Master Constraint Operators in Loop Quantum Gravity

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Abstract

We introduce a master constraint operator $\hat{\mathbf{M}}$ densely defined in the diffeomorphism invariant Hilbert space in loop quantum gravity, which corresponds classically to the master constraint in the programme. It is shown that $\hat{\mathbf{M}}$ is positive and symmetric, and hence has its Friedrichs self-adjoint extension. The same conclusion is tenable for an alternative master operator $\hat{\mathbf{M}}'$, whose quadratic form coincides with the one proposed by Thiemann. So the master constraint programme for loop quantum gravity can be carried out in principle by employing either of the two operators.

Keywords: loop quantum gravity, master constraint, quantum dynamics.

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1 Introduction

It is well known that the quantization programme of loop quantum gravity is based on the connection dynamics of general relativity [1][2][3]. The basic conjugate pairs in the phase space are su(2)-valued connections A_a^i and densitized triads \widetilde{P}_i^a on a 3-manifold Σ . In the case where Σ is a compact set without boundary, the Hamiltonian is a linear combination of constraints as follows:

$$H_{tot} = \mathcal{G}(\Lambda) + \mathcal{V}(\vec{N}) + \mathcal{H}(N). \tag{1}$$

*Email address: mhan1@lsu.edu †Email address: mayg@bnu.edu.cn As an infinite dimensional Poisson algebra, the constraints algebra is not a Lie algebra unfortunately, because the Poisson bracket between the two scalar (Hamiltonian) constraints $\mathcal{H}(N)$ and $\mathcal{H}(M)$ has structure function depending on dynamical variables [1]. This character causes much trouble in solving the constraints quantum mechanically. On the other hand, the algebra generated by the Gaussian constraints $G(\Lambda)$ forms not only a subalgebra but also a 2-side ideal in the full constraint algebra. Thus one can first solve the Gaussian constraints independently. But the subalgebra generated by the diffeomorphism constraints $\mathcal{V}(\vec{N})$ can not form an ideal. Hence the procedures of solving the diffeomorphism constraints and solving the Hamiltonian constraints are entangled with each other. This leads to certain ambiguity in the construction of a Hamiltonian constraint operator [4][5][6]. Thus, although the kinematical Hilbert space \mathcal{H}_{Kin} and the diffeomorphism invariant Hilbert space \mathcal{H}_{Diff} in loop quantum gravity have been constructed rigorously [7], the quantum dynamics of the theory is still an open issue. The regulated Hamiltonian constraint operator $\hat{\mathcal{H}}^{\epsilon}(N)$ can be densely defined in \mathcal{H}_{Kin} and diffeomorphism covariant by certain state-dependent triangulation $T(\epsilon)$, which may naturally give a dual Hamiltonian constraint operator $\mathcal{H}'(N)$ acting on diffeomorphism invariant states [4][8]. Moreover, one may even define a symmetric version of regulated Hamiltonian constraint operator [9]. However, there are still several unsettled problems concerning either form of the (dual) Hamiltonian constraint operators, which are listed below.

• Although the action of the dual commutator of two Hamiltonian constraint operators on $\Psi_{Diff} \in \mathcal{H}_{Diff}$ reads

$$([\hat{\mathcal{H}}(N), \hat{\mathcal{H}}(M)])'\Psi_{Diff} = 0, \tag{2}$$

it is unclear whether the commutator between two Hamiltonian constraint operators resembles the classical Poisson bracket between two Hamiltonian constraints. Hence it is doubtful whether the quantum Hamiltonian constraint produces the correct quantum dynamics with correct classical limit [5][6], so it is in danger of physical quantum anomaly.

• Although the action of the dual commutator between the Hamiltonian constraint operator and finite diffeomorphism transformation operator \hat{U}_{φ} on Ψ_{Diff} gives [8]

$$([\hat{\mathcal{H}}(N), \hat{U}_{\varphi}])'\Psi_{Diff} = \hat{\mathcal{H}}'(\varphi^*N - N)\Psi_{Diff},\tag{3}$$

which almost resembles the classical Poisson bracket between the Hamiltonian constraint and diffeomorphism constraint, one can see that the dual Hamiltonian constraint operator does not leave \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 do not form a Lie algebra. So one cannot employ group average strategy in solving the Hamiltonian constraint quantum mechanically, since the strategy depends on group structure crucially [10].

