Nonperturbative Loop Quantization of Scalar-Tensor Theories of Gravity

Xiangdong Zhang\(^\dagger\) and Yongge Ma\(^\ddagger\)

\(^1\)Department of Physics, Beijing Normal University, Beijing 100875, China

The Hamiltonian formulation of scalar-tensor theories of gravity is derived from their Lagrangian formulation by Hamiltonian analysis. The Hamiltonian formalism marks off two sectors of the theories by the coupling parameter \(\omega(\phi)\). In the sector of \(\omega(\phi) = -\frac{2}{3}\), the feasible theories are restricted and a new primary constraint generating conformal transformations of spacetime is obtained, while in the other sector of \(\omega(\phi) \neq -\frac{2}{3}\), the canonical structure and constraint algebra of the theories are similar to those of general relativity coupled with a scalar field. By canonical transformations, we further obtain the connection dynamical formalism of the scalar-tensor theories with real \(su(2)\)-connections as configuration variables in both sectors. This formalism enables us to extend the scheme of non-perturbative loop quantum gravity to the scalar-tensor theories. The quantum kinematical framework for the scalar-tensor theories is rigorously constructed. Both the Hamiltonian constraint operator and master constraint operator are well defined and proposed to represent quan-

tum dynamics. Thus loop quantum gravity method is also valid for general scalar-tensor theories.

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I. INTRODUCTION

In the past 25 years, loop quantum gravity (LQG), a background independent approach to quantize general relativity (GR), has been widely investigated \[^1\]–\[^4\]. It is remarkable that, as a non-renormalizable theory, GR can be non-perturbatively quantized by the loop quantization procedure. This background-independent quantization method relies on the key observation that classical GR can be cast into the connection dynamical formalism with structure group of \(SU(2)\). Thus one is naturally led to ask whether GR is a unique relativistic theory of gravity with connection dynamical character. It was recently shown in Refs. \[^5\]–\[^6\] that metric \(f(R)\) theories can also be cast into the connection dynamical formalism, and hence LQG has been extended to metric \(f(R)\) theories. In fact, modified gravity theories have recently received increased attention in issues related to "dark Universe" and non-trivial tests on gravity beyond GR. Besides \(f(R)\) theories, a well-known competing relativistic theory of gravity was proposed by Brans and Dicke in 1961 \[^7\], which is apparently compatible with Mach’s principle. To represent a varying "gravitational constant", a scalar field is non-minimally coupled to the metric in Brans-Dicke theory. To interpret the observational results within the framework of a broad class of theories, the Brans-Dicke theory was generalized by Bergmann \[^8\] and Wagoner \[^9\] to general scalar-tensor theories (STT). Scalar-tensor modifications of GR have also become very popular in unification schemes such as string theory (see e.g. \[^10\]–\[^12\] ). On the other hand, since 1998, a series of independent observations, including type Ia supernova, weak lens, cosmic microwave background anisotropy, baryon oscillation, etc, implied that our universe is currently undergoing a period of accelerated expansion \[^13\]. These results have caused the "dark energy" problem in the framework of GR. It is reasonable to consider the possibility that GR is not a valid theory of gravity on a galactic or cosmological scale. The scalar field in STT of gravity is then expected to account for "dark energy", since it can naturally lead to cosmological acceleration in certain models (see e.g. \[^14\]–\[^17\] ). Moreover, some models of STT of gravity may account for the "dark matter" problem \[^18\]–\[^20\] , which was revealed by the observed rotation curve of galaxy clusters.

A large part of the non-trivial tests on gravity theory is related to Einstein’s equivalence principle (EEP) \[^21\]. There exist many local experiments in solar-system supporting EEP, which implies the metric theories of gravity. Actually, STT are a class of representative metric theories, which have been received most attention. Note that the metric \(f(R)\) theories and Palatini \(f(R)\) theories are equivalent to the special kind of STT with the coupling parameter \(\omega(\phi) = 0\) and \(\omega(\phi) = -\frac{2}{3}\) respectively \[^22\] , while the original Brans-Dicke theory is the particular case of constant \(\omega\) and vanishing potential of \(\phi\). Thus it is interesting to see whether this class of metric theories of gravity could be quantized nonperturbatively. In this paper, we will first do Hamiltonian analysis of the STT of gravity. Based on the resulted connection dynamical formalism, we then quantize the STT by extending the nonperturbative
quantization procedure of LQG in the way similar to loop quantum $f(R)$ gravity. Nevertheless, the STT that we are considering are a much more general class of metric theories of gravity than metric $f(R)$ theories. Throughout the paper, we use Greek alphabet for spacetime indices, Latin alphabet a,b,c,..., for spatial indices, and i,j,k,..., for internal indices.

II. HAMILTONIAN ANALYSIS

The most general action of STT reads

$$S(g) = \int d^4x \sqrt{-g} \left[ -\frac{\omega(\phi)}{\phi} \left( \partial_\mu \phi \partial^\mu \phi \right) - \xi(\phi) \right]$$

where $\omega(\phi)$ and $\xi(\phi)$ can be arbitrary functions of scalar field $\phi$. Variations of the action (2.1) with respect to $g_{ab}$ and $\phi$ give equations of motion.

$$\phi G_{\mu\nu} = \nabla_\mu \nabla_\nu \phi - g_{\mu\nu} \Box \phi + \frac{\omega(\phi)}{2} \left[ (\partial_\mu \phi) \partial_\nu \phi - \frac{1}{2} g_{\mu\nu} (\nabla \phi)^2 \right] - g_{\mu\nu} \xi(\phi),$$

$$R + \frac{2\omega(\phi)}{\phi} \Box \phi - \frac{\omega(\phi)}{\phi^2} (\partial_\mu \phi) \partial^\mu \phi + \frac{\omega'(\phi)}{\phi} (\partial_\mu \phi) \partial^\mu \phi - 2\xi'(\phi) = 0,$$

where $\omega(\phi)$ and $\xi(\phi)$ are defined respectively as

$$\omega(\phi) = \frac{\phi G_{\mu\nu} \nabla_\mu \nabla_\nu \phi - g_{\mu\nu} \Box \phi}{\phi},$$

$$\xi(\phi) = \frac{R + \frac{2\omega(\phi)}{\phi} \Box \phi - \frac{\omega(\phi)}{\phi^2} (\partial_\mu \phi) \partial^\mu \phi + \frac{\omega'(\phi)}{\phi} (\partial_\mu \phi) \partial^\mu \phi - 2\xi'(\phi)}{\phi}.$$

where a prime over a letter denotes a derivative with respect to the argument, $\nabla_\mu$ is the covariant derivative compatible with $g_{\mu\nu}$ and $\Box = g^{\mu\nu} \nabla_\mu \nabla_\nu$. By doing 3+1 decomposition of the spacetime, the four-dimensional (4d) scalar curvature can be expressed as

$$R = K_{ab} K^{ab} - K^2 + R + \frac{2}{\sqrt{-g}} \partial_\mu (\sqrt{-g} n^\mu K) - \frac{2}{N \sqrt{h}} \partial_\mu (\sqrt{h} h_{ab} \partial_\nu N)$$

where $K_{ab}$ is the extrinsic curvature of a spatial hypersurface $\Sigma$, $K = K_{ab} h^{ab}$, $R$ denotes the scalar curvature of the 3-metric $h_{ab}$ induced on $\Sigma$, $n^\mu$ is the unit normal of $\Sigma$ and $N$ is the lapse function. By Legendre transformation, the momenta conjugate to the dynamical variables $h_{ab}$ and $\phi$ are defined respectively as

$$p_{ab} = \frac{\partial L}{\partial \dot{h}_{ab}} = \frac{\sqrt{h}}{2} \left[ \phi (K_{ab} - K h^{ab}) - h_{ab} \left( \frac{\phi}{N} - N^c \partial_c \phi \right) \right],$$

$$\pi = \frac{\partial L}{\partial \dot{\phi}} = -\frac{\sqrt{h}}{N} (K - \frac{\omega(\phi)}{\phi} (\phi^2 - N^c \partial_c \phi)), $$

where $N^c$ is the shift vector. Combination the trace of Eq. (2.5) and Eq. (2.6) gives

$$(3 + 2\omega(\phi))(\dot{\phi} - N^a \partial_a \phi) = \frac{2N}{\sqrt{h}} (\dot{\phi} - p).$$

It is easy to see from Eq. (2.7) that one extra constraint $S = p - \phi \pi = 0$ emerges when $\omega(\phi) = -\frac{3}{2}$. Hence it is natural to mark off two sectors of the theories by $\omega(\phi) \neq -\frac{3}{2}$ and $\omega(\phi) = -\frac{3}{2}$.

A. Sector of $\omega(\phi) \neq -3/2$

In the case of $\omega(\phi) \neq -3/2$, the Hamiltonian of STT can be derived as a liner combination of constraints as

