Extension of Loop Quantum Gravity to Metric Theories beyond General Relativity

Yongge Ma
Department of Physics, Beijing Normal University, Beijing 100875, China
E-mail: mayg@bnu.edu.cn

Abstract. The successful background-independent quantization of Loop Quantum Gravity relies on the key observation that classical General Relativity can be cast into the connection-dynamical formalism with the structure group of $SU(2)$. Due to this particular formalism, Loop Quantum Gravity was generally considered as a quantization scheme that applies only to General Relativity. However, we will show that the nonperturbative quantization procedure of Loop Quantum Gravity can be extended to a rather general class of metric theories of gravity, which have received increased attention recently due to motivations coming from cosmology and astrophysics. In particular, we will first introduce how to reformulate the 4-dimensional metric $f(R)$ theories of gravity, as well as Brans-Dicke theory, into connection-dynamical formalism with real $SU(2)$ connections as configuration variables. Through these formalisms, we then outline the nonperturbative canonical quantization of the $f(R)$ theories and Brans-Dicke theory by extending the loop quantization scheme of General Relativity.

1. Introduction
In the recent 25 years, loop quantum gravity (LQG), a background independent approach to quantize general relativity (GR), has been widely investigated [1, 2, 3, 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 relies on the key observation that classical GR can be cast into the connection-dynamical formalism with the structure group of $SU(2)$[5, 6]. Thus one is naturally led to ask the following questions. Does the non-perturbative quantization scheme of LQG apply only to GR? What is the applicable scope of LQG? On this Loops 11 Conference, we just learned from the talks by Thiemann et al that LQG is applicable to GR in arbitrary dimensions, since higher dimensional GR could also be cast into connection dynamics with certain compact structure group. We are going to answer the question: whether GR is a unique relativistic theory of gravity with the desired connection-dynamical character?

In fact, modified gravity theories have recently received increased attention due to motivations coming from cosmology and astrophysics. 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[7]. This result has carried the "dark energy" problem in GR. A large number of phenomenological models for dark energy have been proposed, such as quintessence, phantom, Chaplygin gas, K-essence etc. In all these models, certain scalar fields are added by hand, and their origins are not understood. Moreover, there are indirect evidences suggesting that the bulk of the matter of the universe
is invisible or dark (see e.g. [8]). The strongest evidence comes from the rotational velocity of the isolated stars or hydrogen cloud on the outskirts of galaxies. Although a few candidates for dark matter are proposed, such as sterile neutrinos, neutralinos etc, none of them are satisfying. To explain the accelerated expansion of the universe, as well as dark matter, from fundamental physics is now a great challenge. It is reasonable to consider the possibility that GR is not a valid theory of gravity on a galactic or cosmological scale. Historically, Einstein’s GR is the simplest relativistic theory of gravity with correct Newtonian limit. It is worth pursuing all alternatives, which provide a high chance to new physics.

A large variety of models of \( f(R) \) modified gravity have been proposed to explain the ”dark universe” without recourse to dark energy and dark matter [9]. The action of metric \( f(R) \) theories reads:

\[
S[g] = \frac{1}{2} \int d^4x \sqrt{-g} f(R)
\] (1)

where \( f \) is a general function of the scalar curvature \( \mathcal{R} \), and we set \( 8\pi G = 1 \). Besides \( f(R) \) theories, a well-known competing relativistic theory of gravity was proposed by Brans and Dicke in 1961 [10], which is apparently compatible with Mach’s principle. To represent a varying ”gravitational constant”, a scalar field is non-minimally coupled to the metric as

\[
S[g, \phi] = \int d^4x \sqrt{-g} \left( f(s) - \phi(s - \mathcal{R}) \right).
\] (2)

The scalar field in Brans-Dicke theory (BDT) of gravity is then expected to account for ”dark energy”. It can naturally lead to cosmological acceleration if certain potential term of the scalar is added in the original action (2). It is also possible to account for the dark matter problem. Furthermore, a large part of the non-trivial tests on gravity theory is related to Einstein’s equivalence principle (EEP) [11], which contains the following three elements. (i) The trajectory of a freely falling ”test” body is independent of its internal structure and composition. (ii) The outcome of any non-gravitational experiments is independent of the velocity of the freely falling reference frame in which it is performed. (iii) The outcome of any non-gravitational experiments is independent of where and when in the universe it is performed. There exist many local experiments in solar-system supporting EEP, which implies the metric theories of gravity. In a metric theory of gravity, spacetime is endowed with a metric, and the trajectories of freely falling ”test” bodies are geodesics of that metric. Moreover, in local freely falling reference frames, the non-gravitational laws of physics are those written in the language of Special Relativity. Actually, besides GR, both \( f(R) \) theories and BDT belong to metric theories of gravity. For metric theories, gravity is still geometry with diffeomorphism invariance as in GR. The differences between them are just reflected in dynamical equations and additional variables. Hence, a background-independent and non-perturbative quantization for metric theories of gravity is preferable. Since metric \( f(R) \) theories, as well as BDT, are a class of representative metric theories, which have received most attention, we will take them as examples to carry out the extension of LQG to metric 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.

