Probability Interpretation for Klein-Gordon Fields and the Hilbert Space Problem in Quantum Cosmology

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Abstract

We give an explicit construction of a positive-definite invariant inner-product for the Klein-Gordon fields, thus solving the old problem of the probability interpretation of Klein-Gordon fields without having to restrict to the subspaces of the positive-frequency solutions. Our method has a much wider domain of application and may be used to obtain a general class of invariant inner-product on the solution space of a broad class of Klein-Gordon type evolution equations. We explore its consequences for the solutions of the Wheeler-DeWitt equation associated with the FRW-massive-real-scalar-field models.

1 Introduction

The birth of modern particle physics and the advent of relativistic quantum field theories have their origin in Dirac’s attempts to obtain a consistent probability interpretation for Klein-Gordon fields. These attempts led to the discovery of the Dirac equation, Dirac’s theory of holes, and the positron on the one hand, and the formulation of the method of second quantization on the other hand. Yet, these developments did not provide a satisfactory resolution of the issue of the probability interpretation for Klein-Gordon fields. Because first quantized scalar fields did not play an important role in high energy physics this problem did not attract much attention until the 1960s when John Wheeler and Bryce DeWitt founded quantum cosmology.

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One of the outstanding problems of quantum cosmology is the issue of how to interpret
the wave function of the universe [1, 2, 3, 4, 5, 6]. This is a scalar field satisfying the Wheeler-
DeWitt equation. The latter has the structure of a Klein-Gordon equation and is plagued
among other things with the problem of negative probabilities, if one adopts the invariant but
indefinite Klein-Gordon inner product [1, 7, 8]. Use of the non-invariant $L^2$-inner product
allows for a conditional probability interpretation [9, 2]. But this approach does not lead to
a satisfactory resolution of the problem either [3, 4]. Today, the only successful attempt to
attack this problem consists of Woodard’s [10] proposal of gauge-fixing the Wheeler-DeWitt
symmetry and its variations known as the method of refined algebraic quantization and
group averaging [11]. These could however be applied to certain special models [11].

The basic problem of the construction of invariant positive-definite inner product on the
solution space of the Klein-Gordon type evolution equations has been open for the past 75
years. The purpose of this paper is to report on an application of the theory of pseudo-
Hermitian operators [12, 13, 14, 15, 16] that leads to a complete solution of this problem.
In the following we first recall the basic properties of pseudo-Hermitian Hamiltonians and
then discuss their relevance to the problem of the probability interpretation of the Klein-
Gordon and Wheeler-DeWitt fields. A more detailed treatment that applies to more general
Klein-Gordon type equations is presented in [17].

2 Basic Mathematical Results

A linear operator $H : \mathcal{H} \to \mathcal{H}$ acting in a Hilbert space $\mathcal{H}$ is said to be pseudo-Hermitian
[12] if there is a linear, Hermitian, invertible operator $\eta : \mathcal{H} \to \mathcal{H}$ satisfying
\[
H^\dagger = \eta H \eta^{-1}.
\]
Let $\eta : \mathcal{H} \to \mathcal{H}$ be such an operator and consider $\langle \langle \ , \ \rangle \rangle_\eta : \mathcal{H}^2 \to \mathbb{C}$ defined by
\[
\langle \langle \psi_1 | \psi_2 \rangle \rangle_\eta := \langle \psi_1 | \eta \psi_2 \rangle.
\]

Clearly, $\langle \langle \ , \ \rangle \rangle_\eta$ is a nondegenerate Hermitian sesquilinear form [18], i.e., it is a possibly
indefinite inner product — a pseudo-inner product — on $\mathcal{H}$. A pseudo-Hermitian operator
together with a given operator $\eta$ satisfying (1) is said to be $\eta$-pseudo-Hermitian.