However, if one could 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, then the programme of solving constraints would be much improved at a basic level. Such a constraint Lie algebra was first introduced by Thiemann in Ref.[11]. The central idea is to introduce the master constraint:

$$\mathbf{M} := \frac{1}{2} \int_{\Sigma} d^3 x \frac{|\widetilde{C}(x)|^2}{\sqrt{|\det q(x)|}},\tag{4}$$

where the scalar constraint $\widetilde{C}(x)$ reads

$$\widetilde{C} = \frac{\widetilde{P}_i^a \widetilde{P}_j^b}{\sqrt{|\det q|}} \left[\epsilon_k^{ij} F_{ab}^k - 2(1 + \gamma^2) K_{[a}^i K_{b]}^j \right]. \tag{5}$$

After solving the Gaussian constraint, one gets the master constraint algebra as a Lie algebra:

$$\{\mathcal{V}(\vec{N}), \ \mathcal{V}(\vec{N}')\} = \mathcal{V}([\vec{N}, \vec{N}']),$$

$$\{\mathcal{V}(\vec{N}), \ \mathbf{M}\} = 0,$$

$$\{\mathbf{M}, \ \mathbf{M}\} = 0,$$
 (6)

where the subalgebra of diffeomorphism constraints forms an ideal. So it is possible to define a corresponding master constraint operator on \mathcal{H}_{Diff} . A candidate self-adjoint master constraint operator was first proposed in Ref.[12] from the positive quadratic form on \mathcal{H}_{Diff} introduced in Ref.[11]. In the following section, we will construct two candidate self-adjoint master constraint operators on \mathcal{H}_{Diff} from a different perspective. One of them coincides with the one proposed by Thiemann.

2 Self-adjoint Master Constraint Operators

We first introduce a master constraint operators densely defined in \mathcal{H}_{Diff} , then prove that it is symmetric and positive and hence has its natural self-adjoint extension. Moreover, the Lie algebra property of Eq.(6) is maintained in its quantum version. The other master constraint operator can be constructed in a similar way. The regularized version of the master constraint can be expressed as

$$\mathbf{M}^{\epsilon} := \frac{1}{2} \int_{\Sigma} d^3 y \int_{\Sigma} d^3 x \chi_{\epsilon}(x - y) \frac{\widetilde{C}(y)}{\sqrt{V_{U_y^{\epsilon}}}} \frac{\widetilde{C}(x)}{\sqrt{V_{U_x^{\epsilon}}}}, \tag{7}$$

where $\chi_{\epsilon}(x-y)$ is any 1-parameter family of functions such that $\lim_{\epsilon \to 0} \chi_{\epsilon}(x-y)/\epsilon^3 = \delta(x-y)$ and $\chi_{\epsilon}(0) = 1$. Introducing a partition \mathcal{P} of the 3-manifold Σ into cells C, we have an operator $\hat{H}_{C,\alpha}^{\epsilon}$ acting on any cylindrical function $f_{\alpha} \in Cyl_{\alpha}^{3}(\overline{\mathcal{H}})$ in \mathcal{H}_{Kin} as

$$\hat{H}_{C,\alpha}^{\epsilon} f_{\alpha} = \sum_{\nu \in V(\alpha)} \chi_{C}(\nu) \sum_{\nu(\Lambda) = \nu} \frac{\hat{p}_{\Delta}}{\sqrt{\hat{E}(\nu)}} \hat{h}_{\nu}^{\epsilon, \Delta} \frac{\hat{p}_{\Delta}}{\sqrt{\hat{E}(\nu)}} f_{\alpha}, \tag{8}$$

via a state-dependent triangulation $T(\epsilon)$ on Σ , where $\chi_C(v)$ is the characteristic function of the cell C(v) containing a vertex v of the graph α , we use the triangulation compatible with the symmetric Hamiltonian constraint operator by asking the arcs a_{ij} added by the Hamiltonian-like operator $\hat{h}_v^{\epsilon,\Delta}$ to be smooth exceptional edges defined in Ref.[9], and the tetrahedron projector associated with segments s_1 , s_2 and s_3 is

$$\hat{p}_{\Delta} := \hat{p}_{s_1} \hat{p}_{s_2} \hat{p}_{s_3}
= \theta(\sqrt{\frac{1}{4} - \Delta_{s_1}} - \frac{1}{2})\theta(\sqrt{\frac{1}{4} - \Delta_{s_2}} - \frac{1}{2})\theta(\sqrt{\frac{1}{4} - \Delta_{s_3}} - \frac{1}{2}),$$
(9)

here Δ_{s_i} is the Casimir operator associated with the segment s_i and θ is the distribution on **R** which vanishes on $(-\infty, 0]$ and equals 1 on $(0, \infty)$, which gives the vertex operator $\hat{E}(v) := \sum_{v(\Delta)=v} \hat{p}_{\Delta}$. The expression of $\hat{h}_v^{\epsilon, \Delta}$ reads

