Quantum Mechanics of Klein-Gordon-Type Fields and Quantum Cosmology

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Abstract

With a view to address some of the basic problems of quantum cosmology, we formulate the quantum mechanics of the solutions of a Klein-Gordon-type field equation: 
\[(\partial_t^2 + D)\psi(t) = 0,\] 
where \(t \in \mathbb{R}\) and \(D\) is a positive-definite operator acting in a Hilbert space \(\tilde{\mathcal{H}}\). In particular, we determine all the positive-definite inner products on the space \(\mathcal{H}\) of the solutions of such an equation and establish their physical equivalence. This specifies the Hilbert space structure of \(\mathcal{H}\) uniquely. We use a simple realization of the latter to construct the observables of the theory explicitly. The field equation does not fix the choice of a Hamiltonian operator unless it is supplemented by an underlying classical system and a quantization scheme supported by a correspondence principle. In general, there are infinitely many choices for the Hamiltonian each leading to a different notion of time-evolution in \(\mathcal{H}\). Among these is a particular choice that generates \(t\)-translations in \(\mathcal{H}\) and identifies \(t\) with time whenever \(D\) is \(t\)-independent. For a \(t\)-dependent \(D\), we show that regardless of the choice of the inner product the \(t\)-translations do not correspond to unitary evolutions in \(\mathcal{H}\), and \(t\) cannot be identified with time. We apply these ideas to develop a formulation of quantum cosmology based on the Wheeler-DeWitt equation for a Friedman-Robertson-Walker model coupled to a real scalar field with an arbitrary positive confining potential. In particular, we offer a complete solution of the Hilbert space problem, construct the observables, use a position-like observable to introduce the wave functions of the universe (which differ from the Wheeler-DeWitt fields), reformulate the corresponding quantum theory in terms of the latter, reduce the problem of the identification of time to the determination of a Hamiltonian operator acting in \(L^2(\mathbb{R}) \oplus L^2(\mathbb{R})\), show that the factor-ordering problem is irrelevant for the kinematics of the quantum theory, and propose a formulation of the dynamics. Our method is based on the central postulates of nonrelativistic quantum mechanics, especially the quest for a genuine probabilistic interpretation and a unitary Schrödinger time-evolution. It generalizes to arbitrary minisuperspace (spatially homogeneous) models and provides a way of unifying the two main approaches to the canonical quantum cosmology based on these models, namely quantization before and after imposing the Hamiltonian constraint.

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1 Introduction

The problem of applying the machinery of nonrelativistic quantum mechanics to Klein-Gordon fields has been a subject of interest since late 1920s. It was this problem that led Dirac to the discovery of the wave equation for the electron and the formulation of the method of second quantization. These form the main ingredients of the modern theories of elementary particle physics. The very same problem also arises in canonical quantum gravity \[1\] and in particular quantum cosmology where the trick of considering a first order field equation such as Dirac’s or using the method of second quantization does not provide a satisfactory description \[2, 3, 4\].

It is ironic that despite its enormous impact on the formulation and resolution of a number of fundamental problems of theoretical physics, a satisfactory solution of this problem has been out of reach. The purpose of this article is two-fold. First, it aims at providing a complete solution of the above-mentioned problem for the class of linear field equations of the form

\[
\ddot{\psi}(t) + D\psi(t) = 0, \tag{1}
\]

where \( t \in \mathbb{R} \), a dot denotes a \( t \)-derivative, and \( D : \mathcal{H} \to \mathcal{H} \) is a possibly \( t \)-dependent Hermitian operator acting in a Hilbert space \( \mathcal{H} \) from which one selects the values \( \psi(t) \) of the field \( \psi \), alternatively the initial values of the field \( \psi_0 \) and its \( t \)-derivative \( \dot{\psi}_0 \) at an initial value \( t_0 \) of \( t \).

Second, it employs the resulting theory to devise a formulation of the minisuperspace quantum cosmology that allows for a genuine probabilistic interpretation and a unitary Schrödinger time-evolution.

Equation (1) is a simple generalization of the free Klein-Gordon equation, for the latter corresponds to the choice:

\[
t = \text{time}, \quad \mathcal{H} = L^2(\mathbb{R}^3), \quad D = -\nabla^2 + \mu^2, \tag{2}
\]

where \( \mu := mc/\hbar \) and \( m \) is the mass of the Klein-Gordon field. Therefore, following Ref. \[5\], we call (1) (respectively its solutions \( \psi \)) a Klein-Gordon-type field equation (respectively Klein-Gordon-type fields). The Wheeler-DeWitt equation for a number of minisuperspace cosmological models \[6\] also provides a family of Klein-Gordon-type equations. A well-known example is the Wheeler-DeWitt equation associated with a Friedman-Robertson-Walker (FRW) model coupled to a real scalar field \[7, 8, 9, 10\]:

\[
\left[ -\frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \varphi^2} + \kappa e^{4\alpha} - e^{6\alpha} V(\varphi) \right] \psi(\alpha, \varphi) = 0, \tag{3}
\]

where \( \alpha := \ln a \), \( a \) is the scale factor, \( V = V(\varphi) \) is a real-valued potential for the field \( \varphi \), \( \kappa = -1, 0, 1 \) 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 \[11, 10\]. We can write the Wheeler-DeWitt equation (3) in the form (11), if we identify \( \alpha \) with the variable \( t \), set \( \tilde{H} = L^2(\mathbb{R}) \) and \( D = -\partial^2_\varphi + e^{6\alpha}V(\varphi) - \kappa e^{4\alpha} \). Clearly \( D \) is a Hermitian operator acting in \( L^2(\mathbb{R}) \).

The identification of the Wheeler-DeWitt equation for various minisuperspace models with certain Klein-Gordon-type field equations marks the significance of devising a genuine quantum mechanical treatment of a general Klein-Gordon-type field. This requires the identification of an appropriate Hilbert space (a vector space endowed with a complete positive-definite inner product) that determines the kinematics and a Hermitian Hamiltonian operator that governs the dynamics of the corresponding theory.

The natural choice for the vector space structure of the Hilbert space is the solution space of the corresponding Klein-Gordon-type field equation \[12\]. Endowing this vector space with an ‘appropriate’ positive-definite inner product is a more difficult task. In Ref. \[5\], we constructed a class of positive-definite inner products on the solution space \( \mathcal{H} \) of a Klein-Gordon-type equation. In this article, we give a direct argument clarifying the extent of the generality of the results of \[5\]. In particular, we address the problem of finding the most general positive-definite inner product on \( \mathcal{H} \) that turns it into a Hilbert space. We show that the corresponding Hilbert spaces are physically equivalent. Furthermore, for various choices of the inner product (various realizations of the Hilbert space structure), we discuss in great detail the nature and construction of the possible Hamiltonian operators and other observables of the corresponding quantum systems. The choice of a Hamiltonian operator determines what we mean by ‘time-evolution.’ We show that, similarly to nonrelativistic quantum mechanics, this choice is by no means unique unless one identifies a corresponding classical system and employs a quantization scheme (with specific operator-ordering prescription in canonical quantization or choice of the ‘measure’ in the path-integral quantization).

A direct application of our general results in minisuperspace quantum cosmology provides a way of decoupling the Hilbert space problem and the problem of time. It leads to a resolution of the former and suggests how one should approach the latter. It further shows that the factor-ordering ambiguity associated with the Wheeler-DeWitt equation does not affect the kinematical structure of the corresponding quantum theory. Another remarkable consequence of our method is that in a sense it unifies the two main approaches to the canonical quantization of gravity, namely quantization before and after imposing the constraints \[3\].

The article is organized as follows. In Section 2, we provide a brief review of the results of Ref. \[5\]. In Section 3, we construct the most general positive-definite inner product on \[1\] We will avoid identifying \( \alpha = t \) with a physical time variable. We will show that this choice violates unitarity!
the solution space of a Klein-Gordon-type equation. In Section 4, we study a special class of
Klein-Gordon-type fields, qualified as being stationary, give various equivalent descriptions of
the quantum mechanics for this class, explore the corresponding Hamiltonians, and construct
the observables. In Section 5, we extend the results of Section 4 to general (nonstationary)
Klein-Gordon-type fields. In Section 6, we demonstrate the application of our general results
in the study of the quantum mechanics on the solution space of the equation of motion for a
classical (possibly time-dependent) harmonic oscillator. A particular example of the latter is
the Wheeler-DeWitt equation for a FRW cosmological model with a cosmological constant. In
section 7, we consider the FRW models coupled to a real scalar field with an arbitrary positive
confining potential \( V \). We develop the corresponding quantum cosmology, i.e., construct a
positive-definite inner product on the physical Hilbert space of the solutions of the Wheeler-
DeWitt equation \( \Psi \), define a set of basic observables, introduce a position-like basis for the
Hilbert space and use it to define a wave function \( f \) associated with every Wheeler-DeWitt field
\( \psi \). Using the fact that in our approach Wheeler-DeWitt fields \( \psi \) are treated as vectors belonging
to the abstract Hilbert space \( \mathcal{H} \) of the theory, we explain the conceptual difference between the
functions \( \psi(\alpha, \varphi) \) appearing in the Wheeler-DeWitt equation \( \Psi \) and the wave functions \( f \) that
assign the coefficients of the Wheeler-DeWitt fields \( \psi \) in the position-like basis. This suggests
that it is the wave functions \( f \) that should be identified with the ‘wave functions of the universe’
not the functions \( \psi(\alpha, \varphi) \). We give a formulation of the kinematics and the dynamics in terms
of these wave functions, and reduce the problem of the identification of time to the issue of
selecting a Hamiltonian operator (a linear Hermitian operator) acting in the space \( L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \)
of the wave functions \( f \). Following Dirac’s canonical quantization program, we then argue that
the Hamiltonian operator is to be obtained by quantizing a classical Hamiltonian that governs
the classical ‘dynamics’ of the system after imposing the classical constraint. This requires
the identification of the position-like operator with the quantum analog of a specific classical
observable and a choice for a classical time. The quantization after imposing the constraint
provides the physical meaning of the wave functions of the universe. It is supported by an
analog of the correspondence principle of nonrelativistic quantum mechanics that relates a
quantum system to its classical counterpart. Finally in Section 8, we offer a survey of our main
results and present our concluding remarks. The Appendix includes the calculations that are
useful but not of primary interest.

Throughout this article, we identify the separable Hilbert space defined by an inner product
with the Cauchy completion of the corresponding inner product space and view the operators
acting in this Hilbert space as densely defined \([13]\). Furthermore, we use the terms ‘self-adjoint’
and ‘Hermitian’ interchangeably. One must account for the difference whenever the domain of
the corresponding operator is a proper subset of the Hilbert space \([13]\). This leads to a similar
type of technical complications that are already present in nonrelativistic quantum mechanics and can be dealt with similarly \[14\].

2 Hilbert Space Problem for Klein-Gordon-Type Fields

In order to construct a quantum mechanics of a Klein-Gordon-type field, one needs to promote the vector space

\[ \mathcal{H} := \left\{ \psi : \mathbb{R} \to \tilde{\mathcal{H}} \mid \ddot{\psi}(t) + D\psi(t) = 0 \right\} \] (4)

of solutions of the field equation (1) to a Hilbert space, i.e., construct a positive-definite inner product on \( \mathcal{H} \). One way of doing this is to construct an inner product \( \langle \cdot, \cdot \rangle \) on \( \mathcal{H} \) using the inner product \( \langle \cdot, \cdot \rangle \) on \( \tilde{\mathcal{H}} \), i.e., define the inner product \( \langle \psi, \phi \rangle \) of a pair of fields \( \psi, \phi \in \mathcal{H} \) in terms of their values \( \psi(t) \) and \( \phi(t) \) that belong to \( \tilde{\mathcal{H}} \).

