashtekar, S. Fairhurst, and B. Krishnan, Isolated horizons: Hamiltonian evolution and the first law, Phys. Rev. D **62**, 104025 (2000).

[15] A. Ashtekar, S. Fairhurst, and J. Willis, Quantum gravity, shadow state and quantum mechanics, Class. Quantum Grav. **20**, 1031 (2003).

[16] A. Ashtekar and C. J. Isham, Representation of the holonomy algebras of gravity and non-Abelian gauge theories, Class. Quantum Grav. **9**, 1433 (1992).

[17] A. Ashtekar and J. Lewandowski, Projective techniques and functional integration, J. Math. Phys. **36**, 2170 (1995).

[18] A. Ashtekar and J. Lewandowski, Differential geometry on the space of connections via graphs and projective limits, J. Geom. Phys. **17**, 191 (1995).

[19] A. Ashtekar and J. Lewandowski, Relation between polymer like and Fock excitations, Class. Quantum Grav. **18**, L117 (2001).

[20] A. Ashtekar and J. Lewandowski, Background independent quantum gravity: A status report, Class. Quantum Grav. **21**, R53 (2004), (preprint: gr-qc/0404018).

[21] A. Ashtekar and J. Lewandowski, Quantum theory of geometry I: Area operators, Class. Quantum Grav. **14**, A55 (1997), (preprint: gr-qc/9602046).

[22] A. Ashtekar and J. Lewandowski, Quantum theory of geometry II: Volume operators, Adv. Theor. Math. Phys. **1**, 388 (1997), (preprint: gr-qc/9711031).

[23] A. Ashtekar, A. Corich, and J. A. Zapata, Quantum theory of geometry III: Non-commutativity of Riemannian structures, Class. Quantum Grav. **15**, 2955 (1998).

[24] A. Ashtekar, J. Lewandowski, D. Marolf, J. Mourão, and T. Thiemann, A manifest gauge-invariant approach to quantum theories of gauge fields, (preprint: hep-th/9408108).

[25] A. Ashtekar, J. Lewandowski, D. Marolf, J. Mourão, and T. Thiemann, Quantization of diffeomorphism invariant theories of connections with local degrees of freedom, J. Math. Phys. **36**, 6456 (1995).

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

[27] A. Ashtekar, J. Lewandowski, and H. Sahlmann, Polymer and Fock representations for a scalar field, Class. Quantum Grav. **20**, L11 (2003).

[28] A. Ashtekar, T. Powlowski and P. Singh, Quantum nature of the big bang, Phys. Rev. Lett. **96**, 141301 (2006).

[29] A. Ashtekar, T. Powlowski and P. Singh, Quantum nature of the big bang: improved dynamics, Phys. Rev. D **74**, 084003(2006).

[30] A. Ashtekar, J. Romano, R. Tate, New variables for gravity: Inclusion of matter, Phys. Rev. D **40**, 2572 (1989).

[31] A. Ashtekar, C. Rovelli, and L. Smolin, Weaving a classical geometry with quantum threads, Phys. Rev. Lett. **69**, 237 (1992).

[32] J. C. Baez, Spin networks and quantum gravity, in The Interface of Knots and Physics, ed. L. Kauffman (Providence, RI: American Mathematical Society, 1996).

[33] J. C. Baez, An introduction to spin foam models of quantum gravity and BF theory, Lect. Notes Phys. **543**, 25 (2000).

[34] J. Barbero, Real Ashtekar variables for Lorentzian signature spacetimes, Phys. Rev. D **51**, 5507 (1995).

[35] J. W. Bardeen, B. Carter, and S. W. Hawking, The four laws of black hole mechanics, Commun. Math. Phys. **31**, 161 (1973).

[36] J. W. Barrett and L. Crane, Relativistic spin networks and quantum gravity, J. Math. Phys. **39**, 3296 (1998).

[37] J. W. Barrett and L. Crane, A Lorentzian signature model for quantum general relativity, Class. Quantum Grav. **17**, 3101 (2000).

[38] D. Di Bartolo, R. Gambini, J. Griego, and J. Pullin, Consistent quantization of general relativity in the space of Vassiliev knot invariants, Phys. Rev. Lett. **84**, 2314 (2000).

[39] D. Di Bartolo, R. Gambini, J. Griego, and J. Pullin, Canonical quantum gravity in the Vassiliev knot invariants arena: I. Kinematical structure, Class. Quantum Grav. **17**, 3211 (2000).

