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A note on quantum cosmology through canonical quantization

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Abstract: In spite of huge successes, Einstein's "General theory of Relativity" is plagued with unavoidable singularity. It can not describe the phenomena near and beyond the 'Planck era'. The Planck Era is the very early phase of the universe, lasting from the moment of the Big Bang until approximately 10^{-43} seconds (Planck time). During this extremely hot and compressed situation, the four fundamental forces, (i.e., gravity, strong nuclear, weak nuclear, and electromagnetic) were unified into a single force. To bypass this problem a suitable 'Quantum theory of gravity' is crucial. Despite repeated attempts, full quantum theory of gravity is still far away. At this point, 'Quantum Cosmology' was used, to explore physical insight near and beyond Planck era to some extent. Canonical quantization of gravitational action is one such way to study quantum cosmology. In this article I have discussed this technique and recent advancement in this field.

Keywords: GTR, ADM Formulation, Wheeler-DeWitt Equation, Canonical Quantization

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1. Introduction

One of the well-known discoveries of 20-th century physics, is the 'General Theory of Relativity' (GTR). In 1915, Einstein replaced Newtonian theory of gravitation by the famous GTR, where space and time are dynamical quantities, being shaped by the energy-momentum tensor of the surrounding. GTR is described by the following tensorial field equation (Weinberg, 1972; Misner, 1973)

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 8\pi GT_{\mu\nu} \quad (1)$$

Left part of Equation (1) is called 'Einstein tensor' ($G_{\mu\nu}$) which consists of 'Ricci Tensor' ($R_{\mu\nu}$), 'Ricci scalar' (R) and 'metric tensor' ($g_{\mu\nu}$). The right-hand side of equation (1) consists of energy-momentum tensor of any sort of matter field ($T_{\mu\nu}$), while G is the Newtonian gravitational constant. Here each Greek subscript run from 0 to 3. "0" represents the time part while 1, 2 and 3 represents the spatial part. As stated by Wheeler, the equation of GTR implies "space-time tells matter how to move and matter tells space-time how to curve".

GTR drew attention immediately, because it not only reproduced known observed results, but also predicted lot of new phenomena like bending of light, expansion of the universe, gravitational waves, existence of black holes, gravitational lensing, gravitational time dilation etc.(Dyson, 1920; Pound et al., 1959; Abbott et al., 2016).Further, based on idea of the expanding universe(instead of being static or stationary) following Hubble's discovery (Hubble, 1929), a model of the universe coined using GTR by the name 'Standard Model of Cosmology' which successfully predicts some astrophysical observations having cosmological importance, such as CMBR (Friedmann, 1922; Penzias, 1965). Again, phenomena like nucleosynthesis have been completely understood using standard model. This also estimates the amount of baryonic matter present in the universe (Dodelson, 2003). All these successes established this new theory on a firm footing.

Nevertheless, standard model suffers from an incurable disease, and that is the issue of unavoidable singularity problem (Carroll, 2004). 'General Theory of Relativity' (GTR) is plagued with unavoidable 'singularity'. To circumvent this problem one requires 'Quantum Theory of Gravity' near and beyond Planck era. As, GTR is non-renormalizable (Zumino, 1970; 't Hooft, 1973; 't Hooft, 1974; Deser, 1974), higher-order curvature invariant terms can be included in the Einstein-Hilbert (EH) action to make the theory renormalizable. However, in this case, unitarity is lost (Stelle, 1977).

It was realized that GTR should be treated as weak field approximation of a more general theory (super-gravity, super-string etc.)(Yahalom, 2023). However, successive trials to construct a viable quantum theory of gravity are still in vain (Rovelli, 2000). Under such circumstances, 'Quantum Cosmology'(QC) was invoked to get an insight near and beyond Planck era (Arnowitt, et al., 1962; Padmanabhan, 2004). In Quantum cosmology, ideas of quantum mechanics are applied to

the entire universe, especially its earliest moments. It seeks to answer fundamental questions about the universe's origin, such as the Big Bang singularity, by treating the universe as a single system described by a wave function(Bojowald, 2015;Gielen, 2025).

