Wave Function of the Universe
and Its Meaning

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Abstract

For a FRW-spacetime coupled to an arbitrary real scalar field, we endow the solution space of the associated Wheeler-DeWitt equation with a Hilbert-space structure, construct the observables, and introduce the physical wave functions of the universe that admit a genuine probabilistic interpretation. We also discuss a proposal for the formulation of the dynamics. The approach to quantum cosmology outlined in this article is based on the results obtained within the theory of pseudo-Hermitian operators.

1 Introduction

Quantum cosmology is a natural outcome of the efforts toward a unification of quantum mechanics (QM) and general relativity, i.e., development of a quantum theory of gravity (QG) \[1\, 2\, 3\]. Even in its gravely simplified minisuperspace realizations \[1\, 4\, 2\, 8\], quantum cosmology provides a useful testing ground for various proposals for solving some of the most important problems of QG such as the Hilbert-space problem, the factor-ordering problem, and the problem of time. These problems have been studied extensively.

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for the past four decades. Yet, even for the simplest minisuperspace models, their complete solution could not be found.

This article aims at providing a brief outline of a consistent formulation of quantum cosmology, based on a FRW-spacetime coupled to an arbitrary real scalar field, that offers explicit solutions for some of these problems and provides valuable insight in others.

2 Quantization of the model and the Wheeler-DeWitt equation

Consider a FRW-spacetime coupled to a real scalar field $\varphi$ with an arbitrary real-valued potential $V = V(\varphi)$. The Einstein equations for this model are equivalent to a single differential equation which can be cast in the form of a Hamiltonian constraint $[5]$. Choosing the natural system of units described in $[3]$, the latter takes the form

$$K := -\pi_\alpha^2 + \pi_\varphi^2 - \kappa e^{4\alpha} + e^{6\alpha} V(\varphi) = 0,$$

where $\alpha := \ln a$, $a$ is the scale factor of the FRW model, $\kappa$ is the curvature index with the values $-1, 0, 1$ that respectively correspond to an open, flat, or closed universe, and $\pi_\alpha$ and $\pi_\varphi$ are the canonical momenta conjugate to $\alpha$ and $\varphi$.

The standard canonical quantization of the above model uses Dirac’s method of quantizing constrained systems $[6]$. This involves the canonical quantization of the unconstrained system and the imposition of the constraint as a restriction on the allowed state vectors. For the system described by the phase-space variables ($\alpha, \pi_\alpha; \varphi, \pi_\varphi$) and the constraint (1), this leads to the auxiliary Hilbert space $\mathcal{H}' = L^2(\mathbb{R}^2)$ and the operators ($\hat{\alpha}', \hat{\pi}_\alpha', \hat{\varphi}', \hat{\pi}_\varphi'$) that act in $\mathcal{H}'$ and satisfy the canonical commutation relations $[\hat{\alpha}', \hat{\varphi}'] = [\hat{\pi}_\alpha', \hat{\pi}_\varphi']$ that act in $\mathcal{H}$ and satisfy the canonical commutation relations $[\hat{\alpha}', \hat{\varphi}'] = [\hat{\pi}_\alpha', \hat{\pi}_\varphi'] = 0$ and $[\hat{\alpha}', \hat{\pi}_\alpha'] = [\hat{\varphi}', \hat{\pi}_\varphi'] = i$. Moreover, the quantum analogue of the classical constraint (1) takes the form $\hat{K}'|\psi\rangle = 0$, where $\hat{K}'$ is obtained by quantizing the classical Hamiltonian $\mathcal{K}$ and has, up to the factor-ordering ambiguities, the form: $\hat{K}' = -\pi_\alpha'^2 + \pi_\varphi'^2 + e^{6\alpha'} V(\varphi') - \kappa e^{4\alpha'}$.

