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On quantizing gravity and geometrizing quantum mechanics

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Abstract
We elaborate on some recent results on a solution of the Hilbert-space problem in minisuperspace quantum cosmology and discuss the consequences of making the (geometry of the) Hilbert space of ordinary nonrelativistic quantum systems time-dependent. The latter reveals a remarkable similarity between Quantum Mechanics and General Relativity.

Keywords: quantum gravity, Hilbert-space problem, geometric phase

1. Introduction

Perhaps the most challenging problem facing theoretical physicists since the 1930's has been the formulation of a consistent physical theory that encompasses Quantum Mechanics (QM) and General Relativity (GR). The early steps toward addressing this problem were taken by Dirac who attempted to apply the rules of canonical quantization to GR. The fact that 4 out of 10 components of the Einstein field equation are constraints necessitated the development of a quantization scheme that could handle the presence of constraints. This constituted one of the most significant contributions of Dirac to theoretical physics. It is referred to as Dirac's constrained quantization scheme which he formulated in the 1950's, [1].

The application of Dirac's scheme to GR required a Hamiltonian formulation of GR which was made available in early 1960's [2]. The first concrete steps toward establishing a canonical quantum theory of gravity was subsequently taken by Bryce DeWitt [3] and John Wheeler [4]. The result was an ingenious theory that suffered from severe mathematical as well as interpretational problems [5,6]. These problems have been the subject of numerous research articles for the past 40 years or so. Yet a satisfactory solution of many of them is still unavailable [7]. Among the most important of these is the Hilbert-space problem that we will elude to here.

The severity of the problems associated with canonical quantization of gravity has led a number of researchers to take the opposite root, i.e., rather than trying to quantize GR they tried to geometrize QM, [8]. This was mainly motivated by the idea that perhaps the origin of the above-mentioned difficulties is that QM itself is an approximate theory and that one must put QM in a geometric setting and seek for its nonlinear generalization(s) [9]. The developments in this direction have admittedly failed to lead to a concrete and physically acceptable alternative to QM. Nevertheless, revealing the geometric structure of QM is an interesting endeavor in its own right, especially in connection with geometric phases and their widespread applications and implications [10,11].

Today the most promising candidate for a canonical quantum theory of gravity is the so-called loop quantum gravity [12]. Similarly to its more popular rival, String Theory, loop quantum gravity has not yet produced a concrete experimentally verifiable prediction. Therefore one cannot view it as a physical theory. As a mathematical theory with potential physical applications, however, it enjoys a higher level of rigor in its formulation than the String Theory.

2. Hilbert-space problem in minisuperspace quantum cosmology

Consider a classical system that is time-

Dedicated to the memory of Bryce Dewitt.

reparameterization invariant. Then its classical Hamiltonian K vanishes identically; the system has a first-class constraint $K(q,p)=0$, where $q=(q_1,...,q_n)$ and $p=(p_1,...,p_n)$ are the unconstrained coordinate and momentum degrees of freedom. According to Dirac [1], quantization of this system is performed in two steps. First one quantizes (q, p) as if there were no constraints. This is done according to the well-known rules of canonical quantization: $q_i \to \hat{q}_i$, $p_i \to \hat{p}_i$ where

$$[\hat{q}_i,\hat{q}_j]=[\hat{p}_i,\hat{p}_j]=0\,, \qquad [\hat{q}_i,\hat{p}_j]=i\delta_{ij}\,. \tag{1}$$

Then one imposes the constraint as the condition:

$$K(\hat{p},\hat{q})\left|\psi\right\rangle=0\,. \tag{2}$$

This defines the physical state vectors $\left|\psi\right\rangle$ of the constrained system.

Dirac's scheme involves an auxiliary (unconstrained) Hilbert space $\mathcal{H}'$, that is endowed with the L^2-inner product and furnishes the Heisenberg-Weyl algebra (1) with an irreducible representation, and a physical Hilbert space $\mathcal{H}$, which is defined according to eq. (2) as the kernel (null space) of the quantum constraint $\hat{K}:=K(\hat{p},\hat{q}):\mathcal{H}'\to\mathcal{H}'$,

$$\mathcal{H}:=\left\{\left|\psi\right\rangle\in\mathcal{H}'\,\middle|\,\hat{K}\left|\psi\right\rangle=0\right\}=\mathrm{Ker}(\hat{K}). \tag{3}$$

This equation identities $\mathcal{H}$ with a certain vector subspace of $\mathcal{H}'$. It does not specify the inner product on this subspace. This lack of a prescription to endow $\mathcal{H}$ with an inner product is known as the Hilbert-space problem. Once an appropriate inner product is given to $\mathcal{H}$, one can define the physical observables of the theory (as Hermitian operator acting in $\mathcal{H}$), outline a dynamics by selecting a Hamiltonian operator from among the observables, and employ the axioms of QM to deal with interpretational issues [13].

