Dynamics of a scalar field in a polymer-like representation

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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. We consider the quantum dynamics of a real massless scalar field coupled to gravity in this framework. A Hamiltonian operator for the scalar field can be well defined in the coupled diffeomorphism-invariant Hilbert space, which is both self-adjoint and positive. On the other hand, the Hamiltonian constraint operator for the scalar field coupled to gravity can be well defined in the coupled kinematical Hilbert space. There are one-parameter ambiguities due to scalar field in the construction of both operators. The results heighten our confidence that there is no divergence within this background-independent and diffeomorphism-invariant quantization approach of matter coupled to gravity. Moreover, to avoid possible quantum anomaly, the master constraint programme can be carried out in this coupled system by employing a self-adjoint master constraint operator on the diffeomorphism-invariant Hilbert space.

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1. Introduction

The research on quantum gravity theory is rather active. Many quantization programmes for gravity are being carried out (for a summary see, e.g., [1]). In these different kinds of approaches, the idea of loop quantum gravity is motivated by researchers in the community of general relativity. It follows closely the thoughts of general relativity, and hence it is a quantum theory born with background independence [2]. For recent reviews in this field, we refer to [3–5].

To apply the background-independent quantization technique, one first casts general relativity into the Hamiltonian formalism of a diffeomorphism-invariant Yang–Mills gauge
field theory with a compact internal gauge group [6, 7]. The kinematical Hilbert space \( \mathcal{H}^{\text{GR}}_{\text{kin}} \) of the quantum theory is then constructed rigorously. One can even solve the Gaussian and diffeomorphism constraints to arrive at a diffeomorphism-invariant Hilbert space [8]. Certain geometrical operators are shown to have discrete spectra in the kinematical Hilbert space [9–13]. However, some important elements in this approach are not yet understood. Despite the systematic efforts in constructing the Hamiltonian constraint operator [14, 15] and the master constraint operator [16–18], the dynamics of the quantum theory has not been fully understood, especially if one wants to include all known matter fields. The primary goal of this paper is to apply the loop quantization technique to a scalar field and check whether the quantum dynamics can be well defined. Since we will use the developed polymer-like kinematical description of the scalar field [19, 20], it can be considered as a development of the construction for quantum Higgs fields in [21, 22].

In section 2, the Hamiltonian formalism of a massless real scalar field coupled to gravity is obtained in generalized Palatini formulation. For readers’ convenience, the loop quantum kinematical setting of a real scalar field coupled to gravity is also introduced. We then show in section 3 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. Thus, quantum gravity acts exactly as a natural regulator for the quantum scalar field in the polymer representation. In section 4, 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. Moreover, the contribution of the scalar field to the Hamiltonian constraint can be promoted to a positive self-adjoint operator. Similar to the gravitational Hamiltonian constraint, there is a one-parameter ambiguity in defining both the Hamiltonian operator and the constraint operator due to the scalar field. To avoid possible quantum anomaly and find physical Hilbert space, the programme of master constraint for the coupled system is discussed in section 5. A self-adjoint master operator is obtained in the diffeomorphism-invariant Hilbert space, which assures the feasibility of the programme.

2. Polymer-like representation for scalar field coupled to gravity

First consider the classical dynamics of a real massless scalar field \( \phi \) coupled to gravity on a 4-manifold \( M \). The coupled generalized Palatini action reads

\[
S[e^\beta_K, \omega_{\alpha}^{IJ}, \phi] = S_p[e^\beta_K, \omega_{\alpha}^{IJ}] + S_{KG}[e^\beta_K, \phi],
\]

where

\[
S_p[e^\beta_K, \omega_{\alpha}^{IJ}] = \frac{1}{2\kappa} \int_M d^4x(e) e_i^\alpha e_j^\beta \left( \Omega_{\alpha\beta}^{IJ} + \frac{1}{2\gamma} \epsilon^{IJ}_{KL} \Omega_{\alpha\beta}^{KL} \right),
\]

\[
S_{KG}[e^\beta_K, \phi] = -\frac{\alpha_M}{2} \int_M d^4x(e) \eta^{IJ} e_i^\alpha e_j^\beta \eta^{\phi}(\partial_\alpha \phi) \partial_\beta \phi,
\]

here \( e^\beta_K \) and \( \omega_{\alpha}^{IJ} \) are, respectively, the tetrad and Lorentz connection on \( M \), the real numbers \( \gamma, k \) and \( \alpha_M \) are, respectively, the Barbero–Immirzi parameter, the gravitational constant and the coupling constant. From now on, we use \( \alpha, \beta, \ldots \) for four-dimensional spacetime indices and \( I, J, \ldots \) for internal Lorentz indices, \( a, b, \ldots \) for three-dimensional spatial indices and \( i, j, \ldots \) for internal \( SU(2) \) indices. After 3+1 decomposition and Legendre transformation, similar to the case in the Palatini formalism [23], we obtain the total Hamiltonian of the coupling system on the 3-manifold \( \Sigma \) as

\[
\mathcal{H}_{\text{tot}} = \int_\Sigma \left( \Lambda^i G_i + N^a \mathcal{V}_a + NC \right),
\]
where $\Lambda', N^a$ and $N$ are Lagrange multipliers, and the Gaussian, diffeomorphism and Hamiltonian constraints are expressed, respectively, as

$$G_i = D_a \tilde{P}_i^a := \partial_a \tilde{P}_i^a + \epsilon_{ijk} A^j_a \tilde{P}_k^a,$$

$$\gamma_i = \tilde{P}^i_a F_{ab} - A^j_a G_i + \tilde{\pi} \partial_a \phi,$$

$$C = \frac{\kappa \gamma^2}{2\sqrt{\left| \det q \right|}} \tilde{P}_i^a \tilde{P}_j^b \left[ \epsilon^{ij} \delta^{ab} F_{ab}^k - 2(1 + \gamma^2) K_i^a K_j^b \right]$$

$$+ \frac{1}{\sqrt{\left| \det q \right|}} \left[ \frac{\kappa \gamma^2}{2} \delta^{ij} \tilde{P}_i^a \tilde{P}_j^b \left( \partial_a \phi \right) + \frac{1}{2\alpha_M} \pi^2 \right].$$

Here the conjugate pair for gravity consists of the $SU(2)$ connection $A^j_a$ and the densitized triad $\tilde{P}_i^a$. $F_{ab}^k$ is the curvature of $A^j_a$, and $\tilde{\pi}$ denotes the momentum conjugate to $\phi$. Thus, one has the elementary Poisson brackets

$$\{ A_i^a(x), \tilde{P}_b^j (y) \} = \delta^a_b \delta^i_j \delta(x - y), \quad \{ \phi(x), \tilde{\pi}(y) \} = \delta(x - y).$$

Note that the second term of the Hamiltonian constraint (4) is just the Hamiltonian of the real scalar field.

Now, we introduce the background-independent quantization of a real scalar field coupled to gravity, following the polymer representation of the scalar field [19, 20]. The classical configuration space, $U$, consists of all real-valued smooth functions $\phi$ on $\Sigma$. Given a set of a finite number of points $X = \{ x_1, \ldots, x_N \}$ in $\Sigma$, denote as $Cyl_X$ the vector space generated by finite linear combinations of the following functions of $\phi$:

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

where $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ are arbitrary real numbers. It is obvious that $Cyl_X$ has the structure of a ∗-algebra. The space $Cyl$ of all cylindrical functions on $U$ is defined by

$$Cyl := \cup_X Cyl_X.$$  

Completing $Cyl$ with respect to the sup norm, one obtains a unital Abelian $C^*$-algebra $\overline{Cyl}$. Thus, one can use the GNS structure to construct its cyclic representations. A preferred positive linear functional $\omega_0$ on $\overline{Cyl}$ is defined by

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

which defines a diffeomorphism-invariant faithful Borel measure $\mu$ on $U$ as

$$\int_U d\mu(\Pi_{X, \lambda}) = \begin{cases} 1 & \text{if } \lambda_j = 0 \forall j \\ 0 & \text{otherwise.} \end{cases}$$

Thus, one obtains the Hilbert space, $\mathcal{H}_\text{kin}^{K}\equiv L^2(U, d\mu)$, of square integrable functions on a compact topological space $U$ with respect to $\mu$, where $\overline{Cyl}$ acts by multiplication. The quantum configuration space $U$ is called the Gel’fand spectrum of $\overline{Cyl}$. More concretely, for a single point set $X_0 = \{ x_0 \}$, $Cyl_{x_0}$ is the space of all almost periodic functions on a real line $\mathbb{R}$. The Gel’fand spectrum of the corresponding $C^*$-algebra $\overline{Cyl}_{x_0}$ is the Bohr completion $\overline{\mathbb{R}}_{x_0}$ of $\mathbb{R}$ [19], which is a compact topological space such that $\overline{Cyl}_{x_0}$ is the $C^*$-algebra of all continuous functions on $\overline{\mathbb{R}}_{x_0}$. Since $\mathbb{R}$ is densely embedded in $\overline{\mathbb{R}}_{x_0}$, $\overline{\mathbb{R}}_{x_0}$ can be regarded as a completion of $\mathbb{R}$. 
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 \(\psi(\phi) \in \mathcal{H}_{\text{KG}}\) by

\[
\hat{U}(x_0, \lambda_0)\psi(\phi) = U(x_0, \lambda_0)\psi(\phi).
\]

(7)

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 operator \(\hat{U}(x)\) on \(\mathcal{H}_{\text{KG}}\). The momentum functional smeared on a three-dimensional region \(R \subset \Sigma\) is expressed by

\[
\pi(R) := \int_R d^3 x \bar{\pi}(x).
\]

