Extension of loop quantum gravity to \(f(R)\) theories

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The 4-dimensional metric \(f(R)\) theories of gravity are cast into connection-dynamical formalism with real \(SU(2)\)-connections as configuration variables. Through this formalism, the classical metric \(f(R)\) theories are quantized by extending the loop quantization scheme of general relativity. Our results imply that the non-perturbative quantization procedure of loop quantum gravity is valid not only for general relativity but also for a rather general class of 4-dimensional metric theories of gravity.

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In recent twenty years, loop quantum gravity (LQG), a background independent approach to quantize general relativity (GR), has been widely investigated\([1,2]\). It is remarkable that, as a non-renormalizable theory, GR can be non-perturbatively quantized by the loop quantization procedure\([3]\). 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 \(SU(2)\)\([4,5]\). Thus it is interesting to see whether GR is a unique relativistic theory with the connection-dynamic character. Especially, modified gravity theories have received increasingly attention recently 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\([6,7]\). This result conflicts with the prediction of GR and has carried the "dark energy" problem. Hence it is reasonable to consider the possibility that GR is not a valid theory of gravity on a cosmological scale. Since it was found that a small modification of the Einstein-Hilbert action by adding an inverse term of curvature scalar \(R\) would lead to current acceleration of our universe, a large variety of models of \(f(R)\) modified gravity have been proposed\([8]\). Moreover, some models of \(f(R)\) gravity may account for the "dark matter" problem, which was revealed by the observed rotation curve of galaxy clusters\([9]\). 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. Recall that the precession of Mercury’s orbit was at first attributed to some unobserved planet orbiting in side Mercury’s orbit, but was actually explained only after the passage from Newtonian gravity to GR.

Given the strong motivations to \(f(R)\) gravity, it is desirable to study such kind of theories at fundamental quantum level. For metric \(f(R)\) theories, gravity is still geometry as GR. The differences between them are just reflected in dynamical equations. Hence, a background-independent and non-perturbative quantization for \(f(R)\) gravity is preferable. In this letter, we derive the connection-dynamical formulation of \(f(R)\) gravity by canonical transformations from its geometrical dynamics. The latter was realized by introducing a non-minimally coupled scalar field to replace the original \(f(R)\) action and then doing Hamiltonian analysis. The canonical variables of our Hamiltonian formalism of \(f(R)\) gravity consist of \(SU(2)\)-connection \(A_s^i\) and its conjugate momentum \(E_s^i\), as well as the scalar field \(\phi\) and its momentum \(\pi\). The Gaussian, diffeomorphism and Hamiltonian constraints are also obtained, and they comprise a first-class system. Loop quantization procedure is then naturally employed to quantize \(f(R)\) gravity.

The rigorous kinematical Hilbert space structure of LQG is extended to loop quantum \(f(R)\) gravity by adding a polymer-like quantum scalar field. As in LQG, the Gaussian and diffeomorphism constraints can be solved at quantum level, and the Hamiltonian constraint is promoted to a well-defined operator. We use Greek alphabet for spacetime in indices, Latin alphabet \(a, b, c\ldots\) for spatial indices and \(i, j, k\ldots\) for internal indices.

The original action of \(f(R)\) theories reads:

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

where \(f\) is a general function of \(R\), and we set \(8 \pi G = 1\). By introducing an independent variable \(s\) and a Lagrange multiplier \(\phi\), an equivalent action is proposed as\([10,11]\):

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

The variation of \(S\) with respect to \(s\) yields \(\phi = df(s)/ds \equiv f'(s)\). Assuming \(s\) could be resolved from the above equation, action \(S\) is reduced to

\[
S[g, \phi] = \frac{1}{2} \int d^4 x \sqrt{-g} (\phi R - V(\phi)) \equiv \int d^4 x \mathcal{L} \tag{3}
\]

where \(V(\phi) \equiv \phi s - f(s)\). It is easy to see that the variations of \(S\) give the equations of motion equivalent to that from action \(S\). The virtue of \(S\) is that it admits a treatable Hamiltonian analysis\([10]\). By doing 3+1
decomposition and Legendre transformation:

\[ p^{ab} = \frac{\partial L}{\partial h_{ab}} = \frac{\sqrt{h}}{2} [\phi(K^{ab} - K h^{ab}) - \frac{h^{ab}}{N}(\phi - N \partial_{\phi} \phi)], \]

\[ \pi = \frac{\partial L}{\partial \dot{\phi}} = -\sqrt{h} K, \]

(4)

where \( h_{ab} \) and \( K_{ab} \) are the induced 3-metric and the extrinsic curvature of the spatial hypersurface \( \Sigma \) respectively, and \( K \equiv K_{\alpha}^{\alpha} \), the Hamiltonian of \( f(R) \) gravity can be derived as a liner combination of constraints as \( \mathcal{H}_{\text{total}} = \int_{V} N^a V_a + NH \), where \( N \) and \( N^a \) are the lapse function and shift vector respectively, and the diffeomorphism and Hamiltonian constraints read

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

\[ H = \frac{2}{\sqrt{h}} (p_{ab} \pi^{ab} - \frac{1}{2} \rho^2) + \frac{1}{6} \phi \pi^2 - \frac{1}{3} \rho \pi \]

\[ + \frac{1}{2} \sqrt{h} (V(\phi) - \phi R + 2D_a D^a \phi). \]

(6)

The symplectic structure is given by

\[ \{h_{ab}(x), p^{cd}(y)\} = \delta_b^c \delta^d_x \delta(\mathbf{x}, \mathbf{y}), \]

\[ \{\phi(x), \pi(y)\} = \delta^3(\mathbf{x}, \mathbf{y}). \]

(7)

Straightforward calculations show that the constraints \( 5_{\mathcal{E}} \) and \( 6_{\mathcal{E}} \) comprise a first-class system similar to GR[11]. Although the above Hamiltonian analysis is started with the action \( 3_{\mathcal{E}} \) where a non-minimally coupled scalar field is introduced, one can check that the resulted Hamiltonian formalism is equivalent to the Lagrangian formalism[12].