It is very easy to choose an expression involving \( \psi(t) \) and \( \phi(t) \) that satisfies the defining axioms of an inner product. More difficult is to make sure that such an expression yields a well-defined function \( \langle \cdot, \cdot \rangle : \mathcal{H}^2 \to \mathbb{C} \), i.e., a pair \( \psi, \phi \in \mathcal{H} \) determines \( \langle \psi, \phi \rangle \) uniquely. For example consider setting

\[ \langle \psi, \phi \rangle = \langle \psi(t) | \phi(t) \rangle + \lambda^2 \langle \dot{\psi}(t) | \dot{\phi}(t) \rangle \] (5)

where \( \langle \cdot, \cdot \rangle \) is the inner product of \( \tilde{\mathcal{H}} \) and \( \lambda \in \mathbb{R} - \{0\} \) is a constant having the dimension of \( t \). This expression satisfies all the requirements of an inner product for every choice of \( t \). Yet it fails to yield a well-defined inner product on \( \mathcal{H} \), for one can check by differentiating the right-hand side of (5) that it depends on \( t \). The above method of constructing inner products on \( \mathcal{H} \) will be effective, if despite the explicit appearance of the variable \( t \) in the expression for \( \langle \psi, \phi \rangle \) the latter does not depend on \( t \), i.e., one obtains the same value for any choice of \( t \).

In Ref. \[5\], we employ the above method of using the Hilbert space structure of \( \tilde{\mathcal{H}} \) to construct a class of inner products on \( \mathcal{H} \) for the cases that the value of \( D \) at \( t_0 \) is a positive-definite operator.\[4\] In this article we shall again suppose that \( D \) satisfies this condition. We will comment on the Klein-Gordon-type equations that violate this condition in Section 3.

\[3\]See Ref. \[14\] for a straightforward treatment of the issue of domains in the context of the theory of pseudo-Hermitian operators that is used in Ref. \[5\] and the present work.

\[4\]If one sets \( \lambda = 0 \) in (5), this equation violates the condition that if the norm of a vector vanishes then that vector must be the zero vector. This is because there are nonzero solutions of (1) that vanish at a given \( t \). This problem does not arise for \( \lambda \neq 0 \), because for a nonzero Klein-Gordon-type field the value of the field and its \( t \)-derivative cannot simultaneously vanish.

\[4\]A linear operator is said to be positive-definite if it is a Hermitian (self-adjoint) operator with a positive spectrum. In particular, it is an invertible operator.
If the operator $D$ does not depend on $t$, we will call the field equation (1) (respectively the field $\psi$) stationary. A typical example is the free Klein-Gordon equation (2).

The unique solution of a Klein-Gordon-type equation (1) fulfilling the initial conditions

$$\psi(t_0) = \psi_0, \quad \dot{\psi}(t_0) = \dot{\psi}_0,$$  

is

$$\psi(t) = C(t, t_0)\psi_0 + S(t, t_0)\dot{\psi}_0,$$  

where $C(t, t_0)$ and $S(t, t_0)$ are a pair of linear operators acting in $\tilde{\mathcal{H}}$ and satisfying

$$\ddot{C}(t, t_0) + DC(t, t_0) = 0, \quad C(t_0, t_0) = 1, \quad \dot{C}(t_0, t_0) = 0,$$  

$$\ddot{S}(t, t_0) + DS(t, t_0) = 0, \quad S(t_0, t_0) = 0, \quad \dot{S}(t_0, t_0) = 1.$$  

Here 1 stands for the identity operator of $\tilde{\mathcal{H}}$. If the Klein-Gordon-type equation is stationary, we can easily solve (8) and (9) and obtain

$$C(t, t_0) = \cos\left(\frac{t-t_0}{2}\right) \sum_{\ell=0}^{\infty} \frac{(-1)^\ell(t-t_0)^{2\ell}}{(2\ell)!} D^\ell,$$  

$$S(t, t_0) = \sin\left(\frac{t-t_0}{2}\right) \sum_{\ell=0}^{\infty} \frac{(-1)^\ell(t-t_0)^{2\ell+1}}{(2\ell+1)!} D^\ell.$$  

For a stationary Klein-Gordon-type field with a positive-definite $D$, the positive-definite inner products constructed in (5) have the form

$$\langle \langle \psi_1, \psi_2 \rangle \rangle = \frac{1}{2} \left[ \langle \psi_1(t) | L^+_+ \psi_2(t) \rangle + \langle \dot{\psi}_1(t) | L^+_+ D^{-1} \dot{\psi}_2(t) \rangle + i \langle \psi_1(t) | L^- D^{-1/2} \dot{\psi}_2(t) \rangle - \langle \dot{\psi}_1(t) | L^- D^{-1/2} \dot{\psi}_2(t) \rangle \right],$$  

where $\psi_1, \psi_2 \in \mathcal{H}$, $\langle \cdot | \cdot \rangle$ is the inner product of $\tilde{\mathcal{H}}$, and $L^\pm$ are Hermitian operators acting in $\tilde{\mathcal{H}}$ such that $A^\pm := L^+ \pm L^-$ are positive-definite operators commuting with $D$. For a nonstationary Klein-Gordon-type field, one can construct a class of inner products on $\mathcal{H}$ that depend on the choice of $t_0$, i.e., an initial value of $t$. They have the form

$$\langle \langle \psi_1, \psi_2 \rangle \rangle_{t_0} := \langle \langle \psi_1, \psi_2 \rangle \rangle|_{t=t_0},$$  

where the expression on the right-hand side is obtained by evaluating (12) at $t_0$.

The construction of the inner products (12) is a direct consequence of the following two basic principles.

(I) As a vector space, the Hilbert space $\mathcal{H}$ has a dual interpretation, namely as the space of solutions $\psi$ of the field equation (1) and as the space of all possible initial data $(\psi_0, \dot{\psi}_0)$ for this equation.
(II) In order to identify $\mathcal{H}$ with the Hilbert space of state vectors for a quantum system (admitting a probability interpretation), the inner product that turns $\mathcal{H}$ into a Hilbert space must be positive-definite.

(I) follows from the linearity of the field equation (1) which implies that as a vector space $\mathcal{H}$ is isomorphic to the space $\tilde{\mathcal{H}}^2$ of the initial data $(\psi_0, \dot{\psi}_0)$ or equivalently the space $\mathcal{H} \otimes \mathbb{C}^2$ of the two-component state vectors

$$\Psi_0 := \Psi(t_0),$$

where $\Psi$ is the two-component field

$$\Psi := \begin{pmatrix} \psi + i\lambda \dot{\psi} \\ \psi - i\lambda \dot{\psi} \end{pmatrix},$$

(15)

$\lambda \in \mathbb{R} - \{0\}$ is an arbitrary parameter\footnote{\lambda belongs to the subgroup $GL(1, \mathbb{R})$ of a $GL(2, \mathbb{C})$ symmetry group of the two-component formulation of the Klein-Gordon-type field equations, \[16\].} having the dimension of $t$, $\psi \in \mathcal{H}$, and $\dot{\psi} : \mathbb{R} \to \tilde{\mathcal{H}}$ is defined by $\dot{\psi}(t) = \frac{d}{dt}\psi(t)$.

The identification of $\mathcal{H}$ with $\tilde{\mathcal{H}} \otimes \mathbb{C}^2$ leads to the idea of employing a two-component Schrödinger formulation of the Klein-Gordon-type fields, \[17, 18\]. Using the two-component fields (15) and the Hamiltonian

$$H = \frac{\hbar}{2} \begin{pmatrix} \lambda D + \lambda^{-1} & \lambda D - \lambda^{-1} \\ -\lambda D + \lambda^{-1} & -\lambda D - \lambda^{-1} \end{pmatrix},$$

(16)

we can express the field equation (1) as the Schrödinger equation

$$i\hbar \dot{\Psi}(t) = H \Psi(t).$$

(17)

The values $\Psi(t)$ of the two-component field $\Psi$ belong to $\tilde{\mathcal{H}} \otimes \mathbb{C}^2$. If we endow the latter with the inner product $\langle \cdot, \cdot \rangle$ defined by

$$\langle \xi, \zeta \rangle = \sum_{a=1}^{2} \langle \xi^a | \zeta^a \rangle,$$

(18)

for all

$$\xi =: \begin{pmatrix} \xi^1 \\ \xi^2 \end{pmatrix}, \zeta =: \begin{pmatrix} \zeta^1 \\ \zeta^2 \end{pmatrix} \in \tilde{\mathcal{H}} \otimes \mathbb{C}^2,$$

and denote the corresponding Hilbert space, namely $\tilde{\mathcal{H}} \oplus \tilde{\mathcal{H}}$, by $\mathcal{H}_*$, we can view $\Psi(t)$ as elements of $\mathcal{H}_*$ and identify $H$ with a linear operator acting in $\mathcal{H}_*$. In this article, we will confine our
attention to the two-component state vectors that belong to $H_*$ (have finite $\langle \cdot, \cdot \rangle$-norm) and will define the adjoint $T^\dagger$ of any linear operator $T$ acting in $\mathcal{H} \otimes \mathbb{C}^2$ using the inner product \[13\]. Following this convention, we can easily show that the Hamiltonian \[16\] satisfies

\[ H^\dagger = \sigma_3 H \sigma_3, \] \[19\]

where $\sigma_3$ is the diagonal Pauli matrix (See \[35\] below.) Noting that $\sigma_3^{-1} = \sigma_3$ and recalling that a linear operator $H$ is said to be pseudo-Hermitian if there is an invertible, Hermitian, linear operator $\eta$ such that $H^\dagger = \eta H \eta^{-1}$, we see that the Hamiltonian \[16\] is pseudo-Hermitian.

Moreover, using the assumption that $D$ is a positive-definite operator, we can easily check that $H$ is diagonalizable and has a real spectrum. These observations together with (II) above suggest the use of the characterization theorems of Refs. \[19, 20, 21, 22\] to construct positive-definite inner products $\langle \langle \cdot | \cdot \rangle \rangle_\tilde{\eta}$ on $\mathcal{H} \otimes \mathbb{C}^2$ that are invariant under the time-evolution generated by the Hamiltonian $H$. The equivalence of $\mathcal{H} \otimes \mathbb{C}^2$ with $\mathcal{H}$ then leads one to use the inner products $\langle \langle \cdot | \cdot \rangle \rangle_\eta$ to construct the inner products \[12\] and subsequently \[13\]. In the remainder of this section we sketch the derivation of \[12\] as given in Ref. \[5\]. This allows us to fix the notation and introduce the necessary tools that we will use in the rest of the article.

First, we recall that as any inner product on $\mathcal{H} \otimes \mathbb{C}^2$, $\langle \langle \cdot | \cdot \rangle \rangle_\tilde{\eta}$ may be expressed in the form \[23\]:

\[ \langle \langle \xi | \zeta \rangle \rangle_\tilde{\eta} = \langle \xi, \tilde{\eta} \zeta \rangle, \] \[20\]

where $\xi, \zeta \in \mathcal{H} \otimes \mathbb{C}^2$ and $\tilde{\eta}$ is a positive-definite operator acting in $\mathcal{H} \otimes \mathbb{C}^2$.