It is customary to use the coordinate basis $\left\{\left|q'\right\rangle\right\}$ to represent the state vectors and operators,

$$\left\langle q'\right|\hat{q}_i=q_i'\left\langle q'\right|,\quad \left\langle q'\right|\hat{p}_i=-i\partial_{q_i'}\left\langle q'\right|,\quad \psi(q'):=\left\langle q'|\psi\right\rangle, \tag{4}$$

where $q'=(q_1',...,q_n')\in\mathbb{R}^n$ and $\psi=\psi(q')$ is the coordinate wave function associated with the state vector $\left|\psi\right\rangle$. In this coordinate representation the quantum constraint (2) takes the form of a linear partial differential equation:

$$K(-i\partial_{q'},q')\psi(q')=0 \tag{5}$$

where $\partial_{q'}=(\partial/\partial_{q_1'},...,\partial/\partial_{q_n'})$, and the physical Hilbert space is identified with the solution space of this equation. In effect, the Hilbert-space problem is equivalent to promoting the vector space of solutions of eq. (5) into a Hilbert space.

It is important to note that in general the operators $\hat{q}_i$ and $\hat{p}_i$ do not commute with $\hat{K}$. Therefore they do not leave $\mathcal{H}$ invariant, i.e., there are $\left|\psi\right\rangle\in\mathcal{H}$ such that $\hat{q}_i\left|\psi\right\rangle\notin\mathcal{H}$ and $p_i'\left|\psi\right\rangle\notin\mathcal{H}$. This shows that the coordinate and momentum operators $(\hat{q}_i,\hat{p}_i)$ are not physical observables. In particular, the eigenvalues q_i' of $\hat{q}_i$ are not (measurable) physical quantities, and the wave functions $\psi(q')$ do not represent physically meaningful entities. The attempts to extract a 'probability density' out of the wave function $\psi(q')$ therefore lack a logical basis.

The situation is quite different in the absence of such a constraint. In that case $\mathcal{H}'$ is the physical Hilbert space, and being Hermitian operators acting in $\mathcal{H}'$, $\hat{q}_i$ and $\hat{p}_i$ are physical observables. Therefore, we can identify q' with the result of a $\hat{q}$-measurement whose probability density is proportional to $|\psi(q')|^2$.[1]

When the constraint (2) is present, one must first determine the physical position operator that unlike $\hat{q}$ acts in $\mathcal{H}$ (and leaves it invariant) and then use its eigenvectors to define a new set of wave functions whose modulus-square can be interpreted as the physical probability density of localization of the system. All this cannot be achieved unless one solves the Hilbert-space problem.

In full canonical quantum gravity, in its traditional metric formulation [3], the metric tensor $g_{\mu\nu}$ plays the role of the coordinates q. In the Hamiltonian formulation the diffeomorphism invariance of the theory manifests itself as the presence of a Hamiltonian constraint which is related to time-reparameterization symmetry of the theory and three momentum constraints that are linked with the diffeomorphism symmetry of the spatial hypersurface in the ADM decomposition of the spacetime. Quantization of the Hamiltonian constraint leads to an infinite-dimensional analog of eq. (5) which is known as the Wheeler-DeWitt equation; it is a functional partial differential equation plagued with a number of problems [5,6,7,14].

Imposing the extremely strong and highly unrealistic simplifying assumption of spatial homogeneity, one is led to a finite-dimensional system in which the Wheeler-DeWitt equation may be written as a Klein-Gordon equation with a variable mass term:

$$[\partial_{\alpha'}^2+D]\psi(\alpha',\beta_1',....,\beta_n')=0 \tag{6}$$

where α' and $\beta_1',....,\beta_5'$ correspond to the eigenvalues of the operators obtained by quantizing the 3-metric g_{ij}, β_i' with $i>5$ represent matter degrees of freedom, and D is a second order elliptic differential operator with variable coefficients. We will view eq.(6) as a second