Recall that the non-perturbative loop quantization of GR was based on it’s connection-dynamic formalism. It is very interesting to study whether the previous geometric dynamics of \( f(R) \) modified gravity also has a connection-dynamic correspondence. To this aim, we first introduce the following canonical transformation on the phase space of \( f(R) \) theories. Let

\[ \tilde{K}^{ab} \equiv \phi K^{ab} + \frac{h^{ab}}{2N}(\phi - N \partial_{\phi} \phi), \]

(8)

and \( E^a_i \equiv \sqrt{h} e^a_i \) where \( e^a_i \) is the triad s.t. \( h_{ab} e^a_i e^b_j = \delta_{ij} \). Then we get

\[ p^{ab} = \frac{1}{2} (\tilde{K}^{ab}_i E^b_i - \frac{1}{h} \tilde{K}^{ab}_i E^b_i E^b_j), \]

\[ \pi = -\sqrt{h} (\tilde{K}^c_i - \frac{3}{2N} (\phi - N \partial_{\phi} \phi)), \]

(9)

where \( \tilde{K}^a_i \equiv \tilde{K}^{ab}_i e^b_i \). By the symplectic structure \( 7_{\mathcal{E}} \) we obtain the following Poisson brackets:

\[ \{E^a_i(x), E^b_j(y)\} = \{\tilde{K}^a_i(x), \tilde{K}^b_j(y)\} = 0, \]

\[ \{\tilde{K}^a_i(x), E^b_j(y)\} = \delta^b_j \delta^a_i \delta(\mathbf{x}, \mathbf{y}). \]

(10)

Thus the transformation from conjugate pairs \( (h_{ab}, p^{cd}) \) to \( (E^a_i, \tilde{K}^b_j) \) is canonical. Note that since \( \tilde{K}^{ab} = \tilde{K}^{ba} \), we have an additional constraint:

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

(11)

So we can make a second canonical transformation by defining:

\[ A^a_i = \Gamma^a_i + \gamma \tilde{K}^a_i, \]

(12)

where \( \Gamma^a_i \) is the spin connection determined by \( E^a_i \) and \( \gamma \) is a nonzero real number, since the Poisson brackets among the new variables read

\[ \{A^a_i(x), E^b_j(y)\} = \gamma \delta^a_i \delta^b_j \delta(\mathbf{x}, \mathbf{y}), \]

\[ \{A^a_i(x), A^b_j(y)\} = 0. \]

(13)

Now, the phase space consists of conjugate pairs \( (A^a_i, E^b_j) \) and \( (\phi, \pi) \). Combining Eq. \( 11_{\mathcal{E}} \) with the compatibility condition: \( \partial_a E^a_i + \epsilon_{ijk} A^j_a E^{ak} = 0 \), we obtain the standard Gaussian constraint

\[ G_i = \partial_a E^a_i + \epsilon_{ijk} A^j_a E^{ak}, \]

(14)

which justifies \( A^a_i \) as an \( \mathcal{I} \mathcal{W}(2) \)-connection. Note that, 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

\[ V_a = \frac{1}{\gamma} F^a_{ab} E^b_i + \pi \partial_a \phi, \]

(15)

where \( F^a_{ab} \equiv 2 \partial_{[a} A_{b]} + \epsilon_{ijk} A^k_a A^j_b \) is the curvature of \( A^a_i \). The original Hamiltonian constraint can be written up to Gaussian constraint as

\[ H = \frac{2}{\sqrt{h}}(F^a_{ab} - C_{ijkl} E^b_i E^c_j E^d_k E^e_l) \]

\[ + \frac{1}{2} (\tilde{K}_i E^a_i)^2 + \frac{4}{3} (\tilde{K}_i E^a_i) \pi \]

\[ + \frac{2}{3} \pi^2 + \frac{3}{3 \sqrt{h}} \phi \]

\[ + \sqrt{h}(V(\phi) + \sqrt{h} D_a D^a \phi). \]

(16)

It is easy to check that the smeared Gaussian constraint, \( G(\Lambda) := \int_{\Sigma} d^3 x \Lambda^a(x) G_a(x) \), generates \( SU(2) \) gauge transformations on the phase space, while the smeared constraint \( \mathcal{V}(\tilde{N}) := \int_{\Sigma} d^3 x N^a (V_a - A^a_i G_i) \) generates spatial diffeomorphism transformations. Together with the smeared Hamiltonian constraint \( H(N) = \int_{\Sigma} d^3 x \sqrt{h} H \), the constraints algebra has the following form[12]:

\[ \{G(\Lambda), G(\Lambda')\} = G(\Lambda, \Lambda'), \]

\[ \{G(\Lambda), \mathcal{V}(\tilde{N})\} = -\mathcal{V}(\mathcal{L}_\Lambda \Lambda), \]

\[ \{G(\Lambda), H(N)\} = 0, \]