2. Connection Dynamics of \( f(R) \) and Brans-Dicke Theories

By introducing an independent variable \( s \) and a Lagrange multiplier \( \phi \), an action equivalent to (1) of \( f(R) \) theories is proposed as [12]

\[
S[g, \phi, s] = \frac{1}{2} \int d^4x \sqrt{-g} \left( f(s) - \phi(s - \mathcal{R}) \right).
\] (3)
The variation of (3) with respect to \( s \) yields \( \phi = df(s)/ds \equiv f'(s) \). Assuming \( s \) could be resolved from the above equation, action (3) is reduced to

\[
S[g, \phi] = \frac{1}{2} \int d^4x \sqrt{-g} (\phi R - \xi(\phi)) \equiv \int d^4x \mathcal{L}
\]

(4)

where \( \xi(\phi) \equiv \phi s - f(s) \). Comparing action (4) with (2), it is obvious that metric \( f(\mathcal{R}) \) theories could be regarded as a particular kind of generalized BDT with certain potentials of \( \phi \) and a vanishing coupling parameter \( \omega \). The virtue of (4) is that it admits a treatable Hamiltonian analysis [12]. By doing 3+1 decomposition and Legendre transformation, the Hamiltonian of metric \( f(\mathcal{R}) \) gravity can be derived as a linear combination of first-class constraints as:

\[
H_{\text{total}} = \int_{\Sigma} N^a V_a + N H,
\]

where \( N \) and \( N^a \) are the lapse function and shift vector respectively, and the diffeomorphism and Hamiltonian constraints read respectively

\[
V_a = -2D^b(p_{ab}) + \pi \partial_b \phi,
\]

\[
H = \frac{2}{\sqrt{h}} \left( \frac{p_{ab}p^{ab} - \frac{1}{2}p^2}{\phi} + \frac{1}{6} \phi \pi^2 - \frac{1}{3} \pi^3 \right) + \frac{1}{2} \sqrt{h}(\xi(\phi) - \phi R + 2D^a D^\alpha \phi),
\]

where \( p_{ab} \) and \( \pi \) are the momentum respectively conjugate to the spatial 3-metric \( h_{ab} \) and scalar field \( \phi \) on the spatial manifold \( \Sigma \). Although the above Hamiltonian analysis is started with the action (4) where a non-minimally coupled scalar field is introduced, we can show that the resulted Hamiltonian formalism is equivalent to the Lagrangian formalism. The symplectic structure reads

\[
\{h_{ab}(x), p^{cd}(y)\} = \delta^c_a \delta^d_b \delta^3(x, y), \quad \{\phi(x), \pi(y)\} = \delta^3(x, y).
\]

(5)

To achieve the connection dynamics of metric \( f(\mathcal{R}) \) modified gravity, we let

\[
\tilde{K}^{ab} \equiv \phi K^{ab} + \frac{h_{ab}(\phi - N^c \partial_c \phi)}{2N},
\]

where \( K_{ab} \) is the extrinsic curvature of \( \Sigma \), and introduce

\[
E^a_i \equiv \sqrt{h} e^a_i, \quad \tilde{K}^j_a \equiv \tilde{K}_{ab} e^b_j,
\]

where \( e^a_i \) is the triad such that \( h_{ab}e^a_i e^b_j = \delta_{ij} \). We first extend the phase space of geometry to the space consisting of pairs \( (E^a_i, \tilde{K}^j_a) \). It is then easy to see that the symplectic structure (5) can be derived from the following Poisson brackets:

\[
\{E^a_i(x), E^b_j(y)\} = \{\tilde{K}^j_a(x), \tilde{K}^k_b(y)\} = 0, \quad \{\tilde{K}^j_a(x), E^b_j(y)\} = \delta^b_a \delta^j_k \delta(x, y).
\]

(6)

Thus there is a symplectic reduction from the extended phase space to the original one. Since \( \tilde{K}^{ab} = \tilde{K}^{ba} \), we have an additional constraint:

\[
G_{jk} \equiv \tilde{K}_{a[j} E^a_k] = 0.
\]

(7)

For second step, we make a canonical transformation by defining

\[
A^i_a = \Gamma^i_a + \gamma \tilde{K}^i_a,
\]
where $\Gamma_a^i$ is the spin connection determined by $E_a^a$ and $\gamma$ is a nonzero real number. Then the Poisson brackets among the new variables read
\[
\{ A_a^i(x), E_b^j(y) \} = \gamma \delta_a^i \delta_b^j \delta(x, y), \quad \{ A_a^i(x), A_a^j(y) \} = 0.
\]

Now, the phase space consists of conjugate pairs $(A_a^i, E_b^j)$ and $(\phi, \pi)$. Combining Eq.(7) with the compatibility condition: $\partial_a E_b^j + \epsilon_{ijk} F_a^i E_b^k = 0$, we obtain the standard Gaussian constraint
\[
G_a = D_a E_b^a \equiv \partial_a E_b^a + \epsilon_{ijk} A_a^i E_b^k, \tag{8}
\]
which justifies $A_a^i$ as an Ashtekar-Barbero $su(2)$-connection. Had we let $\gamma = \pm i$, the (anti-)self-dual complex connection formalism would be obtained. The original diffeomorphism constraint can be expressed in terms of new variables up to Gaussian constraint as
\[
V_a = \frac{1}{\gamma} F_a^i E_i^b + \pi \partial_a \phi,
\]
where $F_a^b = 2 \partial_a A_b^i + \epsilon_{kl} A_a^k A_b^l$ is the curvature of $A_a^i$. The original Hamiltonian constraint can be written up to Gaussian constraint as
\[
H_{fR} = \frac{\phi}{2} [F_a^b - (\gamma^2 + 1/\phi^2) \varepsilon_{jmn} \hat{K}_a^m \hat{K}_b^n] \frac{\varepsilon_{jkl} E_k^a E_l^b}{\sqrt{\hbar}}
+ \frac{1}{2} \left( \frac{2}{3\phi} \frac{(K_a^b E^b)^2}{\sqrt{\hbar}} + \frac{4}{3} \frac{(K_a^b E^b)\pi}{\sqrt{\hbar}} + \frac{2\pi^2 \phi}{3\sqrt{\hbar}} + \frac{\phi \xi(\phi)}{\sqrt{\hbar}} + \sqrt{\hbar} D_a D^a \phi \right). \tag{9}
\]