The term ‘pseudo-Hermitian’ was introduced in [12]. But it turns out that mathematicians
[19] had developed similar concepts in the study of vector spaces with an indefinite
metric, and Pauli [20] had made use of these concepts in his study of a formulation of the
quantum electrodynamics due to Dirac [21]. Note however that there is a seemingly unim-
portant but actually quite significant difference between the approach pursued in the context
of spaces with an indefinite metric (including Pauli’s generalization of quantum mechanics to such spaces) and the point of view adopted in [12]. While in the former one considers a space with a given \( \eta \), in the latter one formulates the concept of pseudo-Hermiticity without having to specify a particular \( \eta \). In fact, as emphasized in [15] for a given pseudo-Hermitian Hamiltonian, \( \eta \) is not unique.

The basic properties of pseudo-Hermitian operators are the following [12, 13, 14, 16, 17].

**Theorem I:** \( H \) is \( \eta \)-pseudo-Hermitian if and only if it is Hermitian with respect to the pseudo-inner product \( \langle \langle \cdot, \cdot \rangle \rangle_\eta \), i.e., for all \( \psi_1, \psi_2 \in \mathcal{H} \), \( \langle \langle \psi_1 | H \psi_2 \rangle \rangle_\eta = \langle \langle H \psi_1 | \psi_2 \rangle \rangle_\eta \).

**Theorem II:** Let \( H \) be the Hamiltonian of a quantum system and \( \eta \) be a linear, Hermitian, invertible operator. Suppose that \( \eta \) is time-independent, then \( H \) is \( \eta \)-pseudo-Hermitian if and only if the pseudo-inner product \( \langle \langle \cdot, \cdot \rangle \rangle_\eta \) is a dynamical invariant. That is given any two solutions \( \psi_1(t) \) and \( \psi_2(t) \) of the Schrödinger equation, \( i \hbar d\psi/dt = H \psi \), \( \langle \langle \psi_1(t) | \psi_2(t) \rangle \rangle_\eta \) does not depend on time. If \( \eta \) depends on time, the pseudo-Hermiticity of \( H \) implies

\[
\frac{d}{dt} \langle \langle \psi_1(t) | \psi_2(t) \rangle \rangle_\eta(t) = \langle \psi_1(t) | \frac{d\eta(t)}{dt} \psi_2(t) \rangle = \langle \langle \psi_1(t) | \eta^{-1}(t) \frac{d\eta(t)}{dt} \psi_2(t) \rangle \rangle_\eta(t). \tag{3}
\]

**Theorem III:** Suppose \( H \) is a diagonalizable Hamiltonian with a discrete spectrum. Then the following are equivalent.

1. The eigenvalues of \( H \) are either real or come in complex-conjugate pairs. In this case we shall say that \( H \) has a pseudo-real spectrum.
2. \( H \) is pseudo-Hermitian.
3. \( H \) admits an antilinear symmetry generated by an invertible antilinear operator \( \mathcal{X} \), i.e., \( [H, \mathcal{X}] = 0 \).

**Theorem IV:** Suppose \( H \) is a diagonalizable Hamiltonian with a discrete spectrum. Then the following are equivalent.

1. \( H \) has a real spectrum,
2. \( H \) is \( O^†O \)-pseudo-Hermitian for an invertible operator \( O \).
3. \( H \) is related to a Hermitian operator by a similarity transformation. Following [22], in this case \( H \) is said to be quasi-Hermitian.
4. \( H \) is Hermitian with respect to a positive-definite inner product.
By definition an inner product $\langle \psi, \psi \rangle$ is said to be positive-definite if for all nonzero $\psi \in \mathcal{H}$, $\langle \psi|\psi \rangle > 0$. In this case $\psi$ is called a positive vector. Similarly, $\psi$ is called nonnegative, if $\langle \psi|\psi \rangle \geq 0$.