$$\hat{h}_{v}^{\epsilon,\Delta} = \frac{8}{3i\hbar\kappa^{2}\gamma}\epsilon^{ijk}\mathrm{Tr}\Big(\{\hat{A}(\alpha_{ij}(\Delta))^{-1}, \,\hat{A}(s_{k}(\Delta))^{-1}[\hat{A}(s_{k}(\Delta)), \,\sqrt{\hat{V}_{U_{v}^{\epsilon}}}]\}\Big)$$

$$+2(1+\gamma^{2})\frac{4\sqrt{2}}{3i\hbar^{3}\kappa^{4}\gamma^{3}}\epsilon^{ijk}\mathrm{Tr}\Big(\hat{A}(s_{i}(\Delta))^{-1}[\hat{A}(s_{i}(\Delta)), \,\hat{K}^{\epsilon}]$$

$$\hat{A}(s_{j}(\Delta))^{-1}[\hat{A}(s_{j}(\Delta)), \,\sqrt{\hat{V}_{U_{v}^{\epsilon}}}]\hat{A}(s_{k}(\Delta))^{-1}[\hat{A}(s_{k}(\Delta)), \,\hat{K}^{\epsilon}]\Big). \tag{10}$$

where $\{.,..\}$ denotes the anti-commutator, $\{s_i(\Delta)\}_{i=1,2,3}$ is the segments associated to the tetrahedron Δ , and the arcs and segments constitute loops $\alpha_{ij}(\Delta) := s_i(\Delta) \circ a_{ij}(\Delta) \circ s_j(\Delta)$. Note that $\hat{h}_{\nu}^{\epsilon,\Delta}$ is similar to that involved in the regulated symmetric Hamiltonian constraint operator defined in Ref.[9], while the only difference is that now the volume operator is replaced by its quare-root in Eq.(10). Hence the action of $\hat{H}_{C,\alpha}^{\epsilon}$ on f_{α} adds smooth exceptional arcs $a_{ij}(\Delta)$ with $\frac{1}{2}$ -representation with respect to each $v(\Delta)$ of α . Thus, for each $\epsilon > 0$, $\hat{H}_{C,\alpha}^{\epsilon}$ is a Yang-Mills gauge invariant and diffeomorphism covariant operator defined on $Cyl_{\alpha}^{3}(\overline{\mathcal{A}})$. The family of such operators with respect to different graphs is cylindrically consistent up to diffeomorphisms and hence can give a limit operator \hat{H}_{C} densely defined on \mathcal{H}_{Kin} by the uniform Rovelli-Smollin topology. Moreover, the regulated operators are symmetric with respect to the inner product on \mathcal{H}_{Kin} , i.e.,

$$\langle g_{\gamma'}, \hat{H}^{\epsilon}_{C,\gamma} f_{\gamma} \rangle_{Kin} = \langle \hat{H}^{\epsilon}_{C,\gamma} g_{\gamma'}, f_{\gamma} \rangle_{Kin} = \langle \hat{H}^{\epsilon}_{C,\gamma'} g_{\gamma'}, f_{\gamma} \rangle_{Kin}, \tag{11}$$

which is non-vanishing provided γ , $\gamma' \in \Gamma_e(\gamma_0)$, where $\Gamma_e(\gamma_0)$ denotes the collection of extended graphs obtained by adding only finite number of smooth exceptional edges on an analytic skeleton γ_0 . Eq.(11) can be shown in analogy with the proof for Theorem 3.1 in Ref.[9] using the properties of smooth exception edges. Then a master constraint operator, $\hat{\mathbf{M}}$, acting on any $\Psi_{Diff} \in \mathcal{H}_{Diff}$ can be defined as:

$$(\hat{\mathbf{M}}\Psi_{Diff})[f_{\alpha}] := \lim_{\mathcal{P} \to \Sigma; \epsilon, \epsilon' \to 0} \Psi_{Diff}[\sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_{C,\alpha}^{\epsilon} \hat{H}_{C,\alpha}^{\epsilon'} f_{\alpha}]. \tag{12}$$

Note that the actions of $\hat{H}_{C,\alpha}^{\epsilon}$ on any $f_{\alpha} \in Cyl_{\alpha}^{3}(\overline{\mathcal{A}})$ only add finite smooth exceptional arcs to the graph α , and the newly added vertices do not contribute in the successive

action by the other $\hat{H}_{C,\alpha}^{\epsilon}$. In addition, $\hat{H}_{C,\alpha}^{\epsilon}\hat{H}_{C,\alpha}^{\epsilon'}f_{\alpha}$ is a finite linear combination of spin-network functions on an extended graph with the same analytic skeleton of α , hence the value of $(\hat{\mathbf{M}}\Psi_{Diff})[f_{\alpha}]$ is finite for any given Ψ_{Diff} . Thus $\hat{\mathbf{M}}\Psi_{Diff}$ lies in the algebraic dual \mathcal{D}^* of the space of cylindrical functions. Furthermore, we can show that $\hat{\mathbf{M}}$ leaves the diffeomorphism invariant distributions invariant. For any diffeomorphism transformation φ on Σ ,