$$H_{total} = \int d^3x (N^a V_a + NH),$$
where the smeared diffeomorphism and Hamiltonian constraints read respectively
\[ V(N) = \int_{\Sigma} d^3x N^a V_a = \int_{\Sigma} d^3x N^a (-2D^b(p_{ab}) + \pi \partial_a \phi), \]
\[ H(N) = \int_{\Sigma} d^3x N H = \int_{\Sigma} d^3x N \left[ \frac{2}{\sqrt{h}} \left( \frac{p_{ab}p^{ab} - \frac{1}{2}p^2}{\phi} + \frac{(p - \phi \pi)^2}{2\phi (3 + 2\omega)} \right) + \frac{1}{2\sqrt{h}}(-\phi R + \frac{\omega(\phi)}{\phi} (D_a \phi)D^a \phi + 2D_a D^a \phi + 2\xi(\phi)) \right]. \]
\[ (2.9) \]
\[ (2.10) \]
By the symplectic structure
\[ \{h_{ab}(x), p^{cd}(y)\} = \delta_{ac}^e \delta^d_{bd} \delta^3(x, y), \]
\[ \{\phi(x), \pi(y)\} = \delta^3(x, y), \]
lengthy but straightforward calculations show that the constraints (2.9) and (2.10) comprise a first-class system similar to GR as:
\[ \{V(N), V(N')\} = V([N, N']), \]
\[ \{H(M), V(N)\} = -H[L_N M], \]
\[ \{H(N), H(M)\} = V(ND^a M - MD^a N). \]
\[ (2.11) \]
\[ (2.12) \]
Note that the Hamiltonian formulation of Brans-Dicke theory was studied in Ref. 23 (but the term \( D_a D^a \phi \) of Hamiltonian constraint was missing there). We now show that the above Hamiltonian formalism of STT is equivalent to their initial canonical variables formalism obtained in Ref. 24. In the Hamiltonian formalism, the evolution equations of the basic canonical variables can be derived by taking Poisson brackets with the Hamiltonian (2.8). Thus it is easy to check that the evolution equation of \( h_{ab} \) is just the definition of \( K_{ab} \). Also we have
\[ \dot{\phi} = \{\phi, H_{total}\} = \frac{2N}{(3 + 2\omega)\sqrt{h}}(\phi \pi - p) + N^a \partial_a \phi \]
\[ (2.13) \]
which is nothing but Eq. (2.4). Moreover, it is easy to obtain
\[ \dot{x} = \partial_a (N^a \pi) + \frac{N\sqrt{h}}{2}(K_{ab} K^{ab} - K^2) + \frac{N\sqrt{h}}{2}R - \partial_a (\sqrt{h} h_{ab} h_b N) \]
\[ + \frac{N\omega\sqrt{h}}{2\phi^2} (D_a \phi) D^a \phi + \sqrt{h} \omega D_\phi \left( \frac{N}{\phi} D^a \phi \right) - \frac{N\sqrt{h}}{2\phi^2} (\phi - N^c \partial_c \phi)^2 + \frac{\omega'(\phi)}{2\phi} \left( D_a \phi \right) D^a \phi - \sqrt{h} \xi'(\phi). \]
\[ (2.14) \]
Using Eqs. (2.4), (2.15) and \( n^0 = \frac{1}{N}, n^a = \frac{N^a}{N}, \sqrt{-g} = N \sqrt{h}, \) we can get
\[ \dot{x} - \partial_a (N^a \pi) - \partial_\mu (\sqrt{-g} n^\mu K) = \partial_a (\sqrt{-g} \frac{\omega(\phi)}{\phi} n^\alpha n^a \partial_\alpha \phi) \]
\[ = \frac{\sqrt{-g} R}{2} - \frac{\sqrt{-g} \omega}{2\phi^2} (n^\alpha \partial_\alpha \phi)^2 + \frac{\sqrt{-g} \omega}{2\phi} (D_a \phi) D^a \phi \]
\[ + \frac{\omega}{\phi} \partial_a (\sqrt{-g} h^{ab} h_b \phi) + \frac{\omega'(\phi) N \sqrt{h}}{2\phi} (D_a \phi) D^a \phi - \sqrt{-g} \xi'(\phi), \]
\[ (2.15) \]
which is equivalent to Eq. (2.8). On the other hand, in the Lagrangian formalism, the 00-component of Eq. (2.2) reads
\[ \phi G_{\mu \nu} n^\mu n^\nu = \frac{\phi}{2} (R - K_{ab} K^{ab} + K^2) \]
\[ = D_a D^a \phi - \frac{K}{N} (\phi - N^c \partial_c \phi) + \frac{\omega}{\phi} (D_a \phi) D^a \phi + \frac{\omega}{\phi} (n^\mu \partial_\mu \phi)^2 + \xi(\phi), \]
\[ (2.16) \]
where the fact \( g_{\mu \nu} n^\mu n^\nu = -1, h^{\mu \nu} n_\nu = 0 \) and \( n^\alpha \partial_\alpha \phi = \frac{1}{N} (\phi - N^c \partial_c \phi) \) have been used in the above derivation. Note that the Hamiltonian constraint in (2.10) can be expressed as
\[ 0 = H = \frac{\sqrt{h} \phi}{2} (K_{ab} K^{ab} - K^2 - R) + \frac{\sqrt{h}}{2\phi} (D_a \phi) D^a \phi + 2D_a D^a \phi \]
\[ - \sqrt{h} \frac{K}{N} (\phi - N^c \partial_c \phi) + \frac{\omega \sqrt{h}}{2\phi} (n^\mu \partial_\mu \phi)^2 + \sqrt{h} \xi(\phi). \]
\[ (2.17) \]
So the 00-component of (2.3) is equivalent to the Hamiltonian constraint. Since
\[ \phi G_{\mu \nu} n^\mu h_c^\nu = \phi (D_a K_b^c - D_b K_a^c) \quad \text{and} \quad g_{\mu \nu} n^\mu h_c^\nu = 0, \]  
we can get from the 0a-components of (2.2) that
\[ 0 = D_a (\phi K_b^c - D_b (\phi K_a^c)) + K \phi D_b - D_b \left( \frac{1}{N} (\phi - N^c \partial_c \phi) \right) - (n^\mu \partial_\mu \phi) \phi^2 D_b \phi \\
= 2 \sqrt{\hbar} D_a \left( \frac{\sqrt{\eta}}{2} \phi (K_b^c - K_h^c) - \frac{h_a^c}{N} (\phi - N^c \partial_c \phi) \right) - \frac{\pi}{\sqrt{\hbar}} \partial_b \phi. \]  
(2.19)

This is nothing but the diffeomorphism constraints in (2.9). Now we turn to the ab-components of (2.2), we will show that they are equivalent to the equation of motion of \( p_{ab} \), which reads
\[ \dot{p}_{ab} = \frac{h_{ab} N}{\sqrt{\hbar}} \left( \frac{\rho_{cd} \rho_{id} - \frac{1}{2} p^2}{\phi} + \frac{(p - \phi \pi)^2}{2 \phi (3 + 2 \omega)} \right) + \frac{4 N}{\sqrt{\hbar}} \left( p_{ac} p_{db} - \frac{1}{2} p p_{ab} \right) + \frac{(p - \phi \pi) p_{ab}}{2 \phi (3 + 2 \omega)} \\
+ \frac{N}{4} \sqrt{\hbar} h_{ab} \phi \phi R - \frac{N}{2} \sqrt{\hbar} \phi R_{ab} - \frac{N}{2} \sqrt{\hbar} h_{ab} D_c D^c \phi - D_{(a} N \sqrt{\hbar} D_{b)} \phi - \frac{N \omega}{4 \phi} \sqrt{\hbar} h_{ab} D_c \phi D^c \phi + \frac{N \omega}{2 \phi} \sqrt{\hbar} D_a \phi D_b \phi \\
+ \frac{\sqrt{\eta}}{2} (D_{(a} D_b) (\phi) - h_{ab} D_c D^c (\phi)) + 2 p_{ab} D^c N_b + D_c (p_{ab} N^c) - \frac{1}{2} N \sqrt{\hbar} h_{ab} \xi (\phi). \]  
(2.20)

Since the initial value formalism of STT has been obtained in Ref.[24], we may use Eq.(2.20) to derive the time derivative of the extrinsic curvature:
\[ K_{ab} = \frac{2 (p_{ab} - \frac{1 + \omega}{3 + 2 \omega} p h_{ab})}{\phi \sqrt{\hbar}} - \frac{\pi h_{ab}}{(3 + 2 \omega) \sqrt{\hbar}}. \]  
(2.21)

Straightforward calculations give
\[ \dot{K}_{ab} = 2 N K_{ac} K_b^c - N K K_{ab} + E_{\eta} K_{ab} - N R_{ab} + D_a D_b N + \frac{N}{\phi} D_a D_b \phi \\
+ \frac{N \omega}{\phi^2} (D_a \phi) D_b \phi - \frac{n^\gamma \partial b \phi}{\phi} N K_{ab} + N h_{ab} (\frac{1}{2} \Box \phi + \frac{\xi (\phi)}{\phi}). \]  
(2.22)

It is easy to see that Eq.(2.22) is equivalent to Eq. (69) in Ref.[24]. Note that there is a sign difference between the definition of our extrinsic curvature and that in Ref.[24]. To summarize, we have shown that the Hamiltonian formalism of STT with \( \omega (\phi) \neq -3/2 \) is equivalent to their Lagrangian formalism.

Since the geometric canonical variables of STT in this sector are as same as those of metric \( f(R) \) theories [6], we can use the same canonical transformations of \( f(R) \) theories to obtain the connection dynamical formalism of the STT. Let
\[ \tilde{K}^{ab} = \phi K^{ab} + \frac{h_{ab}}{2 N} (\phi - N^c \partial_c \phi) = \phi K^{ab} + \frac{h_{ab}}{(3 + 2 \omega) \sqrt{\hbar}} (\phi \pi - p). \]  
(2.23)

The new canonical geometric variables are
\[ E_i^a = \sqrt{\eta} e_i^a, \quad A_i^a = \Gamma_i^a + \gamma \tilde{K}_i^a, \]  
(2.24)

where \( e_i^a \) is the triad such that \( h_{ab} e_i^a e_j^b = \delta_{ij} \), \( \tilde{K}_i^a \equiv \tilde{K}^{ab} e_b^i \), \( \Gamma_i^a \) is the spin connection determined by \( E_i^a \), and \( \gamma \) is a nonzero real number. It is clear that our new variable \( A_i^a \) coincides with the Ashtekar-Barbero connection [25, 26] when \( \phi = 1 \). The Poisson brackets among the new variables read:
\[ \{ A_i^a (x), E_k^b (y) \} = \gamma \delta_i^a \delta_k^b \delta (x, y), \]
\[ \{ A_i^a (x), A_k^b (y) \} = \{ E_i^a (x), E_k^b (y) \} = 0. \]  
(2.25)

Now, the phase space of the STT consists of conjugate pairs \( (A_i^a, E^b_j) \) and \( (\phi, \pi) \), with the additional Gaussian constraint
\[ G_i = e_i^a E_i^a \equiv \partial_a E_i^a + \epsilon_{ijk} A_i^j E^{ak}, \]  
(2.26)
which justifies $A^i_a$ as an $su(2)$-connection. Note that, had we let $\gamma = \pm i$, the (anti-)self-dual complex connection formalism would be obtained. The original vector and Hamiltonian constraints can be respectively written up to Gaussian constraint as

$$V_a = \frac{1}{\gamma} F^{ab}_i E^b_i + \pi \partial_a \phi, \quad (2.27)$$

$$H = \frac{\phi}{2} \left[ F^{ij}_a - (\gamma^2 + \frac{1}{\phi^2}) \varepsilon_{jmn} \tilde{K}_a^m \tilde{K}_b^n \right] \frac{\varepsilon_{ijkl} E^k_i E^l_j}{\sqrt{\hbar}} + \frac{1}{3 + 2\omega(\phi)} \left( \frac{\left( \tilde{K}_i^a E^a_i \right)^2}{\phi \sqrt{\hbar}} + 2 \left( \tilde{K}_i^a E^a_i \pi \right) \frac{\pi^2 \phi}{\sqrt{\hbar}} \right)
+ \frac{\omega(\phi)}{2\phi} \sqrt{\hbar} (D_a \phi) D^a \phi + \sqrt{\hbar} D_a D^a \phi + \sqrt{\hbar} \xi(\phi), \quad (2.28)$$