Similar to GR, the constraints are of first class. Thus the total Hamiltonian is a linear combination of the constraints. We have obtained the real $su(2)$-connection dynamical formalism of Lorentz $f(R)$ gravity [13, 14]. Note that a connection dynamical formalism of Euclidean $f(R)$ theories in Einstein frame was derived in [15]

We now turn to the BDT. By doing 3+1 decomposition and Legendre transformation, the Hamiltonian of BDT with $\omega \neq -3/2$ can be derived from the action (2) as a linear combination of first-class constraints as $H_{total} = \int_D N^a V_a + N H$, where the diffeomorphism constraint $V_a$ has the same form as that of metric $f(R)$ theories, while the Hamiltonian constraint reads [16, 17]
\[
H = \frac{2}{\sqrt{\hbar}} \left( p_a p^a - \frac{1}{\phi} \frac{p^2}{2\phi(3 + 2\omega)} \right) + \frac{1}{2} \sqrt{\hbar} \left( -\phi R + \frac{\omega}{\phi} (D_a \phi) D^a \phi + 2D_a D^a \phi \right).
\]

In comparison with metric $f(R)$ theories, there is a new kinetic term $\frac{\omega \sqrt{\hbar}}{2\phi} (D_a \phi) D^a \phi$ of the scalar field in the above Hamiltonian constraint. However, this kinetic term will not affect the canonical transformations to connection dynamics. Following the same canonical transformations in $f(R)$ theories, we obtain new conjugate variables for the geometry as: $A_a^i = \Gamma_a^i + \gamma \hat{K}_a^i$ and $E_a^a = \sqrt{\hbar} e_a^a$, as well as the Gaussian constraint (8). In terms of the new variables, the Hamiltonian constraint reads
\[
H_{BD} = \frac{\phi}{2} [F_a^b - (\gamma^2 + 1/\phi^2) \varepsilon_{jmn} \hat{K}_a^m \hat{K}_b^n] \frac{\varepsilon_{jkl} E_k^a E_l^b}{\sqrt{\hbar}}
+ \frac{1}{3 + 2\omega} \left( \frac{(\hat{K}_a^b E^b)^2}{\phi \sqrt{\hbar}} + 2 \frac{(\hat{K}_a^b E^b)\pi}{\sqrt{\hbar}} + \frac{\pi^2 \phi}{2\phi \sqrt{\hbar}} \right) + \frac{\omega}{2\phi} \sqrt{\hbar} (D_a \phi) D^a \phi + \sqrt{\hbar} D_a D^a \phi. \tag{10}
\]

The special case of $\omega = -3/2$ can also be dealt with [17]. Hence both $f(R)$ theories and BDT can be cast into connection dynamics with $su(2)$-connection as one of configuration variables.
3. Loop Quantization of f(\mathcal{R}) and Brans-Dicke Theories

Based on the connection dynamical formalisms, the nonperturbative loop quantization procedure can be straightforwardly extended to both f(\mathcal{R}) theories and BDT. Since the scalar field in f(\mathcal{R}) theories and BDT still reflects gravity, it is natural to employ the polymer-like representations for both the scalar field and the connection. The following quantum kinematical structure is valid for both f(\mathcal{R}) theories and BDT.

For the geometry sector, we have the unique diffeomorphism and internal gauge invariant representation for the quantum holonomy-flux algebra\(^1\). The kinematical Hilbert space of geometry reads
\[
\mathcal{H}_{\text{kin}}^{\text{geo}} = L^2(\mathcal{A}, d\mu_{AL}),
\]
with the so-called spin-network basis \(T_\alpha(A) \equiv T_{\alpha,j,m,n}(\mathcal{A})\). The spatial geometric operators of LQG, such as the area\(^1\), the volume\(^1\) and the length operators\(^2\) are still valid here. Hence, the important physical result that both the area and the volume are discrete at quantum kinematical level remains true for loop quantum f(\mathcal{R}) gravity as well as loop quantum Brans-Dicke gravity.

For the polymer-like quantization of the scalar field\(^2\), one extends the space \(U\) of smooth scalar fields to the quantum configuration space \(\bar{U}\). A simple element \(U \in \bar{U}\) may be thought as a point holonomy: \(U_\lambda = \exp(i\lambda\phi(x))\) at point \(x \in \Sigma\), where \(\lambda\) is a real number. By GNS structure, there is a natural diffeomorphism invariant measure \(d\mu\) on \(\bar{U}\). Thus the kinematical Hilbert space of scalar field reads
\[
\mathcal{H}_{\text{kin}}^{\text{sca}} = L^2(\bar{U}, d\mu),
\]
with the scalar-network basis
\[
T_X(\phi) = \prod_{x_j \in X} U_{\lambda_j}(\phi(x_j)),
\]
where \(X = \{x_1, \ldots, x_n\}\) is an arbitrary given set of finite number of points in \(\Sigma\). The total kinematical Hilbert space for f(\mathcal{R}) and Brans-Dicke gravity reads \(\mathcal{H}_{\text{kin}} = \mathcal{H}_{\text{kin}}^{\text{geo}} \otimes \mathcal{H}_{\text{kin}}^{\text{sca}}\), with an orthonormal basis
\[
T_{\alpha,X}(A, \phi) \equiv T_\alpha(A) \otimes T_X(\phi).
\]