$$(\hat{U}_{\varphi}'\hat{\mathbf{M}}\Psi_{Diff})[f_{\alpha}] = \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to0} \Psi_{Diff}[\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_{C,\varphi(\alpha)}^{\epsilon}\hat{H}_{C,\varphi(\alpha)}^{\epsilon'}\hat{U}_{\varphi}f_{\alpha}]$$

$$= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to0} \Psi_{Diff}[\hat{U}_{\varphi}\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_{\varphi^{-1}(C),\alpha}^{\varphi^{-1}(\epsilon)}\hat{H}_{\varphi^{-1}(C),\alpha}^{\varphi^{-1}(\epsilon')}f_{\alpha}]$$

$$= \lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to0} \Psi_{Diff}[\sum_{C\in\mathcal{P}} \frac{1}{2}\hat{H}_{C,\alpha}^{\epsilon}\hat{H}_{C,\alpha}^{\epsilon'}f_{\alpha}], \qquad (13)$$

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

$$(\hat{U}_{\alpha}'\hat{\mathbf{M}}\Psi_{Diff})[f_{\alpha}] = (\hat{\mathbf{M}}\Psi_{Diff})[f_{\alpha}]. \tag{14}$$

Thus it is natural to define an inner product between $\hat{\mathbf{M}}\Psi_{Diff}$ and any diffeomorphism invariant cylindrical function $\eta(f_{\alpha})$ as $<\hat{\mathbf{M}}\Psi_{Diff}|\eta(f_{\alpha})>_{Diff}:=(\hat{\mathbf{M}}\Psi_{Diff})[f_{\alpha}]$. Given any diffeomorphism invariant spin-network state $\Pi_{[s]}$ [8][3][1], the norm of the resulted state $\hat{\mathbf{M}}\Pi_{[s]}$ can be calculated as:

$$\|\hat{\mathbf{M}}\Pi_{[s]}\|_{Diff} = \sum_{[s']} |\langle \hat{\mathbf{M}}\Pi_{[s]}|\Pi_{[s']}\rangle_{Diff}|^{2}$$

$$= \sum_{[s']} |\lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \Pi_{[s]} [\sum_{C\in\mathcal{P}} \frac{1}{2} \hat{H}^{\epsilon}_{C,\gamma(s')} \hat{H}^{\epsilon'}_{C,\gamma(s')} \Pi_{s'\in[s']}]|^{2}$$

$$= \sum_{[s']} |\lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \frac{1}{n_{\gamma(s)}} \sum_{\varphi\in Diff/Diff_{\gamma(s)}} \sum_{\varphi'\in GS_{\beta}}$$

$$\langle \hat{U}_{\varphi} \hat{U}_{\varphi'} \Pi_{s\in[s]} |\sum_{C\in\mathcal{P}} \frac{1}{2} \hat{H}^{\epsilon}_{C,\gamma(s')} \hat{H}^{\epsilon'}_{C,\gamma(s')} \Pi_{s'\in[s']}\rangle_{Kin}|^{2}$$

$$= \sum_{[s']} |\lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \frac{1}{n_{\gamma(s)}} \sum_{\varphi\in Diff/Diff_{\gamma(s)}} \sum_{\varphi'\in GS_{\gamma(s)}}$$

$$\langle \hat{U}_{\varphi} \hat{U}_{\varphi'} \sum_{C\in\mathcal{P}} \frac{1}{2} \hat{H}^{\epsilon'}_{C,\gamma(s)} \hat{H}^{\epsilon}_{C,\gamma(s)} \Pi_{s\in[s]} |\Pi_{s'\in[s']}\rangle_{Kin}|^{2}$$

$$= \sum_{[s']} |\lim_{\mathcal{P}\to\Sigma;\epsilon,\epsilon'\to 0} \Pi_{[s']} [\sum_{C\in\mathcal{P}} \frac{1}{2} \hat{H}^{\epsilon'}_{C,\gamma(s)} \hat{H}^{\epsilon}_{C,\gamma(s)} \hat{H}^{\epsilon}_{C,\gamma(s)} \Pi_{s\in[s]} |^{2}, \tag{15}$$

where n_{γ} is the number of the elements of the group, GS_{γ} , of colored graph symmetries of γ , $Diff_{\gamma}$ denotes the subgroup of Diff which maps γ to itself, $\gamma(s)$ is the graph associated with the spin-network function Π_s , and we make use of the fact that $\hat{\mathbf{M}}$ commutes