[40] D. Di Bartolo, R. Gambini, J. Griego, and J. Pullin, Canonical quantum gravity in the Vassiliev knot invariants arena: II. Constraints, habitats and consistency, Class. Quantum Grav. **17**, 3239 (2000).

[41] J. D. Bekenstein, Black holes and entropy, Phys. Rev. D **7**, 2333 (1973).

[42] E. Bianchi, L. Modesto, C. Rovelli, S. Speziale, Graviton propagator in loop quantum gravity, Class.Quantum Grav. **23**, 6989, (2006).

[43] M. Bojowald, Absence of singularity in loop quantum cosmology, Phys. Rev. Lett. **86**, 5227 (2001), (preprint: gr-qc/0102069).

[44] M. Bojowald, Dynamical initial conditions in quantum cosmology, Phys. Rev. Lett. **87**, 121301 (2001).

[45] M. Bojowald, Inflation from quantum geometry, Phys. Rev. Lett. **89**, 261301 (2002).

[46] M. Bojowald, Initial conditions for a universe, Gen. Rel. Grav. **35**, 1877 (2003).

[47] M. Bojowald, Spherically symmetric quantum geometry: States and basic operators, Class. Quantum Grav. **21**, 3733 (2004).

[48] M. Bojowald, Nonsingular black holes and degrees of freedom in quantum gravity, Phys. Rev. Lett. **95**, 061301 (2005).

[49] M. Bojowald, Elements of loop quantum cosmology, preprint: gr-qc/0505057.

[50] M. Bojowald, Loop quantum cosmology, Living Rev. Relativity, **8**, (2005), 11.

[51] M. Bojowald, R. Goswami, R. Maartens, and P. Singh, A black hole mass threshold from non-singular quantum gravitational collapse, Phys. Rev. Lett. **95**, 091302 (2005).

[52] M. Bojowald and H. A. Kastrup, Symmetry reduction for quantized diffeomorphism invariant theories of connections, Class. Quantum Grav. **17**, 3009 (2000).

[53] T. Bröcker and T. Dieck, Representations of Compact Lie Group, (Springer-Verlag, 1985).

[54] J. D. Brown, K. V. Kuchar, Dust as a standard of space and time in canonical quantum gravity, Phys. Rev. D**51**, 5600 (1995), (preprint: gr-qc/9409001).

[55] S. Carlip, Quantum gravity: a progress report, Rept. Prog. Phys. **64**, 885 (2001).

[56] M. Carmeli and S. Malin, Theory of Spinor: An Introduction, (World Scientific, 2000).

[57] Y. Choquet-Bruhat, C. Dewitt-Morette, M. Dillard-Bleick, Analysis, Manifold, and Physics, (North-Holland Publishing Company, 1977).

[58] J. B. Conway, A Course in Functional Analysis, Second Edition, (Springer-Verlag, 1990).

[59] L. Crane, A. Perez, and C. Rovelli, Perturbative finiteness in spin-foam quantum gravity, Phys. Rev. Lett. **87**, 181301 (2001).

[60] G. Date and G. M. Hossain, Genericity of inflation in isotropic loop quantum cosmology, Phys. Rev. Lett. **94**, 011301 (2005).

[61] B. Dittrich, Partial and complete observable for Hamiltonian contrained system, (preprint: gr-qc/0411013).

[62] B. Dittrich, Partial and complete observable for canonical general relativity, (preprint: gr-qc/0507106).

[63] B. Dittrich and T. Thiemann, Testing the master constraint programme for loop quantum gravity I. General framework, Class. Quantum Grav. **23**, 1025 (2006), (preprint: gr-qc/0411138).

[64] B. Dittrich and T. Thiemann, Testing the master constraint programme for loop quantum gravity: II. Finite dimensional systems, Class. Quantum Grav. **23**, 1067 (2006), (preprint: gr-qc/0411139).

[65] B. Dittrich and T. Thiemann, Testing the master constraint programme for loop quantum gravity: III. $SL(2,R)$ models, Class. Quantum Grav. **23**, 1089 (2006), (preprint: gr-qc/0411140).

[66] B. Dittrich and T. Thiemann, Testing the master constraint programme for loop quantum gravity: IV. Free field theories, Class. Quantum Grav. **23**, 1121 (2006), (preprint: gr-qc/0411141).

[67] B. Dittrich and T. Thiemann, Testing the master constraint programme for loop quantum gravity: V. Interecting field theories, Class. Quantum Grav. **23**, 1143 (2006), (preprint: gr-qc/0411142).

[68] M. Domagala and J. Lewandowski, Black hole entropy from quantum gravity, Class. Quantum Grav. **21**, 5233 (2004).