The holonomy \(h_\epsilon(A) = \mathcal{P} \exp \int A_{\alpha} f^\alpha\), flux \(E(S, f) := \int_S \epsilon_{ijk} E^i f^j\), point holonomy \(U_\lambda\), and smeared momentum \(\pi(R) := \int_R d^3x \pi(x)\) of scalar field become basic operators in \(\mathcal{H}_{\text{kin}}\). Their actions read respectively
\[
\hat{h}_\epsilon(A)\Psi(A, \phi) = h_\epsilon(A)\Psi(A, \phi), \quad \hat{E}(S, f)\Psi(A, \phi) = i\hbar\{E(S, f), \Psi(A, \phi)\},
\]
\[
\hat{U}_\lambda(\phi(x))\Psi(A, \phi) = \exp(i\lambda\phi(x))\Psi(A, \phi), \quad \hat{\pi}(R)\Psi(A, \phi) = i\hbar\{\pi(R), \Psi(A, \phi)\}.
\]

As in LQG, it is straightforward to promote the Gaussian constraint \(\mathcal{G}(\Lambda)\) to a well-defined operator. The kernel of \(\hat{\mathcal{G}}(\Lambda)\) in \(\mathcal{H}_{\text{kin}}\) is the internal gauge invariant Hilbert space \(\mathcal{H}_G\), with gauge invariant spin-network basis:
\[
T_{s,c}(A, \phi) \equiv T_{s=(\alpha,j,i)}(A) \otimes T_X(\phi).
\]

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\(^2\). Thus we can also obtain the desired diffeomorphism and gauge invariant Hilbert space \(\mathcal{H}_{\text{Diff}}\) for f(\mathcal{R}) and Brans-Dicke gravity.

The quantum dynamics is a nontrivial issue. To implement the Hamiltonian constraint at quantum level, we need to deal with the metric f(\mathcal{R}) and Brans-Dicke theories separately. The smeared version of the Hamiltonian constraint of metric f(\mathcal{R}) theories consists of seven terms in the order of Eq.(9) as:
\[
H_{fR}(N) = \sum_{i=1}^7 H_i(N).
\]
Comparing it with that of GR in connection formalism, the new ingredients that we have to deal with are \(\phi(x), \phi^{-1}(x), \xi(\phi)\) and the four\(^1\).

---

\(^1\) See e.g. talks by Sahlmann, Giesel, Lewandowski on Loops 11 Conference in Madrid

---
terms: $H_3(N), H_4(N), H_5(N), H_7(N)$. By introducing certain small constant $\lambda_0$, an operator corresponding to the scalar $\phi(x)$ can be defined as

$$\hat{\phi}(x) = \frac{1}{2i\lambda_0}(U_{\lambda_0}(\phi(x)) - U_{-\lambda_0}(\phi(x))).$$

The ambiguity of $\lambda_0$ is the price that we have to pay in order to represent field $\phi$ in the polymer-like representation. To further define an operator corresponding to $\phi^{-1}(x)$, we can use the classical identity

$$\phi^{-1}(x) = sgn(\phi) \left( l^{-1}sgn(\phi)\{\{\phi(x)\}, \pi(R)\} \right)^{1/l}, \quad (11)$$

for any rational number $l \in (0, 1)$. For example, one may choose $l = \frac{1}{2}$ for positive $\phi(x)$ and replace the Poisson bracket by commutator to define

$$\hat{\phi}^{-1}(x) = \left( \frac{2}{i\hbar} |\sqrt{\phi(x)}$, $\hat{\pi}(R)| \right)^2.$$

Then all the functions $\xi(\phi)$ which can be expanded as powers of $\phi(x)$ have been quantized. For other non-trivial types of $\xi(\phi)$, we may replace the argument $\phi$ by $\hat{\phi}$, provided that no divergence would arise after the replacement. In the case where divergence does appear, there remain the possibilities to employ tricks similar to Eq.(11) to deal with it. Hence it is reasonable to believe that most physically interesting functions $\xi(\phi)$ can be quantized. Then it is straightforward to quantize the term $H_6(N)$ in the Hamiltonian constraint as an operator acting on a basis vector $T_{a,X}$ as

$$\hat{H}_6(N) \cdot T_{a,X} = \frac{1}{2} \sum_{v \in V(a)} N(v)\hat{\xi}(\phi(v))\hat{V}_v \cdot T_{a,X}.$$