where $F^{i}_{ab} \equiv 2\partial_i [A^i_a + \epsilon^i_{kl} A^k_a A^l_b]$ is the curvature of $A^i_a$. The total Hamiltonian can be expressed as a linear combination

$$H_{total} = \int_\Sigma A^i_a G_i + N^a V_a + NH, \quad (2.29)$$

It is easy to check that the smeared Gaussian constraint, $G(\Lambda) := \int_\Sigma d^3x A^i(x) G_i(x)$, generates $SU(2)$ gauge transformations on the phase space, while the smeared constraint $V(N) := \int_\Sigma d^3x N^a (V_a - A^i_a G_i)$ generates spatial diffeomorphism transformations on the phase space. Together with the smeared Hamiltonian constraint $H(N) = \int_\Sigma d^3x NH$, we can show that the constraints algebra has the following form:

$$\{G(\Lambda), G(\Lambda')\} = G([\Lambda, \Lambda']), \quad (2.30)$$
$$\{G(\Lambda), V(N)\} = -G(\mathcal{L}_N \Lambda), \quad (2.31)$$
$$\{G(\Lambda), H(N)\} = 0, \quad (2.32)$$
$$\{V(N), V(N')\} = V([N, N']), \quad (2.33)$$
$$\{V(N), H(M)\} = H(\mathcal{L}_N M), \quad (2.34)$$
$$\{H(N), H(M)\} = V(N D^a M - M D^a N)
+ G \left( \left[ (N \partial_a M - M \partial_a N) \hbar a^b A_b \right] \right)
- \frac{\left[ E^a D_a N, E^b D_b M \right]^i}{\hbar} G_i
- \frac{\gamma^2 \left[ E^a D_a (\phi N), E^b D_b (\phi M) \right]^i}{\hbar} G_i. \quad (2.35)$$

One may understand Eqs. (2.30-2.34) by the geometrical interpretations of $G(\Lambda)$ and $V(N)$. The detail calculation on the Poisson bracket (2.35) between the two smeared Hamiltonian constraints will be presented in the Appendix. Hence the constraints are of first class. Moreover, the constraint algebra of GR can be recovered for the special case when $\phi = 1$. To summarize, the STT of gravity in the sector $\omega(\phi) \neq -3/2$ have been cast into the $su(2)$-connection dynamical formalism. The resulted Hamiltonian structure is similar to metric $f(R)$ theories.

**B. Sector of $\omega(\phi) = -3/2$**

In the special case of $\omega(\phi) = -3/2$, Eq. (2.27) implied an extra primary constraint $S = 0$, which we call "conformal" constraint. Hence, as pointed out in Ref. [28], the total Hamiltonian in this case can be expressed as a linear combination of constraints as

$$H_{total} = \int_\Sigma d^3x (N^a V_a + NH + \lambda S), \quad (2.36)$$
where the smeared diffeomorphism $V(\bar{N})$ is as same as (2.4), while the Hamiltonian and conformal constraints read respectively

$$H(N) = \int_\Sigma d^3xNH$$

$$= \int_\Sigma d^3xN \left[ \frac{2}{\sqrt{h}} \left( \frac{p_{ab}p^{ab}}{\phi} - \frac{1}{2}\rho^2 \right) + \frac{1}{2\sqrt{h}}(-\phi R - \frac{3}{2\phi} (D_a \phi) D^a \phi + 2D_a D^a \phi + 2\xi(\phi)) \right],$$

(2.37)

$$S(\lambda) = \int_\Sigma d^3x\lambda S = \int_\Sigma d^3x(\xi - \phi \pi).$$

(2.38)

By the symplectic structure (2.11), detailed calculations show that

$$\{H(M), V(\bar{N})\} = -H(\mathcal{L}_N M), \quad \{S(\lambda), V(\bar{N})\} = -S(\mathcal{L}_N \lambda),$$

(2.39)

$$\{H(N), H(M)\} = V(ND^a M - MD^a N) + S(\frac{D_a \phi}{\phi} (ND^a M - MD^a N)),$$

(2.40)

$$\{S(\lambda), H(M)\} = H(\frac{\lambda M}{2}) + \int_\Sigma N \lambda \sqrt{h} (2\xi(\phi) + \phi \xi'(\phi)).$$

(2.41)

One may understand Eqs. (2.39) by the geometrical interpretations of $V(\bar{N})$. The detail calculations on the Poisson brackets (2.40) and (2.41) will be presented in the Appendix. The Poisson bracket (2.11) implies that, in order to maintain the constraints $S$ and $H$ in the time evolution, we have to impose a secondary constraint

$$-2\xi(\phi) + \phi \xi'(\phi) = 0.$$  

(2.42)

It is easy to see that this constraint is of second-class, and hence one has to solve it. As for the vacuum case that we considered the solutions of Eq. (2.42) are either $\xi(\phi) = 0$ or $\xi(\phi) = C\phi^2$, where $C$ is certain dimensional constant. Thus the consistency strongly restricted the feasible STT in the sector $\omega(\phi) = -3/2$ to only two theories. As pointed out in Ref. 22, for these two theories, the action (2.4) is invariant under the following conformal transformations

$$g_{\mu\nu} \rightarrow e^{\lambda} g_{\mu\nu}, \quad \phi \rightarrow e^{-\lambda} \phi.$$  

(2.43)

Hence, besides diffeomorphism invariance, the two theories are also conformal invariant. Now in the Hamiltonian formalism the constraints $(V, H, S)$ comprise a first-class system. The conformal constraint generates the following transformations on the phase space

$$\{h_{ab}, S(\lambda)\} = \lambda h_{ab}, \quad \{p_{ab}, S(\lambda)\} = -\lambda p_{ab},$$

(2.44)

$$\{\phi, S(\lambda)\} = -\lambda \phi, \quad \{\pi, S(\lambda)\} = \lambda \pi.$$  

(2.45)

It is easy to check that the above transformations coincide with those of spacetime conformal transformations (2.43). Thus all the physical meaning of constraints has been cleared. Because of the extra conformal constraint (2.38), the physical degrees of freedom of this special kind of STT are equal to those of GR.

The connection-dynamical formalism for these special theories can also be obtained by the canonical transformation to the new variables (2.24). Then the total Hamiltonian can be expressed as a linear combination

$$H_{total} = \int_\Sigma \Lambda^i \dot{G}_i + N^a V_a + NH + \lambda S,$$

(2.46)

where the Gaussian and diffeomorphism constraints keep the same form as Eqs. (2.26) and (2.27), while the Hamiltonian and the conformal constraints read respectively

$$H = \frac{\phi}{2} \left[ F^2 - (\gamma^2 + \frac{1}{\phi^2}) \Sigma_{jmn} K_a^m K_b^n \right] \varepsilon_{jkl} E_k^a E_l^b \sqrt{h}$$

$$- \frac{3}{4\phi} \sqrt{h} (D_a \phi) D^a \phi + \sqrt{h} D_a D^a \phi + \sqrt{h} \xi(\phi),$$

(2.47)

$$S = K_a^a E_a^a - \pi \phi.$$  

(2.48)
The constraints algebra in the connection formalism is closed as
\[
\{\mathcal{G}(\Lambda), H(N)\} = 0, \quad \{\mathcal{G}(\Lambda), S(\lambda)\} = 0, \quad \{S(\lambda), H(M)\} = H(\lambda M/2), \quad \{H(N), H(M)\} = \mathcal{V}(ND^a M - MD^a N)
\]
\[+ S(D_\alpha \phi (ND^a M - MD^a N)) \]
\[+ \mathcal{G}((N \partial_\alpha M - M \partial_\alpha N) h^{ab} A_b) \]
\[= \left[\frac{E^a D_\alpha N, E^b D_\alpha (\phi N)}{\hbar}\right] G_i \]
\[= \gamma^2 \frac{[E^a D_\alpha (\phi N), E^b D_\alpha (\phi M)]}{\hbar} G_i. \quad (2.52)
\]

It is obvious that the Poisson bracket among the other constraints are also weakly equal to zero. Since the initial value
formalism in this sector is a delicate issue \cite{22, 23}, we leave the comparison between the Hamiltonian formulation and
the Lagrangian formulation for further work.

III. LOOP QUANTIZATION

Based on the connection dynamical formalism, the nonperturbative loop quantization procedure can be straight-
forwardly extended to the STT. The kinematical structure of STT is as same as that of \( f(R) \) theories \cite{3, 4}. The
kinematical Hilbert space of the system is a direct product of the Hilbert space of geometry and that of scalar field,
\( \mathcal{H}_{\text{kin}} := \mathcal{H}_{\text{kin}}^G \otimes \mathcal{H}_{\text{kin}}^s \), with the orthonormal spin-scalar-network basis
\( T_{\alpha,X}(A, \phi) \equiv T_{\alpha}(A) \otimes T_X(\phi) \) over some graph \( \alpha \cup X \subset \Sigma \). Here \( \alpha \) and \( X \) consist of finite number of curves and points respectively in \( \Sigma \). The basic operators are
the quantum analogue of holonomies \( h_e(A) = P \exp \int_e A_e \) of connections, densitized triads smeared over 2-surfaces
\( E(S, f) := \int_{\Sigma} \epsilon_{abc} E_i^a f^i, \) point holonomis \( U_\lambda = \exp(\alpha_\lambda(x)) \) \cite{27}, and scalar momenta smeared on 3-dimensional regions
\( \pi(R) := \int_\Sigma d^3x \pi(x) \). Note that the spatial geometric operator of LQG, such as the area \cite{28}, the volume \cite{29}
and the length \cite{30, 31} operators, are still valid in \( \mathcal{H}_{\text{kin}}^G \), though their properties in the physical Hilbert space still need
to be clarified \cite{32, 33}. As in LQG, it is straightforward to promote the Gaussian constraint \( \mathcal{G}(\Lambda) \) to a well-defined operator \cite{2, 4}. Its kernel is the internal gauge invariant Hilbert space \( \mathcal{H}_G \) with gauge invariant spin-scalar-network basis. Since the diffeomorphisms of \( \Sigma \) act covariantly on the cylindrical functions in \( \mathcal{H}_G \), the so-called group averaging technique can be employed to solve the diffeomorphism constraint \cite{3, 4}. Thus we can also obtain the desired diffeomorphism and gauge invariant Hilbert space \( \mathcal{H}_{\text{Diff}} \) for the STT.