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

\[ \{\mathcal{V}(\tilde{N}), H(M)\} = \mathcal{H}(\mathcal{L}_\Lambda M), \]

\[ \{H(N), H(M)\} = \mathcal{V}(N^a M - MD^a N). \]

(17)
Hence the constraints are of first class. The total Hamiltonian is a linear combination of constraints as
\[ H = \int_{\Sigma} H(N) + V(\vec{N}) + g(\Lambda). \] (18)

To summarize, \( f(R) \) theories of gravity have been cast into the \( \mathcal{W}(2) \)-connection dynamical formalism. Though a scalar field is non-minimally coupled, the resulted Hamiltonian structure is similar to GR. Note that what we obtain is real \( \mathcal{W}(2) \)-connection dynamics of \( f(R) \) gravity rather than complex connection dynamics of some conformal theories.[13]

Now the non-perturbative loop quantization procedure can be straightforwardly extended to \( f(R) \) theories. Since the configuration space consists of geometry sector and scalar sector, we expect the kinematical Hilbert space of the system to be a direct product of the Hilbert space of geometry and that of scalar field. To construct quantum kinematics for geometry as in LQG, we have to extend the space \( \mathcal{A} \) of smooth connections to space \( \mathcal{A} \) of distributional connections. A simple element \( A \in \mathcal{A} \) may be thought as a holonomy, \( h_c(A) = \mathcal{P} \exp{\int A} \), of a connection along an edge \( e \subset \Sigma \). Through projective techniques, \( \mathcal{A} \) is equipped with a natural measure \( \mu_o \), called the Ashtekar-Lewandowski measure.[3, 4]. In a certain sense, this measure is the unique diffeomorphism and internal gauge invariant measure on \( \mathcal{A} \). The kinematic Hilbert space of geometry then reads \( H_{\text{kin}}^{gr} = L^2(\mathcal{A}, d\mu_0) \). A typical vector \( \Psi_\alpha(A) \in H_{\text{kin}}^{gr} \) is a cylindrical function over some finite graph \( \alpha \subset \Sigma \). The so-called spin-network basis \( T_\alpha(A) \equiv T_{\alpha,j,m,n}(A) \) provides an orthonormal basis for \( H_{\text{kin}}^{gr} \).[3, 4]. Note that the spatial geometric operators of LQG, such as the area, the volume and the length operators[14] are still valid here. Since the scalar field also reflects \( f(R) \) gravity, it is natural to employ the polymer-like representation for it’s quantization.[15, 16] In this representation, one extends the space \( \mathcal{W} \) of smooth scalar fields to the quantum configuration space \( \mathcal{W} \). A simple element \( U \in \mathcal{W} \) may be thought as a point holonomy, \( U_\lambda = \exp(\mathbf{i} \lambda \phi(x)) \), at point \( x \in \Sigma \), where \( \lambda \) is a real number. By GNS structure,[2] there is a natural diffeomorphism invariant measure \( d\mu \) on \( \mathcal{W} \).[15]. Thus the kinematical Hilbert space of scalar field reads \( H_{\text{kin}}^{sc} = L^2(\mathcal{W}, d\mu) \). The following scalar-network functions of \( \phi \),
\[ T_X(\phi) \equiv T_X(\lambda)(\phi(x)) = \prod_{x_j \in X} U_{\lambda,j}(\phi(x_j)) \] (19)
where \( X = \{x_1, \ldots, x_n\} \) is an arbitrary given set of finite number of points in \( \Sigma \), constitute an orthonormal basis in \( H_{\text{kin}}^{sc} \). Thus the total kinematical Hilbert space for \( f(R) \) gravity reads \( H_{\text{kin}} = H_{\text{kin}}^{sc} \otimes H_{\text{kin}}^{gr} \), with an orthonormal basis \( T_{\alpha,X}(A, \phi) \equiv T_{\alpha,j}(A) \otimes T_X(\phi) \). A basic feature of loop quantization is that only holonomies will become configuration operators, rather than the classical configuration variables themselves. Since the holonomy of a connection is smeared over an 1-dimensional curve, the conjugate densitized triad is smeared over 2-surfaces as \( E(S, f) := \int_S \epsilon_{abc} E^a_i f^i \), where \( f^i \) is a \( \mathcal{W}(2) \)-valued function on \( S \). Since the point holonomy of a scalar is defined on an 0-dimensional point, the momentum is smeared on 3-dimensional regions \( R \in \Sigma \) as \( \pi(R) := \int_R d^3x \pi(x) \). Let \( \Psi(A, \phi) \) denote a quantum state in \( H_{\text{kin}} \). Then the actions of basic operators read
\[ \tilde{h}_c(A) \Psi(A, \phi) = h_c(A) \Psi(A, \phi), \]
\[ \hat{E}(S, f) \Psi(A, \phi) = i\hbar \{E(S, f), \Psi(A, \phi)\}, \]
\[ \hat{U}_\lambda(\phi(x)) \Psi(A, \phi) = \exp(i \lambda \phi(x)) \Psi(A, \phi), \]
\[ \hat{\pi}(R) \Psi(A, \phi) = i\hbar (\pi(R), \Psi(A, \phi)). \] (20)

As in LQG, it is straightforward to promote the Gaussian constraint \( g(\Lambda) \) to a well-defined operator in \( H_{\text{kin}}^{gr} \). It’s kernel is the internal gauge invariant Hilbert space \( H_G \) with gauge invariant spin-network basis as well. Since the diffeomorphisms of \( \Sigma \) act covariantly on the cylindrical functions in \( H_G \), the so-called group averaging technique can be employed to solve the diffeomorphism constraint[3, 4]. Thus we can also obtain the desired diffeomorphism and gauge invariant Hilbert space \( H_{\text{Diff}} \) for \( f(R) \) gravity.