1. It is equal to $|\psi(q')|^2$ for a normalized state vector $\left|\psi\right\rangle$.

order ordinary differential equation defined on the Hilbert space $\widetilde{\mathcal{H}} := L^2(\mathbb{R}^n)$ by identifying D with a α'-dependent Hermitian operators $\mathcal{D}$ acting in $\widetilde{\mathcal{H}}'$. Introducing $\psi(\alpha') := \psi(\alpha',.) \in \widetilde{\mathcal{H}}$, we then have

$$[\partial^2_{\alpha'} + \mathcal{D}]\psi(\alpha') = 0. \quad (7)$$

Note that we label the coordinate operators acting in the Hilbert space $\widetilde{\mathcal{H}} = L^2(\mathbb{R}^n)$ by $\hat{\beta}_i$ and identify their common eigenvectors and the corresponding eigenvalues by $|\beta'\rangle$ and β'_i. Then we have

$$\psi(\alpha', \beta'_1, ..., \beta'_n) = \langle \beta' | \psi(\alpha') \rangle,$$

where we use $\langle.|.\rangle$ to denote the L^2-inner product on $\widetilde{\mathcal{H}}$.

As an example, consider an FRW model coupled to a real scalar field φ. Then (in natural units [15]) the classical Hamiltonian constraint has the form

$$K = -p^2_\alpha + p^2_\varphi - \kappa e^{4\alpha} + e^{6\alpha} V(\varphi) = 0, \quad (8)$$

where α is the logarithm of the scale factor: $a = e^\alpha, \kappa$ is the curvature index (= -1, 0, 1 for open, flat, and closed universes, respectively), and V is the self-interaction potential for the field φ. In this case, all β_i, except $\beta_6 = \varphi$ are absent, and the corresponding Wheeler-DeWitt equation is given by eq. (6) with

$$D = -\partial^2_{\varphi'} - \kappa e^{4\alpha'} + e^{6\alpha'} V(\varphi'). \quad (9)$$

Another example is the mixmaster model [16,17] whose Hamiltonian constraint has the form

$$K = -p^2_\alpha + p^2_{\beta_1} + p^2_{\beta_2} + e^{4\alpha}[V(\beta_1, \beta_2) - 1] = 0, \quad (10)$$

where α is again the logarithm of the scale factor $(a = e^\alpha)$ that together with β_1 and β_2 parameterize the 3-metric,

$$(g_{ij}) = e^{2\alpha} \begin{pmatrix} \beta_1 + \sqrt{3}\beta_2 & 0 & 0 \\ 0 & \beta_1 - \sqrt{3}\beta_2 & 0 \\ 0 & 0 & -2\beta_1 \end{pmatrix},$$

β_i with i> 2 are absent, and

$$V(\beta_1, \beta_2) := \frac{1}{3} e^{-8\beta_1} - \frac{4}{3} e^{-2\beta_1} \cosh(2\sqrt{3}\beta_2) + 1 + \frac{2}{3} e^{4\beta_1} [\cosh(4\sqrt{3}\beta_2) - 1]. \quad (11)$$

Again the associated Wheeler-DeWitt equation is given by eq. (6) with

$$D = -\partial^2_{\beta'_1} - \partial^2_{\beta'_2} + e^{4\alpha'} [V(\beta'_1, \beta'_2) - 1]. \quad (12)$$

Note that in these examples, and more generally for other spatially homogeneous cosmological models, the operator D appearing in the Wheeler-DeWitt equation is identical with the standard Hamiltonian operator for a non-relativistic particle moving in $\mathbb{R}^n$ and interacting with a certain α'-dependent potential.

As seen from the form of the classical Hamiltonian constraints (8) and (10), α is a time-like coordinate in the minisuperspace. This has made the variable α' that appears in the Wheeler-DeWitt eq. (6) a popular choice for a time-variable in quantum cosmology. A surprising recent result [18] is that no matter which positive-definite inner product one endows the physical Hilbert space $\mathcal{H}$ with, the α'-translations correspond to non-unitary operators acting in $\mathcal{H}$. This is a concrete evidence that one cannot use α' as a physical time variable. Indeed the rather involved analysis of the Hilbert-space problem for the Wheeler-DeWitt eq. (6) shows that the problem has a rather trivial solution. One can identify the space of solutions $\mathcal{H}$ with the space $L^2(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$ of initial conditions $\psi(\alpha'_0), \partial_{\alpha'}\psi(\alpha'_0)$ of the Wheeler-DeWitt eq. (7) and endow the vector space. $L^2(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$ with a positive-definite inner product. For example one may take the direct sum inner product, i.e., identify $\mathcal{H}$ with $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n)$ The choice of the initial value α'_0 of α' and the choice of the inner product on $L^2(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$ are physically irrelevant, for up to unitary equivalence $\mathcal{H}$ has a unique separable Hilbert space structure [19].