A. Sector of \( \omega(\phi) \neq -3/2 \)

While the kinematical framework of LQG and polymer-like scalar field have been straight-forwardly extended to the
STT, the nontrivial task in the case \( \omega(\phi) \neq -3/2 \) is to implement the Hamiltonian constraint \cite{22, 28} at quantum level. In order to compare the Hamiltonian constraint of STT with that of metric \( f(R) \) theories in connection formalism, we write Eq. (2.28) as \( H(N) = \sum_{j=1}^{8} H_j \) in regular order. It is easy to see that the terms \( H_1, H_2, H_7, H_8 \) just keep the
same form as those in \( f(R) \) theories (see Eq.(39) in Ref.\cite{6}), and the \( H_3, H_4, H_5 \) terms are also similar to the
remaining terms in \( f(R) \) theories. Here the differences are only reflected by the coefficients as a certain functions
of \( \phi \). Now we come to the completely new term, \( H_6 = \int_\Sigma d^3x N_x^{\omega(\phi)} \sqrt{n(D_\alpha \phi)} D^a \phi \). This term is somehow like the
kinetic term of a Klein-Gordon field which was dealt with in Ref.\cite{34}. We can introduce the well-defined operators
\( \phi, \phi^{-1} \) as in Ref. \cite{6}. It is reasonable to believe that function \( \omega(\phi) \) can also be quantized \cite{6}. By the same regularization techniques as in Refs. \cite{6, 34}, we triangulate \( \Sigma \) in adaptation to some graph \( \alpha \) underling a cylindrical function in \( \mathcal{H}_{\text{kin}}^G \) and reexpress connections by holonomies. The corresponding regulated operator acts on a basis vector \( T_{\alpha,X} \) over
some graph $\alpha \cup X$ as

$$
\hat{H}_6^\varepsilon \cdot T_{\alpha,X} = \lim_{\varepsilon \to 0} \frac{2^{17}N(v)\hat{\omega}(\phi)}{36\gamma^4(i\lambda_0)^2(4\hat{\alpha}^4)} \hat{\delta}^{-1}(v) \chi_\varepsilon(v - v') \\
\times \sum_{v \in \alpha(v)} \frac{1}{E(v)} \sum_{v(\Delta) = v} \epsilon(s_L s_M s_N) e_L M N \hat{U}_{\lambda_0}^{-1}(\phi(s_L(\Delta))) \\
\times \left[ \hat{U}_{\lambda_0}(\phi(t_{s_L}(\Delta))) - \hat{U}_{\lambda_0}(\phi(s_L(\Delta))) \right] \\
\times \text{Tr}(\tau_i \hat{h}_{s_M(\Delta)}[\hat{h}_{s_M(\Delta)}, (\hat{V}_{\nu_1})^{3/4}] \hat{h}_{s_N(\Delta)}(\hat{h}_{s_N(\Delta)}, (\hat{V}_{\nu_1})^{3/4})) \\
\times \sum_{v' \in \alpha(v)} \frac{1}{E(v')} \sum_{v(\Delta') = v'} \epsilon(s_I s_J s_K) e_I J K \hat{U}_{\lambda_0}^{-1}(\phi(s_{s_I(\Delta')})) \\
\times \left[ \hat{U}_{\lambda_0}(\phi(t_{s_I}(\Delta'))) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta')})) \right] \\
\times \text{Tr}(\tau_i \hat{h}_{s_J(\Delta')}[\hat{h}_{s_J(\Delta')}, (\hat{V}_{\nu_1'})^{3/4}] \hat{h}_{s_K(\Delta')}(\hat{h}_{s_K(\Delta')}, (\hat{V}_{\nu_1'})^{3/4})) \cdot T_{\alpha,X}.
$$

We refer to \ref{6} for the meaning of notations in Eq. (3.1). It is easy to see that the action of $\hat{H}_6^\varepsilon$ on $T_{\alpha,X}$ is graph changing. It adds a finite number of vertices at $t(s_I(v)) = \varepsilon$ for edges $e_I(t)$ starting from each high-valent vertex of $\alpha$. As a result, the family of operators $\hat{H}_6^\varepsilon(N)$ fails to be weakly convergent when $\varepsilon \to 0$. However, due to the diffeomorphism covariant properties of the triangulation, the limit operator can be well defined via the so-called uniform Rovelli-Smolin topology induced by diffeomorphism-invariant states $\Phi_{Diff}$ as:

$$
\Phi_{Diff}(\hat{H}_6 \cdot T_{\alpha,X}) = \lim_{\varepsilon \to 0} (\Phi_{Diff} | \hat{H}_6^\varepsilon | T_{\alpha,X}).
$$

It is obviously that the limit is independent of $\varepsilon$. Hence both the regulators $\epsilon$ and $\varepsilon$ can be removed. We then have

$$
\hat{H}_6 \cdot T_{\alpha,X} = \sum_{v \in V(\alpha)} \frac{2^{17}N(v)\hat{\omega}(\phi)}{36\gamma^4(i\lambda_0)^2(4\hat{\alpha}^4)} \hat{\delta}^{-1}(v) \\
\times \sum_{v(\Delta) = v(\Delta')} \epsilon(s_L s_M s_N) L M N \hat{U}_{\lambda_0}^{-1}(\phi(s_L(\Delta))) \\
\times \left[ \hat{U}_{\lambda_0}(\phi(t_{s_L}(\Delta))) - \hat{U}_{\lambda_0}(\phi(s_L(\Delta))) \right] \\
\times \text{Tr}(\tau_i \hat{h}_{s_M(\Delta)}[\hat{h}_{s_M(\Delta)}, (\hat{V}_{\nu_1})^{3/4}] \hat{h}_{s_N(\Delta)}(\hat{h}_{s_N(\Delta)}, (\hat{V}_{\nu_1})^{3/4})) \\
\times \epsilon(s_I s_J s_K) L M N \hat{U}_{\lambda_0}^{-1}(\phi(s_{s_I(\Delta')})) \\
\times \left[ \hat{U}_{\lambda_0}(\phi(t_{s_I}(\Delta'))) - \hat{U}_{\lambda_0}(\phi(s_{s_I(\Delta')})) \right] \\
\times \text{Tr}(\tau_i \hat{h}_{s_J(\Delta')}[\hat{h}_{s_J(\Delta')}, (\hat{V}_{\nu_1'})^{3/4}] \hat{h}_{s_K(\Delta')}(\hat{h}_{s_K(\Delta')}, (\hat{V}_{\nu_1'})^{3/4})) \cdot T_{\alpha,X}.
$$

In order to simplify the expression, we introduce $f(\phi) = \frac{1}{\phi}$ for the other terms containing it in $H(N)$, which can also be promoted to a well-defined operator $\hat{f}(\phi)$. Hence, the terms $H_3, H_4$ and $H_5$ can be quantized as

$$
\hat{H}_3 \cdot T_{\alpha,X} = \sum_{v \in V(\alpha)} \frac{4N(v)\hat{f}(\phi(v))}{\gamma^3(h^2)^2} \hat{\delta}^{-1}(v) \\
\times \left[ \hat{H}^E(1), \sqrt{V_{\nu_1}} \right] \hat{H}^E(1), \sqrt{V_{\nu_1}} \right) \cdot T_{\alpha,X},
$$

(3.4)
\( \hat{H}_4 \cdot T_{\alpha, X} = - \sum_{v \in V(\alpha) \cap X} \frac{220N(v)\hat{f}(\phi(v))}{3^{14} \gamma^6 (i\hbar)^6 E^2(v)} \tilde{\pi}(v) \times \sum_{v(\Delta)=v(\Delta')=v} \text{Tr}(\tau_i \hat{h}_{sl}(\Delta)[\hat{h}_{sl}(\Delta), \hat{K}]) \times \epsilon(sLsM) \epsilon^{LMN} \times \text{Tr}(\tau_i \hat{h}_{sm}(\Delta)[\hat{h}_{sm}(\Delta), (\hat{V}_e)^{3/4} \hat{h}_{sn}(\Delta)[\hat{h}_{sn}(\Delta), (\hat{V}_e)^{3/4}]) \times \epsilon(sjsK) \epsilon^{IJK} \times \text{Tr}(\hat{h}_{sl}(\Delta') \hat{h}_{sl}(\Delta'), (\hat{V}_e)^{1/2}) \times \text{Tr}(\hat{h}_{sl}(\Delta') \hat{h}_{sl}(\Delta'), (\hat{V}_e)^{1/2}) \cdot T_{\alpha, X}, \) (3.5)

\( \hat{H}_5 \cdot T_{\alpha, X} = \sum_{v \in V(\alpha) \cap X} \frac{218N(v)\hat{f}(\phi(v))}{3^{14} \gamma^6 (i\hbar)^6 E^2(v)} \phi(v)\tilde{\pi}(v) \times \sum_{v(\Delta)=v(\Delta')=v} \epsilon(sLsM) \epsilon^{LMN} \times \text{Tr}(\tau_i \hat{h}_{sm}(\Delta)[\hat{h}_{sm}(\Delta), (\hat{V}_e)^{1/2} \hat{h}_{sj}(\Delta)[\hat{h}_{sj}(\Delta), (\hat{V}_e)^{1/2}] \times \epsilon(sjsK) \epsilon^{IJK} \times \text{Tr}(\hat{h}_{sl}(\Delta') \hat{h}_{sl}(\Delta'), (\hat{V}_e)^{1/2}) \times \text{Tr}(\hat{h}_{sl}(\Delta') \hat{h}_{sl}(\Delta'), (\hat{V}_e)^{1/2}) \cdot T_{\alpha, X}, \) (3.6)

Therefore, the total Hamiltonian constraint in this sector has been quantized as a well-defined operator \( \hat{H}(N) = \sum_{i=1}^{8} \hat{H}_i \) in \( \mathcal{H}_{\text{kin}} \). It is easy to see that \( \hat{H}(N) \) is internal gauge invariant and diffeomorphism covariant. Hence it is at least well defined in the gauge invariant Hilbert space \( \mathcal{H}_G \). However, it is difficult to define \( \hat{H}(N) \) directly on \( \mathcal{H}_{\text{Diff}} \).

Moreover, as in \( f(R) \) theories the constraint algebra do not form a Lie algebra. This might lead to quantum anomaly after quantization.