The nontrivial task is to implement the Hamiltonian constraint \( H(N) \) at quantum level. As in LQG, we can show by detail and technical analysis that the Hamiltonian constraint can be promoted to a well-defined operator in \( H_{\text{kin}}^{gr} \). The resulted Hamiltonian constraint operator is internal gauge invariant and diffeomorphism covariant. Hence it is at least also well defined in \( H_G \). Comparing Eq.(19) with the Hamiltonian constraint of GR in connection formalism[2], the new ingredients of \( f(R) \) gravity that we have to deal with are \( \phi(x), \phi^{-1}(x), V(\phi) \) and the following four terms
\[ H_3 = \int_{\Sigma} d^3x N \frac{\sqrt{\hat{K}_a^i E^a_i}}{3\hbar}, \]
\[ H_4 = \int_{\Sigma} d^3x \frac{2N \sqrt{\hat{K}_a^i E^a_i}}{3\hbar} \pi, \]
\[ H_6 = \int_{\Sigma} d^3x \frac{N \pi^2 \phi}{3\hbar}, \]
\[ H_7 = \int_{\Sigma} d^3x N \sqrt{\hat{K}} D_a D^a \phi. \] (21)

By introducing certain small constant \( \lambda_0 \), an operator corresponding to the scalar \( \phi(x) \) can be defined as
\[ \tilde{\phi}(x) = \frac{1}{2i\lambda_0}(U_{\lambda_0}(\phi(x)) - U_{-\lambda_0}(\phi(x))). \] (22)

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
\[ \phi^{-1}(x) = \left( \frac{1}{\hbar} (\hat{\phi}(x), \pi(R)) \right)^{-\pi_\lambda}, \] (23)
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

$$\hat{\phi}^{-1}(x) = \left(\frac{2}{i\hbar}[\sqrt{\hat{\phi}(x)}, \hat{\pi}(R)]\right)^2. \quad (24)$$

Similar tricks can be employed to deal with the function $V(\phi)$, provided that it can be expanded as powers of $\phi(x)$. Moreover, by the regularization techniques developed for the Hamiltonian constraint operators of LQG and polymer-like scalar field, all the terms $H_3, H_4, H_6$ and $H_7$ can be quantized as operators acting on cylindrical functions in $\mathcal{H}_{\text{kin}}$ in state-dependent ways. For example, the operator corresponding to $H_3$ acts on a basis vector as

$$\hat{H}_4 \cdot T_{\alpha,X} = \sum_{v \in V(\alpha)} 2^{14} N(v) \frac{\pi_v}{\sqrt{\hbar}} \hat{h}_{s_L(v)}(\hat{h}_{s_L(v)}, \hat{V}_v)^{3/4}$$

$$\times e^{LMN} \text{Tr}(\hat{h}_{s_M(v), \hat{h}_{s_N(v)}} (\hat{V}_v)^{3/4})$$

$$\times \hat{h}_{s_N(v)}(\hat{h}_{s_N(v)}, \hat{V}_v)^{3/4})$$

$$\times e^{JK} \text{Tr}(\hat{h}_{s_J(v), \hat{h}_{s_K(v)}} (\hat{V}_v)^{1/2})$$

$$\times \hat{h}_{s_K(v)}(\hat{h}_{s_K(v)}, \hat{V}_v)^{1/2}) \cdot T_{\alpha,X} \quad (25)$$

where the coefficient $C(v)$ comes from the triangulation ambiguity, and $h_{s_L(v)}$ denotes the holonomy along the segment $s_L$ starting from the vertex $v$ of graph $\alpha$. Note that the action of the volume operator $\hat{V}$ on $T_{\alpha}(A)$ over a graph $\alpha$ can be factorized as $\hat{V} \cdot T_{\alpha} = \sum_{v \in V(\alpha)} \hat{V}_v \cdot T_{\alpha}$. The action of the operator $\pi(R)$ on $T_X(\phi)$ over a graph $X$ can also be factorized as $\pi(R) \cdot T_X = \sum_{x \in X(\mathcal{R})} \hat{\pi}_x \cdot T_X$. It is easy to see from Eq. (25) that the action of $H_4$ on $T_{\alpha,X}$ is graph changing. It adds a finite number of vertices within the edges $e(t)$ starting from each high-valence vertex of $\alpha$. By similar ways, the whole Hamiltonian constraint can be quantized as a well-defined operator $\hat{H}$, which is internal gauge invariant and diffeomorphism covariant. Although $\hat{H}$ 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 in $\mathcal{H}_{\text{Diff}}$. One way out is to employ the master constraint program. By using the structure of $\hat{H}$, we can define also a corresponding master constraint operator in $\mathcal{H}_{\text{Diff}}$. Then it is very possible to solve all the quantum constraints and obtain some physical Hilbert space with observables in it.