A few remarks are in order: 1. The quantum constraint, $\hat{K}'|\psi\rangle = 0$, identifies the space of the physical state vectors of the system with the kernel $\mathcal{V}$ of the operator $\hat{K}'$. In particular, $\mathcal{V}$ is a vector subspace of the auxiliary Hilbert space $L^2(\mathbb{R}^2)$. Because Dirac’s quantization scheme does not endow $\mathcal{V}$ with...
an inner product, one must find a way to construct an inner product on \( V \) and promote it to a genuine Hilbert space \( \mathcal{H} \). This is known as the \textit{Hilbert-space problem}. 2. The observables of the theory are the Hermitian operators acting in \( \mathcal{H} \); 3. The usual formulation of quantum dynamics requires identifying one of the observables with the Hamiltonian operator and defining the evolution parameter \( \tau \) appearing in the corresponding Schrödinger equation with time.

It is usually more instructive to write the quantum constraint as a differential equation. To do this, one first identifies \( \vec{x}' := (\hat{\alpha}', \hat{\varphi}') \) with the position operator acting in \( \mathcal{H}' \) and expresses the state vectors \( |\psi\rangle \) and the relevant operators in the position representation. The \((\delta\text{-function normalized})\) position basis kets \( |\alpha', \varphi'\rangle \) satisfy the defining relations:

\[
\alpha', \varphi'|\alpha' = \alpha'(\alpha', \varphi'), \quad (\alpha', \varphi'|\varphi' = \varphi'(\alpha', \varphi'), \quad (\alpha', \varphi'|\pi'_{\alpha} = -i\partial_{\alpha'}(\alpha', \varphi'), \quad (\alpha', \varphi'|\pi'_{\varphi} = -i\partial_{\varphi'}(\alpha', \varphi').
\]

In this basis, the elements \( |\psi\rangle \) of \( \mathcal{H}' \) are represented by the ‘position’ wave functions

\[
\psi(\alpha', \varphi') := (\alpha', \varphi'|\psi),
\]

and the quantum constraint, \( \hat{K}'|\psi\rangle = 0 \), takes the form of the Wheeler-DeWitt equation \[1, 2, 3\]:

\[
\left[-\partial_{\alpha'}^2 + \partial_{\varphi'}^2 + \kappa e^{4\alpha'} - e^{6\alpha'}V(\varphi')\right] \psi(\alpha', \varphi') = 0.
\]

This in turn implies that one can identify \( \mathcal{V} \) with the (vector) space of solutions of this equation. Indeed, as far as the Dirac’s program of constrained quantization is concerned, the function of the Wheeler-DeWitt equation is to determine \( \mathcal{V} \).

3 \textbf{Hilbert-space problem}

Because \[3\] is a second order hyperbolic equation, its solutions \( \psi \in \mathcal{V} \) may be uniquely determined in terms of two initial conditions. This is done by selecting a time-like coordinate \( \tau' \) for the \((1+1)\)-dimensional Minkowski space parameterized by the coordinates \((\alpha', \varphi')\) and specifying each solution \( \psi \) with a pair of initial data for \[3\] at some initial value \( \tau'_0 \) of \( \tau' \). The choice of the \( \tau' \) and \( \tau'_0 \) is actually arbitrary. Here we will take \( \tau' := \alpha' \), but we should like to emphasize that this does not mean that we identify \( \alpha' \) with a physical time variable. We will determine the latter by requiring that it is an evolution parameter for a Hamiltonian operator acting in the physical Hilbert space \( \mathcal{H} \).
Next, let $\alpha_0 \in \mathbb{R}$ be an arbitrary initial value for $\alpha'$, and for all $\psi \in \mathcal{V}$ and $\alpha' \in \mathbb{R}$ define $\psi(\alpha') : \mathbb{R} \to \mathbb{C}$ according to $\psi(\alpha')[\varphi'] := \psi(\alpha', \varphi')$, where $\varphi' \in \mathbb{R}$ is arbitrary. Then we can view both $\psi(\alpha'_0)$ and $\dot{\psi}(\alpha'_0)$ as elements of $L^2(\mathbb{R})$. In particular, we have $\psi(\alpha'_0), \dot{\psi}(\alpha'_0) \in L^2(\mathbb{R})$. Furthermore, we can express the Wheeler-DeWitt equation (3), in the form