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 \(\Pi_{\gamma(c)}(\phi)\) as

\[
\hat{\pi}(R)\Pi_{\rho, e}(\phi) := i\hbar\{\pi(R), \Pi_{\rho, e}(\phi)\} = i\hbar \sum_{x_j \in X} \lambda_j \chi_R(x_j) \Pi_{\rho, e}(\phi).
\]

It is clear from equation (6) that an orthonormal basis in \(\mathcal{H}_{\text{KG}}\) is given by the so-called scalar-network functions \(\Pi_{\gamma(c)}(\phi)\), where \(c\) denotes \((X(c), \lambda)\) and \(\lambda \equiv (\lambda_1, \lambda_2, \ldots, \lambda_N)\) are non-zero real numbers now. So, the total kinematical Hilbert space \(\mathcal{H}_{\text{kin}}\) is the direct product of the kinematical Hilbert space \(\mathcal{H}_{\text{GR}}\) for gravity and the kinematical Hilbert space for real scalar field, i.e., \(\mathcal{H}_{\text{kin}} := \mathcal{H}_{\text{GR}} \otimes \mathcal{H}_{\text{KG}}\). Let \(\Pi(A)\) be the spin network basis in \(\mathcal{H}_{\text{GR}}\) labelled by \(s\) [11, 24]. Then, the state \(\Pi_{\rho, e} \equiv \Pi_{\rho}(A) \otimes \Pi_{\rho}(\phi) \in \text{Cyl}_y(\mathcal{A}) \otimes \text{Cyl}_{X(c)} \equiv \text{Cyl}_{\gamma(c)}(\mathcal{A}) \otimes \text{Cyl}_{\gamma(c)}(\mathcal{A})\) 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 constitute a complete set of orthonormal basis in \(\mathcal{H}_{\text{kin}}\) as

\[
\langle \Pi_{\gamma(c)}(A, \phi) | \Pi_{\gamma', c}(A, \phi) \rangle_{\mathcal{H}_{\text{kin}}} = \delta_{\gamma, \gamma'} \delta_{c, c'}.
\]

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

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

\[
\hat{U}_\varphi \Pi_{\gamma(x), j}(N, c) = \Pi_{\gamma(\varphi(x)), j}(N, c).
\]

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

\[
\Pi_{\gamma(c), \rho, e} := \frac{1}{n_{\gamma(c), \rho, e}} \sum_{\varphi \in \text{Diff}/\text{Diff}_{\gamma(c), \rho, e}} \sum_{\psi' \in \text{GS}_{\gamma(c), \rho, e}} \hat{U}_\varphi \hat{U}_\psi \Pi_{\gamma(c), \rho, e},
\]

(8)

where \(\text{Diff}_\varphi\) is the set of diffeomorphisms leaving the coloured graph \(\gamma\) invariant, \(\text{GS}_\varphi\) denotes the graph symmetry quotient group \(\text{Diff}_\varphi/T\text{Diff}_\varphi\), where \(T\text{Diff}_\varphi\) is the set of
diffeomorphisms which is trivial on the graph \( \gamma \) and \( n_\gamma \) is the number of elements in \( \text{GS}_\gamma \).

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 such that they form an orthonormal basis as

\[
\langle \Pi_{[s,c]} | \Pi_{[s',c']} \rangle_{\text{Diff}} = \delta_{[s,c],[s',c']}. \tag{9}
\]

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 \( \mathcal{H}_{\text{Diff}} \). In the following sections, we would like to discuss the quantum dynamical properties of the polymer-like scalar field coupled to gravity.

### 3. Diffeomorphism-invariant quantum Hamiltonian of a scalar field

In the present section, we first consider the quantum scalar field on a fluctuating background. A similar idea was considered in [25], where a Hamiltonian operator with respect to a \( U(1) \) group representation of a scalar field is defined on a kinematical Hilbert space \( \mathcal{H}_{\text{kin}} \) of matter coupled to gravity. Then, an effective Hamiltonian operator of the scalar field can be constructed as a quadratic form via

\[
\langle \psi_{\text{matter}}, \hat{H}_{\text{eff \ matter}}(m) \psi_{\text{matter}}' \rangle_{\mathcal{H}_{\text{kin}}'} = \langle \psi_{\text{grav}}(m) \otimes \psi_{\text{matter}}, \hat{H}_{\text{matter}} \psi_{\text{grav}}(m) \otimes \psi_{\text{matter}}' \rangle_{\mathcal{H}_{\text{kin}}'}, \tag{10}
\]

where \( \psi_{\text{grav}}(m) \in \mathcal{H}_{\text{GR} \text{kin}} \) presents a semiclassical state of gravity approximating some classical spacetime background \( m \) where the quantum scalar field lives. Thus, the effective Hamiltonian operator \( \hat{H}_{\text{eff \ matter}}(m) \) of a scalar field also contains information on the fluctuating background metric. In the light of this idea, we will construct a Hamiltonian operator \( \hat{H}_{\text{KG}} \) for a scalar field in the polymer-like representation. It turns out that the Hamiltonian operator can be defined in the Hilbert space \( \mathcal{H}_{\text{Diff}} \) of diffeomorphism-invariant states for a 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 \( \mathcal{H}_{\text{Diff}} \) by defining \( \langle \Psi_{[m]}(A, \phi), \hat{H}_{\text{KG}}(A, \phi) \rangle_{\text{Diff}} \) to be its expectation value on diffeomorphism-invariant states \( \Psi(A, \phi) \) of a scalar field, where the diffeomorphism-invariant semiclassical state \( \Psi_{[m]}(A) \) represents a 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 the theorem in functional analysis.

#### 3.1. Regularization of the Hamiltonian

In a suitable gauge, the classical Hamiltonian for the massless scalar field on the 3-manifold \( \Sigma \) can be given by

\[
\mathcal{H}_{\text{KG}} = \mathcal{H}_{\text{KG, \ phi}} + \mathcal{H}_{\text{KG, \ kin}} = \int_\Sigma d^3x \left[ \frac{\kappa^2 \gamma^2 \alpha_M}{2} \frac{1}{\sqrt{|\det q|}} \delta^{ij} \vec{P}_i^a \vec{P}_j^b (\partial_a \phi) \partial_b \phi + \frac{1}{2\alpha_M} \frac{1}{\sqrt{|\det q|}} \vec{\pi}^2 \right]. \tag{11}
\]

We will employ the following identities:

\[
\vec{P}_i^a = \frac{1}{2k \gamma} \eta^{abc} \epsilon_{ijk} \epsilon_i^j \epsilon_j^k \quad \text{and} \quad \epsilon_i^j(x) = \frac{2}{k \gamma} \{ A_i^a(x), V_{U_i} \},
\]
where $\tilde{\epsilon}_{abc}$ denotes the Levi-Civita tensor tensity and $V_{U_i}$ is the volume of an arbitrary neighbourhood $U_i$ containing the point $x$. By using the point-splitting strategy, the regulated version of the Hamiltonian (11) is obtained as

$$H_{KG,\phi} = \frac{\kappa^2 y^2}{2} \int \sum d^3 y \int dx \chi_s(x-y) \delta^{ij} \frac{1}{\sqrt{V_{U_i}}} \tilde{P}^i(x) \tilde{P}^j(y) \frac{\partial \phi(x)}{\partial x} \frac{\partial \phi(y)}{\partial y}$$

$$= \frac{32\alpha_M}{\kappa^4 y^4} \int \sum d^3 y \int d^3 x \chi_s(x-y) \delta^{ij} \times \tilde{\eta}_{abc} \left( \partial_a \phi(x) \right) Tr \left( \tau_i \left[ A_c(x), \sqrt{V_{U_i}} \right] \left[ A_c(x), \sqrt{V_{U_i}} \right] \right) \times \tilde{\eta}_{bdf} \left( \partial_b \phi(y) \right) Tr \left( \tau_j \left[ A_d(y), \sqrt{V_{U_i}} \right] \left[ A_d(y), \sqrt{V_{U_i}} \right] \right),$$

$$H_{KG,kin} = \frac{1}{2\tilde{\alpha}_M} \int \sum d^3 x \tilde{\tau}(x) \int \sum d^3 y \tilde{\tau}(y) \int \sum d^3 u \tilde{u} \tilde{\tau}(u) \left( \frac{\det \left( e_c^j(u) \right)}{\sqrt{V_{U_i}}} \right)$$

$$= \frac{1}{2\tilde{\alpha}_M} \frac{2^8}{\sqrt{V_{U_i}}} \int \sum d^3 x \tilde{\tau}(x) \int \sum d^3 y \tilde{\tau}(y) \int \sum d^3 u \tilde{u} \tilde{\tau}(u) \left( \frac{\det \left( e_c^j(u) \right)}{\sqrt{V_{U_i}}} \right)$$

$$\times \chi_s(x-y) \chi_s(u-x) \chi_s(w-y),$$

where we denote $A_0 \equiv A_0 \tau_i$, $\chi_s(x-y)$ as the characteristic function of a box containing $x$ with scale $\epsilon$ such that $\lim_{\epsilon \to 0} \chi_s(x-y)/\epsilon^3 = \delta(x-y)$ and $V_{U_i}$ is the volume of the box. In order to quantize the Hamiltonian as a well-defined operator in the polymer-like representation, we have to express the classical formula of $H_{KG}$ in terms of elementary variables with clear quantum analogues. This can be realized 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 the correct limit when $\epsilon \to 0$. Given a tetrahedron $\Delta \in T(\epsilon)$, we use $\{s_1(\Delta)\}_{i=1,2,3}$ to denote the three outgoing oriented segments in $\Delta$ with a common beginning point $v(\Delta) = s(s(\Delta))$ and use $a_i(\Delta)$ to denote the arcs connecting the end points of $s_i(\Delta)$ and $s_j(\Delta)$. Then, several loops $\alpha_i(\Delta)$ are formed by $\alpha_i(\Delta) := s_i(\Delta) \circ a_i(\Delta) \circ s_j(\Delta)^{-1}$. Thus, we have the identities