with diffeomorphism transformations. The cylindrical function $\sum_{C \in \mathcal{P}} \frac{1}{2} \hat{H}_{C,\gamma(s)}^{\epsilon'} \hat{H}_{C,\gamma(s)}^{\epsilon} \Pi_{s \in [s]}$ is a finite linear combination of spin-network functions on extended graph γ' with the same analytic skeleton of $\gamma(s)$. Hence, fixing $\Pi_{[s]}$, there are only finite number of terms which contribute the sum in Eq.(15). Thus the sum will automatically converge. Note that one can give a more extensive account of the terms contributing in Eq.(15), in analogy with the proof of the theorem 3.2 in Ref.[12]. Therefore, the master constraint operator $\hat{\mathbf{M}}$ is densely defined on \mathcal{H}_{Diff} .

We now consider the property of $\hat{\mathbf{M}}$. Given two diffeomorphism invariant spinnetwork functions $\Pi_{[s_1]}$ and $\Pi_{[s_2]}$, the matrix elements of $\hat{\mathbf{M}}$ are calculated as

$$\begin{aligned}
&<\Pi_{[s_{1}]}|\hat{\mathbf{M}}|\Pi_{[s_{2}]}>_{Diff} \\
&= (\hat{\mathbf{M}}\Pi_{[s_{2}]})[\Pi_{s_{1}\in[s_{1}]}] \\
&= \lim_{\varphi \to \Sigma; \epsilon, \epsilon' \to 0} \sum_{C \in \mathcal{P}} \frac{1}{2} \overline{\Pi_{[s_{2}]}[\hat{H}^{\epsilon}_{C,\gamma(s_{1})}\hat{H}^{\epsilon'}_{C,\gamma(s_{1})}\Pi_{s_{1}\in[s_{1}]}]} \\
&= \lim_{\varphi \to \Sigma; \epsilon, \epsilon' \to 0} \sum_{C \in \mathcal{P}} \frac{1}{2} \frac{1}{n_{\gamma(s_{2})}} \sum_{\varphi \in Diff/Diff_{\gamma(s_{2})}} \sum_{\varphi' \in GS_{\gamma(s_{2})}} \\
&< \hat{U}_{\varphi} \hat{U}_{\varphi'} \Pi_{s_{2}\in[s_{2}]}|\hat{H}^{\epsilon}_{C,\gamma(s_{1})}\hat{H}^{\epsilon'}_{C,\gamma(s_{1})}\Pi_{s_{1}\in[s_{1}]} >_{Kin} \\
&= \sum_{s} \lim_{\varphi \to \Sigma; \epsilon, \epsilon' \to 0} \sum_{C \in \mathcal{P}} \frac{1}{2} \frac{1}{n_{\gamma(s_{2})}} \sum_{\varphi \in Diff/Diff_{\gamma(s_{2})}} \sum_{\varphi' \in GS_{\gamma(s_{2})}} \\
&< \hat{U}_{\varphi} \hat{U}_{\varphi'} \Pi_{s_{2}\in[s_{2}]}|\hat{H}^{\epsilon}_{C,\gamma(s_{1})}\Pi_{s} >_{Kin} < \Pi_{s}|\hat{H}^{\epsilon'}_{C,\gamma(s_{1})}\Pi_{s_{1}\in[s_{1}]} >_{Kin} \\
&= \sum_{s} \lim_{\varphi \to \Sigma; \epsilon, \epsilon' \to 0} \sum_{C \in \mathcal{P}} \frac{1}{2} \frac{1}{n_{\gamma(s_{2})}} \sum_{\varphi \in Diff/Diff_{\gamma(s_{2})}} \sum_{\varphi' \in GS_{\gamma(s_{2})}} \\
&< \hat{U}_{\varphi} \hat{U}_{\varphi'} \Pi_{s_{2}\in[s_{2}]}|\hat{H}^{\epsilon}_{C,\gamma(s_{1})}\Pi_{s} >_{Kin} < \Pi_{s}|\hat{H}^{\epsilon'}_{C,\gamma(s_{1})}\Pi_{s_{1}\in[s_{1}]} >_{Kin} \\
&= \sum_{[s]} \sum_{\nu \in V(\gamma(s\in[s]))} \frac{1}{2} \lim_{\epsilon \to 0} \overline{\Pi_{[s_{2}]}[\hat{H}^{\epsilon}_{\nu,\gamma(s)}\Pi_{s\in[s]}]} \sum_{s\in[s]} < \Pi_{s}|\hat{H}^{\epsilon'}_{\nu,\gamma(s_{1})}\Pi_{s_{1}\in[s_{1}]} >_{Kin}, \\
\end{aligned}$$
(16)