We summarize with a few remarks. (i) The connection dynamics of $f(R)$ gravity have been obtained by canonical transformations from it’s geometric dynamics. It is still desirable to find an action for the connection dynamics. (ii) Due to the $\mathcal{G}\mathcal{W}(2)$-connection dynamical formalism, the metric $f(R)$ theories have been successfully quantized by extending LQG scheme. Thus, the non-perturbative loop quantization procedure is not only valid for GR but also valid for a rather general class of 4-dimensional metric theories of gravity. (iii) Classically the scalar fields $\phi$ characterize different $f(R)$ theories of gravity by $f = f'(R)$. Thus for a given $f(R)$ theory, $\phi$ will become a particular function of $R$ while the potential $V(\phi)$ is fixed. Hence our quantum $f(R)$ gravity may be understood as a class of quantum theories representing different choices of the function $f(R)$. However, the other possible and appealing interpretation remains. We may just think different classical $f(R)$ theories as emerging from different classical limits of the quantum observables $\hat{\phi}$ and $\hat{R}$. The latter understanding provides an enlightening mechanism to produce chameleon $f(R)$ theories from one fundamental quantum gravity theory, which might be significant to understand our universe.

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Extension of loop quantum gravity to $f(R)$ theories

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In recent twenty-five 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$^{[5]}$. 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)$$^{[6,7]}$. Thus it is interesting to see whether GR is a unique relativistic theory with the connection-dynamical character. Especially, modified gravity theories have received increasingly attention recently due to motivations coming from cosmology and astrophysics. A series of independent observations, including type Ia supernova, weak lens, cosmic microwave background anisotropy, baryon oscillation, etc, implied that our universe is currently undergoing a period of accelerated expansion$^{[8]}$. This result conflicts with the prediction of GR and has carried the "dark energy" problem. Hence it is reasonable to consider the possibility that GR is not a valid theory of gravity on a cosmological scale. A large variety of models of $f(R)$ modified gravity have been proposed to account for the cosmic acceleration$^{[9]}$. Some models of $f(R)$ gravity may also account for the "dark matter" problem, which was revealed by the observed rotation curve of galaxy clusters$^{[10]}$. Given the strong motivations to $f(R)$ gravity, it is desirable to study such kind of theories at fundamental quantum level. For metric $f(R)$ theories, gravity is still geometry as GR. The differences between them are just reflected in dynamical equations. Hence, a background-independent and non-perturbative quantization for $f(R)$ gravity is preferable.

In contrast to the initial Wheeler-DeWitt canonical quantization of GR, the classical algebra that one wants to represent on the Hilbert space of LQG is based on the holonomies of the gravitational connection. Physically, holonomies are natural variables representing Faraday’s "lines of force", that do not refer to what happens at a point, but rather refer to the relation between different points connected by a line. Mathematically, the quantum configuration space of LQG and the Hilbert space on it can be constructed by the concept of holonomy, since its definition does not depend on an extra background. In this letter, we derive the connection-dynamical formulation of $f(R)$ gravity by canonical transformations from its geometrical dynamics. The latter was realized by introducing a non-minimally coupled scalar field to replace the original $f(R)$ action and then doing Hamiltonian analysis. While the equivalence by canonical transformations at the classical level does not imply equivalence after quantization, our choice of the canonical formalism enables us to carry on the above physical and mathematical ideas of LQG. The canonical variables of our Hamiltonian formalism of $f(R)$ gravity consist of $\mathcal{A}^{\pm}_{\pm}(2)$-connection $A_{\pm}^{\pm}$ and it’s conjugate momentum $E_{\pm}^{\pm}$, as well as the scalar field $\phi$ and it’s momentum $\pi$. The Gaussian, diffeomorphism and Hamiltonian constraints are also obtained, and they comprise a first-class system. Loop quantization procedure is then naturally employed to quantize $f(R)$ gravity. The rigorous kinematical Hilbert space structure of LQG is extended to loop quantum $f(R)$ gravity by adding a polymer-like quantum scalar field. The Hamiltonian constraint can be promoted to a well-defined operator. We use Greek alphabet for spacetime in indices, Latin alphabet $a, b, c, ...$ for spatial indices and $i, j, k, ...$ for internal indices.

The original action of $f(R)$ theories reads:

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

(1)

where $f$ is a general function of $R$, and we set $8\pi G = 1$. By introducing an independent variable $s$ and a Lagrange multiplier $\phi$, an equivalent action is proposed as$^{[10,11]}$:

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

(2)

The variation of (2) with respect to $s$ yields $\phi = df(s)/ds \equiv f'(s)$. Assuming $s$ could be resolved from the above equation, action (2) is reduced to

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

(3)

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where $V(\phi) \equiv \phi s - f(s)$. It is easy to see that the variabilities of (3) give the equations of motion equivalent to that from action (1). The virtue of (3) is that it admits a treatable Hamiltonian analysis (10). By doing 3+1 decomposition and Legendre transformation:

$$p^a = \frac{\partial L}{\partial \dot{h}_{ab}} = \frac{\sqrt{h}}{2}[\phi(K_{ab} - Kh^{ab}) - \frac{\dot{h}_{ab}}{N}(\phi - N^c \partial_c \phi)],$$

$$\pi = \frac{\partial L}{\partial \dot{\phi}} = -\sqrt{h} K,$$  

where $h_{ab}$ and $K_{ab}$ are the induced 3-metric and the extrinsic curvature of the spatial hypersurface $\Sigma$ respectively, and $K \equiv K_{ab}^a$, the Hamiltonian of $f(R)$ gravity can be derived as a linear combination of constraints as $H_{\text{total}} = \int_\Sigma N^a V_a + NH$, where $N$ and $N^a$ are the lapse function and shift vector respectively, and the diffeomorphism and Hamiltonian constraints read

$$V_a = -2D^a(p_{ab}) + \pi \partial_a \phi,$$  

$$H = \frac{2}{\sqrt{h}}(p_{ab}p^{ab} - \frac{1}{3} \pi^2) + \frac{1}{6} \phi \pi^2 - \frac{1}{3}p^a \pi + \frac{1}{2} \sqrt{h} (V(\phi) - \phi R + 2D_a D^a \phi).$$