There are many routes to study quantum cosmology, such as, loop quantum cosmology(Agullo, et al., 2017), loop quantum gravity(Rovelli, 1998; Ashtekar, et al., 2021), string theory(Mukhi, 2011) and causal set theory (Surya, 2019).Another route is canonical quantization of classical theory (Kuchař, 1973; DeWitt, 1967; Witten, 2023). Here, I shall discuss this topic with a detail literature review.Canonical formulation of GTR was first done by Arnowitt, Dese and Mesner (Arnowitt, et al., 1962). It is known as ADM formulation of GTR. In the following chapter, I have discussed properties of Einstein's field equation to find out the canonical variables. This is the first step of ADM formulation of GTR. Throughout this paper, Greek letters used as subscripts and superscripts indicates 0,1,2,3, i.e. 4-dimensions and Latin letters used as subscripts and superscripts indicates 1,2,3, i.e. 3- dimensional hyper surface.

2. Characteristics of Einstein's Equation on GTR

Einstein's equation of gravity is the simplest geometrical theory of gravitation. It may be retrieved from an action containing the simplest curvature invariant term R (The Ricci scalar) and supplemented by the Gibbons-Hawking-York (GHY) boundary term. The action named by Einstein-Hilbert (EH) action is expressed as (Hilbert, 1924; Poisson, 2004),

$$A = \int_{\mathcal{V}} \sqrt{-g} \left(\frac{R}{2\kappa} + \mathcal{L}_m \right) d^4x + \Sigma_R \quad (2)$$

Where, $\kappa = 8\pi G$ and \mathcal{L}_m is the Lagrangian density for any sort of matter fields, as well as barotropic fluids, \mathcal{V} is a hyper-volume in 4-dimensional space-time \mathcal{M} , and Σ_R is the GHY boundary term having the following form(York,1972; Gibbons,1977)

$$\Sigma_R = \frac{1}{\kappa} \oint_{\partial\mathcal{V}} K \sqrt{h} d^3x \quad (3)$$

In the above, $\partial\mathcal{V}$ is the boundary of the region enclosed by \mathcal{V} . In the above equation, h and K are called traces of the 'induced metric' and the 'extrinsic curvature tensor' respectively. These two parameters play an important role in the literature. I shall discuss about them in the next chapter.

The Einstein's field equations (1) may be reduced from equation (2) using metric ($g_{\mu\nu}$) variation technique, as well as with variations of the lapse function (N) and the shift vector (N_i). It has been observed that four of these equations obtained under the variations of N and N_i do not contain second derivatives. Therefore, these are the constraints of the theory, while N and N_i act as Lagrange multipliers. These four equations appear due to re-parametrization and diffeomorphic invariance of the theory, which are artifact of general covariance, one of the building blocks of GTR. These constraints may be identified as the 'Hamiltonian constraint' and the 'momentum constraints' respectively, under 3 + 1 decomposition. Einstein's field equation (1) shows the following characteristics:

- The space-time, as well as, the time-time parts of equation (1) involve \dot{g}_{ij} as the highest order time derivatives only.
- The space-space part of equation (1) contains \dot{g}_{ij} .
- Time derivatives of the parameters, g_{0i} and g_{00} do not appear in equation (1).

These indicates that, instead of $g_{\mu\nu}$, the real dynamics of GTR evolves with g_{ij} , while g_{00} and g_{0i} lead to constraints of the theory as already mentioned. Nevertheless, the covariant description treats the metric as a single entity. In the process, it leads to a wonderful geometrical interpretation of GTR. Now, let us face the issue, whether maintaining the geometrical structure of the theory, one can split the Einstein's equations, along with the dynamical variables, into space and time. This was done by Arnowitt, Deser and Misner by splitting 4-dimensional space-time into space and time which, as mentioned, is called 3 + 1 decomposition of space-time (Arnowitt, et al., 1962). I shall discuss this in the next section in detail.