### B. Sector of \( \omega(\phi) = -3/2 \)

In the case \( \omega(\phi) = -3/2 \), there is an extra conformal constraint (2.48), whose smeared version \( S(\lambda) \) has to be promoted as an operator. Note that both \( \phi \) and \( \pi(R) \) are already well-defined operators. To quantize the conformal constraint \( S(\lambda) \), we use the classical identity

\[ \tilde{K} \equiv \int_{\Sigma} d^3 x \tilde{K}_a^I E_i^a = \gamma^{- \frac{3}{2}} \{ H^E(1), V \} . \] (3.7)

Here the Euclidean scalar constraint \( H^E(1) \) by definition was:

\[ H^E(1) = \frac{1}{2} \int_{\Sigma} d^3 x F_{ab}^I \frac{\varepsilon_{jkl} E_j^a E_k^b}{\sqrt{\hbar}} . \] (3.8)

Both \( H^E \) and the volume \( V \) under consideration have been quantized in LQG. Now it is easy to promote \( S(\lambda) \) as a well-defined operator by acting on a given basis vector \( T_{\alpha, X} \in \mathcal{H}_{\text{kin}} \) as

\[ \hat{S}(\lambda) \cdot T_{\alpha, X} = \left( \sum_{v \in V(\alpha)} \frac{\lambda(v)}{\gamma^{3/2} (i\hbar)} \{ \hat{H}^E(1), \hat{V}_e \} - \sum_{x \in X} \lambda(x)\hat{\phi}(x)\hat{\pi}(x) \right) \cdot T_{\alpha, X} . \] (3.9)
It is easy to see that $\hat{S}(\lambda)$ is internal gauge invariant, diffeomorphism covariant and graph-changing. Thus it is well defined in $\mathcal{H}_G$. Note that the Hamiltonian constraint operator in this sector is similar to that in the sector of $\omega(\phi) \neq -3/2$. The difference is that $\omega(\phi) = -3/2$ now. Hence we write Eq. (2.47) as $H(N) = \sum_{i=1}^{5} \hat{H}_i$ in regular order. It is easy to see that the terms $H_1, H_2, H_4, H_5$ just keep the same form as those in $f(R)$ theories, while the $H_3$ can be quantized as

\[
\hat{H}_3 \cdot T_{\alpha,x} = - \sum_{v \in V(\alpha)} \frac{2^{16} N(v)}{3^{\gamma^4(4\lambda_0)^2(\gamma)^4 E^2(V)}} \phi^{-1}(v) \\
\times \sum_{v(\Delta) = v(\Delta')} \epsilon(s_L s_M s_N) L^{LMN} \hat{U}_{\lambda_0}^{-1}(\phi(s_{sL}(\Delta))) \\
\times [\hat{U}_{\lambda_0}(\phi(t_{sL}(\Delta))) - \hat{U}_{\lambda_0}(\phi(s_{sL}(\Delta)))] \\
\times \text{Tr}(\tau_3 \hat{s}_{sM}(\Delta)[\hat{s}_{sM}(\Delta), (\hat{V}_0)^{-3/4}] \hat{s}_{sK}(\Delta)[\hat{s}_{sK}(\Delta), (\hat{V}_0)^{-3/4}]) \\
\times \epsilon(s_L s_M s_N) \epsilon(L^IJK) \hat{U}_{\lambda_0}^{-1}(\phi(s_{sL}(\Delta'))) \\
\times [\hat{U}_{\lambda_0}(\phi(t_{sL}(\Delta'))) - \hat{U}_{\lambda_0}(\phi(s_{sL}(\Delta')))] \\
\times \text{Tr}(\tau_3 \hat{s}_{sJ}(\Delta') [\hat{s}_{sJ}(\Delta'), (\hat{V}_0)^{-3/4}] \hat{s}_{sK}(\Delta') [\hat{s}_{sK}(\Delta'), (\hat{V}_0)^{-3/4}] \cdot T_{\alpha,x}.
\]

Thus the total Hamiltonian constraint operator $\hat{H}(N) = \sum_{i=1}^{5} \hat{H}_i$ is also well defined in $\mathcal{H}_G$.

IV. MASTER CONSTRAINT

In order to avoid possible quantum anomaly and find the physical Hilbert space, master constraint programme was first introduced into LQG by Thiemann in [32]. This programme can also be applied to the above quantum STT.

A. Sector of $\omega(\phi) \neq -3/2$

In the case $\omega(\phi) \neq -3/2$, we can employ the master constraint to implement the Hamiltonian constraint. By definition the master constraint of the STT classically reads

\[
\mathcal{M} := \frac{1}{2} \int_{\Sigma} d^3 x \frac{|H(x)|^2}{\sqrt{\mathcal{V}}},
\]

where the Hamiltonian constraint $H(x)$ is given by Eq. (2.28). The master constraint can be regulated via a point-splitting strategy [30] as:

\[
\mathcal{M}' = \frac{1}{2} \int_{\Sigma} d^3 y \int_{\Sigma} d^3 x \chi(x - y) \frac{H(x)}{\sqrt{\mathcal{V}_x}} \frac{H(y)}{\sqrt{\mathcal{V}_y}}.
\]

Introducing a partition $\mathcal{P}$ of the 3-manifold $\Sigma$ into cells $C$, we have an operator $\hat{H}_{C,\beta}^{x, \gamma}$ acting on the internal gauge-invariant spin-scalar-network basis $T_{s,v}$ in $\mathcal{H}_G$ via a state-dependent triangulation,

\[
\hat{H}_{C,\alpha}^{x, \gamma} \cdot T_{s,v} = \sum_{v \in V(\alpha)} \chi_C(v) \hat{H}_{C,\beta}^{x, \gamma} \cdot T_{s,v}
\]

where $\alpha$ denotes the underlying graph of the spin-network state $T_s$, $\chi_C$ is the characteristic function over $C$, and

\[
\hat{H}_{v}^{x} = \sum_{v(\Delta) = v} \hat{H}_{G,R,v}^{x, \Delta} + \sum_{i=3}^{8} \hat{H}_{i, v},
\]

with

\[
\hat{H}_{3,0}^{x, \Delta} = \frac{16 \hat{f}(\phi(v))}{\gamma^4(\gamma)^2 \phi^{-1}(v)} \phi^{-1}(v) \\
\times [\hat{H}^{E}(1), (\hat{V}_{U_{v}})^{1/4}][\hat{H}^{E}(1), (\hat{V}_{U_{v}})^{1/4}],
\]

\[
\hat{H}_{3,0}^{x, \Delta} = \frac{16 \hat{f}(\phi(v))}{\gamma^4(\gamma)^2 \phi^{-1}(v)} \phi^{-1}(v) \\
\times [\hat{H}^{E}(1), (\hat{V}_{U_{v}})^{1/4}][\hat{H}^{E}(1), (\hat{V}_{U_{v}})^{1/4}],
\]
\[ \hat{H}_{4,v} = - \sum_{v(\Delta)=v(\Delta')} \frac{2^{18} \hat{f}(\phi)}{3^{3} \gamma^6 (4\pi)^6 E^2(v)} \hat{\pi}(v) \]
\[ \times \text{Tr}(\tau_i \hat{h}_{sl}(\Delta)[\hat{h}_{sl}(\Delta), \hat{\mathbb{K}}]) \]
\[ \times \epsilon(s_{LS}, s_{MN}) \epsilon^{L \bar{M} N} \text{Tr}(\tau_i \hat{h}_{sm}(\Delta)[\hat{h}_{sm}(\Delta), (\hat{V}_v)]^{1/2}) \]
\[ \times \hat{h}_{s,l}(\Delta)[\hat{h}_{s,l}(\Delta), (\hat{V}_v)]^{1/2} \]
\[ \times \epsilon(s_{JS}, s_{NK}) \epsilon^{J \bar{K}} \text{Tr}(\hat{h}_{s,j}(\Delta)[\hat{h}_{s,j}(\Delta), (\hat{V}_v)]^{1/2}) \]
\[ \times \hat{h}_{s,k}(\Delta)[\hat{h}_{s,k}(\Delta), (\hat{V}_v)]^{1/2} \]
\[ \times \epsilon(s_{LS}, s_{MN}) \epsilon^{L \bar{M} N} \text{Tr}(\hat{h}_{s,m}(\Delta)[\hat{h}_{s,m}(\Delta), (\hat{V}_v)]^{1/2}) \]
\[ \times \hat{h}_{s,n}(\Delta)[\hat{h}_{s,n}(\Delta), (\hat{V}_v)]^{1/2} \]
\[ \times \hat{h}_{s,l}(\Delta)[\hat{h}_{s,l}(\Delta), (\hat{V}_v)]^{1/2} \] (4.6)

\[ \hat{H}_{5,v} = \sum_{v(\Delta)=v(\Delta')} \frac{2^{20} \hat{f}(\phi)}{3^{4} \gamma^6 (4\pi)^6 E^2(v)} \hat{\phi}(v) \hat{\pi}(v) \]
\[ \times \epsilon(s_{JS}, s_{NK}) \epsilon^{J \bar{K}} \text{Tr}(\hat{h}_{s,j}(\Delta)[\hat{h}_{s,j}(\Delta), (\hat{V}_v)]^{1/4}) \]
\[ \times \hat{h}_{s,k}(\Delta)[\hat{h}_{s,k}(\Delta), (\hat{V}_v)]^{1/2} \]
\[ \times \epsilon(s_{LS}, s_{MN}) \epsilon^{L \bar{M} N} \text{Tr}(\hat{h}_{s,m}(\Delta)[\hat{h}_{s,m}(\Delta), (\hat{V}_v)]^{1/4}) \]
\[ \times \hat{h}_{s,n}(\Delta)[\hat{h}_{s,n}(\Delta), (\hat{V}_v)]^{1/2} \]
\[ \times \hat{h}_{s,l}(\Delta)[\hat{h}_{s,l}(\Delta), (\hat{V}_v)]^{1/2} \] (4.7)

\[ \hat{H}_{6,v} = \sum_{v(\Delta)=v(\Delta')} \frac{2^{15} \hat{\omega}(\phi)}{3^{2} \gamma^8 (4\pi)^2 (4\pi E^2(v))} \hat{\phi}^{-1}(v) \]
\[ \times \epsilon(s_{LS}, s_{MN}) \epsilon^{L \bar{M} N} \hat{U}_{\lambda_0}^{-1}(\phi(s_{sL}(\Delta))) \]
\[ \times [\hat{U}_{\lambda_0}(\phi(t_{sL}(\Delta))) - \hat{U}_{\lambda_0}(\phi(s_{sL}(\Delta)))] \]
\[ \times \text{Tr}(\tau_i \hat{h}_{s,m}(\Delta)[\hat{h}_{s,m}(\Delta), (\hat{V}_v)]^{3/4}) \hat{h}_{s,k}(\Delta)[\hat{h}_{s,k}(\Delta), (\hat{V}_v)]^{3/4}) \]
\[ \times \epsilon(s_{JS}, s_{NK}) \epsilon^{J \bar{K}} \hat{U}_{\lambda_0}^{-1}(\phi(s_{sJ}(\Delta))) \]
\[ \times [\hat{U}_{\lambda_0}(\phi(t_{sJ}(\Delta))) - \hat{U}_{\lambda_0}(\phi(s_{sJ}(\Delta)))] \]
\[ \times \text{Tr}(\tau_i \hat{h}_{s,j}(\Delta)[\hat{h}_{s,j}(\Delta), (\hat{V}_v)]^{3/4}) \hat{h}_{s,k}(\Delta)[\hat{h}_{s,k}(\Delta), (\hat{V}_v)]^{3/4}) \] (4.8)