The symplectic structure is given by

$$\{h_{ab}(x), p^{cd}(y)\} = \delta^{(c} \delta^{d)} \delta^3(x, y),$$

$$\{\phi(x), \pi(y)\} = \delta^3(x, y).$$  

Straightforward calculations show that the constraints (5) and (6) comprise a first-class system similar to GR (11). Although the above Hamiltonian analysis is started with the action (3) where a non-minimally coupled scalar field is introduced, one can check that the resulted Hamiltonian formalism is equivalent to the Lagrangian formalism (12). Recall that the non-perturbative loop quantization of GR was based on it’s connection-dynamic formalism. To study whether the previous geometric dynamics of $f(R)$ modified gravity also has a connection-dynamic correspondence, we first introduce the following canonical transformation on the phase space of $f(R)$ theories. Let

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

and $E_{i}^a \equiv \sqrt{h}e_{i}^a$ where $e_{i}^a$ is the triad s.t. $h_{ab}e_{i}^a e_{j}^b = \delta_{ij}$. Then we get

$$p^{ab} = \frac{1}{2}(\tilde{K}^{ai} E_a^i - \frac{1}{h} \tilde{K}_a^b E_i^a E_j^b),$$

$$\pi = -\sqrt{h}(\tilde{K}^c_e - \frac{3}{2N}(\phi - N^c \partial_c \phi)),$$

where $\tilde{K}^a_c \equiv \tilde{K}^{ab} e_b^a$. By the symplectic structure (7) we obtain the following Poisson brackets:

$$\{E_{i}^a(x), E_j^b(y)\} = \{\tilde{K}_i^a(x), \tilde{K}_j^b(y)\} = 0,$$

$$\{\tilde{K}_i^a(x), E_j^b(y)\} = \delta_{i}^b \delta_j^a \delta(x, y).$$

Thus the transformation from conjugate pairs $(h_{ab}, p^{cd})$ to $(E_{i}^a, \tilde{K}^{ab})$ is canonical. Note that since $\tilde{K}^{ab} = \tilde{K}^{ba}$, we have an additional constraint:

$$G_{jk} \equiv \tilde{K}_{a[j} E_{k]}^a = 0.$$  

For a second canonical transformation we define

$$A_{i}^a = \Gamma_{a}^i + \gamma \tilde{K}_i^a,$$  

where $\Gamma_a^i$ is the spin connection determined by $E_i^a$ and $\gamma$ is a nonzero real number. Then the Poisson brackets among the new variables read

$$\{A_{i}^a(x), E_{j}^b(y)\} = \gamma \delta_{i}^a \delta_j^b \delta(x, y),$$

$$\{A_{i}^a(x), A_{j}^b(y)\} = 0.$$  

Now, the phase space consists of conjugate pairs $(A_{i}^a, E_{i}^a)$ and $(\phi, \pi)$. Combining Eq.(11) with the compatibility condition: $\partial_a E_i^a + \epsilon_{ijk} \Gamma_a^j E^a_k = 0$, we obtain the standard Gaussian constraint

$$G_{i} = \partial_a E_{i}^a = \partial_a E_{i}^a + \epsilon_{ijk} \Gamma_a^j E^a_k,$$

which justifies $A_{i}^a$ as an $SU(2)$-connection. Note that, had we let $\gamma = \pm i$, the (anti-)self-dual connection formalism would be obtained. The original diffeomorphism constraint can be expressed in terms of new variables up to Gaussian constraint as

$$V_a = \frac{1}{\gamma} F_{ab} A_i^b + \pi \partial_a \phi,$$

where $F_{ab}^a \equiv 2\partial_a A^a_0 + \epsilon_{ijk} A^a_i A^b_j$ is the curvature of $A^a_i$. The original Hamiltonian constraint can be written up to Gaussian constraint as

$$H = \frac{\phi}{2} [F_{ab}^a - (\gamma^2 + \frac{1}{3} \gamma) \epsilon_{i}^{jmn} K^m_a K^n_b E_i^a E_j^b] \frac{\sqrt{h}}{\sqrt{h}} E_i^a E_j^b$$

$$+ \frac{1}{2} \frac{2}{3} \epsilon_{i}^{jmn} \frac{4}{3} \frac{\frac{4}{3} K^a_i E_i^a \pi}{\sqrt{h}} + \frac{2}{3} \frac{\frac{2}{3} \phi}{\sqrt{h}} + \frac{1}{2} \frac{2}{3} \phi \frac{\frac{4}{3} \sqrt{h}}{\sqrt{h}} + \sqrt{h} V(\phi) + \sqrt{h} D_a D^a \phi.$$