$$[\partial^2_{\alpha'} + D]\psi(\alpha') = 0,$$

where $D : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is the Hermitian operator defined by $(D\xi)(\varphi') := [-\partial^2_{\varphi'} + e^{6\alpha'} V(\varphi') - \kappa e^{4\alpha'}] \xi(\varphi')$, with $\xi \in L^2(\mathbb{R})$ and $\varphi' \in \mathbb{R}$.

Having identified the Wheeler-DeWitt equation (3) with the second order equation (4), which is defined in the Hilbert space $L^2(\mathbb{R})$, we can write $\mathcal{V} = \{\psi : \mathbb{R} \to L^2(\mathbb{R}) | [\partial^2_{\alpha'} + D]\psi(\alpha') = 0\}$ and use the initial data: $(\psi(\alpha'_0), \dot{\psi}(\alpha'_0)) \in L^2(\mathbb{R}) \times L^2(\mathbb{R})$ to specify the elements $\psi$ of $\mathcal{V}$. Because (4) is a linear equation, as a complex vector space, $\mathcal{V}$ is isomorphic to $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. On the other hand, endowing $\mathcal{V}$ with any inner product so that it acquires a separable Hilbert-space structure yields a Hilbert space $\mathcal{H}$ that is also isomorphic to $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. This follows from the uniqueness of the structure of separable Hilbert spaces [7]. This observation reduces the Hilbert-space problem for the model considered here to the construction of a positive-definite inner product on $\mathcal{V}$. An explicit example is [8, 9]

$$\langle \psi_1, \psi_2 \rangle := \frac{1}{2} \left[ \langle \psi_1(\alpha'_0), D_0 \psi_2(\alpha'_0) \rangle + \langle \dot{\psi}_1(\alpha'_0), \dot{\psi}_2(\alpha'_0) \rangle \right],$$

where $\langle \cdot, \cdot \rangle$ is the inner product of $L^2(\mathbb{R})$ and $D_0$ is an arbitrary positive-definite operator (a Hermitian operator with a strictly positive spectrum) acting in $L^2(\mathbb{R})$. One can check that (5) is a positive-definite inner product on $\mathcal{V}$ and that any other inner product on this space is unitarily equivalent to (5), [9]. The Hilbert space $\mathcal{H}$, which consists of the physical state vectors of the model and is called the physical Hilbert space, is the Cauchy completion of the inner product space obtained by endowing $\mathcal{V}$ with the inner product (5).

It must be emphasized that although the inner product (5) depends on $\alpha'_0$ and $D_0$, the structure of the Hilbert space $\mathcal{H}$ is insensitive to the choice of $\alpha'_0$ and $D_0$; different choices yield unitarily equivalent Hilbert spaces and consequently the same physical theory.

We conclude this section by noting that the original construction of the inner product (5) and its generalizations [8] have their root in the results
obtained in the context of a recently developed theory of pseudo-Hermitian operators [10].

4 Observables and the wave functions of the universe

The unitary-equivalence of the physical Hilbert space $\mathcal{H}$ and $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ means that there exists a linear (invertible) operator $U: \mathcal{H} \rightarrow L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ such that for all $\psi_1, \psi_2 \in \mathcal{H}$, $\langle \psi_1, \psi_2 \rangle = \langle U \psi_1 | U \psi_2 \rangle$, where $\langle | \cdot \rangle$ stands for the inner product of $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. The operator $U$ is clearly not unique. Explicit form of such an operator is given in [9]. But as we shall see below the form of this operator does not have a physical significance.