Note that \( \hat{H}_{4,v} \) and \( \hat{H}_{5,v} \) keep the same form as the corresponding terms in [6], while \( \hat{H}_{6,v} \) is twice as the corresponding term in [6]. Since the family of operators \( \hat{H}_{C,\alpha} \) are cylindrically consistent up to diffeomorphism, the inductive limit operator \( \hat{H}_C \) is densely defined in \( \mathcal{H}_C \) by the uniform Rovelli- Smolin topology. Then we could define master constraint operator \( \mathcal{M} \) on diffeomorphism invariant states as
\[ (\mathcal{M} \Phi_{\text{Diff}}) T_{s,c} = \lim_{p \to \Sigma_{s,c} \epsilon' \to 0} \Phi_{\text{Diff}} \left[ \frac{1}{2} \hat{H}_{C}^{\epsilon}(\hat{H}_{C}^{\epsilon})^\dagger T_{s,c} \right]. \] (4.9)

Note that our construction of \( \mathcal{M} \) is qualitatively similar to those in [6, 34], although the quantitative actions are different. Similar to those in [6, 34], we can prove that \( \mathcal{M} \) is a positive and symmetric operator in \( \mathcal{H}_{\text{Diff}} \) and hence admits a unique self-adjoint Friedrichs extension. It is then possible to obtain the physical Hilbert space of the quantum STT in this sector by the direct integral decomposition of \( \mathcal{H}_{\text{Diff}} \) with respect to \( \mathcal{M} \).
B. Sector of $\omega(\phi) = -3/2$

In the case $\omega(\phi) = -3/2$, we need to employ the master constraint to implement both the Hamiltonian constraint and conformal constraint. Hence, we define the master constraint for this sector as

$$\mathcal{M} := \frac{1}{2} \int_{\Sigma} d^3x \frac{|H(x)|^2 + |S(x)|^2}{\sqrt{h}},$$

(4.10)

where the Hamiltonian constraint $H(x)$ and the conformal constraint $S(x)$ are given by Eqs. (4.14) and (4.15) respectively. It is obvious that

$$\mathcal{M} = 0 \iff H(N) = 0 \quad \text{and} \quad S(\lambda) = 0 \quad \forall N(x), \lambda(x).$$

(4.11)

Now the constraints also form a Lie algebra. The master constraint can be regulated via a point-splitting strategy as:

$$\mathcal{M}' = \frac{1}{2} \int_{\Sigma} d^3y \int d^3x \frac{H(x)H(y) + S(x)S(y)}{\sqrt{\sqrt{V_{x}} \sqrt{V_{y}}}}.$$  

(4.12)

Introducing a partition $\mathcal{P}$ of the 3-manifold $\Sigma$ into cells $C$, we have an operator $\hat{H}_{C,\delta}^\varepsilon$ acting on spin-scalar-network basis $T_{s,c}$ in $\mathcal{H}_G$ via a state-dependent triangulation as Eq. (4.3). Here, $\hat{H}_{C,\delta}^\varepsilon$ has less terms than in Eq. (4.3) as

$$\hat{H}_{C,\delta}^\varepsilon = \sum_{v(\Delta) = v} \hat{H}_{G,R,v}^{\varepsilon} + \sum_{j=3}^5 \hat{H}_{i,v},$$

(4.13)

where

$$\hat{H}_{3,v}^\varepsilon = -\sum_{v(\Delta) = v} \frac{2^{14}}{3^{3} \gamma^4 (i\lambda_0)^2 (i\hbar)^4 E^2(v)} \hat{\phi}^1 (v) \times \epsilon(s_{LSMSN})^{LMN} \hat{U}^{-1}_{\lambda_0} (\phi(s_{LS}(\Delta))) \times [\hat{U}_{\lambda_0} (\phi(t_{SL}(\Delta))) - \hat{U}_{\lambda_0} (\phi(s_{LS}(\Delta)))] \times \text{Tr}(\tau_1 \hat{h}_{sL}(\Delta) \hat{h}_{sM}(\Delta) \hat{h}_{sN}(\Delta) \hat{h}_{sL}(\Delta) \hat{h}_{sN}(\Delta)^{3/4}) \times \epsilon(s_{LSJSK})^{IJK} \hat{U}^{-1}_{\lambda_0} (\phi(s_{LS}(\Delta))) \times [\hat{U}_{\lambda_0} (\phi(t_{SL}(\Delta))) - \hat{U}_{\lambda_0} (\phi(s_{SL}(\Delta)))] \times \text{Tr}(\tau_1 \hat{h}_{sL}(\Delta) \hat{h}_{sM}(\Delta) \hat{h}_{sN}(\Delta) \hat{h}_{sM}(\Delta) \hat{h}_{sN}(\Delta)^{3/4}),$$

(4.14)

and $H_{4,v}^\varepsilon$ keep the same form as the corresponding terms in $\hat{H}_{4,v}^\varepsilon$, while $H_{5,v}^\varepsilon$ is twice as the corresponding term in $\hat{H}_{5,v}^\varepsilon$. Similarly, the operator corresponding to the conformal constraint can be defined as

$$\hat{S}_{C,\alpha} \cdot T_{s,c} = \sum_{v \in V(\alpha)} \chi_C(v) \hat{S}_{C,\alpha} \cdot T_{s,c}$$

(4.15)

where

$$\hat{S}_{v} = \hat{S}_{1,v} + \hat{S}_{2,v},$$

(4.16)

with

$$\hat{S}_{1,v} = \left[ \frac{2}{\gamma^{3/2} (i\hbar)} \right] \hat{H}^E(1) \sqrt{V_{U}^c},$$

(4.17)

$$\hat{S}_{2,v} = -\sum_{v(\Delta) = v(\Delta) = v} \frac{2^{7}}{3^{3} \gamma^2 (i\hbar)^3 E(v)} \hat{\phi}(v) \hat{\phi}(v) \times \epsilon(s_{sJSK})^{IJK} \text{Tr}(\hat{h}_{sL}(\Delta) \hat{h}_{sM}(\Delta)^{3/4}) \times \hat{h}_{sL}(\Delta) \hat{h}_{sM}(\Delta) \hat{h}_{sM}(\Delta) \hat{h}_{sM}(\Delta)^{3/4}),$$

(4.18)

and $H_{3,v}^\varepsilon$ keep the same form as the corresponding terms in $\hat{H}_{3,v}^\varepsilon$, while $H_{4,v}^\varepsilon$ is twice as the corresponding term in $\hat{H}_{4,v}^\varepsilon$. Similarly, the operator corresponding to the conformal constraint can be defined as

$$\hat{S}_{C,\alpha} \cdot T_{s,c} = \sum_{v \in V(\alpha)} \chi_C(v) \hat{S}_{C,\alpha} \cdot T_{s,c}$$

(4.15)

where

$$\hat{S}_{v} = \hat{S}_{1,v} + \hat{S}_{2,v},$$

(4.16)

with

$$\hat{S}_{1,v} = \left[ \frac{2}{\gamma^{3/2} (i\hbar)} \right] \hat{H}^E(1) \sqrt{V_{U}^c},$$

(4.17)

$$\hat{S}_{2,v} = -\sum_{v(\Delta) = v(\Delta) = v} \frac{2^{7}}{3^{3} \gamma^2 (i\hbar)^3 E(v)} \hat{\phi}(v) \hat{\phi}(v) \times \epsilon(s_{sJSK})^{IJK} \text{Tr}(\hat{h}_{sL}(\Delta) \hat{h}_{sM}(\Delta)^{3/4}) \times \hat{h}_{sL}(\Delta) \hat{h}_{sM}(\Delta) \hat{h}_{sM}(\Delta) \hat{h}_{sM}(\Delta)^{3/4}),$$

(4.18)
Since the family of operators $\hat{H}^\epsilon_c,\alpha$ and $\hat{S}^\epsilon_c,\alpha$ are cylindrically consistent up to diffeomorphism, the inductive limit operator $\hat{H}_C$ and $\hat{S}_C$ are densely defined in $\mathcal{H}_G$ by the uniform Rovelli- Smolin topology. Then we could define master constraint operator $\hat{\mathcal{M}}$ on diffeomorphism invariant states as
\[
(\hat{\mathcal{M}}\Phi_{D iff})_{T_{s,c}} = \lim_{p \to \Sigma,\epsilon' \to 0} \Phi_{D iff} \left[ \frac{1}{2} \sum_{c \in \mathcal{P}} \left( \hat{H}^\epsilon_c (\hat{H}^\epsilon_c)^\dagger + \hat{S}^\epsilon_c (\hat{S}^\epsilon_c)^\dagger \right) \right]_{T_{s,c}}. \tag{4.19}
\]

Similar to those in [5, 34], we can prove that $\hat{\mathcal{M}}$ is a positive and symmetric operator in $\mathcal{H}_{D iff}$ and hence admits a unique self-adjoint Friedrichs extension. It is then also possible to obtain the physical Hilbert space of the quantum STT in this sector by the direct integral decomposition of $\mathcal{H}_{D iff}$ with respect to $\hat{\mathcal{M}}$.

V. CONCLUDING REMARKS

STT have received increased attention in issues of "dark Universe" and nontrivial tests on gravity beyond GR. These kinds of theories have also become popular in unification schemes such as string theory. Hence it is desirable to study the Hamiltonian formulation of general STT. The first achievement in this paper is the detailed Hamiltonian structure and connection dynamics of STT. By doing Hamiltonian analysis, we have derived the Hamiltonian formulation of STT of gravity from their Lagrangian formulation. Two sectors of STT are marked off by the coupling parameter $\omega$. In the sector of $\omega \neq -3/2$, the canonical structure and constraint algebra of STT are similar to those of GR coupled with a scalar field. In the sector of $\omega = -3/2$, the feasible theories are restricted and a new primary constraint generating conformal transformations of spacetime is obtained. The canonical structure and constraint algebra are also obtained. Note that Palatini $f(R)$ theories are equivalent to this sector of STT. The successful background independent LQG relies on the key observation that GR can be cast into the connection dynamics with structure group of $SU(2)$. We have shown that the connection dynamical formalism of the STT can also be obtained by canonical transformations from the geometric dynamics.