Moreover, by the regularization techniques developed for the Hamiltonian constraint operators of LQG and polymer-like scalar field $[2, 23]$, all the terms $H_3(N), H_4(N), H_5(N), H_7(N)$ can be quantized as operators acting on cylindrical functions in $H_{kin}$ in state-dependent ways. The regularization procedure involves re-expressing some variables by Thiemann’s trick, point-splitting, triangulating $\Sigma$ in adaptation to some graph $\alpha \cup X$ underlying a cylindrical function, and replacing connections by holonomies. Replacing the classical variables and Poisson brackets by the corresponding operators and commutators respectively, we can obtain the regulated Hamiltonian constraint operator $\hat{H}_{FR}(N)$. It turns out that the regulators of $\hat{H}_3^N(N), \hat{H}_4^N(N), \hat{H}_5^N(N)$ can be straightforwardly removed. However, the action of $\hat{H}_7^N(N)$ on a basis vector $T_{a,X}$ is graph changing. It adds a finite number of vertices with representation $\lambda_0$ at $t(s_I(v)) = \epsilon$ for edges $e_I(t)$ starting from each high ($\geq 3$)-valent vertex of $\alpha$. The family of operators $\hat{H}_7^N(N)$ fails to be weakly convergent when $\epsilon \rightarrow 0$. 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. The operators corresponding to the four new terms in the Hamiltonian constraint act on a basis vector as follows:

$$\hat{H}_3(N) \cdot T_{a,X} = \frac{4}{\gamma^3} (i\hbar)^4 \sum_{v \in V(a)} N(v)\hat{\phi}^{-1}(v)[\hat{H}^{Euc}(1), \sqrt{\hat{V}_v}] [\hat{H}^{Euc}(1), \sqrt{\hat{V}_v}] \cdot T_{a,X},$$

$$\hat{H}_4(N) \cdot T_{a,X} = - \sum_{v \in V(a) \cap X} \frac{2^{20}N(v)}{3^6\gamma^6(i\hbar)^6E(v)^2} \hat{\pi}(v) \sum_{v(\Delta) = v(\Delta') = v} \varepsilon(s_L, s_M, s_N)\varepsilon(s_I, s_J, s_K)\varepsilon^{LMN} \times Tr(\tau_1\hat{h}_{s_L}(\Delta)'[\hat{h}^{-1}_{s_L}(\Delta), \hat{K}])Tr(\tau_1\hat{h}_{s_M}(\Delta)'[\hat{h}^{-1}_{s_M}(\Delta), (\hat{V}_v)^{3/4}], \hat{h}_{s_N}(\Delta)'[\hat{h}^{-1}_{s_N}(\Delta), (\hat{V}_v)^{3/4}], \hat{h}_{s_K}(\Delta)'[\hat{h}^{-1}_{s_K}(\Delta), (\hat{V}_v)^{3/4}]) \cdot T_{a,X},$$
\[ \hat{H}_S(N) \cdot T_{\alpha,X} = \sum_{v \in V(\alpha) \cap X} \frac{2^{18} N(v)}{35^3 \gamma^6 (i h)^6 E(v)^2} \hat{\pi}(v) \phi(v) \hat{\pi}(v) \sum_{\nu(\Delta) = v} \varepsilon(s_I, s_J, s_K) \varepsilon(s_L, s_M, s_N) \]
\[ \times \epsilon^{IJK} \text{Tr}(\hat{h}_{s_I(\Delta)} \hat{h}_{s_J(\Delta)}^{-1} (\hat{V}_c)^{1/2}) \hat{h}_{s_J(\Delta)} \hat{h}_{s_K(\Delta)} \hat{h}_{s_K(\Delta)}^{-1} (\hat{V}_c)^{1/2}) \epsilon^{LMN} \]
\[ \times \text{Tr}(\hat{h}_{s_L(\Delta')} \hat{h}_{s_M(\Delta')}^{-1} (\hat{V}_c)^{1/2}) \hat{h}_{s_M(\Delta')} \hat{h}_{s_N(\Delta')} \hat{h}_{s_N(\Delta')}^{-1} (\hat{V}_c)^{1/2}) \cdot T_{\alpha,X}, \]

where \( \varepsilon(s_I, s_J, s_K) := \text{sgn}(\det(s_I s_J s_K(v))) \) takes the values \((+1, -1, 0)\) if the tangents of the three segments \( s_I, s_J, s_K \) at \( v \) (in that sequence) form a matrix of positive, negative or vanishing determinant, and \( E(v) \equiv \left( \frac{\pi(v)}{3} \right) \) with \( \pi(v) \) denoting the valence of the vertex \( v \).

Hamiltonian constraint operator \( \hat{H}(N) = \sum_v \hat{H}(N)_v \) is internal gauge invariant and hence also well defined in the gauge invariant Hilbert space \( \mathcal{H}_G \).

Although \( \hat{H}(N) \) can dually act on the diffeomorphism invariant states, there is no guarantee for the resulted states to be still diffeomorphism invariant. Hence it is difficult to define a Hamiltonian constraint operator directly on the diffeomorphism invariant Hilbert space \( \mathcal{H}_{Diff} \). The idea of resolution is to introduce the master constraint as in LQG [24]:

\[ \mathcal{M} := \frac{1}{2} \int_{\Sigma} d^3x \frac{|H(x)|^2}{\sqrt{\text{det}(h(x))}}. \]

One then gets the master constraint algebra as a Lie algebra:

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

where the subalgebra of diffeomorphism constraints forms an ideal. So it is possible to define a corresponding master constraint operator on \( \mathcal{H}_{Diff} \). The master constraint can be regulated via a point-splitting strategy as [25]:

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

Introducing a partition \( \mathcal{P} \) of the 3-manifold \( \Sigma \) into cells \( C \), we have an operator \( \hat{H}_{C,\alpha}^s \) acting on gauge invariant spin-scalar-network basis \( T_{s,c} \) via a state-dependent triangulation as

\[ \hat{H}_{C,\alpha}^s \cdot T_{s,c} = (\hat{H}_{C,G}^s + \sum_{i=3}^7 \hat{H}_{C,i}^s) \cdot T_{s,c} = \sum_{v \in V(\alpha)} \chi_C(v) \left( \sum_{\nu(\Delta) = v} \hat{H}_{G,R,v}^s \right) + \sum_{i=3}^7 \hat{H}_{C,i}^s \cdot T_{s,c}, \]

where \( \alpha \) denotes the underlying graph of the spin-network state \( T_s \). Here,

\[ \hat{H}_{G,R,v}^s = \frac{32}{3E(v)} \varepsilon(s_I, s_J, s_K) \epsilon^{IJK} \hat{\phi}(v) \text{Tr}(\hat{h}_{s_I(\Delta)} \hat{h}_{s_J(\Delta)}^{-1} (\hat{V}_c)^{1/2}), \]

\[ - \frac{1}{(i h)^3} \varepsilon(s_I, s_J, s_K) \epsilon^{IJK} \hat{\phi}(v) \text{Tr}(\hat{h}_{s_I(\Delta)} \hat{h}_{s_J(\Delta)}^{-1} \hat{K} \hat{h}_{s_J(\Delta)} \hat{h}_{s_K(\Delta)}^{-1} (\hat{V}_c)^{1/2} \hat{V}_c). \]
\[
\hat{H}_{3,v}^\varepsilon = \frac{16}{3\gamma^2 (1!h)^4} \phi^{-1}(v)[\hat{H}_{\text{Eucl}}(1), (\hat{V}_{1!})^{1/4}][\hat{H}_{\text{Eucl}}(1), (\hat{V}_{1!})^{1/4}],
\]
and \(\hat{H}_{3,v}^\varepsilon, \hat{H}_{5,v}^\varepsilon, \hat{H}_{6,v}^\varepsilon, \hat{H}_{7,v}^\varepsilon\) can be defined similarly [14]. The family of operators \(\hat{H}_{7}^\varepsilon\) are cylindrically consistent up to diffeomorphisms. The inductive limit operator \(\hat{H}_{C}\) can be well defined by the uniform Rovelli-Smolin topology. Thus we can define master constraint operator \(\mathcal{M}\) on diffeomorphism invariant states as

\[
(\mathcal{M}\Phi_{\text{Diff}}) T_{s,c} = \lim_{p \to \Sigma_{s,c',0}} \Phi_{\text{Diff}}[\frac{1}{2} \sum_{c \in \mathcal{D}} \hat{H}_{C}^{\varepsilon}(\hat{H}_{C}^{\varepsilon})^\dagger T_{s,c}].
\]

It is obvious that \(\mathcal{M}\) is diffeomorphism invariant. For any given diffeomorphism invariant spin-scalar-network state \(T_{s,c}\), the norm \(\|\mathcal{M} T_{s,c}\|_{\text{Diff}}\) is finite. So \(\mathcal{M}\) is densely defined in \(\mathcal{H}_{\text{Diff}}\). Moreover, \(\mathcal{M}\) is positive and symmetric and hence admits a unique self-adjoint Friedrichs extension. It is then possible to obtain the physical Hilbert space of quantum \(f(\mathcal{R})\) gravity by the direct integral decomposition of \(\mathcal{H}_{\text{Diff}}\) with respect to \(\mathcal{M}\).

Now we turn to the quantum dynamics of BDT. Comparing the Hamiltonian constraint (2) of Brans-Dicke gravity with that of metric \(f(\mathcal{R})\) gravity in connection formalism, the only new ingredient that we have to deal with is the kinetic term:

\[
H_{k}(N) = \int_{\Sigma} d^{3}x N \frac{\omega}{2\phi} \sqrt{h(D\phi)} D^{a}\phi.
\]

By the regularization techniques similar to those for \(f(\mathcal{R})\) gravity, it can be quantized as a well-defined operator in \(H_{\text{kin}}\) as [16]

\[
\hat{H}_{k} \cdot T_{a,X} = \sum_{v \in \mathcal{V}(\alpha)} \frac{2^{17} \omega N(v)}{3^{3} \gamma^4 (1!h)^2 (2!h)^4 E(v)^2} \phi^{-1}(v) \sum_{v(\Delta) = v'} \varepsilon(s_l, s_j, s_K) \varepsilon(s_L, s_M, s_N)
\]

\[
\times \left[ e^{LMN} \hat{V}_{0}^{-1}(\phi(s_{sl}(\Delta))) \langle \hat{U}_{0}\phi(t_{sl}(\Delta)) - \hat{U}_{0}\phi(s_{sl}(\Delta)) \rangle \right]
\]

\[
\times Tr(\tau_{1}\hat{h}_{s}^{-1}(\hat{V}_{0})^{3/4}\hat{h}_{s}^{-1}(\hat{V}_{0})^{3/4})
\]

\[
\times \left[ e^{JK} \hat{V}_{0}^{-1}(\phi(s_{sj}(\Delta))) \langle \hat{U}_{0}\phi(t_{sj}(\Delta)) - \hat{U}_{0}\phi(s_{sj}(\Delta)) \rangle \right]
\]

\[
\times Tr(\tau_{2}\hat{h}_{s}^{-1}(\hat{V}_{0})^{3/4}\hat{h}_{s}^{-1}(\hat{V}_{0})^{3/4})
\]

\[
\times Tr(\tau_{3}\hat{h}_{s}^{-1}(\hat{V}_{0})^{3/4}\hat{h}_{s}^{-1}(\hat{V}_{0})^{3/4})
\]

\[
\times \cdot T_{a,X}
\]