One may use $U$ to relate the Hermitian operators acting in $\mathcal{H}$ to those acting in $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. This means that the physical observables $\hat{O}$ of the quantum cosmological model under study have the form $\hat{O} = U^{-1} \delta U$ where $\delta$ is a Hermitian operator acting in $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. For instance, we have the basic observables: $\hat{Q} := U^{-1} \hat{q} U$, $\hat{P} = U^{-1} \hat{p} U$, and $\hat{S}_\mu := U^{-1} \hat{s}_\mu U$, where $\mu = 0, 1, 2, 3$, $s_\mu := \sigma_\mu \otimes \hat{1}$, $\sigma_0$ is the $2 \times 2$ identity matrix, $\sigma_\mu$ with $\mu \neq 0$ are Pauli matrices, and $\hat{1}$, $\hat{q}$ and $\hat{p}$ are respectively the identity, position, and momentum operators acting in $L^2(\mathbb{R})$. In particular, $\hat{Q}$ and $\hat{S}_3$ form a maximal set of commuting observables. Hence the corresponding eigenvectors $\psi^{(q, \nu)}$, with $q \in \mathbb{R}$ and $\nu = \pm 1$, form a 'basis' of $\mathcal{H}$. Clearly $\psi^{(q, \nu)} = U^{-1} | q, \nu \rangle$, where $| q, \nu \rangle$ satisfy the defining relations: $\hat{q} | q, \nu \rangle = q | q, \nu \rangle$ and $\hat{s}_3 | q, \nu \rangle = \nu | q, \nu \rangle$, and the orthonormality and completeness relations $\langle q, \nu | q', \nu' \rangle = \delta(q - q') \delta_{\nu, \nu'}$ and $\sum_{\nu = \pm 1} \int_{-\infty}^{\infty} dq | q, \nu \rangle \langle q, \nu \rangle = \hat{s}_0$, respectively.

We can express any element $\psi$ of $\mathcal{H}$ in the basis $\{ \psi^{(q, \nu)} \}$ as

$$\psi = \sum_{\nu = \pm 1} \int_{-\infty}^{\infty} dq \, \Psi(q, \nu) \psi^{(q, \nu)},$$  

where $\Psi : \mathbb{R} \times \{-1, 1\} \rightarrow \mathbb{C}$ are the coefficient functions. One can easily show that indeed $\Psi$ belong to $\in L^2(\mathbb{R} \times \{-1, 1\})$ which is isomorphic, as a Hilbert space, to $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$.

The arguments $q$ and $\nu$ of $\Psi$ are the eigenvalues of the physical observables $\hat{Q}$ and $\hat{S}_3$. This is not true for the arguments $\alpha'$ and $\varphi'$ of the wave functions $\psi(\alpha', \varphi')$ appearing in the Wheeler-DeWitt equation [3], because these are the eigenvalues of the operators $\hat{\alpha}'$ and $\hat{\varphi}'$ which act in the auxiliary


Hilbert space $\mathcal{H}'$ and do not leave the physical Hilbert space $\mathcal{H}$ invariant, i.e., there are $\psi \in \mathcal{H}$ such that $\alpha'\psi, \varphi'\psi \notin \mathcal{H}$. This shows that the description of the state vectors $\psi$ as functions depending on $(\alpha', \varphi')$ is quite different from the description of the state vectors in ordinary QM in terms of the position wave functions. It is the coefficient functions $\Psi$ that have the eigenvalues of physical observables as their argument and play the role of the familiar position wave functions. Therefore, we propose to refer to them as the physical “Wave Function of the Universe.”