As elucidated in [15], for a given pseudo-Hermitian diagonalizable Hamiltonian $H$ the linear, Hermitian, invertible operators $\eta$ that make $H$ $\eta$-pseudo-Hermitian are, up to the choice of the eigenbasis of $H$, classified by a set of signs $\sigma_{n_0}$; $\eta$ has the general form

$$\eta = \sum_{n_0} \sigma_{n_0} |\phi_{n_0}\rangle \langle \phi_{n_0}| + \sum_{n+} (|\phi_{n+}\rangle \langle \phi_{n-}| + |\phi_{n-}\rangle \langle \phi_{n+}|) \tag{4}$$

where $n_0$, $n+$ and $n-$ are spectral labels associated with eigenvalues with zero, positive, and negative imaginary parts, $|\phi_n\rangle$, with $n = n_0, n+, n-$, are the eigenvectors of $H^\dagger$ that together with the eigenvectors $|\psi_n\rangle$ of $H$ form a complete biorthonormal system, i.e., they satisfy

$$\langle \phi_m|\psi_n \rangle = \delta_{mn}, \quad \sum_n |\psi_n\rangle \langle \phi_n| = 1 \tag{5}$$

Next, observe that in view of (4) and (5), we have $\langle \psi_{n_0}|\psi_{n_0} \rangle_{\eta} = \sigma_{n_0}$, and $\langle \psi_{n+}|\psi_{n+} \rangle_{\eta} = \langle \psi_{n-}|\psi_{n-} \rangle_{\eta} = 0$. Therefore, the eigenvectors with complex eigenvalues have zero pseudo-norm; they are null vectors. Furthermore, the choice $\sigma_{n_0} = +$ for all $n_0$ implies that all the basis vectors $|\psi_n\rangle$ are nonnegative. In particular, if the spectrum is real this choice for the signs $\sigma_{n_0}$ yields a basis for the Hilbert space consisting of positive vectors. This in turn implies that the inner product $\langle \psi, \psi \rangle_{\eta}$ is positive-definite. [19]. This is precisely the inner product whose existence is ensured by Theorem IV.

**Theorem V**: Suppose $H$ is a pseudo-Hermitian Hamiltonian with a discrete spectrum. Then the most general inner product with respect to which $H$ is Hermitian has the form $\langle \psi, \psi \rangle_{\tilde{\eta}}$, where $\tilde{\eta} := A^\dagger \eta A$, $A$ is an invertible linear operator commuting with $H$, and $\eta$ is given by (4). In particular, if the spectrum of $H$ is real, then the most general positive-definite inner product with respect to which $H$ is Hermitian has the form $\langle \psi, \psi \rangle_{\tilde{\eta}+}$, where

$$\tilde{\eta}+ := A^\dagger \eta+ A, \tag{6}$$

$$\eta+ := \sum_n |\phi_n\rangle \langle \phi_n|. \tag{7}$$

Furthermore, if $H$ is a time-independent Hamiltonian with a real discrete spectrum. Then $\langle \psi, \psi \rangle_{\tilde{\eta}+}$ is the most general invariant positive-definite inner product on the Hilbert space.
Here and also in [12, 13, 14, 15] we have given the relevant formulas for the cases that the spectrum of $H$ is discrete. If the spectrum happens not to be discrete we treat the spectral label $n$ as a continuous variable, replace the summations with integrations, and change the Kronecker deltas to Dirac deltas.

3 Invariant Inner Products for Klein-Gordon Fields

Consider the Klein-Gordon equation

$$-\ddot{\psi}(\vec{x}, t) + \nabla^2 \psi(\vec{x}, t) = \mu^2 \psi(\vec{x}, t), \quad (8)$$

where a dot means a derivative with respect to $x^0 := ct$, $c$ is the velocity of light, $\mu := m c / \hbar$, and $m$ is the mass of the Klein-Gordon field $\psi : \mathbb{R}^{3+1} \rightarrow \mathbb{C}$. We can express (8) in the form

$$\ddot{\psi}(\vec{x}, t) + D \psi(\vec{x}, t) = 0, \quad (9)$$

where $D := -\nabla^2 + \mu^2$. Now, introducing the two-component state vector $\Psi$ and the (effective) Hamiltonian $H$,