It is easy to check that the smeared Gaussian constraint, $G(\Lambda) := \int_\Sigma d^3 x \Lambda_i(x) G_i(x)$, generates $SU(2)$ gauge transformations on the phase space, while the smeared constraint $\mathcal{V}(\tilde{N}) := \int_\Sigma d^3 x N^a (V_a - A^a_0 G_0)$ generates spatial diffeomorphism transformations. Together with the smeared Hamiltonian constraint $H(N) = \int_\Sigma d^3 x N H$, the constraints algebra has the following form (12):

$$\{G(\Lambda), G(\Lambda')\} = G(\Lambda, \Lambda'),$$

$$\{G(\Lambda), \mathcal{V}(\tilde{N})\} = -G(\mathcal{L} \tilde{N}, \Lambda),$$

$$\{G(\Lambda), H(N)\} = 0,$$

$$\{\mathcal{V}(\tilde{N}), \mathcal{V}(\tilde{N}')\} = \mathcal{V}(\tilde{N}, \tilde{N}'),$$

$$\{\mathcal{V}(\tilde{N}), H(M)\} = H(\mathcal{L} \tilde{N}, M),$$

$$\{H(N), H(M)\} = \mathcal{V}(ND^a M - MD^a N).$$  

Hence the constraints are of first class. The total Hamiltonian is a linear combination: $\mathcal{H} \equiv \int_{\Sigma} H(N) + \mathcal{V}(\bar{N}) + G(\Lambda)$. To summarize, $f(\mathcal{R})$ theories of gravity have been cast into the $\mathcal{S}\mathcal{W}(2)$-connection dynamical formalism. Though a scalar field is non-minimally coupled, the re

cast into the $\mathcal{H}$ of distributional connections. A simple element $\bar{\lambda}$ quantum kinematics for geometry as in LQG, we have to extend the space $\mathcal{A}$ of smooth connections to space $\mathcal{A}$ of distributional connections. A simple element $\bar{A} \in \mathcal{A}$ may be thought as a holonomy, $\bar{h}(\bar{A}) = \mathcal{P} \exp \int A_{e}$, of a connection along an edge $e \subset \Sigma$. Through projective techniques, $\mathcal{A}$ provides an orthonormal basis for $\mathcal{H}_{\text{kin}}$. In a certain sense, this measure is the unique diffeomorphism and internal gauge invariant measure on $\mathcal{A}$. The kinematical Hilbert space of geometry then reads $\mathcal{H}_{\text{kin}}^{gr} = L^{2}(\mathcal{A}, d\mu_{0})$. A typical vector $\Psi_{\alpha}(A) \in \mathcal{H}_{\text{kin}}^{gr}$ is a cylindrical function over some finite graph $\alpha \subset \Sigma$. The so-called spin-network basis $T_{\alpha}(A) \equiv T_{\alpha,j,m,n}(\bar{A})$ provides an orthonormal basis for $\mathcal{H}_{\text{kin}}^{gr}$. Note that the spatial geometric operators of LQG, such as the area, the volume and the length operators are still valid here. Since the scalar field also reflects $f(\mathcal{R})$ gravity, it is natural to employ the polymer-like representation for it’s quantization. In this representation, one extends the space $\mathcal{U}$ of smooth scalar fields to the quantum configuration space $\mathcal{U}$. A simple element $U \in \mathcal{U}$ 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 $\mathcal{U}$. Thus the kinematical Hilbert space of scalar field reads $\mathcal{H}_{\text{kin}}^{sc} = L^{2}(\mathcal{U}, d\mu)$. The scalar-network functions $T_{X}(\phi) \equiv \prod_{x_{j} \in X} U_{\lambda_{j}}(\phi(x_{j}))$, where $X = \{x_{1}, \ldots, x_{n}\}$ is an arbitrary given set of finite points of $\Sigma$, constitute an orthonormal basis in $\mathcal{H}_{\text{kin}}^{sc}$. Thus the total kinematical Hilbert space for $f(\mathcal{R})$ gravity reads $\mathcal{H}_{\text{kin}} = \mathcal{H}_{\text{kin}}^{gr} \otimes \mathcal{H}_{\text{kin}}^{sc}$ with an orthonormal basis $T_{\alpha,X}(A, \phi) \equiv T_{\alpha}(A) \otimes T_{X}(\phi)$. A basic feature of loop quantization is that only holonomies will become configuration operators, rather than the classical configuration variables themselves. Since the holonomy of a connection is smeared over an 1-dimensional curve, the conjugate densitized triad is smeared over 2-surfaces as $E(S, f) := \int_{S} b_{ab} E_{a} f^{b}$, where $f^{b}$ is a $\mathcal{S}\mathcal{W}(2)$-valued function on $S$. Since the point holonomy of a scalar is defined on an 0-dimensional point, the momentum is smeared on 3-dimensional regions $R$ in $\Sigma$ as $\pi(R) := \int_{R} d^{3}x \pi(x)$. Let $\Psi(A, \phi)$ denote a quantum state in $\mathcal{H}_{\text{kin}}$. Then the actions of basic operators read

$$
\begin{align*}
\hat{h}_{e}(A)\Psi(A, \phi) &= \hat{h}_{e}(A)\Psi(A, \phi), \\
\hat{E}(S, f)\Psi(A, \phi) &= \hat{h}(E(S, f), \Psi(A, \phi)), \\
\hat{U}_{\lambda}(\phi(x))\Psi(A, \phi) &= \exp(i\lambda\phi(x))\Psi(A, \phi), \\
\hat{\pi}(R)\Psi(A, \phi) &= \hat{h}(\pi(R), \Psi(A, \phi)).
\end{align*}
$$