Consider a stationary Klein-Gordon-type field, where $D$ and $H$ are $t$-independent. Then supposing that the operator $\tilde{\eta}$ and consequently the inner product \[20\] do not depend on $t$, one can show \[19, 5\] that the requirement of the invariance ($t$-independence) of $\langle \langle \Psi(t) | \Phi(t) \rangle \rangle_\tilde{\eta}$, for any two solutions $\Psi(t), \Phi(t)$ of the Schrödinger equation \[17\], is equivalent to the condition:

\[ H^\dagger = \tilde{\eta} H \tilde{\eta}^{-1}, \] \[21\]

i.e., $H$ is $\tilde{\eta}$-pseudo-Hermitian \[19\]. According to Refs. \[21, 24\], any positive-definite operator $\tilde{\eta}$ fulfilling \[21\] may be expressed in the form

\[ \tilde{\eta} = \sum_\nu |\tilde{\Phi}_\nu\rangle \langle \tilde{\Phi}_\nu|, \] \[22\]

where $|\tilde{\Phi}_\nu\rangle$ form a complete set of eigenvectors of $H^\dagger$, $\nu$ is a spectral label\(^6\), and for all $\xi, \zeta \in \mathcal{H} \otimes \mathbb{C}^2$, $|\xi\rangle \langle \zeta|$ acts on two-component vectors $\chi \in \mathcal{H} \otimes \mathbb{C}^2$ according to

\[ |\xi\rangle \langle \zeta| \chi = \langle \zeta, \chi \rangle \xi. \] \[23\]

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\(^6\)The summation over $\nu$ means a summation over the discrete spectrum and an integration over the continuous spectrum.
The eigenvalue problem for $H$ and $H^\dagger$ is easily solved \[16, 5\]. The common eigenvalues of $H$ and $H^\dagger$ are

$$E_{\pm,n} = \pm \hbar \omega_n,$$

where $\omega_n$ are the positive square root of the eigenvalues $\omega_n^2 \in \mathbb{R}^+$ of $D$. A set of eigenvectors of $H$ and $H^\dagger$ are respectively given by

$$\Psi_{\pm,n} = \begin{pmatrix} \lambda^{-1} \pm \omega_n \\ \lambda^{-1} \mp \omega_n \end{pmatrix} \phi_n, \quad \Phi_{\pm,n} = \frac{1}{4} \begin{pmatrix} \lambda \pm \omega_n^{-1} \\ \lambda \mp \omega_n^{-1} \end{pmatrix} \phi_n,$$

where $\phi_n$ form a complete set of orthonormal eigenvectors of $D$, i.e.,

$$D \phi_n = \omega_n^2 \phi_n, \quad \langle \phi_n | \phi_n \rangle = \delta_{n,n}, \quad \sum_n |\phi_n \rangle \langle \phi_n| = 1.$$  \hfill (25)

One can check that $\Psi_{\pm,n}$ and $\Phi_{\pm,n}$ form a complete biorthonormal system of eigenvectors of $H$ and $H^\dagger$, i.e., they satisfy

$$H \Psi_{\epsilon,n} = E_{\epsilon,n} \Psi_{\epsilon,n}, \quad H^\dagger \Phi_{\epsilon,n} = E_{\epsilon,n} \Phi_{\epsilon,n},$$

$$\langle \Phi_{\epsilon,n} | \Psi_{\epsilon',n'} \rangle = \delta_{\epsilon,\epsilon'} \delta_{n,n'}, \quad \sum_\epsilon \sum_n |\Psi_{\epsilon,n} \rangle \langle \Phi_{\epsilon,n}| = 1.$$ \hfill (27)

Furthermore, because any other complete set of eigenvectors of $H^\dagger$ may be obtained from $\Phi_{\pm,n}$ through the action of an invertible operator $B$ that commutes with $H^\dagger$, we can express the most general positive-definite operator $\tilde{\eta}$ satisfying (21) as

$$\tilde{\eta} = A^\dagger \eta_+ A,$$ \hfill (30)

where $A = B^\dagger$ is an invertible linear operator commuting with $H$, \[5, 22\]. The latter condition implies that

$$A = \sum_\epsilon \sum_n a_{\epsilon,n} |\Psi_{\epsilon,n} \rangle \langle \Phi_{\epsilon,n}|,$$ \hfill (31)

for some nonzero complex numbers $a_{\epsilon,n}$.\footnote{The eigenvalues $\omega_n^2$ of $D$ may be degenerate. Here we suppress the degeneracy labels and allow for $\omega_n^2$ with different $n$ to coincide.}
In view of (25), we can express the operator $A$ in terms of $D$ and its eigenvectors $\phi_n$ directly. This results in

$$A = A_+ + A_- A',$$

where

$$A_\pm := \frac{1}{2} \sum_n (a_{+,n} \pm a_{-,n}) |\phi_n\rangle \langle \phi_n| \sigma_0,$$

$$A' := \frac{1}{2} \left[ (\sigma_3 + i\sigma_2) \lambda D^{1/2} + (\sigma_3 - i\sigma_2) \lambda^{-1} D^{-1/2} \right],$$

$\sigma_0$ is the $2 \times 2$ unit matrix, and $\sigma_1 = \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right)$, $\sigma_2 = \left( \begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right)$, $\sigma_3 = \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right)$, are the Pauli matrices. Now, substituting (32) and (29) in (30), and carrying out the necessary calculations, we find

$$\tilde{\eta} = \frac{1}{8} \left( \begin{array}{cc} L_+(\lambda^2 + D^{-1}) + 2\lambda L_- D^{-1/2} & L_+ (\lambda^2 - D^{-1}) \\ L_+ (\lambda^2 - D^{-1}) & L_+ (\lambda^2 + D^{-1}) - 2\lambda L_- D^{-1/2} \end{array} \right),$$

where

$$L_\pm := \frac{1}{2} \sum_n (|a_{+,n}|^2 \pm |a_{-,n}|^2) |\phi_n\rangle \langle \phi_n|.$$  

Finally, introducing

$$\langle (\psi_1, \psi_2) \rangle := \lambda^{-2} \langle \Psi_1(t) | \Psi_2(t) \rangle \tilde{\eta},$$

in which $\Psi_i$ are related to $\psi_i$ according to (15), and using (20), we arrive at the expression (12).

One can use the field equation (11) to check that the $t$-derivative of the right-hand side of (12) vanishes identically. Therefore, $\langle (\cdot, \cdot) \rangle$ is a well-defined inner product on $\mathcal{H}$. It can be evaluated at any value of $t$, e.g., at $t_0$:

$$\langle (\psi_1, \psi_2) \rangle = \lambda^{-2} \langle \Psi_1(t_0) | \Psi_2(t_0) \rangle \tilde{\eta}. $$

For a nonstationary Klein-Gordon-type field, $D$ and $H$ depend on $t$. In this case the right-hand side of (12) fails to be $t$-independent, and this relation does not provide a well-defined inner product on $\mathcal{H}$. But there is a well-defined positive-definite inner product on $\mathcal{H}$ which reduces to (12) for the cases where $D$ is $t$-independent [5]. This inner product turns out to be given by a direct generalization of (39), namely (13). It is well-defined provided that a choice of $t_0$ is made. We will elaborate on the general positive-definite inner products on the solution space of nonstationary Klein-Gordon-type fields in Section 3.
Each choice of a positive-definite inner product on $\mathcal{H}$ determines a quantum mechanics of the corresponding Klein-Gordon-type field. The quantum observables are the linear operators $o: \mathcal{H} \to \mathcal{H}$ that are Hermitian with respect to the chosen inner product. A quantum system associated with a Klein-Gordon-type field is uniquely determined by the choice of the Hilbert space (a positive-definite inner product on) $\mathcal{H}$ and an observable called the Hamiltonian. The results reported in Ref. [5] solve the Hilbert space problem for a Klein-Gordon-type field. But they do not explain how one should fix a particular inner product on $\mathcal{H}$. Neither do they provide an explicit construction of the observables or describe the form and meaning of the possible Hamiltonians. The present article aims at addressing these issues. The first step in this direction is to determine the most general positive-definite inner product on $\mathcal{H}$.

3 General Form of an Inner Product on $\mathcal{H}$

In standard nonrelativistic canonical quantum mechanics, the Hilbert space is (up to its dimension if it is finite-dimensional) unique. This follows from the fact that any two separable Hilbert spaces (with the same dimension if they are finite-dimensional) are related by a unitary transformation [13]. Yet in order to specify a physical system one must fix the Hilbert space $\mathcal{H}$ and specify a Hamiltonian operator $H: \mathcal{H} \to \mathcal{H}$. A pair $(\mathcal{H}, H)$ determines a quantum system uniquely, but a quantum system may be described by different (actually infinitely many pairs) $(\mathcal{H}, H)$.

Let $\mathcal{H}_i$, with $i \in \{1, 2\}$, be Hilbert spaces with inner products $\langle \cdot, \cdot \rangle_i$, $H_i: \mathcal{H}_i \to \mathcal{H}_i$ be Hermitian operators, and $S_i$ be the quantum system determined by the pair $(\mathcal{H}_i, H_i)$. Suppose that there exists a time-independent unitary linear transformation $^8 U: \mathcal{H}_1 \to \mathcal{H}_2$ such that $H_2 = U H_1 U^{-1}$. Then $S_1$ and $S_2$ are physically equivalent, i.e., there is a one-to-one correspondence between the states and observables of $S_1$ and $S_2$ such that all the physically measurable quantities, namely the transition amplitude between the states and the expectation values of the observables, are invariant under this correspondence. Clearly, the observables $O_2: \mathcal{H}_2 \to \mathcal{H}_2$ of $S_2$ are related to the observables $O_1: \mathcal{H}_1 \to \mathcal{H}_1$ of $S_1$ via the unitary similarity transformation $O_2 = U O_1 U^{-1}$.

Next, suppose that a quantum system $S_2$ is determined by a Hilbert space $\mathcal{H}_2$ and a Hamiltonian $H_2$. Let $\mathcal{H}_1$ be a vector space which is isomorphic to $\mathcal{H}_2$, i.e., there is an invertible linear transformation $U: \mathcal{H}_1 \to \mathcal{H}_2$. Then one can use $U$ to induce a Hilbert space structure on $\mathcal{H}_1$ and define a Hermitian operator $H_1 := U^{-1} H_2 U$ such that the quantum system $S_1$ correspond-

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$^8$This means [13] that for all $\psi_1, \phi_1 \in \mathcal{H}$, $\langle U \psi_1, U \Phi_1 \rangle_2 = \langle \psi_1 | \phi_1 \rangle_1$, alternatively for all $\psi_1 \in \mathcal{H}_1$ and $\psi_2 \in \mathcal{H}_2$, $\langle U \psi_1, \psi_2 \rangle_2 = \langle \psi_1, U^{-1} \psi_2 \rangle_1$, i.e., $U^\dagger = U^{-1}$. 

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ing to the pair \((H_1, H_1)\) is physically equivalent to \(S_2\). The inner product \(\langle \cdot, \cdot \rangle_1 : H_1^2 \to \mathbb{C}\) induced by \(U\) is defined by

\[
\langle \psi_1, \phi_1 \rangle_1 := \langle U\psi_1, U\phi_1 \rangle_2,
\]

where \(\psi_1, \phi_1\) are arbitrary elements of \(H_1\) and \(\langle \cdot, \cdot \rangle_2\) is the inner product of \(H_2\). By construction \(U\) is a unitary transformation and the quantum system \(S_1\) is physically equivalent to \(S_2\). The observables \(O_1\) of \(S_1\) are clearly related to the observables \(O_2\) of \(S_2\) via \(O_1 = U^{-1}O_2U\).

As we shall demonstrate below, the construction of the inner products \((13)\) given in \([5]\) and reviewed in the preceding section is an example of the application of the above method of inducing an inner product on a vector space from an isomorphic Hilbert space.