[69] W. Fairbain and C. Rovelli, Separable Hilbert space in loop quantum gravity, J. Math. Phys. **45**, 2802 (2004).

[70] E. E. Flanagan and R. M. Wald, Does backreaction enforce the averaged null energy condition in semiclassical gravity, Phys. Rev. D**54**, 6233 (1996).

[71] L. Freidel and E. Livine, Spin networks for non-Compact groups, J. Math. Phys. **44**, 1322 (2003).

[72] R. Gambini, J. Lewandowski, D. Marolf, and J. Pullin, On the consistency of the constraint algebra in spin network quantum gravity, Int. J. Mod. Phys. D **7**, 97 (1998).

[73] R. Gambini and J. Pullin, Loops, Knots, Gauge Theories and Quantum Gravity, (Cambridge University Press, Cambridge, 1996).

[74] R. Gambini and J. Pullin, Canonical quantization of general relativity in discrete spacetimes, Phys. Rev. Lett. **90**, 021301 (2003).

[75] R. Gambini and J. Pullin, Consistent discretization and loop quantum geometry, Phys. Rev. Lett. **94**, 101302 (2005).

[76] R. Gambini and J. Pullin, Discrete spacetime, Preprint: gr-qc/0505023.

[77] K. Giesel and T. Thiemann, Consistency check on volume and triad operator quantisation in loop quantum gravity I, (preprint: gr-qc/0507036).

[78] K. Giesel and T. Thiemann, Consistency check on volume and triad operator quantisation in loop quantum gravity II, (preprint: gr-qc/0507037).

[79] K. Giesel and T. Thiemann, Algebraic quantum gravity (AQG) I. Conceptual setup, preprint: gr-qc/0607099.

[80] K. Giesel and T. Thiemann, Algebraic quantum gravity (AQG) II. Semiclassical analysis, preprint: gr-qc/0607100.

[81] K. Giesel and T. Thiemann, Algebraic quantum gravity (AQG) III. Semiclassical perturbation theory, preprint: gr-qc/0607101.

[82] R. Giles, Reconstruction of gauge potentials from Wilson loops, Phys. Rev. D **24**, 2160 (1981).

[83] J. Glimm and A. Jaffe, Quantum Physics, (Springer-Verlag, New York, 1987).

[84] N. Guilini and D. Marolf, On the generality of refined algebraic quantization, Class. Quantum Grav. **16**, 2479, (1999).

[85] R. Haag, Local Quantum Physics, 2nd ed. (Springer-Verlag, Berlin, 1996).

[86] B. C. Hall, The Segal-Bergmann coherent state transformation for compact Lie groups, J. Funct. Anal. **122**, 103 (1994).

[87] M. Han, Y. Ma, Y. Ding, and L. Qin, Hamiltonian Analysis of $n$-dimensional Palatini Gravity with Matter, Mod. Phys. Lett. A**20** 725 (2005), (preprint: gr-qc/0503024).

[88] M. Han and Y. Ma, Master constraint operators in loop quantum gravity, Phys. Lett. B**635**, 225 (2006), (preprint: gr-qc/0510014).

[89] M. Han and Y. Ma, Dynamics of a scalar field in a polymer-like representation, Class. Quantum Grav. **23**, 2741 (2006).

[90] M. Han, W. Huang and Y. Ma, Fundamental structure of loop quantum gravity, preprint: gr-qc/0509064.

[91] S. W. Hawking, and G. F. R. Ellis, The large scale structure of space-time, (Cambridge University Press, 1973).

[92] S. Hollands, R. M. Wald, On the renormalization group in curved spacetime, Commun. Math. Phys. **237** 123 (2003).

[93] S. Holst, Barbero's Hamiltonian derived from a generalized Hilbert-Palatini action, Phys. Rev. D **53**, 5966 (1996) (preprint: gr-qc/9511026).

[94] R. K. Kaul and P. Majumdar, Logarithmic corrections to the Bekenstein-Hawking entropy, Phys. Rev. Lett. **84**, 5255 (2000).

[95] J. Lewandowski and D. Marolf, Loop constraints: a habitate and their algebra, Int. J. Mod. Phys. D **7**, 299 (1998).

[96] J. Lewandowski, A. Okolow, H. Sahlmann, T. Thiemann, Uniqueness of diffeomorphism invariant states on holonomy-flux algebras, (preprint: gr-qc/0504147).

[97] C. Liang, Introductory differential geometry and general relativity I, II, (Beijing Normal University Press, 2000, in Chinese).