$$\Psi := \begin{pmatrix} \psi + i\lambda \dot{\psi} \\ \psi - i\lambda \dot{\psi} \end{pmatrix}, \quad H := \frac{1}{2} \begin{pmatrix} \lambda D + \lambda^{-1} & \lambda D - \lambda^{-1} \\ -\lambda D + \lambda^{-1} & -\lambda D - \lambda^{-1} \end{pmatrix}, \quad (10)$$

with $\lambda$ being an arbitrary nonzero real parameter, we may express the Klein-Gordon equation in the Schrödinger form $i\dot{\Psi} = H \Psi$, [23, 24]. It is not difficult to solve the eigenvalue problem for the Hamiltonian $H$, [23]. The eigenvectors $\Psi_{\vec{k}}$ and the corresponding eigenvalues $E_{\vec{k}}$ are given by

$$\Psi_{\vec{k}} = \begin{pmatrix} \lambda^{-1} + E_{\vec{k}} \\ \lambda^{-1} - E_{\vec{k}} \end{pmatrix} \phi_{\vec{k}}, \quad E_{\vec{k}} = \pm \sqrt{k^2 + \mu^2}, \quad (11)$$

where $\phi_{\vec{k}} := \langle \vec{x}|\vec{k} \rangle = (2\pi)^{-3/2} e^{i\vec{k} \cdot \vec{x}}$ and $\vec{k} \in \mathbb{R}^3$.

The Hamiltonian $H$ of [10] is not Hermitian with respect to the $L^2$ inner-product on the space of two-component state vectors. It is however easy to check that $H$ is $\sigma_3$-pseudo-Hermitian where $\sigma_3$ is the Pauli matrix diag$(1, -1)$. In view of Theorem III, the pseudo-Hermiticity of $H$ was to be expected as it is diagonalizable and has a real spectrum. The pseudo-inner product $\langle \ , \ \rangle_{\sigma_3}$ is nothing but the well-known Klein-Gordon inner product [23], for one can easily check that $\langle \Psi_1, \Psi_2 \rangle_{\sigma_3} = 2i\lambda (\psi_1^* \dot{\psi}_2 - \psi_2^* \dot{\psi}_1)$. Here the two-component state vectors $\Psi_i$ are related to one-component state vectors $\psi_i$ according to [10]. The invariance of the Klein-Gordon inner product may therefore be viewed as a manifestation of Theorem II. The much more interesting observation is that according to Theorem IV, $H$ must
be $\eta_+$-pseudo-Hermitian for a positive $\eta_+$ of the form $O^\dagger O$. The corresponding pseudo-inner product is in fact a positive-definite inner product. Then according to Theorems I and II, $H$ is Hermitian with respect to this new positive-definite inner product and that this inner product is invariant provided that $\eta_+$ does not depend on time. It is this inner product that we wish to construct for the effective Hamiltonian $H$ of (10).

Having obtained the eigenvectors $\Psi_{k}$ of this Hamiltonian, we can easily compute the biorthonormal dual vectors $\Phi_{k}$ and use (4) to obtain the positive operator $\eta_+$,

$$\Phi_{k} = \frac{1}{4} \left( \lambda + E_k^{-1} \right) \phi_{k},$$

$$\eta_+ = \frac{1}{8} \int d^3 k \left( \begin{array}{c} \lambda^2 + (k^2 + \mu^2)^{-1} \\ \lambda^2 - (k^2 + \mu^2)^{-1} \end{array} \right) |k\rangle \langle k|$$

$$= \frac{1}{8} \left( \begin{array}{cc} \lambda^2 + D^{-1} & \lambda^2 - D^{-1} \\ \lambda^2 - D^{-1} & \lambda^2 + D^{-1} \end{array} \right).$$