Since all the other terms in the Hamiltonian constraint are equal to the corresponding terms of metric \(f(\mathcal{R})\) theories up to coefficients, the whole Hamiltonian constraint operator of BDT with \(\omega \neq -3/2\) has been well defined. The quantum dynamics for the special case \(\omega \neq -3/2\) of BDT can also be well defined [17]. For the same reason as in \(f(\mathcal{R})\) gravity, we also wish to define a master constraint operator for Brans-Dicke gravity. The "square root" of the new term in the regulated master constraint can be quantized as

\[
\hat{H}_{k,v}^{\varepsilon} = \sum_{v(\Delta) = v'} \frac{2^{15} \omega}{3^{3} \gamma^4 (1!h)^2 (2!h)^4 E(v)^2} \varepsilon(s_l, s_j, s_K) \varepsilon(s_L, s_M, s_N)
\]

\[
\times \left[ \phi^{-1}(v) e^{LMN} \hat{V}_{0}^{-1}(\phi(s_{sl}(\Delta))) \langle \hat{U}_{0}\phi(t_{sl}(\Delta)) - \hat{U}_{0}\phi(s_{sl}(\Delta)) \rangle \right]
\]

\[
\times Tr(\tau_{1}\hat{h}_{s}^{-1}(\hat{V}_{0})^{1/2}\hat{h}_{s}^{-1}(\hat{V}_{0})^{1/2})
\]

\[
\times \left[ e^{JK} \hat{V}_{0}^{-1}(\phi(s_{sj}(\Delta))) \langle \hat{U}_{0}\phi(t_{sj}(\Delta)) - \hat{U}_{0}\phi(s_{sj}(\Delta)) \rangle \right]
\]

\[
\times Tr(\tau_{2}\hat{h}_{s}^{-1}(\hat{V}_{0})^{1/2}\hat{h}_{s}^{-1}(\hat{V}_{0})^{1/2})
\]

\[
\times Tr(\tau_{3}\hat{h}_{s}^{-1}(\hat{V}_{0})^{1/2}\hat{h}_{s}^{-1}(\hat{V}_{0})^{1/2})
\]

from which a positive and self-adjoint master constraint operator can be defined on \(\mathcal{H}_{\text{Diff}}\). Thus the master constraint program is also valid for BDT.
4. Summary and Outlook

Based on the above loop quantization procedure of metric \( f(R) \) theories and BDT, we can propose a general quantization scheme for 4-dimensional metric theories of gravity. The prerequisite is that the theories should have well-defined geometrical dynamics, which means a Hamiltonian formalism with 3-metric \( h_{ab} \) as one of configuration variables and a closed (first-class) constraint algebra (perhaps after solving some second-class constraints). Without loss of generality, we assume that the classical phase space of the theory consists of conjugate pairs \((h_{ab}, p^{ab})\) and \( (\phi_A, \pi^A) \), where \( \phi_A \) could be a rather arbitrary scalar, vector, tensor or spinor field. Then the quantization scheme consists of the following steps. (i) To obtain a connection dynamical formalism, we first enlarge the phase space by transforming to the triad formulation as

\[
(h_{ab}, p^{ab}) \rightsquigarrow (E^a_i \equiv \sqrt{h} h^{ab} e_{aj}, \tilde{K}_a^j = \tilde{K}_{ab} e^{bj}),
\]

where \( \tilde{K}_{ab} = \frac{2}{\sqrt{h}} (\tilde{p}_{ab} - \frac{1}{2} \sqrt{h} \tilde{h}_{ab}) \) and \( \tilde{K}_a[iE^a_i] = 0 \). Then we make a canonical transformation to connection formulation as:

\[
(E^a_i, \tilde{K}_a^j) \rightsquigarrow (E^a_i, A^j_a \equiv \Gamma^j_a + \gamma \tilde{K}_a^j),
\]

with the Gaussian constraint, \( D_a E^a_i = \partial_a E^a_i + \epsilon_{ijk} A^j_a E^a_k = 0 \), appeared by construction. It is straightforward to write all the constraints in terms of the new variables. (ii) For loop quantization, we first find the polymer-like representation of the fields \( (\phi_A, \pi^A) \), together with the LQG representation of the holonomy-flux algebra. Then the kinematical Hilbert space reads \( \mathcal{H}_{kin} := \mathcal{H}_{kin}^{geo} \otimes \mathcal{H}_{kin}^{\phi} \), where the basic operators and geometrical operators could be well defined. By implementing the Gaussian and diffeomorphism constraints as in standard LQG, we could get the gauge and diffeomorphism invariant Hilbert space as: \( \mathcal{H}_{kin} \rightsquigarrow \mathcal{H}_{G} \rightsquigarrow \mathcal{H}_{Diff} \).

To implement quantum dynamics, one may first construct the Hamiltonian constraint operator at least in \( \mathcal{H}_G \). Usually it could not be well defined on \( \mathcal{H}_{Diff} \). Then we can construct master constraint operator in \( \mathcal{H}_{Diff} \) by using the structure of the Hamiltonian operator. (iii) One may try to understand the physical Hilbert space by the direct integral decomposition of \( \mathcal{H}_{Diff} \) with respect to the master constraint operator. (iv) One may also do certain semiclassical analysis in order to confirm the classical limits of the Hamiltonian and master constraint operators as well as the constraint algebra. The low energy physics is also expected in the analysis. (v) Finally, to complement above canonical approach, we can also try the covariant path integral (spin foam) quantization. It should be noted that in the present work we only finished steps (i) and (ii) for metric \( f(R) \) theories and BDT.