$$\left\{ \int_{s(\Delta)} \text{d} t \ A_0 \delta^a t \left( V_{U_i}^{3/4} \right) \right\} = -A \left( s(\Delta) \right)^{-1} \left\{ A \left( s(\Delta) \right), V_{U_i}^{3/4} \right\} + o(\epsilon),$$

and

$$\int_{s(\Delta)} \text{d} t \ A_0 \delta^a t = \frac{1}{i\lambda} U \left( s(s(\Delta)), \lambda \right)^{-1} \left[ U \left( t(s(\Delta)), \lambda \right) - U \left( s(s(\Delta)), \lambda \right) \right] + o(\epsilon)$$

for non-zero $\lambda$, 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 classical Hamiltonian of the scalar field reads
\[ \mathcal{H}_{K,\phi} = -\frac{4\alpha_M}{9\kappa^4\pi^2} \sum_{\Delta \in T(e)} \sum_{\Delta' \in T(e)} \chi_c(v(\Delta) - v(\Delta')) \delta^{ij} \]
\[ \times e^{inn} \frac{1}{\lambda} U(v(\Delta), \lambda)^{-1} [U(t(s_i(\Delta)), \lambda) - U(v(\Delta), \lambda)] \]
\[ \times \text{Tr} \left( \tau_i A(s_m(\Delta))^{-1} \left\{ A(s_m(\Delta)), V_{\lambda i}^{3/4} \right\} A(s_n(\Delta))^{-1} \left\{ A(s_n(\Delta)), V_{\lambda j}^{3/4} \right\} \right) \]
\[ \times e^{ipq} \frac{1}{\lambda} U(v(\Delta'), \lambda)^{-1} [U(t(s_i(\Delta')), \lambda) - U(v(\Delta'), \lambda)] \]
\[ \times \text{Tr} \left( \tau_j A(s_p(\Delta'))^{-1} \left\{ A(s_p(\Delta')), V_{\lambda i}^{3/4} \right\} A(s_q(\Delta'))^{-1} \left\{ A(s_q(\Delta')), V_{\lambda j}^{3/4} \right\} \right) \],
where the overall numerical factors are got from the scale of a tetrahedron to an octahedron.

3.2. Quantization of the Hamiltonian

Since all constituents in expression (12) have clear quantum analogues, one can quantize it as an operator by replacing the constituents by the corresponding operators and Poisson brackets by canonical commutators. Then, the regulator should be removed by \( \epsilon \rightarrow 0 \) with respect to a suitable operator topology. Now, we begin to construct the Hamiltonian operator. Given a spin–scalar–network function \( \Pi_{s,c} \), in order to ensure that the final operator is diffeomorphism covariant, and cylindrically consistent (up to diffeomorphisms), one can make the triangulation \( T(\epsilon) \) adapted to the graph \( \gamma(s, c) \) of \( \Pi_{s,c} \) according to the strategy developed in [14] with the following properties:

- The graph \( \gamma(s, c) \) is embedded in \( T(\epsilon) \) for all \( \epsilon \), so that every vertex \( v \) of \( \gamma(s, c) \) coincides with a vertex \( v(\Delta) \) in \( T(\epsilon) \).
- For every triple of edges \( (e_1, e_2, e_3) \) of \( \gamma(s, c) \) such that \( v = s(e_1) = s(e_2) = s(e_3) \), there is a tetrahedron \( \Delta \in T(\epsilon) \) such that \( v = v(\Delta) \) and \( s_1(\Delta) \subset e_i, \forall i = 1, 2, 3 \). We denote such a tetrahedron as \( \Delta_{e_1,e_2,e_3}^0 \).
For each tetrahedron $\Delta_{s_1,s_2,s_3}^0$, one can construct seven additional tetrahedra $\Delta_{s_1,s_2,s_3}^{\epsilon}$, $\epsilon = 1, \ldots, 7$, by backward analytic extensions of $s_i(\Delta)$ so that $U_{s_1,s_2,s_3} = \cup_{\epsilon=1}^7 \Delta_{s_1,s_2,s_3}^{\epsilon}$ is a neighbourhood of $v$.

The triangulation must be fine enough so that the neighbourhoods $U(v) := \cup_{s_i(s^{(1)} \gamma)} U_{s_1,s_2,s_3}(v)$ are disjoint for different vertices $v$ and $v'$ of $\gamma(s, c)$. Thus, for any open neighbourhood $U_{y(s,c)}$ of the graph $\gamma(s, c)$, there exists a triangulation $T(\epsilon)$ such that $\cup_{\epsilon=1}^7 U_{y(s,c)}(v) \subseteq U_{y(s,c)}$.

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 analytically diffeomorphic with each other.

With the triangulation $T(\epsilon)$, the integral over $\Sigma$ is replaced by the Riemann sum:

\[
\int_{\Sigma} = \int_{U_{y(s,c)}} + \int_{\Sigma-U_{y(s,c)}},
\]

\[
\int_{U_{y(s,c)}} = \sum_{v \in V(y(s,c))} \int_{U(v)} + \int_{U_{y(s,c)}-U_{y(s,c)}},
\]

\[
\int_{U(v)} = \frac{1}{C_n(s_1,s_2,s_3)} \sum_{v \in V(y(s,c))} \left[ \int_{U_{1,s_2,s_3}(v)} + \int_{U(v)-U_{1,s_2,s_3}(v)} \right],
\]

where $n(v)$ is the valence of the vertex $v = s(s_1) = s(s_2) = s(s_3)$ and $C_n = \binom{n}{3}$ denotes the binomial coefficient. One then observes that

\[
\int_{U_{1,s_2,s_3}(v)} = 8 \int_{\Delta_{s_1,s_2,s_3}^0},
\]

in the limit $\epsilon \to 0$.

The triangulation for the regions

\[
U(v) = U_{s_1,s_2,s_3}(v), \quad U_{y(s,c)} = \cup_{v \in V(y(s,c))} U(v), \quad \Sigma = U_{y(s,c)}
\]

(13)

is arbitrary. These regions do not contribute to the construction of the operator, since the commutator terms like $[\hat{A}(s_i(\Delta)), \hat{V}_{y(s,c)}]\Pi_{\epsilon,\gamma}$ would vanish for all tetrahedron $\Delta$ in the regions (13).

Note that there are many possible ways of choosing a triangulation. The motivation for the above choice has been fully discussed in [14]. Introducing a partition $\mathcal{P}$ of the 3-manifold $\Sigma$ into cells $C$, we can smear the ‘square roots’ of $\mathcal{H}_{KG,\phi}$ and $\mathcal{H}_{KG,\mathrm{kin}}$ in one cell $C$ respectively and promote them as regulated operators in $\mathcal{H}_{\mathrm{kin}}$ with respect to the state-dependent triangulation $T(\epsilon)$ as

\[
\hat{W}_{y(s,c),\phi,\epsilon}^C = \sum_{v \in V(y(s,c))} \chi_C(v) \sum_{\epsilon(\Delta)=v} \frac{\hat{p}_\Delta}{\sqrt{E(v)}} \hat{h}_{\phi,\epsilon,\Delta}^C \frac{\hat{p}_\Delta}{\sqrt{E(v)}},
\]

\[
\hat{W}_{y(s,c),\mathrm{kin}}^C = \sum_{v \in V(y(s,c))} \chi_C(v) \sum_{\epsilon(\Delta)=v} \frac{\hat{p}_\Delta}{\sqrt{E(v)}} \hat{h}_{\epsilon,\mathrm{kin},\Delta} \frac{\hat{p}_\Delta}{\sqrt{E(v)}},
\]

(14)

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

\[
\hat{h}_{\phi,\epsilon,\Delta}^C := \frac{1}{h^2} \lim_{\epsilon \to 0} \int_{U(v)} \nu(v, \lambda(v))^{-1} \left[ \hat{U}(t(s_i(\Delta)), \lambda(v)) - \hat{U}(v, \lambda(v)) \right]
\]

\[
\times \text{Tr} \left( \tau(\hat{A}(s_m(\Delta)))^{-1} [\hat{A}(s_n(\Delta)), \hat{V}_{U_c}^{1/4}] [\hat{A}(s_n(\Delta)))^{-1} [\hat{A}(s_n(\Delta)), \hat{V}_{U_c}^{1/4}] \right),
\]
\[ \hat{H}^{\text{kin},i} := \frac{1}{(2\pi)^3} \int \mathcal{D}(v) e^{i\mathcal{L}(\Psi,v)} \text{Tr}(\hat{A}(s_{j}(\Delta)))^{-1} \left[ \hat{\mathcal{A}}(s_{j}(\Delta)), \sqrt{\hat{V}_{U_{j}}} \right] \times \hat{A}(s_{m}(\Delta))^{-1} \left[ \hat{\mathcal{A}}(s_{m}(\Delta)), \sqrt{\hat{V}_{U_{m}}} \right] \hat{A}(s_{n}(\Delta))^{-1} \left[ \hat{\mathcal{A}}(s_{n}(\Delta)), \sqrt{\hat{V}_{U_{n}}} \right]. \]  

Note that the tetrahedron projector \( \hat{p}_{\Delta} \) associated with segments \( s_{1}, s_{2} \) and \( s_{3} \) reads

\[
\hat{p}_{\Delta} := \hat{p}_{s_{1}} \hat{p}_{s_{2}} \hat{p}_{s_{3}} \\
= \theta(\frac{1}{2} - \Delta_{s_{1}} - \frac{1}{2}) \theta(\frac{1}{2} - \Delta_{s_{2}} - \frac{1}{2}) \theta(\frac{1}{2} - \Delta_{s_{3}} - \frac{1}{2}) \tag{16}
\]

where \( \Delta_{s_{i}} \) is the Casimir operator associated with the segment \( s_{i} \) and \( \theta \) is the distribution on \( \mathbb{R} \) which vanishes on \( (-\infty, 0] \) and equals 1 on \( [0, \infty) \), and the tetrahedron projector related to a same vertex constitutes the vertex operator \( \hat{E}(v) := \sum_{v(\Delta)=v} \hat{p}_{\Delta} \). Also note that the partition \( \mathcal{P} \) is not required to coincide with the triangulation \( T(\epsilon) \). We have arranged the operator \( \hat{p}_{\Delta} / \sqrt{\hat{E}(v)} \) in such a way that both operators in (14) and their adjoint operators are cylindrically consistent up to diffeomorphisms. Thus, there are two densely defined operators \( \hat{W}^{C}_{\gamma,\phi,i} \) and \( \hat{W}^{C}_{\xi,\phi,i} \) in \( \mathcal{H}_{\text{kin}} \) associated with the two consistent families of (14). We now give several remarks on their properties.