where we have used the resolution of identity trick in the fourth step. Since only finite number of terms in the sum over spin-networks s, cells $C \in \mathcal{P}$, and diffeomorphism transformations φ are non-zero respectively, we can interchange the sums and the limit. In the fifth step, since only the spin-network functions with $\gamma(s)$, $\gamma(s_1) \in \Gamma_{e}(\gamma_0)$ contribute the sum over s, we can change $\hat{H}^{\epsilon}_{C,\gamma(s_1)}$ to $\hat{H}^{\epsilon}_{C,\gamma(s)}$. In the sixth step, we take the limit $C \to v$ and split the sum \sum_{s} into $\sum_{[s]} \sum_{s \in [s]}$, where [s] 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 φ transforming the graph associated with $\hat{H}^{\epsilon}_{v,\gamma(s)}\Pi_{s}$ ($v \in \gamma(s)$) to that of $\hat{H}^{\epsilon}_{v',\gamma(s')}\Pi_{s'}$ ($v' \in \gamma(s')$) with $\varphi(v) = v'$, hence $\Pi_{[s_2]}[\hat{H}^{\epsilon}_{v,\gamma(s)}\Pi_{s \in [s]}]$ is constant for different $s \in [s]$.

Note that the term $\sum_{s \in [s]} < \prod_s |\hat{H}^{\epsilon'}_{\nu, \gamma(s_1)} \Pi_{s_1 \in [s_1]} >_{Kin}$ in Eq.(16) is free of the choices of the parameter ϵ' up to diffeomorphisms. We thus use $[\epsilon']$ instead of ϵ' to represent

an arbitrary state-dependent triangulation $T(\epsilon')$ in the diffeomorphism equivalent class. Hence we get

$$\sum_{s \in [s]} < \Pi_{s} | \hat{H}_{v, \gamma(s_{1})}^{\epsilon'} \Pi_{s_{1} \in [s_{1}]} >_{Kin} = \sum_{\varphi} < \hat{H}_{v, \varphi(\gamma(s))}^{[\epsilon']} U_{\varphi} \Pi_{s} | \Pi_{s_{1} \in [s_{1}]} >_{Kin} \\
= \sum_{\varphi} < U_{\varphi} \hat{H}_{\varphi^{-1}(v), \gamma(s)}^{[\epsilon']} \Pi_{s} | \Pi_{s_{1} \in [s_{1}]} >_{Kin} \\
= \overline{\Pi_{[s_{1}]} [\hat{H}_{v \in V(\gamma(s)), \gamma(s)}^{\epsilon'} \Pi_{s}]}, \tag{17}$$

where φ 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 $\varphi(\gamma(s))$, $\gamma(s_1) \in \Gamma_e(\gamma_0)$ and $v \in V(\varphi(\gamma(s)))$. Then the matrix elements (16) are resulted as:

$$<\Pi_{[s_{1}]}|\hat{\mathbf{M}}|\Pi_{[s_{2}]}>_{Diff}$$

$$=\sum_{[s]}\sum_{v\in V(\gamma(s\in[s]))}\frac{1}{2}\lim_{\epsilon,\epsilon'\to 0}\overline{\Pi_{[s_{2}]}[\hat{H}^{\epsilon}_{v,\gamma(s)}\Pi_{s\in[s]}]}\Pi_{[s_{1}]}[\hat{H}^{\epsilon'}_{v,\gamma(s)}\Pi_{s\in[s]}]$$

$$=\sum_{[s]}\sum_{v\in V(\gamma(s\in[s]))}\frac{1}{2}\overline{(\hat{H}'_{v}\Pi_{[s_{2}]})[\Pi_{s\in[s]}]}(\hat{H}'_{v}\Pi_{[s_{1}]})[\Pi_{s\in[s]}]. \tag{18}$$

From Eq.(18) 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 [13]. The closure of $Q_{\mathbf{M}}$ is the quadratic form of a unique self-adjoint operator $\overline{\hat{\mathbf{M}}}$, called the Friedrichs extension of $\hat{\mathbf{M}}$. We relabel $\overline{\hat{\mathbf{M}}}$ to be $\hat{\mathbf{M}}$ for simplicity. From the construction of $\hat{\mathbf{M}}$, the qualitative description of the kernel of the symmetric Hamiltonian constraint operator in Ref.[9] 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 (4), 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. Eq.(14) assures that the master constraint operator commutes with finite diffeomorphism transformations, i.e.,

$$[\hat{\mathbf{M}}, \hat{U}'_{\alpha}] = 0. \tag{19}$$

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

$$[\hat{\mathbf{M}}, \hat{\mathbf{M}}] = 0. \tag{20}$$

So the quantum constraint algebra is consistent with the classical constraint algebra (6) 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.