The expression (6) provides a one-to-one correspondence between the state vectors $\psi$ and the wave functions $\Psi$. This is a manifestation of the unitary-equivalence of $\mathcal{H}$ and $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. Indeed one may use (6) to define $U : \mathcal{H} \rightarrow L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ according to $U\psi := \begin{pmatrix} \Psi(q,+) \\ \Psi(q,-) \end{pmatrix}$ with $\Psi(q, \nu) := \langle \langle \psi(q, \nu), \psi \rangle \rangle$, and check that $U$ is a unitary operator. An immediate implication of the existence and unitarity of $U$ is that, similarly to ordinary QM, we can formulate our quantum cosmological theory in terms of the wave functions $U\psi$ which belong to the well-known Hilbert space $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. We can express the inner product of two state vectors $\psi_1, \psi_2 \in \mathcal{H}$ in terms of their wave functions $\Psi_1$ and $\Psi_2$ as $\langle \psi_1, \psi_2 \rangle = \sum_{\nu=\pm 1} \int_{-\infty}^{\infty} dq \Psi_1(q, \nu)^* \Psi_2(q, \nu)$.

Similarly, we can express the action of an observable $\hat{O}$ on a state vector $\psi \in \mathcal{H}$ in terms of the corresponding wave function $\Psi$ by defining $\hat{\Omega} := U \hat{O} U^{-1} : L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ and checking that indeed $\hat{O} \psi = \sum_{\nu=\pm 1} \int_{-\infty}^{\infty} dq [\hat{\Omega} \Psi(q, \nu)] \psi(q, \nu)$. For example, we have $\hat{Q} \psi = \sum_{\nu=\pm 1} \int_{-\infty}^{\infty} dq q \Psi(q, \nu) \psi(q, \nu)$. The converse of the above argument also holds: Every observable $\hat{\Omega}$ acting in $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ defines an observable $\hat{O} := U^{-1} \hat{\Omega} U$ acting in $\mathcal{H}$.

5 Physical Interpretation and the Dynamics

So far we have constructed the Hilbert space and obtained the form of the observables, but failed to describe how the latter connect with the classical observables or discuss their physical meaning. Another crucial issue that we have not treated is the dynamics.

We propose to associate physical meaning to the basic observables $\hat{Q}$ and $\hat{S}_3$ and consequently the variables $q$ and $\nu$ by identifying the former with quantum analogues of a pair of observables for the reduced (constrained) classical system $(\mathcal{C})$. This means that we intend to perform a quantization
of $C$ that leads to a quantum theory having $\mathcal{H}$ as its Hilbert space. Similarly, we propose to determine a Hamiltonian operator by selecting a classical time variable, obtaining a classical Hamiltonian that describes the dynamics of $C$, and carrying out the above-mentioned quantization.

A widely used classical time is the logarithm of the scale factor, i.e., $\alpha$, which is acceptable if the classical universe is ever-expanding. There are classical universes that violate this assumption. It is also obvious that one cannot make such an assumption in a quantum mechanical treatment of the universe. An alternative to taking $\alpha$ as a classical time-variable that avoids this assumption is $\tau := \epsilon \alpha$, where $\epsilon := (d\alpha(t)/dt)/|d\alpha(t)/dt|$. Clearly $\tau$ is a monotonically increasing function of the physical time $t$.

If we choose $\tau$ as a classical time-variable, we can generate the dynamics of $C$ using the classical Hamiltonian $H = \sqrt{\pi^2_{\varphi} + e^{6\epsilon \tau} V(\varphi) - \kappa e^{4\epsilon \tau}}$. As seen from this relation $C$ has $\varphi$ and $\epsilon$ as configuration variables. This suggests the following quantization rule: $\varphi \rightarrow \hat{\varphi}$, $\pi_{\varphi} \rightarrow \hat{P}$, and $\epsilon \rightarrow \hat{S}_3$. For convenience, we introduce: $\hat{\varphi} := \hat{Q}$, $\hat{\pi}_{\varphi} := \hat{P}$, and $\hat{\epsilon} := \hat{S}_3$, which in turn suggest the following identifications: $q = \varphi$ and $\nu = \epsilon$.