- **Removal of regulator \( \epsilon \)**

  It is not difficult to see that the action of the operator \( \hat{W}^{C}_{\gamma,\phi,i} \) on a spin-scalar-network function \( \Pi_{\gamma,\phi} \) is graph changing. It adds a finite number of vertices with representation \( \lambda(v) \) at \( t(s_{j}(\Delta)) \) 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 \( \hat{W}^{C}_{\gamma,\phi,i} \) also fails to be weakly convergent 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 \( \mathcal{H}_{\text{Diff}} \) invariant.

- **Quantization ambiguity**

  As a main difference of the dynamics in polymer-like representation from that in \( U(1) \) group representation [22], a continuous label \( \lambda(\Delta) \) appears explicitly in the expression of (14). Hence, there is a one-parameter quantization ambiguity due to the real scalar field. Recall that the construction of the 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 [26]. We will come back to this point in a future publication [27]. Since the regulator is removed in a diffeomorphism-invariant way, the quadratic form, which we are going to construct, will be independent of the initial triangulation \( T \) in the sense that it depends only on the diffeomorphism class of \( T \), as is the case of the gravitational Hamiltonian constraint operator [14].

Since our quantum field theory is expected to be diffeomorphism invariant, we would like to define the Hamiltonian operator of the polymer scalar field in the diffeomorphism-invariant Hilbert space \( \mathcal{H}_{\text{Diff}} \). 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 [16, 17]. We first construct a quadratic form in the light of a new inner product defined in [17] on the algebraic dual \( D^{*} \) of the space of cylindrical functions. Then, we prove that the quadratic form is closed. Note that, although the calculation by employing this inner product is formal, it can lead to a well-defined expression of the desired quadratic form (equation (22)). Since an arbitrary element of \( D^{*} \) is of the form \( \Psi = \sum_{s, c} c_{s,c} \langle \Pi_{s,c}, \cdot \rangle_{\text{kin}} \), one can formally
define an inner product \( \langle \cdot | \cdot \rangle \) on \( \mathcal{D}^* \) via
\[
\langle \Psi | \Psi' \rangle_\star := \left( \sum_{\alpha, \beta} \langle \Pi_{\alpha, \beta} | \cdot \rangle_\text{kin} \right) \left( \sum_{\alpha', \beta'} \langle \Pi_{\alpha', \beta'} | \cdot \rangle_\text{kin} \right)^* \sum_{\alpha, \beta} \sum_{\alpha', \beta'} \langle \Pi_{\alpha, \beta} | \Pi_{\alpha', \beta'} \rangle_\text{kin} \frac{1}{\sqrt{N(s, c)N(s', c')}}
\]
\[
= \sum_{s, c} c_{s, c}^* c_{s', c'} \left( \sum_{\alpha, \beta} \frac{1}{8([s, c])} \right),
\]
(17)

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 [17], so that the inner product
\( \langle \Psi_\text{Diff} | \Psi'_\text{Diff} \rangle \), reduces to \( \langle \Psi_\text{Diff} | \Psi'_\text{Diff} \rangle \) for any \( \Psi_\text{Diff}, \Psi'_\text{Diff} \in \mathcal{H}_\text{Diff} \). 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 with some positive and symmetric operator in
analogy with the classical expression of (12). 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 \( \mathcal{H}_\text{Diff} \subset \mathcal{H}_\star \) as
\[
Q_{KG, \phi}(\Psi_\text{Diff}, \Psi'_\text{Diff}) := \lim_{P \to \Sigma} \sum_{C \in \mathcal{P}} 64 \times \frac{4 \alpha_M}{9 \kappa^4 \gamma^2} \delta C (\hat{W}^C_{\phi, j} \Psi_\text{Diff} | \hat{W}^C_{\phi, j} \Psi'_\text{Diff})^* \Psi_\text{Diff}, \Psi'_\text{Diff} \rangle_\text{kin} \langle \Pi_{\alpha, \beta} | \cdot \rangle_\text{kin}
\]
\[
= \lim_{P \to \Sigma} \sum_{C \in \mathcal{P}} 8 \times \frac{4 \alpha_M}{9 \kappa^4 \gamma^2} \delta C \sum_{s, c} \frac{1}{N([s, c])} \sum_{s', c'} \langle \Pi_{\alpha, \beta} | \hbar_{\alpha, \beta} \rangle_\text{kin} \langle \Pi_{\alpha', \beta'} | \hbar_{\alpha', \beta'} \rangle_\text{kin} \frac{1}{8([s, c])} \left( \sum_{\alpha, \beta} \frac{1}{8([s, c])} \right)
\]
(18)

To show that the quadratic forms are well defined, we write
\[
\hat{W}^C_{\phi, j} \Psi_\text{Diff} = \sum_{s, c} w_{\phi, j, s, c}(C) \langle \Pi_{\alpha, \beta} | \cdot \rangle_\text{kin} \Rightarrow \Psi_\text{Diff} = \left( \hat{W}^C_{\phi, j} \Psi_\text{Diff} \right) | \Pi_{\alpha, \beta} \rangle
\]
\[
\hat{W}^C_{\phi, j} \Psi_\text{Diff} = \sum_{s, c} w_{\phi, j, s, c}(C) \langle \Pi_{\alpha, \beta} | \cdot \rangle_\text{kin} \Rightarrow \Psi_\text{Diff} = \left( \hat{W}^C_{\phi, j} \Psi_\text{Diff} \right) | \Pi_{\alpha, \beta} \rangle
\]

Then, by using the inner product (17), the quadratic forms in (18) become
\[
Q_{KG, \phi}(\Psi_\text{Diff}, \Psi'_\text{Diff})
\]
\[
= \lim_{P \to \Sigma} \sum_{C \in \mathcal{P}} 64 \times \frac{4 \alpha_M}{9 \kappa^4 \gamma^2} \delta C \sum_{s, c} \frac{1}{N([s, c])} \sum_{s', c'} \langle \Pi_{\alpha, \beta} | \hbar_{\alpha, \beta} \rangle_\text{kin} \langle \Pi_{\alpha', \beta'} | \hbar_{\alpha', \beta'} \rangle_\text{kin} \frac{1}{8([s, c])} \left( \sum_{\alpha, \beta} \frac{1}{8([s, c])} \right)
\]
(19)

Note that, since \( \Psi_\text{Diff} \) is a finite linear combination of the diffeomorphism-invariant spin-scalar-
network basis, taking the operational property of \( \hat{W}^C_{\phi, j} \) into account there is only a finite number

of terms in the summation \( \sum_{[r,c]} \) contributing to (20). Hence, we can interchange \( \sum_{[r,c]} \) and \( \lim_{\mathcal{P} \to \Sigma} \sum_{C \in \mathcal{P}} \) in the 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 \( \sum_{s,c \in [r,c]} \) and \( \lim_{\mathcal{P} \to \Sigma} \sum_{C \in \mathcal{P}} \) to obtain

\[
Q_{\text{KG, } \Psi}(\Psi_{\text{Diff}}, \Psi_{\text{Diff}}') = 64 \times \frac{4\alpha_M}{9k^2\gamma^2} \sum_{[r,c]} \frac{1}{\mathcal{N}(s, c)} \sum_{s,c \in [r,c]} \lim_{\mathcal{P} \to \Sigma} \sum_{C \in \mathcal{P}} w_{\phi, i, r, c}(C) w_{\phi, i, r, c}'(C)
\]

\[
= 64 \times \frac{4\alpha_M}{9k^2\gamma^2} \sum_{[r,c]} \frac{1}{\mathcal{N}(s, c)} \sum_{s,c \in [r,c]} \sum_{v \in V(\gamma(s, c))} \times (\frac{\hat{W}_{\psi, i}^v}{\text{Diff}}) [\Pi_{s,c} (\frac{\hat{W}_{\psi, j}^v}{\text{Diff}}) ] \Pi_{s,c} '.
\]

\[
Q_{\text{KG, kin}}(\Psi_{\text{Diff}}, \Psi_{\text{Diff}}') = 8^4 \times \frac{16}{81 \alpha_M (\kappa \gamma)^6} \sum_{[r,c]} \frac{1}{\mathcal{N}(s, c)} \sum_{s,c \in [r,c]} \lim_{\mathcal{P} \to \Sigma} \sum_{C \in \mathcal{P}} w_{\psi, i, r, c}(C) w_{\psi, i, r, c}'(C)
\]

\[
= 8^4 \times \frac{16}{81 \alpha_M (\kappa \gamma)^6} \sum_{[r,c]} \frac{1}{\mathcal{N}(s, c)} \sum_{s,c \in [r,c]} \sum_{v \in V(\gamma(s, c))} \times (\frac{\hat{W}_{\psi, i}^v}{\text{Diff}}) [\Pi_{s,c} (\frac{\hat{W}_{\psi, j}^v}{\text{Diff}}) ] \Pi_{s,c} '.
\]