We notice that, similar to the non-symmetric Hamiltonian operator [4], one can define a non-symmetric version of Eq.(8) as

$$\hat{H'}_{C,\alpha}^{\epsilon} f_{\alpha} = \sum_{v \in V(\alpha)} \chi_{C}(v) \sum_{v(\Delta) = v} \frac{\hat{p}_{\Delta}}{\sqrt{\hat{E}(v)}} \hat{h'}_{v}^{\epsilon, \Delta} \frac{\hat{p}_{\Delta}}{\sqrt{\hat{E}(v)}} f_{\alpha}, \tag{21}$$

where the operator $\hat{p}_{\Delta}/\sqrt{\hat{E}(\nu)}$ is suitably arranged such that both $\hat{H'}_{C,\alpha}^{\epsilon}$ and its adjoint are cylindrically consistent up to diffeomorphisms, and

$$\hat{h'}_{v}^{\epsilon,\Delta} = \frac{16}{3i\hbar\kappa^{2}\gamma} \epsilon^{ijk} \operatorname{Tr} \left(\hat{A}(\alpha_{ij}(\Delta))^{-1} \hat{A}(s_{k}(\Delta))^{-1} [\hat{A}(s_{k}(\Delta)), \sqrt{\hat{V}_{U_{v}^{\epsilon}}}] \right)$$

$$+2(1+\gamma^{2}) \frac{4\sqrt{2}}{3i\hbar^{3}\kappa^{4}\gamma^{3}} \epsilon^{ijk} \operatorname{Tr} \left(\hat{A}(s_{i}(\Delta))^{-1} [\hat{A}(s_{i}(\Delta)), \hat{K}^{\epsilon}] \right)$$

$$\hat{A}(s_{j}(\Delta))^{-1} [\hat{A}(s_{j}(\Delta)), \hat{K}^{\epsilon}] \hat{A}(s_{k}(\Delta))^{-1} [\hat{A}(s_{k}(\Delta)), \sqrt{\hat{V}_{U_{v}^{\epsilon}}}]$$

$$(22)$$

via a state-dependent triangulation. The adjoint operator $(\hat{H'}_{C,\alpha}^{\epsilon})^{\dagger}$ can be well defined in \mathcal{H}_{kin} as

$$(\hat{H'}_{C,\alpha}^{\epsilon})^{\dagger} = \sum_{v \in V(\alpha)} \chi_C(v) \sum_{v(\Delta) = v} \frac{\hat{p}_{\Delta}}{\sqrt{\hat{E}(v)}} (\hat{h'}_v^{\epsilon,\Delta})^{\dagger} \frac{\hat{p}_{\Delta}}{\sqrt{\hat{E}(v)}},\tag{23}$$

such that the limit operators $\hat{H}'_{C,\alpha}$ and $(\hat{H}'_{C,\alpha})^{\dagger}$ in the uniform Rovelli-Smolin topology satisfy

$$\langle g_{\alpha'}, \hat{H}'_{C} f_{\alpha} \rangle_{kin} = \langle g_{\alpha'}, \hat{H}'_{C,\alpha} f_{\alpha} \rangle_{kin} = \langle (\hat{H}'_{C,\alpha})^{\dagger} g_{\alpha'}, f_{\alpha} \rangle_{kin}$$

$$= \langle (\hat{H}'_{C})^{\dagger} g_{\alpha'}, f_{\alpha} \rangle_{kin} = \langle (\hat{H}'_{C})^{\dagger} g_{\alpha'}, f_{\alpha} \rangle_{kin}, \qquad (24)$$

where $\hat{H'}_C$ and $(\hat{H'}_C)^{\dagger}$ are respectively the inductive limits of $\hat{H'}_{C,\alpha}$ and $(\hat{H'}_{C,\alpha})^{\dagger}$. Then an alternative master constraint operator can be defined as [8]

$$(\hat{\mathbf{M}}'\Psi_{Diff})[f_{\alpha}] := \lim_{\mathcal{P} \to \Sigma; \epsilon, \epsilon' \to 0} \Psi_{Diff}[\sum_{C \in \mathcal{D}} \frac{1}{2} \hat{H'}_{C}^{\epsilon} (\hat{H'}_{C}^{\epsilon'})^{\dagger} f_{\alpha}]. \tag{25}$$

In analogy with the previous discussion, we can show that $\hat{\mathbf{M}}'$ is also qualified as a positive self-adjoint operator on \mathcal{H}_{Diff} . Note that the construction of $\hat{\mathbf{M}}'$ can be based only on the analytic category of graphs. Moreover, the quadratic form of this operator coincides with the quadratic form on (a dense form domain of) \mathcal{H}_{Diff} defined by Thiemann in Ref.[11]. Thus $\hat{\mathbf{M}}'$ is equivalent to the master constraint operator in Ref.[12].