The second achievement of this paper is the nonperturbative loop quantization of STT. Based on the $su(2)$-connection dynamical formalism, LQG has been successfully extended to the STT by coupling to a polymer-like scalar field. The quantum kinematical structure of STT is as same as that of loop quantum $f(R)$ theories. Thus the important physical result that both the area and the volume are discrete at kinematic level remains valid for quantum STT of gravity. While the dynamics of STT is more general than that of $f(R)$ theories, the Hamiltonian constraint operator and master constraint operator for STT can also be well defined in both sectors. In particular, in the sector $\omega = -3/2$, the conformal constraint can also be quantized as a well-defined operator. Hence the classical STT in both sectors have been successfully quantized non-perturbatively. This guarantees the existence of the STT of gravity at fundamental quantum level. Meanwhile, besides GR and metric $f(R)$ theories, LQG method is also valid for general STT of gravity.

It should be noted that there are still many aspects of the connection formalism and loop quantization of STT which deserve discovering. For examples, it is still desirable to derive the connection dynamics of STT by variational principle. The semiclassical analysis of loop quantum STT is yet to be done. To further explore the physical contents of the loop quantum STT, we would like to study its applications to cosmology and black holes in future works. Moreover, one would also like to quantize STT by the covariant spin foam approach.

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Appendix A

We first use $(\tilde{K}^a_i, E^b_j)$ and $(\phi, \pi)$ as canonical variables to derive the Poisson bracket (2.35) of STT with $\omega \neq -3/2$. The Hamiltonian constraint (2.28) can also be written as
\[
H = \frac{1}{2\sqrt{\hbar}} (\tilde{K}^a_i \tilde{E}^b_j - \tilde{K}^a_i E^b_j) - \frac{1}{2} \phi \sqrt{\hbar} R + \sqrt{\hbar} \xi(\phi) + \frac{1}{(3 + 2\omega)\phi \sqrt{\hbar}} (\tilde{K}^a_i E^b_j + \pi \phi)^2 + \frac{\omega}{2\phi} \sqrt{\hbar} D_a \phi D^a \phi. \tag{5.1}
\]
To calculate the Poisson bracket between two smeared Hamiltonian constraints, we notice that the non-vanishing contributions come only form the terms which contain the derivative of canonical variables. Those terms are $\int \Sigma N \sqrt{\hbar} \int D_\alpha \phi D^\alpha \phi$, which only contains the derivative of $\phi$, and $\int \Sigma x N \sqrt{\hbar} \int D_\alpha D^\alpha \phi$, which contains both the derivative of $E^\alpha_j$ and the derivative of $\phi$, and $\int \Sigma - \frac{1}{2} \phi N \sqrt{\hbar} \mathcal{R}$, which only contain the derivative of $E^\alpha_j$. Hence we first use $\{ \phi(x), \pi(y) \} = \delta^\alpha(x, y)$ to calculate

$$
\{ \int N \sqrt{\hbar} D_\alpha \phi D^\alpha \phi, \int \frac{M}{\Sigma (3 + 2\omega) \phi \sqrt{\hbar}} (\tilde{K}_d^i E_i^a + \pi \phi)^2 \} (\phi, \pi) - M \leftrightarrow N
$$

$$
= \int \left( M D_\alpha D^\alpha N - N D_\alpha D^\alpha M \right) - \frac{2}{(3 + 2\omega)} (\tilde{K}_d^i E_i^a + \pi \phi)
$$

$$
= \frac{2}{(3 + 2\omega)} \int (N D^\alpha M - M D^\alpha N) D_\alpha (\pi \phi + \tilde{K}_d^i E_i^a),
$$

(5.2)

and

$$
\{ \int N \sqrt{\hbar} D_\alpha \phi D^\alpha \phi, \int \frac{M}{\Sigma (3 + 2\omega) \phi \sqrt{\hbar}} (\tilde{K}_d^i E_i^b + \pi \phi)^2 \} (\phi, \pi) - M \leftrightarrow N
$$

$$
= \int \left( M D_\alpha N - N D_\alpha M \right) \omega D_\alpha \phi - \frac{2}{(3 + 2\omega)} (\tilde{K}_d^i E_i^b + \pi \phi)
$$

$$
= \frac{2\omega}{(3 + 2\omega)} \int (N D^\alpha M - M D^\alpha N) (\pi \phi + \tilde{K}_d^i E_i^b) D_\alpha \phi.
$$

(5.3)

Note also that

$$
N \sqrt{\hbar} D_\alpha D^\alpha \phi = N \sqrt{\hbar} h^{ab}(\partial_a \partial_b \phi - \Gamma^c_{ab} \partial_c \phi).
$$

(5.4)

Since only $\Gamma^c_{ab}$ contains the derivative of $E^\alpha_j$ in above equation, we consider

$$
N \sqrt{\hbar} h^{ab} \Gamma^c_{ab} \partial_c \phi = \frac{N}{2} \sqrt{\hbar} h^{ab} (\partial_d \phi (h^{cd}(-\partial_a h_{bd} - \partial_b h_{ad} + \partial_d h_{ab})))
$$

$$
= \frac{N}{2} \sqrt{\hbar} (\partial_c \phi) (2\partial_a h^{ac} - h_{ab} \partial^a \phi)
$$

$$
= \frac{N}{2} \sqrt{\hbar} (\partial_c \phi) (2\partial_a (\frac{E_i^a E_i^c}{h}) - h_{ab} \partial^a (\frac{E_i^a E_i^b}{h})).
$$

(5.5)

Therefore, we use $\{ \tilde{K}_d^i(x), E_i^b(y) \} = \delta_i^b \delta_d^i \delta(x, y)$ to calculate

$$
\{ \int \sqrt{\hbar} (\partial_c \phi) \partial_a \phi \left( \frac{E_i^a E_i^c}{h} \right), \int \frac{M}{2 \sqrt{\hbar}} \left( \frac{1}{\phi} \left( \tilde{K}_d^i E_i^a \tilde{K}_d^i E_i^b - \frac{1}{3 + 2\omega} \tilde{K}_d^i E_i^a \tilde{K}_d^i E_i^b \right) + \frac{4}{3 + 2\omega} \tilde{K}_d^i E_i^a \pi \right) \} (\phi, \pi) - M \leftrightarrow N
$$

$$
= \int \frac{1}{2} M (\partial_a N) (D_\alpha \phi) \frac{2 E_i^c}{h} \left( \frac{2}{\phi} (\tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c - \frac{1}{3 + 2\omega} \tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c) + \frac{4}{3 + 2\omega} \tilde{K}_d^i E_i^a \pi \right)
$$

$$
+ \frac{1}{2} M (\partial_a N) (D_\alpha \phi) \left( - \frac{E_i^c}{h} \frac{2}{\phi} (\tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c - \frac{1}{3 + 2\omega} \tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c) + \frac{4}{3 + 2\omega} \tilde{K}_d^i E_i^a \pi \right) - M \leftrightarrow N
$$

(5.6)

and

$$
\{ \int - \frac{N}{2} \sqrt{\hbar} (\partial_c \phi) h_{ac} \partial^a \phi \left( \frac{E_i^a E_i^c}{h} \right), \int \frac{M}{2 \sqrt{\hbar}} \left( \frac{1}{\phi} \left( \tilde{K}_d^i E_i^a \tilde{K}_d^i E_i^b - \frac{1}{3 + 2\omega} \tilde{K}_d^i E_i^a \tilde{K}_d^i E_i^b \right) + \frac{4}{3 + 2\omega} \tilde{K}_d^i E_i^a \pi \right) \} (\phi, \pi) - M \leftrightarrow N
$$

$$
= \int \left( - \frac{1}{4} M \delta^c N D_\alpha \phi \frac{2 E_i^c}{h} \left( \frac{2}{\phi} (\tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c - \frac{1}{3 + 2\omega} \tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c) + \frac{4}{3 + 2\omega} \tilde{E}_j^a \pi \right)
$$

$$
- \frac{1}{4} M \delta^c N D_\alpha \phi \frac{E_i^c}{h} (-3 \tilde{E}_d^a \frac{2}{\phi} (\tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c - \frac{1}{3 + 2\omega} \tilde{E}_j^a \tilde{K}_d^i E_j^b E_i^c) + \frac{4}{3 + 2\omega} \tilde{E}_j^a \pi \right) \} - M \leftrightarrow N.
$$

(5.7)

The combination of above two Poisson brackets equals to

$$
\int (N D^\alpha M - M D^\alpha N) (- \frac{1}{3 + 2\omega} \pi D_\alpha \phi - \frac{2}{\phi} (\tilde{K}_d^i E_i^b h_{ac} \phi - \frac{1}{3 + 2\omega} \tilde{K}_d^i E_i^b D_\alpha \phi)).
$$

(5.8)
The variation of the terms containing a derivative in $\int_{\Sigma} -\frac{1}{2}\phi N \sqrt{h} R$ reads

$$\int_{\Sigma} \frac{1}{\sqrt{h}} (-D^a D^b (\phi N) + h^{ab} D_c D^c (\phi N)) \delta h_{ab}$$

$$= \int_{\Sigma} \frac{1}{\sqrt{h}} (D_a D_b (\phi N) - h_{ab} D_c D^c (\phi N)) \delta h_{ab}$$

$$= \int_{\Sigma} \frac{1}{\sqrt{h}} (D_a D_b (\phi N) - h_{ab} D_c D^c (\phi N)) \delta \left( \frac{E^a E^b}{h} \right).$$

Thus we have

$$\{ \int_{\Sigma} \frac{1}{\phi} \phi N \sqrt{h} R, \int_{\Sigma} \frac{1}{\sqrt{h}} \left( \frac{1}{\phi} (\tilde{K}^a E_a^i) \tilde{K}^b E_b^i - \frac{1 + 2\omega}{3 + 2\omega} \tilde{K}^a E_a^i \tilde{E}^i + \frac{4}{3 + 2\omega} \tilde{K}^a E_a^i (\pi) \right) \} - M \leftrightarrow N$$

$$= \int_{\Sigma} \frac{1}{\phi} \left( \frac{2}{\phi} \left( \tilde{K}^a E_a^i \tilde{E}^i - \frac{1 + 2\omega}{3 + 2\omega} \tilde{K}^a E_a^i \tilde{E}^i + \frac{4}{3 + 2\omega} E^a (\pi) \right) \right) - M \leftrightarrow N$$

$$= \int_{\Sigma} - \frac{1}{4} (M D_a D_b (\phi N) - h_{ab} M D_c D^c (\phi N)) h^{bc} \frac{1}{\phi} \tilde{K}^a E_a^i + \frac{2}{\phi (3 + 2\omega)} \tilde{K}^a E_a^i - \frac{2}{3 + 2\omega} \tilde{K}^a E_a^i - M \leftrightarrow N$$

$$= \int_{\Sigma} - M D_a D^b (\phi N) \frac{1}{\phi} \tilde{K}^a E_a^i + M D_c D^c (\phi N) (\frac{1 + 2\omega}{\phi (3 + 2\omega)} \tilde{K}^a E_a^i - \frac{2}{3 + 2\omega} \tilde{K}^a E_a^i - M \leftrightarrow N$$

$$= \int_{\Sigma} \left( (N D_a D^b (\phi N) - M D_a D^b (\phi N)) \frac{1}{\phi} \tilde{K}^a E_a^i + (N D_c D^c (\phi N) - M D_c D^c (\phi N)) (\frac{2}{3 + 2\omega} \tilde{K}^a E_a^i - \frac{1 + 2\omega}{\phi (3 + 2\omega)} \tilde{K}^a E_a^i) \right)$$

$$= \int_{\Sigma} \left( (N D_a D^b (\phi M) - M D_a D^b (\phi N)) \frac{2}{3 + 2\omega} \tilde{K}^a E_a^i - \frac{1 + 2\omega}{3 + 2\omega} \tilde{K}^a E_a^i + (N D_a M - M D_a N) D^a \phi (\frac{4}{3 + 2\omega} \tilde{K}^a E_a^i - \frac{2}{3 + 2\omega} \tilde{K}^a E_a^i) \right)$$