To summarize, our main results are in two folds. First, the 4-dimensional connection dynamics of metric \( f(R) \) theories, as well as Brans-Dicke theory, have been obtained by canonical transformations from their geometrical dynamics. Thus GR is not the unique theory of gravity with connection dynamical character. Second, due to the \( su(2) \)-connection dynamical formalism, the 4-dimensional metric \( f(R) \) theories and Brans-Dicke theory have been nonperturbatively quantized by extending LQG scheme. Hence, the non-perturbative loop quantization procedure is not only valid for GR but also valid for a general class of metric theories of gravity. In fact, it is not difficult to extend LQG further to general scalar-tensor theories of gravity [17]. Moreover, since higher dimensional scalar-tensor theories of gravity have well-defined Hamiltonian geometrical dynamics, and the symplectic reduction of Bodendorfer-Thiemann-Thurn connection formalism to metric formalism does not depend on dynamics, LQG may also be extended to higher (\( > 4 \)) dimensional scalar-tensor theories of gravity [26].

Of course, there are still many open issues on the extension of LQG. It is desirable to find suitable actions for the connection dynamics of \( f(R) \) theories and that of Brans-Dicke theory.
We will explore the applications of loop quantum $f(R)$ and Brans-Dicke theories to cosmology and black holes in future work [27]. It is also desirable to quantize metric theories of gravity by the covariant spin foam approach [28]. To conclude, our conservative observation is that LQG could be applicable to metric theories of gravity (with well-defined geometrical dynamics) in arbitrary dimensions. However, a caution arises from the difference between the 4(or 3)-dimensional and higher-dimensional connection dynamical formulations of GR. In particular, in 4-dimensional case, we have both Ashtekar-Barbero connection dynamics and Bodendorfer-Thiemann-Thurn connection dynamics of GR. Are the quantum theories corresponding to them unitary equivalent to each other? If the answer is negative, are there any theoretical criteria for judging them? Is Bodendorfer-Thiemann-Thurn connection dynamics only preferable in higher dimensions? Another interesting question is whether LQG can be extended to non-metric theories, e.g., metric-affine $f(R)$ theories. All these open issues are fascinating and deserve future investigating.

Acknowledgments
The author would like to thank Thomas Thiemann and Xiangdong Zhang for helpful discussion and fruitful collaboration and acknowledge the organizers of Loops 11 conference for the financial support. This work is supported in part by NSFC (Grant No.10975017) and the Fundamental Research Funds for the Central Universities.

References
[1] C. Rovelli, Quantum Gravity, (Cambridge University Press, 2004).
[2] T. Thiemann, Modern Canonical Quantum General Relativity, (Cambridge University Press, 2007).
[3] A. Ashtekar and J. Lewandowski 2004 Class. Quant. Grav. 21 R53
[4] M. Han, Y. Ma and W. Huang 2007 Int. J. Mod. Phys. D 16 1397
[5] A. Ashtekar 1986 Phys. Rev. Lett. 57 2244
[6] J. Barbero 1995 Phys. Rev. D 51 5507
[7] J. Friemann, M. Turner, D. Huterer 2008 Ann. Rev. Astron. Astrophys. 46 385
[8] W. Freedman and M. Turner 2003 Rev. Mod. Phys. 75 1433
[9] T. P. Sotiriou and V. Faraoni 2010 Rev. Mod. Phys. 82 451
[10] C. Brans and R. H. Dicke 1961 Phys. Rev. 124 925
[11] C. M. Will 2006 Living Rev. Rel. 9 3
[12] N. Deruelle, Y. Sendouda, and A. Youssef 2009 Phys. Rev. D 80 084032
[13] X. Zhang and Y. Ma 2011 Phys. Rev. Lett. 106 171301
[14] X. Zhang and Y. Ma 2011 Phys. Rev. D 84 064040
[15] L. Fatibene, M. Ferraris, M. Francaviglia 2010 Class. Quant. Grav. 27 185016
[16] X. Zhang and Y. Ma 2011 Loop quantum Brans-Dicke theory (To appear in Journal of Physics: Conference Series).
[17] X. Zhang and Y. Ma 2011 Phys. Rev. D 84 104045
[18] C. Rovelli and L. Smolin 1995 Nucl. Phys. B 442 593
[19] A. Ashtekar and J. Lewandowski 1998 Adv. Theor. Math. Phys. 1 388
[20] T. Thiemann 1998 J. Math. Phys. 39 3372
[21] Y. Ma, C. Soo, J. Yang 2010 Phys. Rev. D 81 124026
[22] A. Ashtekar, J. Lewandowski, H. Sahlmann 2003 Class. Quant. Grav. 20 L11
[23] M. Han and Y. Ma 2006 Class. Quant. Grav. 23 2741
[24] T. Thiemann 2006 Class. Quant. Grav. 23 2211
[25] M. Han and Y. Ma 2006 Phys. Lett. B 635 225
[26] Y. Han, X. Zhang and Y. Ma 2011 (in preperation).
[27] H. Guo, X. Wu, X. Zhang and Y. Ma 2011 (in preperation).
[28] Z. Zhou, X. Zhang and Y. Ma 2011 (in preperation).

See the talk by Thomas Thiemann on Loops 11 Conference in Madrid