[98] Y. Ma, Quantization of static spacetimes, Phys. Rev. D **65**, 064012 (2002).

[99] Y. Ma and Y. Ling, Classical geometry from a physical state in canonical quantum gravity, Phys. Rev. D **62**, 064030 (2000).

[100] Y. Ma and Y. Ling, $\hat{Q}$ operator for canonical quantum gravity, Phys. Rev. D **62**, 104021 (2000).

[101] L. Modesto, Disappearance of the black hole singularity in loop quantum gravity, Phys. Rev. D **70**, 124009 (2004).

[102] L. Modesto, The Kantowski-Sachs space-time in loop quantum gravity, preprint: gr-qc/0411032.

[103] L. Modesto, Quantum gravitational collapse, (preprint: gr-qc/0504043).

[104] M. Nakahara, Geometry, Topology, and Physics, Second Edition (Institute of Physics Publishing, 2003).

[105] A. Okolow, Hilbert space built over connections with a non-compact structure group, Class. Quant. Grav. **22**, 1329 (2005).

[106] A. Okolow, Quantization of diffeomorphism invariant theories of connections with a non-compact structure group - an example, (preprint: gr-qc/0605138).

[107] P. Peldàn, Actions for gravity, with generalizations: A review, Class. Quantum Grav. **11**, 1087 (1994), (preprint: gr-qc/9305011).

[108] A. Perez, Finiteness of a spin foam model for Euclidean quantum general relativity, Nucl. Phys. B **599**, 427, (2001).

[109] A. Perez, Spin foam models for quantum gravity, Class. Quantum Grav. **20**, R43 (2003).

[110] A. Perez, On the regularization ambiguities in loop quantum gravity, Phys.Rev. D **73**, 044007 (2006).

[111] A. Perez and C. Rovelli, Spin foam model for Lorentzian general relativity, Phys. Rev. D **63**, 041501 (2001).

[112] A. Perez and C. Rovelli, Physical effects of the Immirzi parameter, Phys.Rev. D **73**, 044013 (2006).

[113] M. Reed, and B. Simon, Methods of Modern Mathematical Phycics I: Functional Analysis, (Academic Press, 1973).

[114] M. Reed and B. Simon, Methods of Modern Mathematical Physics II: Fourer Analysis, Self-adjointness, (Academic Press, 1975), Page 177.

[115] M. Reisenberger and C. Rovelli, Spacetime states and covariant quantum theory, Phys. Rev. D **65**, 125016 (2002).

[116] C. Rovelli, What is observable in classical and quantum gravity, Class. Quantum Grav. **8**, 1895 (1991).

[117] C. Rovelli, Black hole entropy from loop quantum gravity, Phys. Rev. Lett. **14**, 3288 (1996).

[118] C. Rovelli, Loop quantum gravity, Living Rev. Relativity **1** (1998), 1.

[119] C. Rovelli, A note on the foundation of relativistic mechanics. I: Relativistic observables and relativistic states, (preprint: gr-qc/0111037).

[120] C. Rovelli, A note on the foundation of relativistic mechanics. II: Covariant Hamiltonian general relativity, (preprint: gr-qc/0202079).

[121] C. Rovelli, Partial observables, Phys. Rev. D **65**, 124013 (2002).

[122] C. Rovelli, Quantum Gravity, (Cambridge University Press, 2004).

[123] C. Rovelli and L. Smolin, Loop representation for quantum general relativity, Nucl. Phys. B **331**, 80 (1990).

[124] C. Rovelli and L. Smolin, The physical Hamiltonian in nonperturbative quantum gravity, Phys. Rev. Lett **72**, 446 (1994).

[125] C. Rovelli and L. Smolin, Discreteness of area and volume in quantum gravity, Nucl. Phys. B **442**, 593, (1995).

[126] C. Rovelli and L. Smolin, Spin networks and quantum gravity, Phys. Rev. D **52**, 5743, (1995).

[127] C. Rovelli, Graviton propagator from background-independent quantum gravity, Phys.Rev.Lett. **97**, 151301, (2006).

[128] H. Sahlmann and T. Thiemann, Towards the QFT on curved spacetime limit of QGR: I. A general scheme, Class. Quantum Grav. **23**, 867 (2006), (preprint: gr-qc/0207030).

[129] H. Sahlmann and T. Thiemann, Towards the QFT on curved spacetime limit of QGR: II. A concrete implementation, Class. Quantum Grav. **23**, 909 (2006), (Preprint: gr-qc/0207031).