3. Decomposition of Space-time

Geometrically this corresponds to a foliation of 4-dimensional space-time \mathcal{M} , by a family of non-intersecting 3-dimensional sub-manifolds. These are known as space-like hyper-surfaces Σ_t , one for each instant of time. Now, $t(x^\alpha)$ is another parameter such that, $t = \text{constant}$. This describes a family of non-intersecting space-like hyper-surfaces Σ_t . It is completely arbitrary. The only requirements are: $t(x^\alpha)$ be a single valued function of x^α and $n_\alpha \propto \partial_\alpha t$ where n_α is the 'unit normal' to the hypersurfaces. The nature of a hypersurface is

described by a constant ϵ as,

$$\epsilon = n^\mu n_\mu = \begin{cases} +1 & \text{if } \Sigma_t \text{ is timelike} \\ -1 & \text{if } \Sigma_t \text{ is spacelike} \end{cases} \quad (4)$$

The metric which is intrinsic to the hypersurface Σ_t , is obtained by restricting the line element to displacements confined to the hypersurface. This is the 'induced metric', or 'first fundamental form', of the hypersurface. It is a scalar with respect to transformations $x^\alpha \rightarrow x^{\alpha'}$ of the spacetime coordinates. At the same time, it behaves as a tensor under transformations $y^i \rightarrow y^{i'}$ of the hypersurface coordinates, where $x^\alpha = x^\alpha(t, y^i)$. It is now possible to construct a general vector t^α as,

$$t^\alpha = \left(\frac{\partial x^\alpha}{\partial t} \right)_{y^i} \quad (5)$$

which is related to the normal vector n^α and the tangential vector $e_i^\alpha = \left(\frac{\partial x^\alpha}{\partial y^i} \right)_t$ with the hypersurface Σ_t , by the following relationship

$$t^\alpha = N n^\alpha + N^i e_i^\alpha \quad (6)$$

Specifically, the lapse function (N) and shift vector (N_i) relates the coordinates on a 3-surface to the preceding and following 3-manifolds. In terms of lapse and shift, unit normal vector may be expressed as,

$$n_\mu = (\epsilon N, 0, 0, 0) \quad \text{and} \quad n^\mu = \left(\frac{1}{N}, -\frac{N^i}{N} \right) \quad (7)$$

Now, $g_{\mu\nu}$, can be written in terms of h_{ij} , N^i and N , where h_{ij} , is concerned with displacements within Σ_t while N^i and N away from Σ_t . The relation amongst these variables is

$$g_{\mu\nu} = \begin{pmatrix} \epsilon N^2 + N_i N^i & N_j \\ N_i & h_{ij} \end{pmatrix} \quad (8)$$

In this decomposed space-time, ds^2 takes the form,

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = -(N^2 - N_i N^i)dt^2 + 2N_i dx^i dt + h_{ij}dx^i dx^j \quad (9)$$

Again,

$$g_{\mu\nu} = h_{\mu\nu} + \epsilon n_\mu n_\nu \quad (10)$$

Now, we are in a position to carry out Hamiltonian formulation of GTR. Let us define covariant derivative, \mathcal{D}_μ which acts on the three-dimensional vector tangent to Σ_t . \mathcal{D}_μ of any vector X_μ that satisfies the condition $X_\mu n^\mu = 0$ (this indicates X_μ is tangential to Σ_t), is given by

$$\mathcal{D}_\mu X_\nu = h_\mu^\alpha h_\nu^\beta \nabla_\alpha X_\beta \quad (11)$$

To gather a detail information about the space-time structure, we have to know how Σ_t are embedded in the four-dimensional geometry. This can be extracted from the manner in which the normal to Σ_t varies from event to event. This is described by the following parameter named the 'extrinsic curvature' of Σ_t ,

$$K_{\mu\nu} = -\nabla_\mu n_\nu - n_\mu a_\nu \quad (12)$$

where a_ν is the 'acceleration' due to the normal vector. It is defined as, $a_\nu = n^\alpha \nabla_\alpha n_\nu$. In view of equation (12), covariant 'spatial' components of $K_{\mu\nu}$ may be defined as (Poisson, 2004; Barth, 1985)

$$K_{ij} = -\nabla_i n_j = \frac{1}{2N} (\mathcal{D}_j N_i + \mathcal{D}_i N_j - \partial_0 h_{ij}) \quad (13)$$

Thus, for a specific structure of the space-time; h_{ij} and K_{ij} have all the necessary information related to the intrinsic and extrinsic properties of Σ_t . Next section, I shall deduce the form of Einstein-Hilbert in 3+1 decomposed space-time.