3 Discussions

We have constructed two candidate self-adjoint master constraint operators $\hat{\mathbf{M}}$ and $\hat{\mathbf{M}}'$ on \mathcal{H}_{Diff} . As a candidate master operator $\hat{\mathbf{M}}$ is different from that proposed in Ref.[12]. In our construction the structure of the kinematical Hilbert space \mathcal{H}_{Kin} is crucially employed, while in Ref.[12] the structure of the diffeomorphism invariant Hilbert space

 \mathcal{H}_{Diff} plays a key role. In Ref.[12], the definition of the master operator depends crucially on a quadratic form on \mathcal{H}_{Diff} , and a new inner product is introduced on the algebra dual \mathcal{D}^* of the space of cylindrical functions in order to have a well-defined quadratic form. Our construction shows that, in a different perspective, master constraint operators can be well defined on \mathcal{H}_{Diff} without employing an inner product on \mathcal{D}^* and a quadratic form. Both approaches can be used to construct master constraint operators for background independent quantum matter fields coupled to gravity [14].

The aim of both Hamiltonian constraint programme and master constraint programme is to seek for the physical Hilbert space \mathcal{H}_{phys} . Since the master constraint operator \mathbf{M} (or \mathbf{M}') is self-adjoint and a separable \mathcal{H}_{Diff} can be introduced by suitable extension of diffeomorphism transformations [15][1], one can use the direct integral decomposition (DID) of \mathcal{H}_{Diff} associated with $\hat{\mathbf{M}}$ to obtain \mathcal{H}_{phys} [11][16]. The physical Hilbert space is just the (generalized) eigenspace of $\hat{\mathbf{M}}$ with the eigenvalue zero, i.e., $\mathcal{H}_{phys} = \mathcal{H}_{\lambda=0}^{\oplus}$ with the induced physical inner product $\langle | \rangle_{\mathcal{H}_{\lambda=0}^{\oplus}}$. The issue of quantum anomaly is expected to be represented in terms of the size of \mathcal{H}_{phys} and the existence of sufficient semi-classical states. The master constraint programme has been well tested in various examples [17][18][19][20][21]. It is an exciting result that the master constraint can be well defined as self-adjoint operators in the framework of loop quantum gravity. However, since the Hilbert spaces \mathcal{H}_{Kin} , \mathcal{H}_{Diff} , and the master operators 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 algebra have correct classical limits with respect to suitable semiclassical states. It is also possible to select a preferred master operator from the alternative candidates by the semiclassical analysis. However, to do the semiclassical analysis, one still needs diffeomorphism invariant coherent states in \mathcal{H}_{Diff} . The research in this aspect is now in progress [22][23].

Assume that the semiclassical analysis confirmed our master constraint operator $\hat{\mathbf{M}}$. Since $\hat{\mathbf{M}}$ is self-adjoint, it is a practical problem to find the DID of \mathcal{H}_{Diff} and the physical Hilbert space \mathcal{H}_{phys} . However, the expression of master constraint operator is so complicated that it is difficult to obtain the DID representation of \mathcal{H}_{Diff} directly. Fortunately, the subalgebra generated by master constraints is an Abelian Lie algebra in the master constraint algebra. So one can employ group averaging strategy to solve the master constraint. Since $\hat{\mathbf{M}}$ is self-adjoint, by Stone's theorem there exists a strong continuous one-parameter unitary group,

$$\hat{U}(t) := \exp[it\hat{\mathbf{M}}],\tag{26}$$

on \mathcal{H}_{Diff} . Then, given any diffeomorphism invariant cylindrical functions $\Psi_{Diff} \in Cyl_{Diff}^{\star}$, one can obtain algebraic distributions of \mathcal{H}_{Diff} by a rigging map η_{phys} from Cyl_{Diff}^{\star} to Cyl_{phys} , which are invariant under the action of $\hat{U}(t)$ and constitute a subset of the algebraic dual of Cyl_{Diff}^{\star} . The rigging map is formally defined as

$$\eta_{phys}(\Psi_{Diff})[\Phi_{Diff}] := \int_{\mathbf{R}} \frac{dt}{2\pi} < \hat{U}(t)\Psi_{Diff}|\Phi_{Diff}>_{Diff}. \tag{27}$$

The physical inner product is then defined formally as

$$<\eta_{phys}(\Psi_{Diff})|\eta_{phys}(\Phi_{Diff})>_{phys}:=\eta_{phys}(\Psi_{Diff})[\Phi_{Diff}]$$

$$= \int_{\mathbf{R}} \frac{dt}{2\pi} < \hat{U}(t) \Psi_{Diff} |\Phi_{Diff}>_{Diff}. \tag{28}$$

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