This in turn implies

$$\lambda^{-2} \langle \Psi_1|\Psi_2\rangle_{\eta_+} = \lambda^{-2} \langle \Psi_1|\eta_+\Psi_2\rangle = \frac{1}{2} \left( \int dx^3 \psi_1(\vec{x},t)^* \psi_2(\vec{x},t) + \int dk^3 \frac{\langle \psi_1|\vec{k}\rangle \langle \vec{k} |\psi_2\rangle}{k^2 + \mu^2} \right) =: \langle \psi_1, \psi_2 \rangle,$$

where we have denoted the $L^2$-inner product on the space of two-component state vectors by $\langle | \rangle$, made use of the first equation in (10) and (12), and introduced the inner product $\langle , \rangle$ on the set of solutions of the Klein-Gordon equation (8). As seen from (13), $\langle , \rangle$ is a positive-definite inner product. Furthermore, according to (12) $\eta_+$ is time-independent. Therefore, in view of Theorem II, $\langle | \rangle_{\eta_+}$ and consequently $\langle , \rangle$ are dynamical invariants.

One can perform the Fourier integral in (13) and obtain

$$\langle \psi_1, \psi_2 \rangle = \frac{1}{2} \left( \int dx^3 \psi_1(\vec{x},t)^* \psi_2(\vec{x},t) + \int dy^3 \dot{\psi}_1(\vec{x},t)^* G(\vec{x} - \vec{y}) \dot{\psi}_2(\vec{y},t) \right),$$

where $G(\vec{u}) := \exp(-\mu|\vec{u}|)/(4\pi|\vec{u}|)$ is a Green’s function for $D$. Indeed, it is not difficult to see that according to (13),

$$\langle \psi_1, \psi_2 \rangle = \frac{1}{2} \left( \langle \psi_1|\psi_2 \rangle + \langle \dot{\psi}_1|D^{-1}|\dot{\psi}_2 \rangle \right),$$

where $\langle | \rangle$ is the usual $L^2$-inner-product, $\langle \psi_1|\psi_2 \rangle := \int dx^3 \psi_1(\vec{x},t)^* \psi_2(\vec{x},t)$. The expression (15) for the inner-product $\langle , \rangle$ is quite convenient as it is manifestly positive-definite and invariant; taking the time-derivative of the right-hand side of (13) and using the Klein-Gordon equation (8) one finds zero.
Next, we make use of Theorem V to obtain a wide class of positive-definite inner product \( \langle \cdot, \cdot \rangle \) on the solution space \( \tilde{H} \) of the Klein-Gordon equation. Then, after a lengthy calculation \cite{17}, we find
\[
\langle \psi_1, \psi_2 \rangle = \frac{1}{2} \left[ \langle \psi_1 | L_+ | \psi_2 \rangle + \langle \psi_1 | L_+ D^{-1} | \dot{\psi}_2 \rangle + i \left( \langle \psi_1 | L_- D^{-1/2} | \dot{\psi}_2 \rangle - \langle \dot{\psi}_1 | L_- D^{-1/2} | \psi_2 \rangle \right) \right],
\]
where \( L_\pm \) are Hermitian linear operators acting in \( \tilde{H} \) such that \( A_\pm = L_+ \pm L_- \) are positive operators commuting with \( D \).

Expression (16) has two important properties. First, one can impose the physical condition of relativistic (Lorentz) invariance and find out that there is a one-parameter family of the inner products (16) that are relativistically invariant. And that the inner product obtained by Woodard in \cite{10} belongs to this family, \cite{17}. Second, one can explore the non-relativistic limit of these inner products and show that they indeed tend to the \( L^2 \)-inner product in this limit. This is a clear indication (besides the invariance and positivity properties) that one can use the inner-product \( \langle \cdot, \cdot \rangle \) to devise a probability interpretation for the Klein-Gordon fields.