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 \( \hat{W}_{\gamma(s,c), \text{Diff}}^v \Pi_{s,c} (v \in \gamma(s, c)) \) to that of \( \hat{W}_{\gamma'(s',c'), \text{Diff}}^v \Pi_{s,c} (v' \in \gamma'(s', c')) \) with \( \varphi(v) = v' \), \( (\frac{\hat{W}_{\psi, i}^v}{\text{Diff}}) [\Pi_{s,c} (\frac{\hat{W}_{\psi, j}^v}{\text{Diff}}) ] \Pi_{s,c} ' \) is constant for different \( (s, c) \in [s, c] \), i.e., all the \( \mathcal{N}(s, c) \) 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

\[
Q_{\text{KG, } \Psi}(\Psi_{\text{Diff}}, \Psi_{\text{Diff}}') = 64 \times \frac{4\alpha_M}{9k^2\gamma^2} \sum_{[r,c]} \sum_{v \in V(\gamma(s, c))} (\frac{\hat{W}_{\psi, i}^v}{\text{Diff}}) [\Pi_{s,c} (\frac{\hat{W}_{\psi, j}^v}{\text{Diff}}) ] \Pi_{s,c} '.
\]

\[
Q_{\text{KG, kin}}(\Psi_{\text{Diff}}, \Psi_{\text{Diff}}') = 8^4 \times \frac{16}{81 \alpha_M (\kappa \gamma)^6} \sum_{[r,c]} \sum_{v \in V(\gamma(s, c))} (\frac{\hat{W}_{\psi, i}^v}{\text{Diff}}) [\Pi_{s,c} (\frac{\hat{W}_{\psi, j}^v}{\text{Diff}}) ] \Pi_{s,c} '.
\]

Note that both quadratic forms in (22) have finite results and hence their form domains are dense in \( \mathcal{H}_{\text{Diff}} \). Moreover, both of them are obviously positive, and the following theorem will demonstrate their closeness.

**Theorem.** Both \( Q_{\text{KG, } \Psi} \) and \( Q_{\text{KG, kin}} \) are densely defined, positive and closed quadratic forms on \( \mathcal{H}_{\text{Diff}} \), which are uniquely associated with two positive self-adjoint operators, respectively, on \( \mathcal{H}_{\text{Diff}} \) such that

\[
Q_{\text{KG, } \Psi}(\Psi_{\text{Diff}}, \Psi_{\text{Diff}}') = (\Psi_{\text{Diff}} | \hat{\mathcal{H}}_{\text{KG, } \Psi} | \Psi_{\text{Diff}}')_{\text{Diff}}
\]

\[
Q_{\text{KG, kin}}(\Psi_{\text{Diff}}, \Psi_{\text{Diff}}') = (\Psi_{\text{Diff}} | \hat{\mathcal{H}}_{\text{KG, kin}} | \Psi_{\text{Diff}}')_{\text{Diff}}.
\]

Therefore, the Hamiltonian operator

\[
\hat{\mathcal{H}}_{\text{KG}} := \hat{\mathcal{H}}_{\text{KG, } \Psi} + \hat{\mathcal{H}}_{\text{KG, kin}}
\]

is positive and also has a unique self-adjoint extension.
\textbf{Proof.} We follow the strategy developed in [17, 18] to prove that both $Q_{KG, \phi}$ and $Q_{KG, \text{kin}}$ are closable and uniquely induce two positive self-adjoint operators $\hat{H}_{KG, \phi}$ and $\hat{H}_{KG, \text{kin}}$. One can formally define $\hat{H}_{KG, \phi}$ and $\hat{H}_{KG, \text{kin}}$ acting on diffeomorphism-invariant spin-scalar-network functions via

\begin{align}
\hat{H}_{KG, \phi} \Pi_{[t_1, c_1]} &:= \sum_{[t_2, c_2]} Q_{KG, \phi}(\Pi_{[t_2, c_2]}, \Pi_{[t_1, c_1]}) \Pi_{[t_2, c_2]}, \\
\hat{H}_{KG, \text{kin}} \Pi_{[t_1, c_1]} &:= \sum_{[t_2, c_2]} Q_{KG, \text{kin}}(\Pi_{[t_2, c_2]}, \Pi_{[t_1, c_1]}) \Pi_{[t_2, c_2]}.
\end{align}

Then, we need to show that both of the above operators are densely defined on the Hilbert space $\mathcal{H}_{\text{Diff}}$, i.e.,

\begin{align}
\| \hat{H}_{KG, \phi} \Pi_{[t_1, c_1]} \|_{\text{Diff}} &= \sum_{[t_2, c_2]} |Q_{KG, \phi}(\Pi_{[t_2, c_2]}, \Pi_{[t_1, c_1]})|^2 < \infty, \\
\| \hat{H}_{KG, \text{kin}} \Pi_{[t_1, c_1]} \|_{\text{Diff}} &= \sum_{[t_2, c_2]} |Q_{KG, \text{kin}}(\Pi_{[t_2, c_2]}, \Pi_{[t_1, c_1]})|^2 < \infty.
\end{align}

Given a diffeomorphism-invariant spin-scalar-network function $\Pi_{[t_1, c_1]}$, there are only finite number of terms $\Pi_{[t_1, c_1]}[\hat{W}^{c, \phi}_{\gamma(t), \epsilon} \Pi_{\epsilon, \epsilon(t)}]$, which are non-zero in the sum over equivalent classes $[s, c]$ in (22). On the other hand, given one spin-scalar-network function $\Pi_{s, c}$, there is also only a finite number of possible $\Pi_{[t_2, c_2]}$ such that the terms $\Pi_{[t_2, c_2]}[\hat{W}^{c, \phi}_{\gamma(t), \epsilon} \Pi_{\epsilon, \epsilon(t)}]$ are non-zero. As a result, only a finite number of terms survives in both sums over $[s_2, c_2]$ in equations (26) and (27). Hence, both $\hat{H}_{KG, \phi}$ and $\hat{H}_{KG, \text{kin}}$ are well defined. Then, it follows from equations (22), (24) and (25) that they are positive and symmetric operators densely defined in $\mathcal{H}_{\text{Diff}}$, whose quadratic forms coincide with $Q_{KG, \phi}$ and $Q_{KG, \text{kin}}$ on their form domains. Hence, both $Q_{KG, \phi}$ and $Q_{KG, \text{kin}}$ have positive closures and uniquely induce self-adjoint (Friedrichs) extensions of $\hat{H}_{KG, \phi}$ and $\hat{H}_{KG, \text{kin}}$, respectively [28], which we denote by $\hat{H}_{KG, \phi}$ and $\hat{H}_{KG, \text{kin}}$ as well. As a result, the Hamiltonian operator $\hat{H}_{KG}$ defined by equation (23) is also positive and symmetric. Hence, it has a unique self-adjoint (Friedrichs) extension.

We note that, from a different perspective, one can construct the same Hamiltonian operator $\hat{H}_{KG}$ without introducing an inner product on $\mathcal{D}^*$. The construction is sketched as follows. Using the two well-defined operators $\hat{W}^{c, \phi}_{\phi, \phi}$ and $\hat{W}^{c, \phi}_{\text{kin}}$ as in (14), as well as their adjoint operators $(\hat{W}^{c, \phi}_{\phi, \phi})^\dagger$ and $(\hat{W}^{c, \phi}_{\text{kin}})^\dagger$, one may define two operators on $\mathcal{H}_{\text{Diff}}$ corresponding to the two terms in (12) by

\begin{align}
(\hat{H}_{KG, \phi} \Psi_{\text{Diff}})[f_y] &= \lim_{\epsilon, \epsilon' \to 0, \beta} \Psi_{\text{Diff}} \left[ \sum_{C \in \mathcal{P}} 64 \times \frac{4\alpha_M}{9\kappa^{-4} \gamma^2} \delta^{ij} \hat{W}^{c, \phi}_{\phi, j} (\hat{W}^{c, \phi}_{\phi, i})^\dagger f_y \right], \\
(\hat{H}_{KG, \text{kin}} \Psi_{\text{Diff}})[f_y] &= \lim_{\epsilon, \epsilon' \to 0, \beta} \Psi_{\text{Diff}} \left[ \sum_{C \in \mathcal{P}} 8^4 \times \frac{16}{81\alpha_M(\kappa')^{-6}} \hat{W}^{c, \phi}_{\text{kin}} (\hat{W}^{c, \phi}_{\text{kin}})^\dagger f_y \right].
\end{align}

In analogy with the discussion in section 5 and [18], it can be shown that both the above operators leave $\mathcal{H}_{\text{Diff}}$ invariant and are densely defined on $\mathcal{H}_{\text{Diff}}$. Moreover, the quadratic forms associated with them coincide with the quadratic forms in (22). Thus, the Hamiltonian operator $\hat{H}_{KG} := \hat{H}_{KG, \phi} + \hat{H}_{KG, \text{kin}}$ coincides with the one constructed in the quadratic form approach.
In summary, we have constructed a positive self-adjoint Hamiltonian operator on $H_{\text{Diff}}$ for the polymer-like scalar field, depending on a chosen parameter $\lambda$. Thus, there is a one-parameter ambiguity in the construction. However, there is no UV divergence in this quantum Hamiltonian without renormalization, since quantum gravity is presented as a natural regulator for the polymer-like scalar field.