Consider an arbitrary positive-definite inner product \(\langle \cdot, \cdot \rangle\) on the vector space \(H\) of \((4)\), and let for all \(t \in \mathbb{R}\), \(U_t : H \to \tilde{H} \otimes \mathbb{C}^2\) be defined by

\[
U_t \psi := \lambda^{-1}\Psi(t),
\]

where \(\psi \in H\) is arbitrary and \(\Psi(t)\) is the two-component field \((15)\) evaluated at \(t\). It is not difficult to see that \(U_t\) is an invertible linear map. If \(\langle \cdot, \cdot \rangle\) denotes the inner product on \(\tilde{H} \otimes \mathbb{C}^2\) induced by \(U_t^{-1}\), then for all \(\psi_1, \psi_2 \in H\)

\[
\langle U_t \psi_1, U_t \psi_2 \rangle = \langle \psi_1, \psi_2 \rangle.
\]

In view of \((10)\), we can write \((11)\) in the form

\[
\langle \Psi_1(t), \Psi_2(t) \rangle = \lambda^2 \langle \psi_1, \psi_2 \rangle,
\]

where \(\Psi_i\) is the two-component field \((15)\) associated with \(\psi_i\) for \(i \in \{1, 2\}\). By construction, \(\Psi_i(t)\) are solutions of the Schrödinger equation \((17)\). Furthermore, because the right-hand side of \((12)\) does not depend on \(t\), the inner product \(\langle \cdot, \cdot \rangle\) is invariant under the dynamics generated by the Hamiltonian \((16)\).

As we mentioned earlier, being an inner product on \(\tilde{H} \otimes \mathbb{C}^2\), \(\langle \cdot, \cdot \rangle\) has the form

\[
\langle \cdot, \cdot \rangle = \langle \cdot \mid \cdot \rangle_\eta = \langle \cdot, \eta \cdot \rangle,
\]

for some positive-definite operator \(\eta\) acting in \(\tilde{H} \otimes \mathbb{C}^2\). Next we enforce the condition that the dynamics generated by the Hamiltonian \(H\) leaves the inner product \((13)\) of any two evolving two-component state vectors \(\Psi_i(t)\) invariant. Considering the possibility that \(\eta\) may depend on \(t\), we then find

\[
\langle \Psi_1(t), \eta(t)\Psi_2(t) \rangle = \langle \Psi_1(t'), \eta(t')\Psi_2(t') \rangle, \quad \forall t, t' \in \mathbb{R}.
\]
In terms of the evolution operator

\[ U(t, t_0) = \mathcal{T} \, e^{-\frac{i}{\hbar} \int_{t_0}^t H(t') dt'}, \]  

(45)

for the Hamiltonian (16), where \( \mathcal{T} \) is the time-ordering operator, (44) takes the form

\[ U(t, t')^\dagger \eta(t) U(t, t') = \eta(t'), \quad \forall t, t' \in \mathbb{R}. \]  

(46)

If we differentiate both sides of this equation with respect to \( t \), we find, using the Schrödinger equation

\[ i \hbar \frac{\partial}{\partial t} U(t, t') = H \, U(t, t'), \]  

(47)

that \( \eta \) satisfies\(^9\)

\[ i \hbar \dot{\eta} = H^\dagger \eta - \eta H. \]  

(48)

It is not difficult to check that the general solution of this equation is given by fixing \( t' \) and \( \eta(t') \) in (46), i.e., we have \[^5\]

\[ \eta(t) = U(t, t_0)^{-1} \eta_0 U(t, t_0)^{-1}, \]  

(49)

where \( t_0 \) is an initial value of \( t \) and \( \eta_0 \) is a \( t \)-independent positive-definite operator acting in \( \tilde{\mathcal{H}} \otimes \mathbb{C}_2 \).

Substituting (49) in (43) and using (42), we have

\[ \langle \psi_1, \psi_2 \rangle = \lambda^{-2} \langle \langle \Psi_1(t_0) | \Psi_2(t_0) \rangle \rangle_{\eta_0}. \]  

(50)

Therefore, every positive-definite inner product on \( \mathcal{H} \) is determined by a \( t_0 \) and a \( t \)-independent positive-definite operator \( \eta_0 \) that yields a solution (49) of (48). This equation has a constant (\( t \)-independent) solution if and only if \( H \) is \( \eta \)-pseudo-Hermitian with respect to a \( t \)-independent positive-definite operator \( \eta \). This is the case for the stationary Klein-Gordon-type fields where \( H \) is \( t \)-independent and \( \eta = \tilde{\eta} \) has the general form (36). In view of (38) and (42), we see that in this case the inner product \( \langle \cdot, \cdot \rangle \) coincides with the inner product \( \langle \cdot, \cdot \rangle \) given by (12).

If we set \( t = t_0 \) in (49) we find that \( \eta(t_0) = \eta_0 \). This provides yet another characterization of the general positive-definite inner products \( \langle \cdot, \cdot \rangle \) on \( \mathcal{H} \), namely that the latter are given by the functions \( \mathcal{F} \) mapping \( \mathbb{R} \) into the set of all positive-definite operators acting in \( \tilde{\mathcal{H}} \otimes \mathbb{C}_2 \). Every such function provides an assignment of a \( t \)-independent positive-definite operator \( \eta_0 \) to each \( t_0 \in \mathbb{R} \) according to \( \eta_0 = \mathcal{F}(t_0) \).

\(^9\)Equation (48) is the defining relation for a dynamical invariant \[^25\] of a non-Hermitian Hamiltonian. This is to be expected as the invariance of the inner product (43) means that the matrix elements of \( \eta \) in an evolving basis of the Hilbert space are constant. \[^{26}\]
The inner products (12) and (13) correspond to a function \( F \) that assigns to each \( t_0 \) the value \( \eta_0 \) of the operator \( \eta \) of (38) at \( t_0 \), i.e., set \( \eta_0 = \eta_0 \), so that

\[
\langle \psi_1, \psi_2 \rangle = \lambda^{-2} \langle \langle \Psi_1(t_0) | \Psi_2(t_0) \rangle \rangle_{\eta_0} = \langle \langle \psi_1, \psi_2 \rangle \rangle_{t_0}.
\]  \( \text{(51)} \)

Clearly, \( F \) is not the most general choice for \( F \). It is however a distinguished choice, for it leads to a constant solution of (18) and consequently defines a \( t \)-independent inner product on \( \tilde{H} \otimes \mathbb{C}^2 \) for the stationary Klein-Gordon-type fields.

In the remainder of this article we shall only be concerned with the inner products (13) that reduce to (12) for stationary Klein-Gordon-type fields. We can justify this restriction by noting that every other inner product leads to the same Hilbert space structure on \( \mathcal{H} \), i.e., the corresponding Hilbert spaces are related by unitary maps. The latter are actually easy to construct.

Let \( \langle \cdot, \cdot \rangle \) be the inner product associated with an arbitrary choice for the positive-definite operator \( \eta_0 \) and \( \langle \langle \cdot, \cdot \rangle \rangle_{t_0} \) be an inner product of the form (13). Then

\[
\langle \psi_1, \psi_2 \rangle = \lambda^{-2} \langle \langle \Psi_1(t_0) | \Psi_2(t_0) \rangle \rangle_{\eta_0} = \lambda^{-2} \langle \Psi_1(t_0), \eta_0 \Psi_2(t_0) \rangle,
\]  \( \text{(52)} \)

\[
\langle \langle \psi_1, \psi_2 \rangle \rangle_{t_0} = \lambda^{-2} \langle \langle \Psi_1(t_0) | \Psi_2(t_0) \rangle \rangle_{\tilde{\eta}_0} = \lambda^{-2} \langle \Psi_1(t_0), \tilde{\eta}_0 \Psi_2(t_0) \rangle.
\]  \( \text{(53)} \)

where \( \tilde{\eta}_0 = \tilde{\eta}(t_0) \) is a \( t \)-independent positive-definite operators acting in \( \tilde{H} \otimes \mathbb{C}^2 \) such that \( H(t_0) \) is \( \tilde{\eta}_0 \)-pseudo-Hermitian. Because \( \eta_0 \) (respectively \( \tilde{\eta}_0 \)) is a positive-definite operator, it has a positive-definite square root \( \rho_0 \) (respectively \( \tilde{\rho}_0 \)). Clearly, \( \mathcal{U} := \tilde{\rho}_0^{-1} \rho_0 \) is an invertible operator acting in \( \tilde{H} \otimes \mathbb{C}^2 \),

\[
\mathcal{U}^\dagger \tilde{\eta}_0 \mathcal{U} = \rho_0 \tilde{\rho}_0^{-1} \tilde{\rho}_0 \rho_0^{-1} \rho_0 = \eta_0,
\]

and for all \( \xi, \zeta \in \tilde{H} \otimes \mathbb{C}^2 \)

\[
\langle \langle \xi | \zeta \rangle \rangle_{\eta_0} = \langle \xi, \eta_0 \zeta \rangle = \langle \xi, \mathcal{U}^\dagger \tilde{\eta}_0 \mathcal{U} \zeta \rangle = \langle \mathcal{U} \xi, \tilde{\eta}_0 \mathcal{U} \zeta \rangle = \langle \langle \mathcal{U} \xi | \mathcal{U} \zeta \rangle \rangle_{\tilde{\eta}_0}. \]  \( \text{(54)} \)

Next, consider the invertible operator \( U_1 := U_{t_0} \), i.e.,

\[
U_1 \psi := \lambda^{-1} \Psi_0,
\]  \( \text{(55)} \)

where \( U_t \) is defined in (40) and \( \Psi_0 \) is the initial two-component state vector (43), and let \( \mathcal{U}' := U_{t_0}^{-1} \mathcal{U} U_1 \). Then Because both \( \mathcal{U} : \tilde{H} \otimes \mathbb{C}^2 \to \tilde{H} \otimes \mathbb{C}^2 \) and \( U_1 : \mathcal{H} \to \tilde{H} \otimes \mathbb{C}^2 \) are invertible, \( \mathcal{U}' \) is an invertible linear operator acting in \( \mathcal{H} \). Furthermore, in view of (52) – (55), we have for all \( \psi_1, \psi_2 \in \mathcal{H} \)

\[
\langle \psi_1, \psi_2 \rangle = \langle \langle U_1 \psi_1(t_0) | U_1 \psi_1 \rangle \rangle_{\eta_0} = \langle \langle \mathcal{U} U_1 \psi_1(t_0) | \mathcal{U} U_1 \psi_1 \rangle \rangle_{\tilde{\eta}_0} = \langle \langle \mathcal{U}' \psi_1, \mathcal{U}' \psi_2 \rangle \rangle_{t_0}.
\]
This shows that $\mathcal{U}'$ is a unitary operator relating the inner products (52) and (53). Therefore, as far as the physical content of a quantum mechanics of a Klein-Gordon-type field is concerned, these inner products are equivalent, and we can suppose, without loss of generality, that the operator $\eta_0$ appearing in (50) is such that $H(t_0)$ is $\eta_0$-pseudo-Hermitian, i.e., $\eta_0 = \tilde{\eta}_0$.

The above discussion of the most general positive-definite inner product on $\mathcal{H}$ may be extended with minor revisions to the cases that the operator $D$ appearing in the field equation (11) is Hermitian but not positive-definite. If $D$ is still invertible, i.e., its spectrum does not include zero, then we can pursue using the inner product (13) provided that we let $D_0$ stand for the value of $\sqrt{D^2}$ at $t_0$ and substitute $D_0$ for $D$ in (12) and consequently (13). Clearly, in this case $D^2$ is a positive-definite operator possessing a unique positive-definite square root $\sqrt{D^2}$. We can also use the argument given in the preceding paragraph to relate any other inner product on $\mathcal{H}$ to the inner product (13) constructed in this way. If $D$ is a general Hermitian operator with a nontrivial null space, then we can still use the inner product (13) provided that we replace the operator $D$ appearing in (12) by a positive-definite operator $D'$. Again all the choices for $D'$ would lead to unitarily equivalent Hilbert spaces.

As we noted in Section 2, in this paper we consider the cases where $D$ is a positive-definite operator and study, without loss of generality, the consequences of endowing $\mathcal{H}$ with the inner product (13).