The explicit form of an inner product on $\mathcal{H}$ can be easily written down [18] and physical observables may be constructed. For example, there is an observable $\hat{\varepsilon}$ that squares to 1, i.e., it has ±1 as eigenvalues. A much more difficult task is to formulate a correspondence principle that would associate classical observables to the obtained quantum mechanical observables. This requires certain amount of speculation. In Ref. [18], we have outlined a proposal in which the classical analog of the quantum observable $\hat{\varepsilon}$ is the sign of the derivative of the classical scale factor with respect to any classical physical time variable. In this formulation the eigenvalues ±1 of $\hat{\varepsilon}$ correspond to the expanding and retracting universes, and in general the state vector for the universe will have expanding and retracting components.

In [18] we also outline a proposal for the formulation of the dynamics of the theory. It is based on the Schrödinger time-evolution determined by a Hamiltonian operator H acting in $\mathcal{H}$ that is obtained by quantizing an associated reduced classical Hamiltonian. In practice, this involves selecting a classical time-variable, finding a corresponding reduced classical Hamiltonian that would yield the classical dynamical equation for this time-variable, and finally quantizing the latter to obtain H.

We wish to emphasize that the Hilbert space problem is not a major obstacle in quantizing minisuperspace models. The difficulty lies in the formulation of a correspondence principle that associates to each quantum observable a classical counterpart. This is also of basic importance for our proposal [18] for defining the dynamics. The theory is still far from satisfactory for it is plagued with the notorious multiple choice problem [5,6]: Different choices for the classical time variable seem to lead to different quantum systems, and it is not clear how one should avoid or interpret this apparent violation of the time-reparameterization invariance. A possible way out is to identify an equivalence relation between these quantum systems and associate physical reality to the quantities that are common to all members of a given equivalence class. The feasibility of this approach can be decided only after a detailed investigation of some concrete models. Unfortunately, this has not been possible even for the simple models such as eqs.(8) and (10) for technical reasons.

3. Hilbert space with changing geometry

What made Albert Einstein the most influential scientist of the 20th century was that not only he had the courage to unify the concepts of time and space, but he was willing to consider the revolutionary idea of making the geometry of spacetime dynamical.

Recently, within a totally remote subject, it was discovered that one could devise a unitary quantum system using a seemingly non-Hermitian Hamiltonian, such as $H = p^2 + ix^3$, provided that its spectrum was real [20,21]. This was only possible at the expense of adopting a non-standard inner product on the Hilbert space of the system. The ensuing theory is termed as pseudo-Hermitian quantum mechanics [20, 22, 23, 24, 25, 26]. It provides a general method of constructing the most general inner product that renders the Hamiltonian self-adjoint and consequently restores the unitarity of the dynamics. It has direct applications in relativistic quantum mechanics of scalar fields and quantum cosmology [18, 27, 28] and many other areas [29]. In particular, in its application in quantum cosmology, one is forced to deal with explicitly time-dependent Hamiltonians which would generate unitary time-evolutions provided that the inner product of the Hilbert space be made time-dependent as well. This observation subsequently led the present author to investigate the consequences of having a quantum system defined on a Hilbert space with a time-dependent inner product and hence a dynamical geometry [30]. The resemblance to the passage from special to general relativity needs no clarification.

The geometry of a Hilbert space is determined by its inner product. It is well-known [31] that any inner product $(.|.)$ on a given vector space $\mathcal{V}$ may be obtained from a given inner product $\langle .|.\rangle$ according to

$$(.|.) = \langle .|\eta .\rangle =: \langle .,.\rangle_\eta , \tag{13}$$

where $\eta : \mathcal{V} \to \mathcal{V}$ is an invertible operator satisfying

$$\langle .|\eta .\rangle = \langle \eta .|.\rangle . \tag{14}$$

That is if we label the inner product (Hilbert) space obtained by endowing $\mathcal{V}$ with $\langle .|.\rangle$ by $\mathcal{H}$, then as an operator acting in $\mathcal{H}$, η is self-adjoint or Hermitian. Furthermore, the requirement that $\langle .,.\rangle_\eta$ be positive-definite, i.e., for all nonzero $|\psi\rangle \in \mathcal{H}, \langle \psi,\psi\rangle_\eta > 0$, implies that η must be a positive-definite operator (its spectrum must be strictly positive.)