4. Quantum Hamiltonian constraint equation

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 energy–momentum, is ambiguous and it is extremely difficult to calculate the backreaction of quantum fields to the background spacetime [29]. This is reflected by the fact that the semiclassical Einstein equation,

$$R_{\alpha\beta}\left[g\right] - \frac{1}{2}R\left[g\right]g_{\alpha\beta} = \kappa \langle \hat{T}_{\alpha\beta}\left[g\right]\rangle,$$

is inconsistent and ambiguous [1, 30]. One could speculate that the difficulty is related to the fact that the present formulation of quantum field theories is background dependent. According to this speculation, if the quantization programme is by construction non-perturbative and background independent, it is 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 the quantum theory of pure gravity, since all the physical states have to satisfy a certain version of the quantum Wheeler–DeWitt constraint equation. However, the situation would be improved when the matter field is coupled to gravity. In the following construction, we impose the quantum Hamiltonian constraint on $H_{\text{kin}}$, 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 backreaction of the quantum scalar field is included in the framework of loop quantum gravity.

Recall that the gravitational Hamiltonian constraint operator $\hat{H}_{\text{GR}}(N)$ can be well defined in $H_{\text{GR}}^{\text{kin}}$ by the uniform Rovelli–Smolin topology [5, 14]. Hence, it is also well defined in the coupled kinematical Hilbert space $H_{\text{kin}}$. Its regulated version via a state-dependent triangulation $T(\epsilon)$ reads

$$\hat{H}_{\text{GR}}^\epsilon(N) = \hat{H}_E^\epsilon(N) - 2(1 + \gamma^2)\hat{T}^\epsilon(N),$$

$$\hat{H}_{E,\alpha}^\epsilon(N) = \frac{16}{3\hbar^2\gamma} \sum_{v \in V(\alpha)} N(v) \sum_{v(\Delta) = v} \epsilon^{ijk} \times \text{Tr} \left( \hat{A}(\alpha_{ij}(\Delta))^{-1} \hat{A}(s_k(\Delta))^{-1} [\hat{A}(s_k(\Delta)), \hat{V}_\alpha]\right) \frac{\hat{p}_\lambda}{E(v)},$$

$$\hat{T}_\alpha^\epsilon(N) = - \frac{4\sqrt{2}}{3\hbar^2\gamma^3} \sum_{v \in V(\alpha)} N(v) \sum_{v(\Delta) = v} \epsilon^{ijk} \times \text{Tr} \left( \hat{A}(s_i(\Delta))^{-1} [\hat{A}(s_i(\Delta)), \hat{K}^\epsilon] \hat{A}(s_j(\Delta))^{-1} [\hat{A}(s_j(\Delta)), \hat{K}^\epsilon] \right) \times \hat{A}(s_k(\Delta))^{-1} \left[ \hat{A}(s_k(\Delta)), \hat{V}_\alpha \right] \frac{\hat{p}_\lambda}{E(v)}. \quad (30)$$

We now define an operator in $H_{\text{kin}}$ corresponding to the scalar field part $H_{\text{KG}}(N)$ of the total Hamiltonian constraint functional, which can be read out from equations (1) and (4) as

$$H_{\text{KG}}(N) = H_{\text{KG,\phi}}(N) + H_{\text{KG,kin}}(N).$$
where

\[ \mathcal{H}_{\text{KG}, \phi}(N) = \frac{k^2 \gamma^2 \alpha_M}{2} \int_{\Sigma} d^3x N \frac{1}{\sqrt{|\det q|}} \delta^i_j \tilde{P}_i^a \tilde{P}_j^b (\partial_x \phi) \partial_y \phi, \]

\[ \mathcal{H}_{\text{KG}, \text{kin}}(N) = \frac{1}{2 \alpha_M} \int_{\Sigma} d^3x N \frac{1}{\sqrt{|\det q|}} \pi^2. \]

In analogy with the regularization and quantization in the previous section, the regulated version of the quantum Hamiltonian constraint \( \hat{\mathcal{H}}_{\text{KG}}(N) \) of the scalar field is expressed via a state-dependent triangulation \( T(\epsilon) \) as

\[ \hat{\mathcal{H}}_{\text{KG}, \gamma}(N) := \sum_{v \in V(\gamma)} N(v) \left[ \delta^{ij} \left( \hat{W}_{\gamma, \phi, i}^{e, v} \right)^\dagger \hat{W}_{\gamma, \phi, j}^{e, v} + \left( \hat{W}_{\gamma, \text{kin}}^{e, v} \right)^\dagger \hat{W}_{\gamma, \text{kin}}^{e, v} \right], \quad (31) \]

where the operators

\[ \hat{W}_{\gamma, \phi, i}^{e, v} := \sum_{v(\Delta) = v} \frac{\hat{P}_{\Delta}^{\phi, \Delta}}{\sqrt{E(v)}} \left( \hat{\delta}_{e, \phi, i}^{\Delta} \right)^\dagger \frac{\hat{P}_{\Delta}}{\sqrt{E(v)}}, \]

\[ \hat{W}_{\gamma, \text{kin}}^{e, v} := \sum_{v(\Delta) = v} \frac{\hat{P}_{\Delta}}{\sqrt{E(v)}} \left( \hat{\delta}_{e, \phi, i}^{\Delta} \right)^\dagger \frac{\hat{P}_{\Delta}}{\sqrt{E(v)}} \]

are all cylindrically consistent up to diffeomorphisms. Hence, the family of Hamiltonian constraint operators (31) is also cylindrically consistent up to diffeomorphisms, and the regulator \( \epsilon \) can be removed via the uniform Rovelli–Smolin topology or equivalently the limit operator dually acts on diffeomorphism-invariant states as

\[ \langle \hat{\mathcal{H}}_{\text{KG}}'(N) \Psi_{\text{Diff}} \rangle[f_{\gamma}] = \lim_{\epsilon \to 0} \langle \Psi_{\text{Diff}} [\hat{\mathcal{H}}_{\text{KG}, \gamma}(N)] f_{\gamma} \rangle, \quad (32) \]

for any \( f_{\gamma} \in \text{Cyl}_{\gamma}(\mathcal{A}) \otimes \text{Cyl}_{\gamma}(\mathcal{T}) \). Similar to the dual of \( \hat{\mathcal{H}}_{\text{GR}}(N) \), the operator \( \hat{\mathcal{H}}_{\text{KG}}'(N) \) fails to commute with the dual of finite diffeomorphism transformation operators, unless the smearing function \( N(x) \) is a constant function over \( \Sigma \). Note that the diffeomorphism-invariant Hamiltonian operator \( \hat{\mathcal{H}}_{\text{KG}} \) defined in the previous section is actually \( \hat{\mathcal{H}}_{\text{KG}}(1) \). From equation (31), it is not difficult to prove that for positive \( N(x) \) the Hamiltonian constraint operator \( \hat{\mathcal{H}}_{\text{KG}}(N) \) of the scalar field is positive and symmetric in \( \mathcal{H}_{\text{kin}} \) and hence has a unique self-adjoint extension. It is pointed out in [31] that there can be problems associated with symmetric constraint operators for systems where the constraints are close with structure functions as in the present case. However, not all the assumptions underlying this conclusion are valid in the framework of loop quantum gravity. For example, it is assumed in [31] that all the classical canonical variables and constraints could be promoted as well-defined operators in the kinematical Hilbert space. However, it is well known that the classical connection and diffeomorphism constraint cannot be represented as well-defined operators in loop quantum gravity. This issue related to the symmetric Hamiltonian constraint operator was fully discussed in [14].

Our construction of \( \hat{\mathcal{H}}_{\text{KG}}(N) \) is similar to that of the Higgs field Hamiltonian constraint in [22]. However, like the case of \( \hat{\mathcal{H}}_{\text{KG}} \), there is a one-parameter ambiguity in our construction of \( \hat{\mathcal{H}}_{\text{KG}}(N) \) due to the real scalar field, which is manifested as the continuous parameter \( \lambda \) in the expression of \( \hat{W}_{\gamma, \phi, i}^{e, v} \) in (15). Note that now \( \lambda \) is not required to be a constant, i.e., its value can be changed from one point to another. This issue of ambiguity will be discussed again in a future publication [27]. Thus, the total Hamiltonian constraint operator of scalar field coupled to gravity has been obtained as

\[ \hat{\mathcal{H}}(N) = \hat{\mathcal{H}}_{\text{GR}}(N) + \hat{\mathcal{H}}_{\text{KG}}(N). \quad (33) \]
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 $\epsilon$ artificially. Now $\epsilon$ has naturally disappeared from the expressions of (23) and (33). So, renormalization is not needed for the polymer-like scalar field coupled to gravity, since quantum gravity has been presented as a natural regulator. Together with the result in the previous section, this heightens our confidence that the issue of divergence in quantum field theory can be cured in the framework of loop quantum gravity. The desired matter-coupled Wheeler–DeWitt equation can be well imposed as

$$\left(-\hat{H}'_{KG}(N)\Psi_{Diff}\right)[f_{\gamma}] = \left(\hat{H}'_{GR}(N)\Psi_{Diff}\right)[f_{\gamma}].$$

(34)

Note that the scalar field part $\hat{H}_{KG}(N)$ acts nontrivially on gravitational quantum states. This can be regarded as the ‘backreaction’ of the quantum matter field to the quantum gravitational field. On the other hand, comparing equation (34) with the well-known Schrödinger equation for a particle,

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

where $\psi(x, t) \in L^2(\mathbb{R}, dx)$ and $t$ is a parameter labelling time evolution, one may take the viewpoint that the matter field constraint operator $\hat{H}'_{KG}(N)$ plays the role of $i\hbar \frac{\partial}{\partial t}$. Then, $\phi$ appears as the parameter labelling the evolution of the gravitational field state. In the reverse viewpoint, the gravitational field would become the parameter labelling the evolution of the quantum matter field.