4 Quantum Mechanics of Stationary Klein-Gordon-Type Fields

In this section we study the quantum mechanics of stationary Klein-Gordon-type fields, i.e., suppose that $D$ does not depend on $t$. First, we introduce the following notation:

$q_{L\pm} =$ the quantum mechanics defined by the Hilbert space $\mathcal{H}$ having (12) as its inner product;

$\mathcal{H}_{L\pm} =$ the Hilbert space obtained by endowing $\tilde{\mathcal{H}} \otimes \mathbb{C}^2$ with the inner product given by (20) where $\tilde{\eta}$ has the form (36);

$Q_{L\pm} =$ the quantum mechanics defined by the Hilbert space $\mathcal{H}_{L\pm}$;

$S_{L\pm} =$ the quantum system determined by the Hilbert space $\mathcal{H}_{L\pm}$ and the Hamiltonian (16).
4.1 Equivalence of $q_{L\pm}$ and $Q_{L\pm}$

In Section 3, we used the operator $U_t$ of (40) to relate the one- and two-component Klein-Gordon-type fields. This operator is clearly $t$-dependent. For stationary Klein-Gordon-type fields one can use a $t$-independent invertible operator to relate one- and two-component fields, namely the operator $U_1 : \mathcal{H} \rightarrow \tilde{\mathcal{H}} \otimes \mathbb{C}^2$ defined in (55). As we mentioned in Section 3, $U_1$ is an invertible linear operator. $U_1^{-1} : \tilde{\mathcal{H}} \otimes \mathbb{C}^2 \rightarrow \mathcal{H}$ is the operator that maps each two-component state vector

$$\xi = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} \in \tilde{\mathcal{H}} \otimes \mathbb{C}^2$$

into the solution $\psi$ of the field equation (1) satisfying the initial conditions

$$\psi(t_0) = \frac{1}{2} (\xi^1 + \xi^2), \quad \dot{\psi}(t_0) = \frac{1}{2i} (\xi^1 - \xi^2).$$

By virtue of (7), we have (for all $t$)

$$\frac{1}{2} \left\{ \cos[(t - t_0)D_1/2](\xi^1 + \xi^2) - i \sin[(t - t_0)D_1/2]D_{1/2}(\xi^1 - \xi^2) \right\}$$

$$= V(t)\xi^1 + V(t)^\dagger\xi^2,$$

where

$$V(t) := \frac{1}{2} \left\{ \cos[(t - t_0)D_1/2] - i \sin[(t - t_0)D_1/2]D_{1/2} \right\}.$$  \hspace{1cm} (56)

Furthermore, we can use (39) to show that for all $\psi_1, \psi_2 \in \mathcal{H}$,

$$\langle \psi_1, \psi_2 \rangle = \lambda^{-2} \langle \lambda U_1 \psi_1, \lambda U_1 \psi_2 \rangle = \langle U_1 \psi_1, U_1 \psi_2 \rangle.$$  \hspace{1cm} (57)

Hence $U_1$ is a unitary operator, and $q_{L\pm}$ and $Q_{L\pm}$ are equivalent.

4.2 Hamiltonians for a stationary Klein-Gordon-type field

Having established the unitarity of $U_1$, we can use $S_{L\pm}$ to define a quantum system $s_{L\pm}$ with the Hilbert space $\mathcal{H}$ and the Hamiltonian

$$h := U_1^{-1}HU_1.$$  \hspace{1cm} (59)

Note that because $H$ is a Hermitian operator with respect to the inner product (20) and $U_1$ is unitary, $h$ is Hermitian with respect to the inner product (12) on $\mathcal{H}$.

It is interesting to see how the Hamiltonian operator $h$ acts on the (one-component) Klein-Gordon-type fields $\psi$. Letting

$$\phi := h\psi$$  \hspace{1cm} (60)

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and making use of (15), (55), and $U_1 h = HU_1$ which is equivalent to (55), we find\(^\text{10}\)
\[
\phi(t_0) = i\hbar \dot{\psi}(t_0), \quad \dot{\phi}(t_0) = -i\hbar D\psi(t_0).
\]
By construction, $\phi$ is a solution of the field equation \((\text{i})\) satisfying the initial conditions \((\text{ii})\). Because $D$ is $t$-independent, $\tilde{\psi} := i\hbar \dot{\psi}$ satisfies both the field equation \((\text{i})\) and the initial conditions
\[
\tilde{\psi}(t_0) = i\hbar \dot{\psi}(t_0), \quad \dot{\tilde{\psi}}(t_0) = -i\hbar D\psi(t_0).
\]
Therefore, by the uniqueness of the solution \((\text{iii})\) of the initial-value problem for equation \((\text{i})\), we have
\[
\begin{align*}
\phi(t) &= i\hbar \dot{\psi}(t), \\
\dot{\phi}(t) &= -i\hbar D\psi(t),
\end{align*}
\]
for all $t$.\(^\text{11}\) According to \((\text{vi})\) and \((\text{vii})\),
\[
h\dot{\psi} = i\hbar \dot{\psi}.
\]
The fact that $\dot{\psi}(t)$ satisfies the field equation \((\text{i})\), i.e., $\dot{\psi} \in \mathcal{H}$, is consistent with the requirement that $h$ maps $\mathcal{H}$ into itself.

The remarkable resemblance of \((\text{vi})\) to the time-dependent Schrödinger equation of non-relativistic quantum mechanics is actually misleading. Unlike the latter which determines the $t$-dependence of an evolving state vector, \((\text{vi})\) describes the action of the operator $h$ on the space $\mathcal{H}$ of the solutions of the field equation \((\text{i})\), i.e., it is the definition of $h$. Because $h$ is obtained through a unitary transformation from the Hamiltonian $H$, one might expect that it should be possible to determine the $t$-dependence of the value $\psi(t)$ of the field\(^\text{12}\) using a Schrödinger-like equation involving $h$. In order to see that this is actually not the case, we evaluate both sides of \((\text{vi})\) at $t$. This yields
\[
i\hbar \frac{d}{dt} \psi(t) = (h\psi)(t),
\]
where the action of $h$ on $\psi$ is determined by \((\text{vi})\). Now, we compare \((\text{vi})\) with a time-dependent Schrödinger equation that is satisfied by $\psi(t) \in \mathcal{H}$. The latter would have the form
\[
i\hbar \frac{d}{dt} \psi(t) = \tilde{h} \psi(t),
\]
\(^\text{10}\)It is remarkable that the free parameter $\lambda$ that enters the expressions for $H$ and the initial two-component fields associated with $\psi$ and $\phi$ disappears in the final result of this calculation.
\(^\text{11}\)The consistency of \((\text{vi})\) and \((\text{vii})\) is equivalent to the field equation \((\text{i})\).
\(^\text{12}\)It is the value of the field $\psi$ (and note $\psi$ itself) that depends on $t$. 

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for a Hamiltonian operator $\tilde{h}$ acting in the Hilbert space $\tilde{H}$.

Equations (66) and (67) are fundamentally different. One cannot solve (66) for $\psi(t)$ without using the field equation (1). This is because, by construction, the domain of the definition of $h$ is the space of solutions of (1).

In terms of $h$, (64) takes the form

$$h\dot{\psi} = -i\hbar D\psi,$$

where again $\psi \in \mathcal{H}$ is an arbitrary solution of (1) and $D\psi$ is the element of $\mathcal{H}$ defined by $(D\psi)(t) := D\psi(t)$. Combining (68) and (65), we find $\hbar^2 \psi = \hbar^2 D\psi$. Therefore, as operators acting in $\mathcal{H}$, $\hbar^2$ and $\hbar^2 D$ coincide,

$$\hbar^2 = \hbar^2 D.$$  \hspace{1cm} (69)

Next, we apply $\tilde{h}$ to both sides of (67). If we now assume that $\tilde{h}$ is $t$-independent and $\psi(t)$ appearing in (67) is an arbitrary solution of the field equation (1), we obtain

$$\tilde{h}^2 \psi(t) = \hbar^2 D\psi(t).$$  \hspace{1cm} (70)

It is essential to observe that this equation only holds if $\psi(t)$ satisfies the field equation (1). As an operator equation in $\tilde{H}$, $\tilde{h}^2 = \hbar^2 D$ does not hold. For if it did, we could use the fact that $D$ is a positive-definite operator to infer that $\tilde{h} = \hbar \Delta$ where $\Delta$ is a square root of $D$. The resulting Schrödinger equation (67), with any choice for $\Delta$, is not equivalent to the Klein-Gordon-type equation (1). This is because we may choose the initial data $(\psi_0, \dot{\psi}_0)$ so that $\dot{\psi}_0 \neq i\Delta \psi_0$. In this case the Schrödinger equation (67) with $\tilde{h} = \hbar \Delta$ and any square root $\Delta$ of $D$ is violated at $t = t_0$. This argument is a manifestation of the rather obvious fact that the $t$-dependence of Klein-Gordon-type fields cannot be described by a time-dependent Schrödinger equation defined in the Hilbert space $\tilde{H}$.

The Hamiltonian $h$ does not determine the $t$-dependence of the value $\psi(t)$ of a given field $\psi$. It generates a time-evolution in the space $\mathcal{H}$ of fields. The corresponding time-dependent Schrödinger equation reads

$$i\hbar \frac{d}{dt} \psi_t = h\psi_t,$$  \hspace{1cm} (71)

$$\psi_{t_0} = \phi,$$  \hspace{1cm} (72)

where for each value of $t \in \mathbb{R}$, $\psi_t \in \mathcal{H}$. We will denote by $\psi_t(t')$ the value of the field $\psi_t$ at $t'$. Clearly $\psi_t(t') \in \tilde{H}$.

\footnote{Because $D$ is assumed to be $t$-independent, for all $\psi \in \mathcal{H}$, $(D\psi)(t) = D\psi(t)$ also satisfies (1). Hence $D\psi \in \mathcal{H}$, and $D$ may be viewed as a linear operator acting in $\mathcal{H}$.}
Before we explore the consequences of the Schrödinger equation (71), we wish to comment on the precise meaning of the term ‘time’ used in this article. We will identify a real variable with a time-parameter if and only if it is the evolution-parameter associated with a (Hermitian) Hamiltonian operator acting in the Hilbert space $\mathcal{H}$. It is the choice of a Hamiltonian operator that decides whether a real parameter is to be qualified as a measure of time. For example the parameter $t$ appearing in the Schrödinger equation (71) is a time-parameter whereas the parameter $t$ appearing in the argument of the value $\psi(t)$ of a Klein-Gordon-type field $\psi \in \mathcal{H}$ cannot be termed as ‘time’ unless we adopt a Hamiltonian operator acting in $\mathcal{H}$ that generates $t$-translations of the fields.\textsuperscript{14} \textit{A priori} such a (Hermitian) Hamiltonian may or may not exist.

The above definition of time is consistent provided that one does not apply it in a discussion of the two-component fields. This is justified by noting that the two-component formulation of a Klein-Gordon-type equation, in which the argument $t$ of the value $\psi(t)$ of the fields $\psi$ is the evolution-parameter for the Hamiltonian (16), involves the arbitrary unphysical parameter $\lambda$.\textsuperscript{15}

Next, we evaluate both sides of (71) at $t'$, i.e., substitute $t'$ for $t$ and $\psi(t')$ for $\psi(t)$ in (66). We also replace the ordinary derivatives with partial derivatives as $t$ and $t'$ are independent variables. Then using (65) we find

$$\frac{\partial}{\partial t} \psi_t(t') = \frac{\partial}{\partial t'} \psi_t(t').$$

This together with (72) yields

$$\psi_t(t') = \phi(t' + t - t_0).$$

(73)

The particularly simple mixing of the parameters $t$ and $t'$ suggests that the argument $t'$ of the value $\phi(t')$ of the field $\phi$ has the same physical meaning as the time-parameter $t$.

Moreover, if we write the Schrödinger equation (71) in the form

$$\psi_t = u(t, t_0) \phi,$$

(74)

with

$$u(t, t_0) := e^{-i(t-t_0)\hbar},$$

(75)

and let $\delta t := t - t_0$, we can express (73) in the form

$$e^{-i(t')\hbar} \phi(t') = \phi(t' + \delta t).$$

(76)

\textsuperscript{14}This point is not properly taken into account in the terminology used in Ref. 5. There the Klein-Gordon-type equation (1) is viewed as an evolution equation and the parameter $t$ appearing in this equation is called time to reflect this point of view.