4. Hamiltonian for Einstein-Hilbert action under 3+1 decomposition

Einstein-Hilbert action depicted in equation (2) has three parts,

$$A_{geometry} = \frac{1}{2\kappa} \int_{\mathcal{V}} \sqrt{-g} R d^4x \quad (14a)$$

$$A_{matter} = \int_{\mathcal{V}} \mathcal{L}(\phi, \phi_{,\alpha}, g_{\alpha\beta}) \sqrt{-g} d^4x \quad (14b)$$

$$\Sigma_R = \frac{1}{2\kappa} \oint_{\partial\mathcal{V}} K \sqrt{h} d^3x \quad (14c)$$

Here ϕ denotes any matter variable. In case of metric variation(Carroll,2004),

$$\delta\sqrt{-g} = \frac{1}{2}\sqrt{-g}g^{\alpha\beta}\delta g_{\alpha\beta} = -\frac{1}{2}\sqrt{-g}g_{\alpha\beta}\delta g^{\alpha\beta} \quad (15)$$

In view of equation (15), variation of equation (14a) with respect to $g_{\mu\nu}$, and considering $\delta g_{\mu\nu}|_{\delta\mathcal{V}} = 0 = \delta g^{\mu\nu}|_{\delta\mathcal{V}}$ one obtains(Guarnizo,et al., 2010),

$$\delta A_{geometry} = \frac{1}{2\kappa} \int_{\mathcal{V}} \left(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R \right) \delta g^{\mu\nu} \sqrt{-g} d^4x + \frac{1}{2\kappa} \oint_{\delta\mathcal{V}} h^{\mu\nu} n^\gamma \partial_\gamma (\delta g_{\mu\nu}) \sqrt{h} d^3x \quad (16a)$$

$$\delta A_{matter} = \int_{\mathcal{V}} \left(\frac{\partial \mathcal{L}}{\partial g^{\mu\nu}} - \frac{1}{2}g_{\mu\nu} \mathcal{L} \right) \delta g^{\mu\nu} \sqrt{-g} d^4x = -\frac{1}{2} \int_{\mathcal{V}} T_{\mu\nu} \delta g^{\mu\nu} \sqrt{-g} d^4x \quad (16b)$$

$$\text{where } T_{\mu\nu} = \left(g_{\mu\nu} \mathcal{L} - 2 \frac{\partial \mathcal{L}}{\partial g^{\mu\nu}} \right)$$

$$\delta \Sigma_R = \frac{1}{\kappa} \oint_{\delta\mathcal{V}} \delta K \sqrt{h} d^3x = -\frac{1}{2\kappa} \oint_{\delta\mathcal{V}} h^{\mu\nu} n^\gamma \partial_\gamma (\delta g_{\mu\nu}) \sqrt{h} d^3x \quad (16c)$$

Combining the above results, the field equation corresponding to EH action supplemented by GHY boundary term reduces to Einstein's equation (1). Under 3+1 decomposition Ricci scalar, R may be expressed as(Padmanabhan,2004)

$$R = {}^{(3)}R + K_{ij}K^{ij} - K^2 - 2\nabla_\gamma(a^\gamma + n^\gamma K) \quad (17)$$

With the help of the above relation, EH action (2) can be expressed as,

$$\begin{aligned} A &= \frac{1}{2\kappa} \int N dt \int ({}^{(3)}R + K_{ij}K^{ij} - K^2) \sqrt{h} d^3x \\ &= \frac{1}{2\kappa} \int_{\mathcal{V}} N \mathcal{L}_{ADM} \sqrt{h} d^4x = f(N, N^i, h_{ij}, \dot{h}_{ij}) \end{aligned} \quad (18)$$

Where,

$$\mathcal{L}_{ADM} = {}^{(3)}R + K_{ij}K^{ij} - K^2 \quad (19)$$

Action, A is cyclic in terms of N and N^i . So, we can infer that the canonical momenta conjugate to them vanish identically. This suggests that unlike h_{ij} , N and N^i are not a dynamical variable. Actually, these are the reparameterization and the diffeomorphic invariance of N and N^i respectively. The momenta conjugate to h_{ij} becomes,

$$p^{ij} = \frac{\partial}{\partial \dot{h}_{ij}} (N \sqrt{h} \mathcal{L}_{ADM}) \equiv \frac{\Pi_{ij}}{2\kappa} \quad (20)$$