5. Master constraint programme

In order to avoid possible quantum anomaly and find the physical Hilbert space of quantum gravity, the master constraint programme was first introduced by Thiemann in [16]. The central idea is to construct an alternative classical constraint algebra, giving the same constraint phase space, which is a Lie algebra (no structure function) and where the subalgebra of diffeomorphism constraints forms an ideal. Self-adjoint master constraint operators for loop quantum gravity are then proposed in [17, 18]. 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 strategy in [18]. By this approach, one not only avoids a possible quantum anomaly 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

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

(35)

where $C(x)$ is the Hamiltonian constraint in (4). After solving the Gaussian constraint, one gets the master constraint algebra as a Lie algebra:

$$\{\mathcal{V}(\tilde{N}), \mathcal{V}(\tilde{N}')\} = \mathcal{V}([\tilde{N}, \tilde{N}']), \quad \{\mathcal{V}(\tilde{N}), M\} = 0, \quad \{M, M\} = 0,$$

(36)

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 $M$ 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

$$\mathbf{M}^e := \frac{1}{2} \int_\Sigma d^3y \int_\Sigma d^3x \chi_e(x - y) \frac{C(v)}{\sqrt{V_U}} \frac{C(x)}{\sqrt{V_U'}}.$$  (37)

Introducing a partition $\mathcal{P}$ of the 3-manifold $\Sigma$ into cells $C$, we have an operator $\hat{H}^e_{C,\gamma}$ acting on any cylindrical function $f_\gamma \in \text{Cyl}_1^\gamma(\mathcal{A}) \otimes \text{Cyl}_1^\gamma(\mathcal{T})$ via a state-dependent triangulation $T(\epsilon)$,

$$\hat{H}^{e,\Delta}_{C,\gamma} = \sum_{v \in V(\gamma)} \chi_C(v) \sum_{t(\Delta) = v} \frac{\hat{p}_\Delta}{\epsilon E(v)} \hat{H}^{e,\Delta}_{C,R,v} + \frac{\hat{p}_\Delta}{\epsilon E(v)}$$

$$\sum_{v \in V(\gamma)} \chi_C(v) \left[ \delta^{ij} \left( \hat{w}_{\gamma,\phi,i}^e \right) \hat{w}_{\gamma,\phi,j}^e + \left( \hat{w}_{\gamma,\phi,j}^e \right)^\dagger \hat{w}_{\gamma,\phi,i}^e \right].$$  (38)

where

$$\hat{H}^{e,\Delta}_{C,R,v} = \frac{16}{3h k^4 \gamma^2 \epsilon^{2i}} \text{Tr} \left( \hat{A}(\alpha_{ij}^{(\Delta)})^{-1} \hat{A}(s_k^{(\Delta)})^{-1} \left[ \hat{A}(s_k^{(\Delta)}), \sqrt{V_U} \right] \right)$$

$$+ (1 + \gamma^2) \frac{8 \sqrt{2}}{3h k^4 \gamma^2 \epsilon^{2i}} \text{Tr} \left( \hat{A}(s_j^{(\Delta)})^{-1} \left[ \hat{A}(s_j^{(\Delta)}), \hat{K}^e \right] \right) \times \hat{A}(s_j^{(\Delta)})^{-1} \left[ \hat{A}(s_j^{(\Delta)}), \sqrt{V_U} \right],$$

$$\hat{w}_{\gamma,\phi,i}^e = \frac{i}{\sqrt{h}} \sum_{t(\Delta) = v} \frac{\hat{p}_\Delta}{\epsilon E(v)} \frac{1}{\lambda} U(v, \lambda)^{-1} \left[ \hat{U}(v, \lambda) - \hat{U}(t(\Delta), \lambda) - \hat{U}(v, \lambda) \right]$$

$$\times \text{Tr} \left( \delta \hat{A}(s_m^{(\Delta)})^{-1} \left[ \hat{A}(s_m^{(\Delta)}), \hat{V}_{U^e_i}^{s_m^{(\Delta)}} \right] \hat{A}(s_m^{(\Delta)})^{-1} \left[ \hat{A}(s_m^{(\Delta)}), \hat{V}_{U^e_i}^{s_m^{(\Delta)}} \right] \right) \frac{\hat{p}_\Delta}{\sqrt{E(v)}},$$

$$\hat{w}_{\gamma,\phi,j}^e = \frac{1}{(2h)} \sum_{t(\Delta) = v} \frac{\hat{p}_\Delta}{\epsilon E(v)} \frac{1}{\lambda} U(v, \lambda)^{-1} \left[ \hat{U}(v, \lambda) - \hat{U}(t(\Delta), \lambda) - \hat{U}(v, \lambda) \right]$$

$$\times \text{Tr} \left( \delta \hat{A}(s_n^{(\Delta)})^{-1} \left[ \hat{A}(s_n^{(\Delta)}), \hat{V}_{U^e_i}^{s_n^{(\Delta)}} \right] \hat{A}(s_n^{(\Delta)})^{-1} \left[ \hat{A}(s_n^{(\Delta)}), \hat{V}_{U^e_i}^{s_n^{(\Delta)}} \right] \right) \frac{\hat{p}_\Delta}{\sqrt{E(v)}},$$  (39)

The notation here is same as in section 3. Note that $\hat{H}^{e,\Delta}_{C,\gamma}$ is similar to the Hamiltonian constraint operator $\hat{H}(1)$ defined in the last section, but is now divided by the square root of volume operator. Hence, the action of $\hat{H}^{e,\Delta}_{C,\gamma}$ on a cylindrical function $f_\gamma$ adds analytical arcs $a_{ij}(\Delta)$ with $j$-representation (or arbitrary chosen spin $j$-representation of $SU(2)$ if one uses non-fundamental representations to express the holonomies in (30)) and points at $t(s_i^{(\Delta)})$ with representation $\lambda$ with respect to each vertex $v(\Delta)$ of $\gamma$. Thus, for each $\epsilon > 0$, $\hat{H}^{e,\Delta}_{C,\gamma}$ is a $SU(2)$ gauge invariant and diffeomorphism covariant operator defined on $\text{Cyl}_1^\gamma(\mathcal{A}) \otimes \text{Cyl}_1^\gamma(\mathcal{T})$. The family of such operators with respect to different graphs is cylindrically consistent up to diffeomorphisms. So, the inductive limit operator $\hat{H}_C$ is densely defined on $\mathcal{H}_{kin}$ by the uniform Rovelli–Smolin topology. Moreover, the adjoint operators of $\hat{H}^{e,\Delta}_{C,\gamma}$, which are also cylindrically consistent up to diffeomorphisms, read

$$\left( \hat{H}^{e,\Delta}_{C,\gamma} \right)^\dagger = \sum_{v \in V(\gamma)} \chi_C(v) \sum_{t(\Delta) = v} \frac{\hat{p}_\Delta}{\epsilon E(v)} \left( \hat{H}^{e,\Delta}_{C,R,v} \right)^\dagger + \frac{\hat{p}_\Delta}{\epsilon E(v)}$$

$$\sum_{v \in V(\gamma)} \chi_C(v) \left[ \delta^{ij} \left( \hat{w}_{\gamma,\phi,i}^e \right)^\dagger \hat{w}_{\gamma,\phi,j}^e + \left( \hat{w}_{\gamma,\phi,j}^e \right)^\dagger \hat{w}_{\gamma,\phi,i}^e \right].$$  (40)
The inductive limit operator of (40) is denoted by $(\hat{H}_C^\epsilon)^\dagger$, which is adjoint to $\hat{H}_C$ as
\[
(\langle g, \hat{H}_C^\epsilon f \rangle)_\text{kin} = (\langle \langle g^\epsilon, \hat{H}_C, f \rangle \rangle)_\text{kin} = (\langle \hat{H}_C^\epsilon g^\epsilon, f \rangle)_\text{kin}
\]
(41)

Then, a master constraint operator, $\hat{M}$, in $\mathcal{H}_{Diff}$ can be defined as
\[
(\hat{M}\Psi_{Diff})(\Pi_{s,c}) := \lim_{\mathcal{P} \to \Sigma, \epsilon \to 0} \Psi_{Diff} \left[ \sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_C^\epsilon (\hat{H}_C^\epsilon)^\dagger \right].
\]
(42)

Since $\hat{H}_C^\epsilon (\hat{H}_C^\epsilon)^\dagger$ is a finite linear combination of spin-scalar-network functions on an extended graph with skeleton $\gamma$, the value of $(\hat{M}\Psi_{Diff})(\Pi_{s,c})$ is finite for a given $\Psi_{Diff} \in \mathcal{H}_{Diff}$. So, $\hat{M}\Psi_{Diff}$ is in the algebraic dual of the space of cylindrical functions. Moreover, we can show that it is diffeomorphism invariant. For any diffeomorphism transformation $\varphi$,
\[
(\hat{U}_\varphi \hat{M}\Psi_{Diff})(f) = \lim_{\mathcal{P} \to \Sigma, \epsilon \to 0} \Psi_{Diff} \left[ \sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_C^\epsilon (\hat{H}_C^\epsilon)^\dagger \hat{U}_\varphi f \right]
\]
(43)

for any cylindrical function $f$, 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
\[
(\hat{U}_\varphi \hat{M}\Psi_{Diff})(f) = (\hat{M}\Psi_{Diff})(f).
\]
(44)