\textsuperscript{15}As pointed out in 16, the freedom in the choice of $\lambda$ is related to a $GL(1, \mathbb{C})$ symmetry of the two-component formulation of the Klein-Gordon-type fields. Indeed, one may consider $t$-dependent $\lambda$’s in which case the corresponding gauge symmetry is local. Physically it signifies a $t$-reparameterization symmetry of the two-component formalism.
This equation shows that the time-evolution generated by the Hamiltonian \( h \) corresponds to \( t \)-translations of the stationary Klein-Gordon-type fields. In other words, \( h \) is the generator of the \( t \)-translations in the space \( \mathcal{H} \). This is another indication that the choice of \( h \) as the Hamiltonian is equivalent to identifying the parameter \( t \) appearing in the defining field equation \( (\text{I}) \) with time.

Next, we use the expression \( (65) \) for the Hamiltonian \( h \) to determine the energy eigenstates of the system. Substituting this expression in the eigenvalue equation

\[
 h\psi_n = e_n\psi_n, \quad (77)
\]

we obtain \( i\hbar \dot{\psi}_n = e_n\psi_n \). Consequently, \( \psi_n(t) = e^{-ie_n(t-t_0)/\hbar}\psi_n(t_0) \). Now imposing the condition that \( \psi_n \) is a solution of the field equation \( (\text{I}) \) with a \( t \)-independent \( D \), we find that \( \psi_n(t_0) \) is an eigenvector of \( D \) with eigenvalue \( e_n^2/\hbar^2 \). Hence, in light of \( (26) \), \( e_n = \pm \hbar \omega_n \), and \( \psi_n(t_0) \) is an eigenvector of \( D \) with eigenvalue \( \omega_n^2 \). In particular, \( \psi_{\pm,n} \in \mathcal{H} \) defined by

\[
 \psi_{\pm,n}(t) := N_{\pm,n} e^{\mp\hbar \omega_n t} \phi_n, \quad (78)
\]

form a set of energy eigenvectors, where \( N_{\pm,n} \in \mathbb{C} - \{0\} \) are arbitrary normalization constants.

We have obtained the Hamiltonian \( h \) and consequently the quantum system \( s_{L\pm} \) by using a particular unitary operator mapping \( \mathcal{H} \) onto \( \mathcal{H}_{L\pm} \), namely \( U_1 \). If we choose another unitary operator \( \tilde{U}_1 : \mathcal{H} \to \mathcal{H}_{L\pm} \) to induce a quantum system in \( q_{L\pm} \) from \( S_{L\pm} \), we will obtain an equivalent quantum system to \( s_{L\pm} \). However, if we select a quantum system \( \tilde{S}_{L\pm} \) in \( Q_{L\pm} \) that is not equivalent to \( S_{L\pm} \), i.e., a Hamiltonian \( \tilde{H} : \mathcal{H}_{L\pm} \to \mathcal{H}_{L\pm} \) that is not related to \( H \) by a unitary similarity transformation, and use \( U_1 \) or \( \tilde{U}_1 \) to induce a quantum system \( \tilde{s}_{L\pm} \) from \( \tilde{S}_{L\pm} \), then obviously \( s_{L\pm} \) and \( \tilde{S}_{L\pm} \) will not be physically equivalent. The choice of \( h \) as the Hamiltonian of a quantum system having \( \mathcal{H} \) as its Hilbert space is by no means unique. Different choices for the Hamiltonian define different notions of time-evolution in \( \mathcal{H} \).

In summary, we have shown that there is a canonical quantum system \( s_{L\pm} \) whose Hamiltonian \( h \) generates \( t \)-translations in \( \mathcal{H} \) so that \( t \) plays the role of time, and that this is not the only quantum system associated with a stationary Klein-Gordon-type field, i.e., one can consider other Hamiltonians with other choices for a time-parameter.

### 4.3 Formulating the quantum mechanics of a stationary Klein-Gordon-type field using the Hilbert space \( \mathcal{H}_\ast \)

In Section 4.2 we constructed a canonical quantum system \( s_{L\pm} \) for stationary Klein-Gordon-type fields that was by construction physically equivalent to \( S_{L\pm} \). In this section we show that the systems \( S_{L\pm} \) (and consequently \( s_{L\pm} \)) corresponding to all possible choices for the operators
\(L_{\pm}\) are also physically equivalent. This involves constructing various unitary operators between the corresponding Hilbert spaces and allows for a formulation of the quantum mechanics of a stationary Klein-Gordon-type field having \(\mathcal{H}_*\) as its Hilbert space.

It is useful to introduce the notation \(\mathcal{H}_0\) for the Hilbert space \(\mathcal{H}_{L_{\pm}}\) with the choice \(L_+ = 1\) and \(L_- = 0\) and \(S_0\) for the quantum system \(S_{L_{\pm}}\) corresponding to this choice. The inner product on \(\mathcal{H}_0\) is \(\langle \cdot | \cdot \rangle_{\eta_+}\) where \(\eta_+\) is given by (29).

Now, consider the operator \(A\) of (31). This is an invertible operator acting in \(\tilde{\mathcal{H}} \otimes \mathbb{C}^2\). In view of (20) and (30), it satisfies, for all \(\xi, \zeta \in \tilde{\mathcal{H}} \otimes \mathbb{C}^2\),

\[
\langle \langle A^\dagger \eta_+ A \xi | A^\dagger \eta_+ A \zeta \rangle \rangle_{\eta_+} = \langle \eta_+ A A^\dagger \eta_+ A \xi, A^\dagger \eta_+ A \zeta \rangle = \langle \eta_+ A \xi, \tilde{\eta} \zeta \rangle = \langle \xi, (\tilde{A}^\dagger \eta_+ A) \zeta \rangle = \langle \xi, \tilde{\eta} \zeta \rangle.
\]

This equation shows that \(A\) is a unitary operator mapping \(\mathcal{H}_{L_{\pm}}\) to \(\mathcal{H}_0\). It also commutes with \(H\). Hence, the quantum systems \(S_{L_{\pm}}\) with all possible choices for \(L_{\pm}\) are actually equivalent to \(S_0\).

Next, we recall that the operator \(\eta_+\) defining the inner product of \(\mathcal{H}_0\) is a positive-definite operator. Therefore, it has a unique positive-definite square root \(\rho := \sqrt{\eta_+}\) namely

\[
\rho = \frac{1}{4} \begin{pmatrix} \lambda + D^{-1/2} & \lambda - D^{-1/2} \\ \lambda - D^{-1/2} & \lambda + D^{-1/2} \end{pmatrix}.
\]

(79)

One can check that \(\rho\) is a Hermitian operator acting in \(\tilde{\mathcal{H}} \otimes \mathbb{C}^2\) and satisfying

\[
\rho^2 = \eta_+.
\]

(80)

This, in particular, implies that \(\rho\) is an invertible operator. The inverse of \(\rho\) has the form

\[
\rho^{-1} = \begin{pmatrix} \lambda^{-1} + D^{1/2} & \lambda^{-1} - D^{1/2} \\ \lambda^{-1} - D^{1/2} & \lambda^{-1} + D^{1/2} \end{pmatrix}.
\]

(81)

We can also use \(\rho^{-1}\) to induce a new quantum system \(S_*\). This is determined by the Hilbert space obtained by endowing \(\tilde{\mathcal{H}} \otimes \mathbb{C}^2\) with the inner product

\[
\langle \langle \xi | \Phi \rangle \rangle_{\eta_*} := \langle \rho^{-1} \xi | \rho^{-1} \Phi \rangle_{\eta_+} = \langle \rho^{-1} \xi, \eta_+ \rho^{-1} \Phi \rangle = \langle \eta_+ \rho^{-1} \xi, \rho^{-1} \Phi \rangle = \langle \xi, \rho \Phi \rangle = \langle \xi, \Phi \rangle,
\]

i.e., the Hilbert space \(\mathcal{H}_* = \tilde{\mathcal{H}} \oplus \mathcal{H}\), and the Hamiltonian

\[
H_* = \rho H \rho^{-1} = \hbar \begin{pmatrix} D^{1/2} & 0 \\ 0 & -D^{1/2} \end{pmatrix} = \hbar D^{1/2} \sigma_3,
\]

(83)

which is clearly Hermitian with respect to the inner product \(\langle \cdot, \cdot \rangle\) of \(\mathcal{H}_*\).
By construction $S_0$ and $S_*$ are physically equivalent. This in turn implies that the quantum systems $S_{L \pm}$ (and subsequently $s_{L \pm}$) are physically equivalent to $S_*$. The Hilbert spaces $\mathcal{H}_{L \pm}$ are mapped to $\mathcal{H}_*$ by the unitary operator

$$U_2 := \rho A,$$

and the Hilbert space $\mathcal{H}$ with inner product (12) is related to $\mathcal{H}_*$ by the unitary operator

$$U := U_2 U_1 = \rho AU_1,$$

where $U_1$ is defined by (55). The following chain of unitary mappings summarizes the above constructions:

$$\mathcal{H} \xrightarrow{U_1} \mathcal{H}_{L \pm} \xrightarrow{A} \mathcal{H}_0 \xrightarrow{\rho} \mathcal{H}_*.$$

It further demonstrates the equivalence of $q_{L \pm}$ with any possible choice for $L_\pm$ with the quantum mechanics $Q_*$ on the Hilbert space $\mathcal{H}_*$.

In fact, the operator $U$ turns out to have a relatively simple form. In order to see this, first we use (31) – (34), (79), and (84) to establish the following useful identity:

$$U_2 = \rho A = A \rho,$$

where

$$A := \begin{pmatrix} A_+ & 0 \\ 0 & A_- \end{pmatrix},$$

$$A_\pm := A_\pm = \sum_n a_{\pm,n} |\phi_n \rangle \langle \phi_n|.$$

Because the coefficients $a_{\pm,n}$ do not vanish, the operators $A_\pm$ and consequently $A$ are invertible. Clearly $A^{-1}$ has the form

$$A^{-1} = \begin{pmatrix} A_+^{-1} & 0 \\ 0 & A_-^{-1} \end{pmatrix},$$

where

$$A_\pm^{-1} = \sum_n a_{\pm,n}^{-1} |\phi_n \rangle \langle \phi_n|.$$

In terms of $A_\pm$, the operators $L_\pm$ appearing in the expression for the inner product (12) take the form

$$L_\pm = \frac{1}{2} \left( A_\pm^\dagger A_\pm \pm A_\pm A_\mp^\dagger \right).$$

We can use (86) to obtain the following expression describing the action of the operator $U$ on a given field $\psi \in \mathcal{H}$:

$$U \psi = \frac{1}{2} \left( A_+ (\psi_0 + iD^{-1/2}\dot{\psi}_0) \pm A_- (\psi_0 - iD^{-1/2}\dot{\psi}_0) \right).$$
It is remarkable that unlike $U_1$ and $U_2$, the operator $U$ does not depend on the arbitrary parameter $\lambda$. This is also the case for the Hamiltonian $H_*$ of (83). Therefore, similarly to $s_{L\pm}$, the quantum system $S_*$ is also independent of the unphysical free parameter $\lambda$. This in turn means that we can use $S_*$ to describe the quantum mechanics of stationary Klein-Gordon-type fields and the corresponding dynamics generated by the Hamiltonian $h$.