The operator η may be conveniently used to quantify the choice of the geometry of the Hilbert space; it is referred to as a metric operator. In the following we will take the inner product $\langle .|.\rangle$ of $\mathcal{H}$ as a time-independent reference inner product and characterize the dynamical geometries of the Hilbert space in terms of time-dependent metric operators.

Now, suppose that the dynamics of a quantum system is determined through the Schrödinger equation:

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle , \tag{15}$$

where $H : \mathcal{H} \to \mathcal{H}$ is a given possibly time-dependent and not necessarily Hermitian operator. Then the condition that H generates a unitary time-evolution for a time-dependent inner product defined by the metric operator $\eta(t)$ i.e., requiring that for any pair $(|\xi(t)\rangle, |\zeta(t)\rangle)$ of solutions of eq. (15), $\frac{d}{dt}\langle \xi,\zeta\rangle_{\eta(t)} = 0$, we find

$$i\frac{d}{dt}\eta(t) = H^\dagger \eta(t) - \eta(t) H. \tag{16}$$

This is the non-Hermitian extension of the Liouville-von Neumann equation. It reduces to the following Liouville-von Neumann equation for a Hermitian Hamiltonian H:

$$i\frac{d}{dt}\eta(t) = [H,\eta]. \tag{17}$$

This equation has two interesting ramifications.

1. The invertible mixed states (density matrices) used in quantum statistical mechanics define acceptable metric operators, for they are positive-definite solutions of the Liouville-von Neumann equation.

2. Each acceptable metric operator (that satisfies eq. (17)) is a dynamical invariant in the sense of Lewis and Riesenfeld, [32]. In particular, the eigenvalues of η(t) are time-independent and one can obtain a complete set of solutions of the Schrödinger eq. (15) out of eigenvectors of $\eta(t)$.

The connection between metric operators and dynamical invariants is particularly interesting because there is a well-known formulation of geometric phases in terms of dynamical invariants [33]. In view of results of [34], it is the metric operator $\eta(t)$ that determines the geometric phases. This observation reveals, in a rather direct manner, the geometric nature of these phases without appealing to the conventional geometric formulation based on the classifying U(1) principal bundle over the projective Hilbert space [11, 35].

Another interesting conclusion that may be drawn out of the above-described connection is that one can postulate a different or more general dynamical equation for the metric operator, determine the geometric phases for evolving states using the eigenvectors of the solution of this equation, and postulate a method to identify the dynamical phases for an evolving state. This would lead to a generalization of quantum mechanics which shares the same geometric structure. In Ref. [30] we offer a proposal for such a generalization based on Lindbald's master equation [36].

Finally, given a Hamiltonian there are an infinity of acceptable metric operators (parameterized by the initial value η_0 of $\eta(t)$). There is a permutation group G that relates this metric operators. The freedom to choose η_0 is a rather trivial quantum mechanical analogue of the diffeomorphism invariance of GR. Similarly, the permutation group G plays in QM a similar role as the diffeomorphism group does in GR.

The natural extension of the ideas presented above is to attempt at introducing a particular type of nonlinearity in QM by allowing the metric operator to be state-dependent. Whether and how this can be achieved is the subject of a future investigation.

4. Conclusion

Quantization of GR and geometrization of QM are both as attractive and intriguing subjects for research as they were initially considered in the 1960s and 1970s. In this paper we elaborated on some recent developments in these subjects.

In connection with canonical quantization of GR, we argued that at least for the simplified quantum cosmological models the Hilbert-space problem may be avoided by trying to directly endow the solution space of the Wheeler-DeWitt equation with an arbitrary inner product. The difficulty lies with interpreting the quantum observables or alternatively relating them via a correspondence principle to the classical observables. This approach is the opposite of the one taken in the so-called group-averaging scheme [37]. It has the advantage of being explicit and easy to compute [18].

On the subject of the geometrization of QM, we elucidated the role of the geometry of the Hilbert space and showed that it was possible to consider quantum systems with dynamical Hilbert spaces. After all, the geometry of the Hilbert space is as unobservable as the state vectors themselves. What is observable is the transition amplitudes and expectation values which involve both the state vector and the metric operator. Promoting the role of the geometry of the Hilbert space from an idle observer to a real player in the quantum game reveals some remarkable resemblances between QM and GR. It also opens up the way to formulate a nonlinear extension of QM which might be more convenient to be unified with GR in a yet-to-be-discovered consistent quantum theory of gravity.

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