Furthermore, one can proceed along the lines suggested in Theorem IV and similarity transform the Hamiltonian \cite{10} to a Hamiltonian that is Hermitian with respect to the \( L^2 \)-inner-product on the space of two-component state vectors. This provides the passage from the pseudo-unitary (or rather quasi-unitary) quantum mechanics defined by the Hamiltonian \cite{10} to the ordinary unitary quantum mechanics in the (spinorial) Hilbert space \( \mathbb{C}^2 \otimes L^2(\mathbb{R}^3) \). One can identify the observables in the latter and use the inverse of the similarity transformation to define the observables for the two-component Klein-Gordon fields. These are the \( \eta_+ \)-pseudo-Hermitian linear operators acting on the space of two-component state vectors. Because \( \eta_+ \) is a positive operator these observables have a real spectrum. Alternatively, one may define the Hilbert space \( \mathcal{H}_{KG} \) of single-component Klein-Gordon fields as the set of solutions \( \psi : \mathbb{R}^{3+1} \to \mathbb{C} \) of (5), equivalently the set of initial conditions, that have finite norm: \( \|(\psi | \psi)\|^{1/2} < \infty \), and identify the observables as linear operators \( O : \mathcal{H}_{KG} \to \mathcal{H}_{KG} \) that are Hermitian with respect to the inner product \( \langle \cdot, \cdot \rangle \). It should be emphasized that in the former approach neither the passage from the single to two-component state vectors nor the similarity transform that maps \( H \) to a Hermitian Hamiltonian is unique. As the physical content lies in the original single-component Klein-Gordon fields \( \psi \), one must only consider the observables whose expectation values are uniquely determined in terms of \( \psi \) (and \( \dot{\psi} \)). These will be the physical observables of the true quantum mechanics of Klein-Gordon fields and coincide with the linear Hermitian operators acting in \( \mathcal{H}_{KG} \). Note also that the nonuniqueness of the two-component form of the Klein-Gordon fields that we have
considered manifests in the presence of the arbitrary parameter $\lambda$. As we have argued in [25], this arbitrariness may be identified with a nonphysical gauge freedom.

An explicit construction of the observables for the Klein-Gordon fields is provided in [26]. A comprehensive treatment of the most general positive-definite inner product on the solution space of the more general class of Klein-Gordon-type fields, the fact that all these inner product are unitarily equivalent and define the same Hilbert space structure, and the nature of the observables for these fields are discussed in [27].

4 Hilbert Space Problem for Minisuperspace Wheeler-DeWitt Equation

Consider the Wheeler-DeWitt equation for a FRW minisuperspace model with a real massive scalar field,

$$
-\frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \varphi^2} + \kappa e^{4\alpha} - m^2 e^{6\alpha} \varphi^2 \psi(\alpha, \varphi) = 0,
$$

where $\alpha := \ln a$, $a$ is the scale factor, $\varphi$ is a real scalar field of mass $m$, $\kappa = -1, 0, 1$ determines whether the FRW model describes an open, flat, or closed universe, respectively, and we have chosen a particularly simple factor ordering and the natural units, [2, 5]. The Wheeler-DeWitt equation (17) is clearly a Klein-Gordon-type equation in $1 + 1$ dimensions. It can be written in the form (9), if we identify a derivative with respect to $\alpha$ by a dot and let

$$
D := -\frac{\partial^2}{\partial \varphi^2} + m^2 e^{6\alpha} \varphi^2 - \kappa e^{4\alpha}.
$$

In view of this identification we shall take $\alpha$ as the time-coordinate. Moreover, we can use (10) to obtain a two-component formulation for the Wheeler-DeWitt equation (17). Again the corresponding effective Hamiltonian is diagonalizable. Its eigenvectors $\Psi_{n\pm}$ and the corresponding eigenvalues $E_{n\pm}$ are given by [28]

$$
\Psi_{n\pm} = \left( \frac{\lambda^{-1} + E_{n\pm}}{\lambda^{-1} - E_{n\pm}} \right) \phi_n, \quad E_{n\pm} = \pm \sqrt{m e^{3\alpha} (2n + 1) - \kappa e^{4\alpha}},
$$

where $n = 0, 1, 2, \cdots$, $\phi_n := \langle \varphi | n \rangle = N_n H_n(m^{1/2} e^{3\alpha/2} \varphi) e^{-m e^{3\alpha} \varphi^2/2}$ are the energy eigenfunctions of a simple harmonic operator with unit mass and frequency $m e^{3\alpha}$, $H_n$ are Hermite polynomials, and $N_n := [m e^{3\alpha}/(\pi 2^n n!)^{1/2}]^{1/4}$ are normalization constants.