### 4.4 Quantum observables for a stationary Klein-Gordon-type field

Having obtained the explicit form of the unitary operator $U$ and established the $\lambda$-independence of $Q_*$, we can construct the observables of $q_{L\pm}$ from those of $Q_*$. The latter are Hermitian operators acting in $H_\star$. In view of the fact that $H_\star = \tilde{H} \oplus \tilde{H}$, any Hermitian operator acting in $H_\star$ has the form

$$O_\star = \begin{pmatrix} \tilde{O}_1 & \tilde{O} \\ \tilde{O}^\dagger & \tilde{O}_2 \end{pmatrix},$$

(93)

where $\tilde{O}_1, \tilde{O}_2$, and $\tilde{O}$ are linear operators acting in $\tilde{H}$, and $\tilde{O}_1, \tilde{O}_2$ are Hermitian.

We can express the observables $o$ of $q_{L\pm}$ in terms of the observables $O_\star$ of $Q_\star$ according to

$$o = U^{-1}O_\star U = U_1^{-1}U_2^{-1}O_\star U_1 U_2,$$

(94)

where $U$ is the unitary operator (85) mapping $H$ to $H_\star$ and $U_1$ and $U_2$ are respectively given by (55) and (84).

Before deriving the explicit form of the observables $o$, we wish to comment on the interpretation of $o$ and $O_\star$ as the Schrödinger- or Heisenberg-picture observables for the quantum systems $s_{L\pm}$ and $S_*$, respectively. Because $U_1$ maps a field $\psi$ to the initial two-component state vector $\lambda^{-1}\Psi_0$, there is no difference between viewing $O_\star$ as a Schrödinger- or Heisenberg-picture observable. This follows from the observation that at the initial time $t_0$ the Schrödinger- and Heisenberg-picture observables coincide. If we identify $O_\star$ with a Schrödinger-picture observable $O^{(S)}_\star$ and denote the corresponding Heisenberg-picture observable by $O^{(H)}_\star$, we have, for all $t \in \mathbb{R}$,

$$O^{(S)}_\star = O_\star, \quad O^{(H)}_\star(t) = U_\star(t, t_0)^{-1}O_\star U_\star(t, t_0),$$

(95)

where

$$U_\star(t, t_0) := e^{-i(t-t_0)H_*} = \begin{pmatrix} U(t, t_0) & 0 \\ 0 & U(t, t_0)^{-1} \end{pmatrix},$$

(96)

$$U(t, t_0) := e^{-i(t-t_0)D^{1/2}}.$$
In this case we can use the physical equivalence of $Q_*$ and $q_{L\pm}$ to identify the Schrödinger-picture observables $o^{(S)}$ and Heisenberg-picture observables $o^{(H)}$ for $q_{L\pm}$ according to

$$o^{(S)} = o, \quad o^{(H)}(t) = u(t, t_0)^{-1} o u(t, t_0),$$

where $u(t, t_0)$ is given by (92). Similarly, if we identify $O_*$ with a Heisenberg-picture observable, we find

$$O_*^{(S)} = U_*(t, t_0) O_*(t) U_*(t, t_0)^{-1}, \quad O_*^{(H)}(t) = O_*(t),$$

$$o^{(S)} = u(t, t_0) o(t) u(t, t_0)^{-1}, \quad o^{(H)}(t) = o(t).$$

Next, we obtain the explicit form of the observables $o$ of $q_{L\pm}$ by computing their action on an arbitrary $\psi \in \mathcal{H}$. In order to do so, first we employ (94), (93), (55), (85), (84), (89), (79), (81), and (6) to determine the initial conditions for $o\psi$. After a lengthy calculation we find

$$\langle o\psi \rangle(t_0) = (J_+ + K_+)\psi_0 + i(J_- + K_-)D^{-1/2}\dot{\psi}_0,$$

$$\frac{d}{dt}\left[\langle o\psi \rangle(t)\right]_{t=t_0} = D^{1/2}\left[i(-J_+ + K_+)\psi_0 + (J_- - K_-)D^{-1/2}\dot{\psi}_0\right],$$

where

$$J_\pm := \frac{1}{2}\left(A_+^{-1}\hat{O}_1 A_+ \pm A_-^{-1}\hat{O}_2 A_-\right), \quad K_\pm := \frac{1}{2}\left(A_-^{-1}\hat{O}_1 A_+ \pm A_-^{-1}\hat{O}_2 A_-\right).$$

Using (90), we then obtain, for all $t$,

$$\langle o\psi \rangle(t) = \left[U(t, t_0) J_+ + U(t, t_0)^\dagger K_+\right] \psi_0 + i \left[U(t, t_0) J_- + U(t, t_0)^\dagger K_-\right] D^{-1/2}\dot{\psi}_0,$$

where $U(t, t_0)$ is given by (97). Equation (104) provides the general form of the observables of $q_{L\pm}$.

As a consistency check of our analysis, we compute the observable $o$ of $q_{L\pm}$ associated with the Hamiltonian $H_*$ of $S_*$. Setting $O_* = H_*$ in (93), we find $\hat{O}_1 = -\hat{O}_2 = \hbar D^{1/2}$ and $\hat{O} = 0$. These in turn imply $J_\pm = \mp K_\pm = \hbar D^{1/2}/2$. Substituting these relations and (97) in (104) and doing the necessary algebra, we find the expected result: $o = \hbar$.

Next, we calculate the matrix element $\langle \langle \psi, o\phi \rangle \rangle$ associated with a pair $\psi, \phi$ of elements of $\mathcal{H}$. In view of the fact that $U$ is a unitary operator and using (92), we have

$$\langle \langle \psi, o\phi \rangle \rangle = \langle U \psi, O_* U \phi \rangle = \langle \psi_0 | (J_+ + K_+) \phi_0 \rangle + \langle \psi_0 | D^{-1/2}(J_- - K_-)D^{-1/2}\dot{\phi}_0 \rangle + i \left[\langle \psi_0 | (J_+ + K_-)D^{-1/2}\phi_0 \rangle + \langle \psi_0 | D^{-1/2}(-J_+ + K_+)\dot{\phi}_0 \rangle\right],$$

where $(\psi_0, \dot{\psi}_0)$ and $(\phi_0, \dot{\phi}_0)$ are respectively the initial date for the fields $\psi$ and $\phi$, and

$$J_\pm := \frac{1}{2}\left(A_+^\dagger \hat{O}_1 A_+ \pm A_-^\dagger \hat{O}_2 A_-\right), \quad K_\pm := \frac{1}{2}\left(A_-^\dagger \hat{O}_1 A_+ \pm A_-^\dagger \hat{O}_2 A_-\right).$$
It is not difficult to check that \( (\psi, o\phi)^* = (\phi, o\psi) \). This confirms the fact that \( o \) is Hermitian with respect to the inner product \( (\cdot, \cdot) \).

In the Appendix, we explore the form of the observables of \( q_{L_{\pm}} \) for a particular two-parameter family of \( L_{\pm} \)'s that is of importance in the study of Klein-Gordon fields in a Minkowski spacetime. [5]

5 Quantum Mechanics of Nonstationary Klein-Gordon-Type Fields

Consider the case where the operator \( D \) depends on \( t \). Then again the solutions \( \psi \) of the field equation (11) are given by (7). However, the operators \( C(t, t_0) \) and \( S(t, t_0) \) no longer satisfy (10) and (11). In fact, a closed-form formula for \( C(t, t_0) \) and \( S(t, t_0) \) is not known. They may be expressed as infinite series involving certain time-ordered products of \( D \).

As we discussed in Section 3, we can adopt, without loss of generality, the positive-definite inner product (13) on \( H \). We can express it more explicitly as

\[
(\langle \psi, \phi \rangle)_{\eta(t)} = \frac{1}{2} \left[ \langle \psi_0 | L_{0+} \phi_0 \rangle + \langle \dot{\psi}_0 | L_{0+} D_0^{-1/2} \dot{\phi}_0 \rangle + i(\langle \psi_0 | L_{0-} D_0^{-1/2} \dot{\phi}_0 \rangle - \langle \dot{\psi}_0 | L_{0-} D_0^{-1/2} \psi_0 \rangle) \right],
\]

(107)

where \( \psi, \phi \in \mathcal{H} \), \( D_0 := D(t_0) \), and \( L_{0\pm} \) are arbitrary Hermitian operators such that \( A_{0\pm} := L_{0+} \pm L_{0-} \) are positive-definite operators commuting with \( D_0 \). Clearly, \( L_{0\pm} = L_{\pm}(t_0) \) and \( A_{0\pm} = A_{\pm}(t_0) \), where \( L_\pm \) and \( A_\pm \) are respectively given by (37) and (33).

In Section 3, we showed that the inner product (107) was obtained from an invariant inner product \( \langle \langle \cdot | \cdot \rangle \rangle_{\eta(t)} \) on \( \tilde{\mathcal{H}} \otimes \mathbb{C}^2 \) where

\[
\eta(t) := U(t, t_0)^{-11} \tilde{\eta}_0 U(t, t_0)^{-1},
\]

\( \tilde{\eta}_0 = \tilde{\eta}(t_0) \) and \( \tilde{\eta} \) is given by (36). In this section we attempt to extend the analysis of Section 4 to the nonstationary Klein-Gordon-type fields. Again, we begin our presentation by introducing some useful notation:

\[
\mathcal{H} = \text{the Hilbert space obtained by endowing the space of solutions of the field equation (11) with the inner product (107)};
\]

\( q_{L_{0\pm}} \) = the quantum mechanics determined by the Hilbert space \( \mathcal{H} \);

\[
\mathcal{H}_{L_{0\pm}} = \text{the Hilbert space obtained by endowing } \tilde{\mathcal{H}} \otimes \mathbb{C}^2 \text{ with the inner product } \langle \langle \cdot | \cdot \rangle \rangle_{\eta(t)};
\]

\( Q_{L_{0\pm}} \) = the quantum mechanics determined by the Hilbert space \( \mathcal{H}_{L_{0\pm}} \).
\( S_{L_0\pm} \) = the quantum system determined by the Hilbert space \( \mathcal{H}_{L_0\pm} \) and the Hamiltonian \( H \) of (16).

We also wish to recall that, by definition [24], an invertible linear operator \( X \) acting in a Hilbert space is said to be \( \eta' \)-pseudo-unitary for a Hermitian, invertible, linear operator \( \eta' \) acting in the same space, if \( X^{-1} = \eta'^{-1}X^\dagger \eta' \) or alternatively \( X^\dagger \eta X = \eta' \).

5.1 Equivalence of \( q_{L_0\pm} \) and \( Q_{L_0\pm} \)

Let \( \tilde{\eta}_0 = \tilde{\eta}(t_0) \) where \( \tilde{\eta} \) is given by (30), i.e., \( \tilde{\eta}_0 : \mathcal{H} \otimes \mathbb{C}^2 \to \mathcal{H} \otimes \mathbb{C}^2 \) is the most general positive-definite operator such that \( H(t_0) \) is \( \tilde{\eta}_0 \)-pseudo-Hermitian. Suppose that \( V : \mathcal{H} \otimes \mathbb{C}^2 \to \mathcal{H} \otimes \mathbb{C}^2 \) is an arbitrary (possibly time-dependent) \( \tilde{\eta}_0 \)-pseudo-unitary operator, so that

\[ V^\dagger \tilde{\eta}_0 V = \tilde{\eta}_0, \quad (108) \]

and \( U'_1 : \mathcal{H} \to \mathcal{H}_{L_0\pm} \) is defined by

\[ U'_1 := U(t,t_0)VU_1, \quad (109) \]

where \( U(t,t_0) \) is the evolution operator [45] for the Hamiltonian \( H \). Then because \( U(t,t_0) \), \( V \), and \( U_1 \) are invertible linear operators, so is \( U'_1 \). Furthermore, a straightforward calculation shows that, for all \( \psi, \phi \in \mathcal{H} \),

\[ \langle \langle U'_1 \psi | U'_1 \phi \rangle \rangle_{\eta(t)} = \lambda^{-2} \langle \langle U(t,t_0)V\Psi_0 | U(t,t_0)V\Phi_0 \rangle \rangle_{\eta(t)} = \lambda^{-2} \langle \Psi_0 | V^\dagger \tilde{\eta}_0 V \Phi_0 \rangle = \lambda^{-2} \langle \Psi_0 | \tilde{\eta}_0 \Phi_0 \rangle = \lambda^{-2} \langle \langle \Psi_0 | \Phi_0 \rangle \rangle_{\tilde{\eta}_0} = \langle \langle \psi, \phi \rangle \rangle_{t_0}, \quad (110) \]

where we have made use of (109), (53), and (51). As seen from (110), \( U'_1 \) is a unitary operator manifesting the equivalence of \( q_{L_0\pm} \) and \( Q_{L_0\pm} \).