Thus, canonical Hamiltonian can be expressed as,

$$H = N \left(\frac{2\kappa}{\sqrt{h}} \left(p^{ij} p_{ij} - \frac{1}{2} p^2 \right) - \frac{\sqrt{h}}{2\kappa} {}^{(3)}R \right) - 2N_i \mathcal{D}_j p^{ij} = N\mathcal{H} + N_i \mathcal{H}^i \quad (21)$$

Where,

$$\mathcal{H} = \frac{2\kappa}{\sqrt{h}} \left(p^{ij} p_{ij} - \frac{1}{2} p^2 \right) - \frac{\sqrt{h}}{2\kappa} {}^{(3)}R \quad (22)$$

$$\mathcal{H}^i = 2 \mathcal{D}_j p^{ij} \quad (23)$$

where \mathcal{H} and \mathcal{H}^i are known as super-Hamiltonian and super-momenta respectively. At last, the action reduces to

$$A = \int (\dot{h}_{ij} p^{ij} - N\mathcal{H} - N_i \mathcal{H}^i) d^3x dt \quad (24)$$

Here, the metric variation of the above action yields $\mathcal{H} = 0$ and $\mathcal{H}^i = 0$. $\mathcal{H} = 0$ is called the 'Hamiltonian constraint equation'. This represents the re-parameterization invariance of GTR with respect to time. On the other hand, $\mathcal{H}^i = 0$ is called the 'momentum constraint equation'. This equation represents the diffeomorphic invariance of GTR (DeWitt, 1967). These two invariances are related with the time-time and the time-space part of Einstein's equation respectively. Thus, the Hamiltonian constraint informs the intrinsic (i.e., coordinate-independent) properties of the gravitational field. In the next section, I shall derive the quantum equation of GTR.

5. Quantization of GTR: Wheeler DeWitt Equation

The first step towards quantization of GTR, is to derive Hamilton-Jacobi (HJ) equation. It attempts to reformulate classical theory in such a way that it behaves like quantum theory using semi-classical approximation. HJ equation may be derived from the Hamiltonian constraint equation $\mathcal{H} = 0$, having the following form (Padmanabhan, 2004; DeWitt, 1967)

$$\mathcal{H} = \frac{2\kappa}{\sqrt{h}} \left(p^{ij} p_{ij} - \frac{1}{2} p^2 \right) - \frac{\sqrt{h}}{2\kappa} {}^{(3)}R = 2\kappa \left[G_{ijkl} p^{ij} p^{kl} - \frac{\sqrt{h}}{(2\kappa)^2} {}^{(3)}R \right] \quad (25)$$

Where,

$$G_{ijkl} = \frac{1}{2\sqrt{h}} (h_{ik} h_{jl} + h_{il} h_{jk} - h_{ij} h_{kl}) \quad (26)$$

Quantizing the Hamiltonian constraint equation, one may derive the following expression (Padmanabhan, 2004; DeWitt, 1967)

$$\mathcal{H}|\psi\rangle = - \left[G_{ijkl} \frac{\delta}{\delta h_{ij}} \frac{\delta}{\delta h_{kl}} + \frac{1}{(2\kappa)^2} \sqrt{h} {}^{(3)}R \right] |\psi\rangle = 0 \quad (27)$$

Here, $|\psi\rangle$ represents the cosmological wave-function of the whole universe. This is known as the 'Wheeler-DeWitt' (WDW) equation. It is considered as the fundamental equation of QC in connection with GTR. Wheeler described the physical interpretation of the above three-dimensional wave-function ('t Hooft, 1973). It is clear from the above expression that the WDW

equation is a second order hyperbolic differential equation. It represents the dynamical evolution of $|\psi\rangle$ in super-space. However, unlike Schrodinger equation, time is absent in this case.

6. Solution of Wheeler DeWitt Equation

WDW equation was first studied by C. Misner (Misner, 1969; Misner, 1972). In this case, the universe has been narrated using the geometry of the three spatial dimensions, as well as, any sort of matter field, ϕ present, i.e., $|\psi\rangle = \psi(h_{ij}, \phi)$, which may be derived by solving the WDW equation. The WDW equation is a hyperbolic equation and may have infinite number of solutions. For a unique solution, one has to specify the boundary conditions for the corresponding wave-function, ψ .