Aside from the usual factor-ordering ambiguities that are also present in ordinary QM, the above quantization rule leads to the Hamiltonian operator

$$\hat{H} = \sqrt{\pi^2_{\varphi} + e^{6\epsilon \tau} V(\hat{\varphi}) - \kappa e^{4\epsilon \tau}}.$$  (7)

The dynamics of the quantum universe is then determined by the Schrödinger equation $i d\psi_{\tau}/d\tau = \hat{H}\psi_{\tau}$, where we have expressed the time-dependence of the evolving state vector $\psi_{\tau}$ using the index $\tau$. We can also express the dynamics in terms of the physical wave functions $\Psi$ whose arguments $q$ and $\nu$ are respectively identified with the scalar field $\varphi$ and the expansion index $\epsilon$. Letting $\Psi(\varphi, \epsilon; \tau) := \langle \psi^{(\varphi, \epsilon)}; \psi_{\tau} \rangle$, we have [9]

$$i \partial_{\tau} \Psi(\varphi, \epsilon; \epsilon \tau) = \epsilon \sqrt{-\partial^2_{\varphi} + e^{6\epsilon \tau} V(\varphi) - \kappa e^{4\epsilon \tau}} \Psi(\varphi, \epsilon; \epsilon \tau).$$ (8)

As seen from (7), the quantum theory described by the Hilbert space $\mathcal{H}$ and the Hamiltonian $\hat{H}$ is a unitary theory admitting a probabilistic interpretation, if the operator appearing in the square root in (7) (alternatively in (8)) is a positive operator. This is always the case for the class of open and flat FRW models coupled to a real scalar field with a positive confining potential, i.e., whenever $\kappa \neq 1$, $V(\varphi) \geq 0$ for all $\varphi \in \mathbb{R}$, and $\lim_{|\varphi| \to \infty} V(\varphi) = \infty$. Various models that allow for classical inflationary expansions belong to this
class. Typical examples are open and flat FRW models coupled to a massive real scalar field \[3\].

In general \( \hat{H} \) fails to be a Hermitian operator for a range of values of the time-variable. Outside this range the quantum theory is unitary. The description of the physics of crossing the boundary of this range is still open to both quantitative and qualitative investigation.

\section{Conclusion}

In this article we presented a summary of our recent attempts to overcome some of the most fundamental problem of quantum cosmology for a large family of cosmological models. Perhaps the most important feature of our method is its formulation of the Wheeler-DeWitt equation as a second order ordinary differential equation defined in a Hilbert space \( \mathcal{H} \). This is equivalent to a first order equation defined in \( \mathcal{H} \oplus \mathcal{H} \) which may be identified with a Schrödinger equation with a generally non-Hermitian but pseudo-Hermitian Hamiltonian. It is the basic spectral properties of the pseudo-Hermitian Hamiltonians \[10\] that lead to the results reported here.

The following are our concluding remarks: 1. The construction of the Hilbert space and subsequently the observables is insensitive to the particular factor-ordering prescription chosen to write down the Wheeler-DeWitt equation \(3\). The factor-ordering problem only arises while quantizing the Hamiltonian of the (reduced) classical system. It is effective to the same extend as in the ordinary QM; 2. A notable feature of our investigation is the introduction of the physical wave functions \( \Psi(\varphi, \pm \tau) \) of the universe that effectively describe the expanding and retracting components of the quantum state of the universe. The whole theory may be described in terms of these wave functions; 3. Our approach may be viewed as providing a link between the traditional approaches of quantization before and after imposing the constraints. Its kinematic aspects uses the former while its interpretation and dynamical aspects involve the latter; 4. As it stands, our method suffers from the multiple-choice problem and is plagued with the problems related to the non-Hermiticity of the quantum Hamiltonian for typical closed universes \[2\]. In our opinion these problems cannot be viewed as insurmountable obstacles unless a comprehensive investigation is performed and a concrete evidence (such as a no-go theorem) shows otherwise.
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