As in LQG, it is straightforward to promote the Gaussian constraint $G(\Lambda)$ to a well-defined operator. It’s kernel is the internal gauge invariant Hilbert space $\mathcal{H}_{G}$ with gauge invariant spin-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. Thus we can also obtain the desired diffeomorphism and gauge invariant Hilbert space $\mathcal{H}_{\text{Diff}}$ for $f(\mathcal{R})$ gravity. The nontrivial task is to implement the Hamiltonian constraint $H(N)$ at quantum level. As in LQG, we can show by detail and technical analysis that the Hamiltonian constraint can be promoted to a well-defined operator in $\mathcal{H}_{\text{kin}}$. The resulted Hamiltonian constraint operator is internal gauge invariant and diffeomorphism covariant. Hence it is at least also well defined in $\mathcal{H}_{G}$. Comparing Eq. (15) with the Hamiltonian constraint of GR in connection formalism, the new ingredients of $f(\mathcal{R})$ gravity that we have to deal with are $\phi(x), \phi^{-1}(x), V(\phi)$ and the following four terms

$$
\begin{align*}
H_{3} &= \int_{\Sigma} d^{3}x \frac{N}{3} \left( \frac{\sqrt{g}}{\hbar} \right)^{2}, \\
H_{4} &= \int_{\Sigma} d^{3}x \frac{2N}{3} \left( \frac{\sqrt{g}}{\hbar} \right)^{2}, \\
H_{6} &= \int_{\Sigma} d^{3}x \frac{\pi^{2} \phi}{3 \hbar}, \\
H_{7} &= \int_{\Sigma} d^{3}x N \sqrt{\hbar} D_{\alpha} D_{\alpha} \phi.
\end{align*}
$$

By introducing certain small constant $\lambda_{0}$, an operator corresponding to the scalar $\phi(x)$ can be defined as

$$
\hat{\phi}(x) = \frac{1}{2\ii \lambda_{0}} (U_{\lambda_{0}}(\phi(x)) - U_{-\lambda_{0}}(\phi(x))).
$$

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

$$
\phi^{-1}(x) = (\frac{1}{2\ii} \{ \phi(x), \pi(R) \})^{\perp},
$$

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

$$
\hat{\phi}^{-1}(x) = (\frac{2}{\ii \hbar} [\sqrt{\phi(x)}, \hat{\pi}(R)])^{2}.
$$
Thus all the functions $V(\phi)$ which can be expanded as powers of $\phi(x)$ have been quantized. For other non-trivial types of $V(\phi)$, we may replace the argument $\phi$ by $\phi$ in Eq. (20), 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. (21) to deal with it. Hence it is reasonable to believe that most physically interesting functions $V(\phi)$ can be quantized. Moreover, by the regularization techniques developed for the Hamiltonian constraint operators of LQG [2] and polymer-like scalar field [16], all the techniques developed for the Hamiltonian constraint operator $H_{\text{kin}}$ in state-dependent ways [12]. For example, the operator corresponding to $H_4$ acts on a basis vector as

$$\hat{H}_4 \cdot T_{\alpha,\chi} = - \sum_{v \in v(\alpha)} \frac{2^{16} N(v)}{3^4 \gamma_6 (\hbar)^6} C(v) \hat{\pi}_v \times \text{Tr} (\tau_i \hat{h}_{s_L(v)}^{-1} [\hat{h}_{s_L(v)}, \hat{K}]) \times e^{6 \alpha \nu} \text{Tr} (\tau_i \hat{h}_{s_M(v)}^{-1} [\hat{h}_{s_M(v)}, (\hat{V}_v)^{3/4}]) \times \hat{h}_{s_N(v)}^{-1} [\hat{h}_{s_N(v)}, (\hat{V}_v)^{3/4}]) \times e^{12 \kappa} \text{Tr} (\hat{h}_{s_R(v)}^{-1} [\hat{h}_{s_R(v)}, (\hat{V}_v)^{1/2}]) \times \hat{h}_{s_s(v)}^{-1} [\hat{h}_{s_s(v)}, (\hat{V}_v)^{1/2}]) \cdot T_{\alpha,\chi}$$

(23)

where the coefficient $C(v)$ comes from the triangulation ambiguity, and $h_{s_f(v)}$ denotes the holonomy along the segment $s_f$ starting from the vertex $v$ of graph $\alpha$. By similar ways, the whole Hamiltonian constraint can be quantized as a well-defined operator $\hat{H}$, which is internal gauge invariant and diffeomorphism covariant. Although $\hat{H}$ 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 in $H_{\text{Diff}}$. One way out is to employ the master constraint program [17, 18]. By using the structure of $\hat{H}$, we can define also a corresponding master constraint operator in $H_{\text{Diff}}$ [12].

We summarize with a few remarks. (i) The connection dynamics of $f(R)$ gravity has been obtained by canonical transformations from it’s geometric dynamics. It is still desirable to find an action for the connection dynamics. (ii) Due to the $\mathcal{W}(2)$-connection dynamical formalism, the metric $f(R)$ theories have been successfully quantized by extending LQG scheme. Thus, the non-perturbative loop quantization procedure is not only valid for GR but also valid for a rather general class of 4-dimensional metric theories of gravity. The important physical result that both the area and the volume are discrete remains valid for quantum $f(R)$ gravity. (iii) Classically the scalar fields $\phi$ characterize different $f(R)$ theories of gravity by $f = f(R)$. Thus for a given $f(R)$ theory, $\phi$ may become a particular function of $R$ while the potential $V(\phi)$ is fixed. Hence our quantum $f(R)$ gravity may be understood as a class of quantum theories representing different choices of the function $f(R)$. (iv) It is also desirable to quantize $f(R)$ theories by the covariant spin foam approach. Besides trying to quantize an original $f(R)$ action directly by the spin foam techniques, one may also try to start with the action (20). The ideas in Ref. [16], where a 3-dimensional spin foam model with a non-minimally coupled scalar field was studied, may provide some insights to construct the $f(R)$ spinfoams.

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