Taking account of Eqs. (5.2) - (5.10), we obtain

$$\{ H(N), H(M) \}$$

$$= \int_{\Sigma} (N D_c D^c M - M D_c D^c N) (-\tilde{K}^a E_a^i) + (N D^a M - M D^a N) (\pi D_a \phi)$$

$$+ (N D_a D^b M - M D_a D^b N) \tilde{K}^a E_a^i$$

$$= \int_{\Sigma} (N D^a M - M D^a N) (D_a (\tilde{K}^a E_a^i) - D_b (\tilde{K}^b E_b^i) + \pi D_a \phi) - (D_a M D^b N - D^b M D_a N) \tilde{K}^a E_a^i$$

$$= \int_{\Sigma} (N D^a M - M D^a N) V_a + \left( \frac{E^a D_a N, E^b D_b M}{h} \right)^i \mathcal{G}_i,$$  \hspace{1cm} (5.11)

where we used the following identity

$$- [D_a M) D^b N - (D^b M) D_a N] \tilde{K}^a E_a^i = - ((D_a M) D_c N - (D_c M) D_a N) h^{bc} E^i \tilde{K}^b$$

$$= -2 (D_a M) (D_c N) E^i h E^i \tilde{K}^b$$

$$= -2 (D_a M) (D_c N) E^i E^i \tilde{K}^b$$

$$= \epsilon^{ijk} (D_M N) \epsilon^{i} E^i \tilde{K}^b E^k$$

$$= - \left( \frac{E^a D_a N, E^b D_b M}{h} \right)^i \mathcal{G}_i.$$  \hspace{1cm} (5.12)

Using above result and shift conjugate pair $(\tilde{K}^i, E^i)$ to $(A^i, E^i)$, we can easily get the Poisson bracket between the smeared Hamiltonian constraints.
Thus we calculate of canonical variables. Those terms are structure (2.11), we notice that the non-vanishing contributions come only from the terms which contain the derivative (2.38) respectively. To calculate the Poisson bracket between two smeared Hamiltonian constraints by the symplectic sector \( \omega \)

On the other hand, the variation of the terms containing the derivative in

Thus we have

Since only \( \Gamma_{ab}^c \) contains the derivative of \( h_{ab} \) in above equation, we consider

Thus we calculate

and

The combination of above two Poisson brackets gives

On the other hand, the variation of the terms containing the derivative in \( \int \phi N \sqrt{h} R \) reads

Thus we have

Now we use \( (h_{ab}, p^{cd}) \) and \( (\phi, \pi) \) as canonical variables to derive the Poisson brackets (2.40) and (2.41) in the sector \( \omega(\phi) = -3/2 \). The Hamiltonian constraint and conformal constraint can be read from Eqs. (2.37) and (2.38) respectively. To calculate the Poisson bracket between two smeared Hamiltonian constraints by the symplectic structure (2.11), we notice that the non-vanishing contributions come only form the terms which contain the derivative of canonical variables. Those terms are \( \int d^3 x \sqrt{h} D_a D^a \phi \), which contains both the derivative of \( h_{ab} \) and the derivative of \( \phi \), and \( \int \phi N \sqrt{h} R \), which only contain the derivative of \( h_{ab} \). Hence we first notice that

\[
N \sqrt{h} D_a D^a \phi = N \sqrt{h} h^{ab} (\partial_a \partial_b \phi - \Gamma^{c}_{ab} \partial_c \phi).
\]

(5.13)

Since only \( \Gamma_{ab}^c \) contains the derivative of \( h_{ab} \) in above equation, we consider

\[
-N \sqrt{h} h^{ab} \Gamma^{c}_{ab} \partial_c \phi = \frac{N}{2} \sqrt{h} h^{ab} (\partial_a \partial_b \phi) (h^{cd} (-\partial_d h_{bd} - \partial_b h_{ad} + \partial_d h_{ab})) = \frac{N}{2} \sqrt{h} (\partial_c \phi) (2 \partial_a h^{ac} - h_{ab} \partial^c h^{ab}).
\]

(5.14)

Thus we calculate

\[
\{ \int \Sigma N \sqrt{h} (\partial_c \phi) \partial_a (h^{ac}), \int \Sigma \sqrt{h} (\frac{p_{cd} p^{bd} - \frac{1}{2} p^2}{\phi}) \} (h, p) - M \leftrightarrow N
\]

\[
= \int \Sigma (2 M \partial_a N - N \partial_a M) (D_c \phi) (\frac{2 (p^{ac} - \frac{1}{2} p h^{ac})}{\phi}),
\]

(5.15)

and

\[
\{ \int \Sigma - \frac{N}{2} \sqrt{h} (\partial_c \phi) h_{ac} \partial^c (h^{ac}), \int \Sigma \sqrt{h} (\frac{p_{cd} p^{bd} - \frac{1}{2} p^2}{\phi}) \} (h, p) - M \leftrightarrow N
\]

\[
= \int \Sigma (M \partial^c N - N \partial^c M) (D_c \phi) \frac{p^c}{\phi}.
\]

(5.16)

The combination of above two Poisson brackets gives

\[
\{ \int \Sigma N \sqrt{h} D_a D^a \phi, \int \Sigma \sqrt{h} (\frac{p_{cd} p^{bd} - \frac{1}{2} p^2}{\phi}) \} (h, p) - M \leftrightarrow N
\]

\[
= \int \Sigma (M \partial_a N - N \partial_a M) (D_c \phi) (\frac{4 (p^{ac} - \frac{1}{2} p h^{ac})}{\phi}).
\]

(5.17)

On the other hand, the variation of the terms containing the derivative in \( \int \phi N \sqrt{h} R \) reads

\[
\int \Sigma \frac{1}{2} \sqrt{h} (-D^a D^b (\phi N) + h^{ab} D_c D^c (\phi N)) \delta h_{ab} = \int \Sigma \frac{1}{2} \sqrt{h} (D_a D_b (\phi N) - h_{ab} D_c D^c (\phi N)) \delta h_{ab}.
\]

Thus we have

\[
\{ \int \Sigma - \frac{1}{2} \phi N \sqrt{h} R, \int \Sigma \sqrt{h} (\frac{p_{ab} p^{ab} - \frac{1}{2} p^2}{\phi}) \} - M \leftrightarrow N
\]

\[
= - \int \Sigma (M D_a D_b (\phi N) - h_{ab} M D_c D^c (\phi N)) \frac{2 (p^{ab} - \frac{1}{2} p h^{ab})}{\phi} - M \leftrightarrow N
\]

\[
= \int \Sigma (N D^a M - M D^a N) (-2 D^b p_{ab} + 4 D^b \phi \frac{p_{ab}}{\phi}).
\]

(5.18)
Combining Eqs. (5.20)-(5.24), we have
\[ H(N), H(M) = \int_{\Sigma} (ND^a M - MD^a N)(-2D^b p_{ab} + \pi D_a \phi + \frac{D_a \phi}{\phi} (p - \phi \pi)) \]
\[ = V(ND^a M - MD^a N) + S\left(\frac{D_a \phi}{\phi} (ND^a M - MD^a N)\right) . \]  

(5.19)

Now, we calculate the Poisson bracket between conformal constraint and Hamiltonian constraint. For this aim, we calculate the following terms respectively
\[ \left\{ \int_{\Sigma} \lambda (p - \phi \pi), \int_{\Sigma} \frac{2N}{\sqrt{h}} \left( \frac{p_{ab} p^{ab} - \frac{1}{2} p^2}{\phi} \right) \right\} = \int_{\Sigma} \frac{N \lambda}{\sqrt{h}} \left( \frac{p_{ab} p^{ab} - \frac{1}{2} p^2}{\phi} \right) \]
\[ (5.20) \]
\[ \left\{ \int_{\Sigma} \lambda (p - \phi \pi), \int_{\Sigma} \frac{N \sqrt{h}}{2} (-\phi R) \right\} = \int_{\Sigma} \frac{N \lambda \sqrt{h}}{4} (-\phi R) - \int_{\Sigma} \lambda \sqrt{h} D_a D_a (\phi N) \]
\[ (5.21) \]
\[ \left\{ \int_{\Sigma} \lambda (p - \phi \pi), -\int_{\Sigma} \frac{3N \sqrt{h}}{4 \phi} (D_a \phi) D_a \phi \right\} = -\int_{\Sigma} \frac{3N \lambda \sqrt{h}}{8 \phi} (D_a \phi) D_a \phi + \int_{\Sigma} \frac{3 \lambda \sqrt{h}}{2} D_a (ND^a N) \]
\[ (5.22) \]
\[ \left\{ \int_{\Sigma} \lambda (p - \phi \pi), -\int_{\Sigma} (D_a N) \sqrt{h} D^a \phi \right\} = \int_{\Sigma} \frac{\lambda}{2} (D_a N) \sqrt{h} D^a \phi + \int_{\Sigma} \lambda \sqrt{h} \phi (D_a D^a N) \]
\[ (5.23) \]
\[ \left\{ \int_{\Sigma} \lambda (p - \phi \pi), \int_{\Sigma} N \sqrt{h} \xi (\phi) \right\} = \int_{\Sigma} \left( -\frac{3}{2} \lambda \phi N \sqrt{h} \xi (\phi) + \lambda \phi N \sqrt{h} \xi' (\phi) \right) \]
\[ (5.24) \]

Combining Eqs. (5.20)-(5.24), we have
\[ \{ S(\lambda), H(M) \} = H \left( \frac{\lambda M}{2} \right) + \int_{\Sigma} N \lambda \sqrt{h} (\phi - 2 \xi (\phi) + \phi \xi' (\phi)) . \]
\[ (5.25) \]

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