On the other hand, given any diffeomorphism-invariant spin-scalar-network state $\Pi_{s,c}$, the norm of the result state $\hat{M}\Pi_{s,c}$ can be expressed as
\[
\|\hat{M}\Pi_{s,c}\|_{\text{Diff}}^2 = \sum_{[s', c']^2 \}} \left| (\langle \hat{M}\Pi_{s,c} | \Pi_{s', c'} \rangle)_{\text{Diff}} \right|^2
\]
(45)

\[
= \sum_{[s', c']^2 \}} \left| \lim_{\mathcal{P} \to \Sigma, \epsilon \to 0} \Pi_{s,c} \left[ \sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_C^\epsilon (\hat{H}_C^\epsilon)^\dagger \right] \right|^2
\]
(46)

\[
= \sum_{[s', c']^2 \}} \left| \lim_{\mathcal{P} \to \Sigma, \epsilon \to 0} \frac{1}{h_{\gamma(s,c)}} \sum_{\psi \in \text{Diff}(s,c)} \sum_{\psi' \in \text{GB}(s,c)} \times \hat{U}_\psi \hat{U}_{\psi'} \Pi_{s', c'} \left[ \sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_C^\epsilon (\hat{H}_C^\epsilon)^\dagger \right] \right|^2
\]
(47)

\[
= \sum_{[s', c']^2 \}} \left| \lim_{\mathcal{P} \to \Sigma, \epsilon \to 0} \frac{1}{h_{\gamma(s,c)}} \sum_{\psi \in \text{Diff}(s,c)} \sum_{\psi' \in \text{GB}(s,c)} \times \hat{U}_\psi \hat{U}_{\psi'} \Pi_{s', c'} \left[ \sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_C^\epsilon (\hat{H}_C^\epsilon)^\dagger \right] \right|^2
\]
where we make use of the fact that $\hat{M}$ commutes with diffeomorphism transformations. Note that the cylindrical function $\sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_C^e (\hat{H}_C^e) | \Pi_{s,c} \in [s,c] \rangle \rangle_{\text{kin}}$ is a finite linear combination of spin-scalar-network functions on some extended graph, so that there is only a finite number of terms contributing to the sum in equation (45). Hence, it automatically converges. So, the master constraint operator $\hat{M}$ defined by equation (42) is densely defined on $\mathcal{H}_{\text{Diff}}$.

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

$$\langle \Pi_{[s_1,c_1]} | \hat{M} | \Pi_{[s_2,c_2]} \rangle_{\text{Diff}} = \langle M \Pi_{[s_1,c_1]} | \Pi_{[s_1,c_1]} \rangle_{\text{Diff}}$$

$$= \lim_{P \to \Sigma, e \to 0} \sum_{C \in \mathcal{P}} \frac{1}{2} \Pi_{[s_2,c_2]} \langle \hat{H}_C^e (\hat{H}_C^e) | \Pi_{s,c_1} \in [s_1,c_1] \rangle_{\text{kin}}$$

$$= \lim_{P \to \Sigma, e \to 0} \sum_{C \in \mathcal{P}} \frac{1}{2} n_{y(s',c')} \sum_{\varphi \in \text{Diff}(\Sigma, e \to 0)} \sum_{\psi \in \text{GS}_{y(s',c')}}$$

$$\times \langle \hat{U}_\varphi \hat{U}_\psi \Pi_{s,c_1} \in [s,c_1] | \hat{H}_C^e (\hat{H}_C^e) \Pi_{s_1,c_2} \in [s_1,c_2] \rangle_{\text{kin}}$$

$$= \sum_{s,c} \lim_{P \to \Sigma, e \to 0} \sum_{C \in \mathcal{P}} \frac{1}{2} n_{y(s',c')} \sum_{\varphi \in \text{Diff}(\Sigma, e \to 0)} \sum_{\psi \in \text{GS}_{y(s',c')}}$$

$$\times \langle \hat{U}_\varphi \hat{U}_\psi \Pi_{s,c} \in [s,c] | \hat{H}_C^e (\hat{H}_C^e) \Pi_{s_1,c_1} \in [s_1,c_1] \rangle_{\text{kin}}$$

$$= \sum_{[s,c] \in V_{[s,c]}} \sum_{e \to 0} \frac{1}{2} \lim_{P \to \Sigma, e \to 0}$$

$$\times \Pi_{[s,c]} | \hat{H}_C^e (\hat{H}_C^e) \Pi_{s_1,c_1} \rangle_{\text{kin}},$$

where Diff$_y$ is the set of diffeomorphisms leaving the coloured graph $y$ invariant, GS$_y$ denotes the graph symmetry quotient group Diff$_y$ / T Diff$_y$, where T Diff$_y$ is the diffeomorphism which is trivial on the graph $y$ and $n_y$ is the number of elements in GS$_y$. 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 $\sum_{s,c} \sum_{[s,c] \in V_{[s,c]}}$ into $\sum_{s,c} \sum_{e \to 0} \frac{1}{2} \lim_{P \to \Sigma, e \to 0}$, where $[s,c]$ denotes the diffeomorphism equivalent class associated with $(s,c)$. Here, we also use the fact that, given $y(s,c)$ and $y(s',c')$ which are different up to a diffeomorphism transformation, there is always a diffeomorphism $\varphi$ transforming the graph associated with $\hat{H}_{C,y(s,c)} \Pi_{s,c} (v \in y(s,c))$ to that of $\hat{H}_{C,y(s',c')} \Pi_{s',c'} (v' \in y(s',c'))$ with $\varphi(v) = v'$, hence $\Pi_{[s,c]} | \hat{H}_{C,y(s,c)} \Pi_{s,c} \rangle_{\text{kin}}$ is constant for different $(s,c) \in [s,c]$.
Since the term \( \sum_{s,c} \langle \Pi_{s,c} | (\hat{H}_c^\epsilon) | \Pi_{s,c} \rangle_{\text{kin}} \) is independent of the parameter \( \epsilon' \), one can see that, by fixing an arbitrary state-dependent triangulation \( T(\epsilon') \),

\[
\sum_{s,c} \langle \Pi_{s,c} | (\hat{H}_c^\epsilon) | \Pi_{s,c} \rangle_{\text{kin}} = \sum_{s,c} \langle U_{\epsilon'} \Pi_{s,c} | (\hat{H}_c^\epsilon) | U_{\epsilon'} \Pi_{s,c} \rangle_{\text{kin}} = \sum_{s,c} \langle U_{\epsilon'} \hat{H}_{\epsilon',\gamma(s,c)} \Pi_{s,c} | \Pi_{s,c} \rangle_{\text{kin}} = \sum_{s,c} \langle U_{\epsilon'} \hat{H}_{\epsilon',\gamma(s,c)} \Pi_{s,c} | \Pi_{s,c} \rangle_{\text{kin}} = \langle \Pi_{[s,c]} | \hat{M} | \Pi_{[s,c]} \rangle_{\text{Diff}}
\]

(47)

where \( \varphi \) are the diffeomorphism transformations spanning the diffeomorphism equivalent 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 a certain skeleton \( \gamma(s_1, c_1) \) by the action of \( (\hat{H}_c^\epsilon)^\dagger \) and \( v \in V(\varphi(\gamma(s, c))) \), i.e., the scale \( \varphi^{-1}(\epsilon') \) of the diffeomorphism images of the tetrahedra added by the action coincides with the scale of certain tetrahedra in \( \gamma(s, c) \) and \( \varphi^{-1}(v) \) is a vertex in \( \gamma(s, c) \). Then, we can express the matrix elements (46) as

\[
\langle \Pi_{[s,c]} | \hat{M} | \Pi_{[s,c]} \rangle_{\text{Diff}} = \sum_{\{s,c\} \in \mathcal{V}(\gamma(s,c))} \sum_{\varphi \in \mathcal{V}(\gamma(s,c))} \frac{1}{2} \lim_{\epsilon, \epsilon' \to 0} \langle \Pi_{[s,c]} | (\hat{H}_{\epsilon,\gamma(s,c)} \Pi_{s,c} \varphi(s,c)) | \Pi_{[s,c]} \rangle_{\text{kin}}
\]

(48)

From equation (48) and the result that the master constraint operator \( \hat{M} \) is densely defined on \( \mathcal{H}_{\text{Diff}} \), it is obvious that \( \hat{M} \) is a positive and symmetric operator on \( \mathcal{H}_{\text{Diff}} \). Hence, it is associated with a unique self-adjoint operator \( \hat{M} \), called the Friedrichs extension of \( \hat{M} \). We relabel \( \hat{M} \) to be \( \hat{M} \) for simplicity. In conclusion, there exists a positive and self-adjoint operator \( \hat{M} \) on \( \mathcal{H}_{\text{Diff}} \) corresponding to the master constraint (35). It is then possible to obtain the physical Hilbert space of the coupled system by the direct integral decomposition of \( \mathcal{H}_{\text{Diff}} \) with respect to \( \hat{M} \).

Note that the quantum constraint algebra can be easily checked to be anomaly free. Equation (44) assures that the master constraint operator commutes with finite diffeomorphism transformations, i.e.,

\[
[\hat{M}, \hat{U}_\epsilon] = 0.
\]

(49)

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

\[
[\hat{M}, \hat{M}] = 0.
\]

(50)

So, the quantum constraint algebra is precisely consistent with the classical constraint algebra (36) 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.

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