[130] H. Sahlmann and T. Thiemann, Irreducibility of the Ashtekar-Isham-Lewandowski representation, (preprint: gr-qc/0303074).

[131] J. Samuel, Is Barbero's Hamiltonian formulation a gauge throry of Lorentzian gravity? Class. Quantum Grav. **17**, L141 (2000), (Preprint: gr-qc/0005095).

[132] S. Sternberg, Group Theory and Physics, (Cambridge University Press, 1994).

[133] lecture notes given by T. Thiemann at Beijing Normal University.

[134] T. Thiemann, Quantum spin dynamics (QSD), Class. Quantum Grav. **15**, 839 (1998).

[135] T. Thiemann, Quantum spin dynamics (QSD): II. The kernel of the Wheeler - DeWitt constraint operator, Class. Quantum Grav. **15**, 875 (1998).

[136] T. Thiemann, Quantum spin dynamics (QSD): III. Quantum constraint algebra and physical scalar product in quantum general relativity, Class. Quantum Grav. **15**, 1207 (1998).

[137] T. Thiemann, Quantum spin dynamics (QSD): IV. Euclidean quantum gravity as a model to test Lorentzian quantum gravity, Class. Quantum Grav. **15**, 1249 (1998).

[138] T. Thiemann, Quantum spin dynamics (QSD): V. Quantum gravity as the natural regulator of the Hamiltonian constraint of matter quantum field theories, Class. Quantum Grav. **15**, 1281 (1998).

[139] T. Thiemann, Quantum spin dynamics (QSD): VI. Quantum Poincare algebra and a quantum positivity of energy theorem for canonical quantum gravity, Class. Quantum Grav. **15**, 1463 (1998).

[140] T. Thiemann, Quantum spin dynamics (QSD): VIII. The master constraint, Class. Quantum Grav. **23**, 2249 (2006).

[141] T. Thiemann, A length operator for canonical quantum gravity, J. Math. Phys. **39**, 3372 (1998).

[142] T. Thiemann, Gauge field theory coherent states (GCS): I. General properties, Class. Quantum Grav. **18**, 2025 (2001).

[143] T. Thiemann and O. Winkler, Gauge field theory coherent states (GCS): II. Peakedness properties, Class. Quantum Grav. **18**, 2561 (2001).

[144] T. Thiemann and O. Winkler, Gauge field theory coherent states (GCS): III. Ehrenfest theorems, Class. Quantum Grav. **18**, 4629 (2001).

[145] T. Thiemann and O. Winkler, Gauge field theory coherent states (GCS): IV. Infinite tensor product and thermodynamical limit, Class. Quantum Grav. **18**, 4997 (2001).

[146] T. Thiemann, Modern Canonical Quantum General Relativity, (Cambridge University Press, in press), Draft preprint: gr-qc/0110034.

[147] T. Thiemann, Complexifier coherent states for quantum general relativity, Class. Quantum Grav. **23**, 2063 (2006), (preprint: gr-qc/0206037).

[148] T. Thiemann, Lectures on loop quantum gravity, Lect. Notes Phys. 631 (2003) 41, (preprint: gr-qc/0210094).

[149] T. Thiemann, The phoenix project: Master constraint programme for loop quantum gravity, Class. Quantum Grav. **23**, 2211 (2006), (preprint: gr-qc/0305080).

[150] T. Thiemann, Reduced phase space quantization and Dirac observables, Class. Quantum Grav. **23**, 1163 (2006), (preprint: gr-qc/0411031).

[151] T. Thiemann, Loop quantum gravity: an inside view, preprint: hep-th/0608210.

[152] M. Varadarajan, Fock representation from $U(1)$ holonomy agebras, Phys. Rev. D **61**, 104001 (2000).

[153] M. Varadarajan, Photons from quantized electric flux representations, Phys. Rev. D **64**, 104003 (2001).

[154] M. Varadarajan, Gravitons from a loop representation of linearized gravity, Phys. Rev. D **66**, 024012 (2002).

[155] J. M. Velhinho, A groupoid approach to spaces of generalized connections, J. Geom. Phys. **41**, 166 (2002).

[156] R. M. Wald, General Relativity, (The University of Chicago Press, 1984).

[157] R. M. Wald, Quantum Field Theory in Curved Spacetime and Black Hole Thermodynamics, (The University of Chicago Press, 1994).

[158] S. Weinberg, The Quantum Theory of Fields I, II, III, (Cambridge University Press, New York, 1995.)

[159] C. M. Will, The Confrontation between general relativity and experiments, Living Rev. Relativity **4** (2001), 4.

# Vita

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