As seen from (19), the spectrum of $H$ is discrete and pseudo-real. Hence according to Theorem III, it is pseudo-Hermitian, [12]. In particular, it is $\sigma_3$-pseudo-Hermitian. The indefinite inner-product $\langle \cdot, \cdot \rangle_{\sigma_3}$ is the invariant Klein-Gordon inner product that is often
used in the probability interpretation of the semiclassical Wheeler-DeWitt fields. Also note that for the open and flat universes the spectrum of $H$ is real. Therefore, $H$ is quasi-Hermitian and there is a positive linear Hermitian invertible operator $\eta_+$ such that $H$ is $\eta_+$-pseudo-Hermitian. In fact, $\eta_+$ is given by Eq. (12) where $D$ has the form (18).

Following the above treatment of the Klein-Gordon equation, we can use this $\eta_+$ to obtain a positive-definite inner product on the space of the Wheeler-DeWitt fields. The latter is given by Eq. (15) where the $L^2$-inner product has the form $\langle \psi_1 | \psi_2 \rangle := \int_{-\infty}^{\infty} d\varphi \psi_1(\alpha, \varphi)^* \psi_2(\alpha, \varphi)$. Eq. (15) involves the inverse of $D$ which is well-defined for the open and flat universes where $\kappa = -1$ or 0. For these cases, $D^{-1} = \sum_{n=0}^{\infty} [m e^{3a}(2n + 1) - \kappa e^{4a}]^{-1} |n\rangle \langle n|$. For the closed universe the above construction works only for $a = e^a < m$ where all the eigenvalues are real. For $a > m$, the complex-conjugate imaginary eigenvalues are also present and the corresponding eigenvectors will be null.

For the cases that the spectrum is real ($H$ is quasi-Hermitian), we can follow the statement of Theorem IV to perform a similarity transformation to map the effective Hamiltonian to a Hamiltonian that is Hermitian in the $L^2$-inner product on the space of two-component state vectors, i.e., $\mathbb{C}^2 \otimes L^2(\mathbb{R})$. This is in complete analogy with the case of Klein-Gordon equation (8). However, there is an important distinction between the Klein-Gordon equation (8) and the Wheeler-DeWitt equation (17), namely that for the latter equation the operators $D$ and $\eta_+$ are ‘time-dependent.’ This in particular means that the associated positive inner product $\langle \ , \ \rangle$ is not invariant. Instead, as a consequence of (3) or alternatively (15) and (9), it satisfies,

$$\frac{d}{d \alpha} \langle \psi_1, \psi_2 \rangle = \frac{1}{2} \langle \psi_1 | d(D^{-1}) | \psi_2 \rangle.$$

Note that the similarity transformation that maps $H$ into a Hermitian effective Hamiltonian is ‘time-dependent’ as well. This makes it fail to preserve the form of the associated Schrödinger equation, i.e., it is not a pseudo-canonical transformation [14]. Therefore, although this similarity transformation may be used to related the observables of the two systems, they do not relate the solutions of the corresponding Schrödinger equations.

In Ref. [17], we have outlined a method to define a unitary quantum evolution for the cases that the Hilbert space has a time-dependent inner product structure. Using this method and the above results for time-independent Hamiltonians, one can obtain the general form of an invariant positive-definite inner product on the solution space of the Wheeler-DeWitt equation (17) for the case of a flat or open universe or when the initial value of the scale factor $a$ is less than $m$. A rather comprehensive treatment is provided in [27].
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