In general, boundary conditions are decided upon the physical conditions external to the system under consideration. However, in QC nothing external to the universe. So, here a boundary condition should be added as an independent physical law. In the literature, two classes of thoughts regarding the boundary conditions are most popular. One is the 'tunneling boundary condition' (Vilenkin, 1986). It was inspired by the idea that the universe is tunneling from nothing. It states that at the boundaries of super-space should include only outgoing waves.

The other proposal was presented by Hartle and Hawking (HH) (Hartle, et al., 1983). It states that the $\psi(h_{ij}, \phi)$, should be given by a Euclidean path integral over compact 4-geometries bounded by the 3-geometry h_{ij} , with the field configuration ϕ . This is expressed as

$$\psi(h_{ij}, \phi) = \int d[g_{\mu\nu}] d[\phi] e^{A_E(g, \phi)} \quad (28)$$

where $A_E(g, \phi)$ is the corresponding Euclidean action. HH boundary condition is also known as 'No Boundary proposal'. Let us explain it more elaborately. History of the gravitational field in general depicted by the specific four-dimensional space-time, in which three spatial dimensions evolves. So, the path integral is the total of all possible four-dimensional space-time geometries that interpolate between the initial and final three-dimensional geometries. In a nut-shell, it is a sum over all possible four-dimensional space-times with two three dimensional boundaries. In this case the boundaries should match the initial and final conditions. The Hartle-Hawking

proposal considers the only the four-dimensional geometries that match onto the final three geometries.

In reality, estimation of probabilities in QC using the full path integral is too much difficult. Therefore, the usual process is to take help of semi-classical approximation. Thus, QC might give some insight at and beyond Planck's era. As full quantum theory of gravity is still to achieve, our primary attempt therefore, is to study the fate of ultra-violet catastrophe related with very early universe using QC.

7. Application of canonical quantization technique in quantum cosmology

Thus, canonical quantization of higher-order theories of gravity is a technique used to quantize gravity by shaping it into a Hamiltonian framework with additional degrees of freedom beyond the standard metric and extrinsic curvature. In this case, Dirac's constraint analysis plays an important role. The steps are transforming the classical theory into canonical variables to get a Hermitian Hamiltonian operator. Then quantizing it to derive corresponding Wheeler DeWitt equation. Solving the quantum equation, explore phenomena like early universe inflation and many other aspects. Although challenges remain in handling the non-linearity and potential inconsistencies that arise in the quantum domain, particularly when total derivative terms are involved.

This particular technique is based on a firm mathematical ground and is being used to discuss phenomena of the early universe very frequently. We have also done some works in this field. We recently done canonical quantization of an gravitational action related with minimally coupled scalar-tensor theory of gravity in Robertson-Walker mini-super-space (Ruz, 2013). Here, quantum, semi-classical, and classical wormhole solutions under back-reaction have been explored for a class of potentials. The result is --- not all type of potentials admits wormhole solutions. This implies, attempt to avoid the singularity problem by invoking wormhole is beyond the scope of GTR. It is expected that the situation might improve under modification of GTR by including higher order curvature invariant terms. In our works (Ruz, 2013; Ruz, 2015; Sanyal, 2012; Debnath, 2014), we have explored a viable canonical quantization scheme for scalar curvature squared (R^2) term, in addition to EH action. The same technique has been applied for quantization of various modified gravity models (Ruz, 2016, Debnath, 2017).

Some authors have applied this technique to explore phenomena of early universe for $f(Q)$ and $f(T)$ gravity (Dimakis, et al., 2021; Saha, et al., 2025; De, et al., 2024). It was also applied in supergravity theory (D'Eath,1984) and modified scalar-tensor theory to explore phenomena of early universe (Mandal, et al., 2018; Mandal, et al., 2020; Mandal, et al., 2021). Recently it has been used to analyse constructive QFT trades quantum fields for random variables (Thiemann,2020).

8. Conclusion

While a complete, non-perturbative quantization of gravity is not yet achieved, there has been progress in constructing a mathematical framework for canonical quantum gravity. New methods are being developed to handle the complexities of quantization and define the theory's physical observables and properties, paving the way for future breakthroughs. The ultimate goal is a theory that can explain the universe's origin, black hole interiors, and unify all fundamental forces.

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