5.2 Hamiltonians for a nonstationary Klein-Gordon-type field

We can use \( U'_1 \) to induce a Hamiltonian operator \( h' : \mathcal{H} \to \mathcal{H} \) from the Hamiltonian \( H \) of \( S_{L_0\pm} \). However note that unlike the operator \( U_1, U'_1 \) is generally \( t \)-dependent. This implies that the requirement that the dynamics generated by \( h' \) in \( \mathcal{H} \) is mapped to the dynamics generated by \( H \) in \( \mathcal{H}_{L_0\pm} \) is equivalent to the condition [26]:

\[ h' = U'^{-1}_1 H U'_1 - i\hbar U'^{-1}_1 \dot{U}'_1. \]

Substituting (109) in this equation, we find

\[ h' = U^{-1}_1 V U_1, \quad (111) \]
where

\[ V := -i\hbar V^{-1}\dot{V}. \]  

(112)

We shall denote the quantum system associated with the Hilbert space \( \mathcal{H} \) and the Hamiltonian \( h' \) by \( s'_{L,\pm} \).

As seen from the above construction, the fact that \( U'_1 \) is unitary follows from the condition that \( \mathcal{V} \) is \( \tilde{\eta}_0 \)-pseudo-unitary. It is not difficult to observe that the converse is also true. Therefore all the unitary operators mapping \( \mathcal{H} \) to \( \mathcal{H}_{L,\pm} \) have the form (109) for some \( \tilde{\eta}_0 \)-pseudo-unitary operator \( V \). The latter form a pseudo-unitary group \( G_{\tilde{\eta}_0} \), [24]. In fact, because \( \tilde{\eta}_0 \) is a positive-definite operator, this group is isomorphic to the unitary group \( U(\mathcal{H}_0) \) of all the unitary operators acting in the Hilbert space \( \mathcal{H}_0 \), [24].

The unitary operator \( U'_1 \) and consequently the Hamiltonian \( h' \) are determined by the operators \( \mathcal{V} \) belonging to the group \( G_{\tilde{\eta}_0} \). For a stationary Klein-Gordon-type field, where \( D = D_0 \) and \( \tilde{\eta} = \tilde{\eta}_0 \), the Hamiltonian \( H \) of \( S_{L,\pm} \) is \( \tilde{\eta}_0 \)-pseudo-Hermitian [19]. This is sufficient to deduce that the evolution operator \( U(t, t_0) \) is \( \tilde{\eta}_0 \)-pseudo-unitary [24], i.e., \( U(t, t_0) \in G_{\tilde{\eta}_0} \). As a result, \( U(t, t_0)^{-1} \in G_{\tilde{\eta}_0} \), and we can take

\[ \mathcal{V} = U(t, t_0)^{-1}. \]  

(113)

This yields \( U'_1 = U_1 \), \( V = H \), and \( h' = h \). Clearly (113) is not the only choice for \( \mathcal{V} \). However, it is this choice that identifies the Hamiltonian \( h' \) with the generator \( h \) of the \( t \)-translations in \( \mathcal{H} \) and consequently makes \( t \) the time-parameter for a stationary Klein-Gordon-type field. This observation leads to the natural question if there is a choice for \( \mathcal{V} \) that makes \( h' \) the generator of \( t \)-translations in \( \mathcal{H} \) (equivalently identifies \( t \) with time) for a nonstationary Klein-Gordon-type field. We will next show that the answer to this question is negative.

Consider the case that \( D \) does depend on \( t \) and let \( h : \mathcal{H} \to \mathcal{H} \) be the operator defined by (59). Then substituting (55) and (16) in (59), we find that the action of \( h \) on a given field \( \psi \in \mathcal{H} \) is described by the expressions (61) for the initial data of \( \phi := h\psi \). Note however that, unlike for a stationary Klein-Gordon-type field, the operator \( D \) appearing in these relations depends on \( t \). Therefore, acting \( h \) on a field \( \psi \) yields a one-parameter family of fields \( \phi_t \), parameterized by \( t \).

16This is similar to the quantum mechanical analog [26] of the dynamical canonical transformation used in the Hamilton-Jacobi formulation of classical mechanics.

17This is a manifestation of the fact that being obtained via a \( t \)-independent unitary transformation from a...
Next, we explore the time-evolution generated by the operator $h$. If we denote by $\tilde{u}(t, t_0)$ the time-evolution operator associated with $h$, namely

$$\tilde{u}(t, t_0) := T e^{-\frac{i}{\hbar} \int_{t_0}^t h(t') dt'},$$

we can use (59) to show that

$$U_1 \tilde{u}(t, t_0) = U(t, t_0) U_1.$$  \hspace{1cm} (115)

Applying both sides of this equation on an initial field $\psi_{t_0} \in \mathcal{H}$, denoting the evolving Klein-Gordon-type field by $\psi_t := \tilde{u}(t, t_0) \psi_{t_0}$, and using (55), we find

$$\lambda U_1 \psi_t = \Psi_t(t_0) = \Psi_{t_0}(t),$$  \hspace{1cm} (116)

where for all $t_1, t_2 \in \mathbb{R}$, $\Psi_{t_1}(t_2)$ stands for the value of the two-component field associated with $\psi_{t_1}$ at $t_2$. In view of (15) and (116),

$$\psi_t(t_0) = \psi_{t_0}(t), \quad \dot{\psi}_t(t_0) := \left. \frac{\partial}{\partial t'} \psi_t(t') \right|_{t'=t_0} = \dot{\psi}_{t_0}(t).$$  \hspace{1cm} (117)

Furthermore, we can check that the field $\psi_{t_0}'$ defined by $\psi_{t_0}'(t') := \psi_{t_0}(t' + t - t_0)$ also satisfies the initial conditions (117). Hence by the uniqueness of the solution of the initial-value problem for (1), we have $\psi_t(t') = \psi_{t_0}(t' + t - t_0)$ for all $t'$. This equation shows that the time-evolution generated by $h$ is a $t$-translation of the fields; the choice of $h$ as the Hamiltonian is equivalent to identifying $t$ with time. However note that a time-translation does not correspond to a unitary time-evolution in $\mathcal{H}$, unless for all $t$ the Hamiltonian $H$ happens to be $\bar{\eta}_0$-pseudo-Hermitian. If this condition holds, we can choose (113) and obtain $h' = h$. As we mentioned above, this is the case for a stationary Klein-Gordon-type field. In general this condition is not fulfilled, $h$ is not a Hermitian operator acting in $\mathcal{H}$, and $t$-translations are not unitary operators in this space.

This argument is valid even if we choose an arbitrary positive-definite inner product on $\mathcal{H}$ that is not necessarily of the form (13). Suppose that $h$ is Hermitian with respect to some inner product $\langle \cdot, \cdot \rangle$ on $\mathcal{H}$. As we have shown in Section 3, such an inner product is obtained from an invariant inner product $\langle \cdot, \cdot \rangle_\eta$ on $\tilde{\mathcal{H}} \otimes \mathbb{C}^2$ that is defined by a general $t$-independent positive-definite operator $\eta_0$ according to (43) and (49). In light of the fact that the operator $U_t = U(t, t_0) U_1$ defined by (10) is a unitary operator mapping $\mathcal{H}$ equipped with the inner product $\langle \cdot, \cdot \rangle$ to $\tilde{\mathcal{H}} \otimes \mathbb{C}^2$ with inner product $\langle \cdot, \cdot \rangle_\eta$, the operator

$$H_t := U_t h U_t^{-1} = U(t, t_0) U_1 h U_1^{-1} U(t, t_0)^{-1} = U(t, t_0) H(t) U(t, t_0)^{-1},$$  \hspace{1cm} (118)

t-dependent operator (namely $H$), $h$ is $t$-dependent.
must be Hermitian with respect to $\langle \cdot, \cdot \rangle_\eta$. This is equivalent to saying that $H_t$ is $\eta$-pseudo-Hermitian: $H_t^\dagger = \eta H_t \eta^{-1}$. Substituting (119) and (118) in this equation then yields $H(t)^\dagger = \eta_0 H(t) \eta_0^{-1}$. Hence, demanding that $h$ be Hermitian with respect to some inner product on $\mathcal{H}$ implies that for all $t$, $H(t)$ is $\eta_0$-pseudo-Hermitian: $H(t)^\dagger = \eta_0 H(t) \eta_0^{-1}$. Substituting (49) and (118) in this equation then yields $H(t_0)^\dagger = \eta_0 H(t_0) \eta_0^{-1}$. Hence, demanding that $h$ be Hermitian with respect to some inner product on $\mathcal{H}$ implies that for all $t$, $H(t)$ is $\eta_0$-pseudo-Hermitian for some $t$-independent positive-definite operator $\eta_0$.\(^{18}\) The necessary and sufficient condition for the latter is that $H(t_0)$ be $\eta_0$-pseudo-Hermitian and the eigenvectors of $H(t)$ do not depend on $t$. In view of (24) – (26), this holds if and only if $D$ is $t$-independent. Therefore, for a nonstationary Klein-Gordon-type field, one cannot identify $t$ with a time-parameter associated with the dynamics generated by a Hermitian Hamiltonian.\(^{19}\)

As we mentioned above, it is a $t$-dependent element $V$ of the group $G_{\eta_0}$ that determines the Hamiltonian $h'$ and consequently the quantum system $s_{L_0}$. There are infinitely many choices for $V$. Among them are certain choices that make $h'$ $t$-independent. For example, letting

$$V_0 := e^{i (t - t_0)/\hbar} H(t_0)$$

(119) yields $h' = h_0' := \hbar U_1 H(t_0) U_1^{-1} = h(t_0)$, where $H(t_0)$ and $h(t_0)$ are respectively the Hamiltonians (10) and (32) evaluated at $t = t_0$. Clearly for stationary Klein-Gordon-type fields, (119) coincides with (113).

We can use the analysis of Section 4.2 to solve the eigenvalue problem for the Hamiltonian $h_0'$. The eigenvalues have the form $\pm \hbar \omega_{0n}$ where $\omega_{0n}$ are the positive square roots of the eigenvalues of $D_0$. A complete set of eigenvectors $\psi_{\pm,n}$ of $h'$ (with eigenvalues $\pm \hbar \omega_{0n}$) are given by the following initial conditions

$$\psi_{\pm,n}(t_0) = N_{\pm,n} \phi_{0n}, \quad \dot{\psi}_{\pm,n}(t_0) = \mp i N_{\pm,n} \omega_{0n} \phi_{0n}.$$ 

Here $N_{\pm,n} \in \mathbb{C}$ are normalization constants and $\phi_{0n}$ are linearly independent eigenvectors of $D_0$ corresponding to the eigenvalue $\omega_{0n}^2$.

We conclude this section by emphasizing that for both stationary and nonstationary Klein-Gordon-type fields the choice of a Hamiltonian acting in $\mathcal{H}$ is not unique. Choosing nonequivalent Hermitian operators as Hamiltonians acting in $\mathcal{H}$ and using the unitary operator $U_1'$ with any choice of $V \in G_{\eta_0}$ to induce a corresponding Hamiltonian acting in $\mathcal{H}$ yield nonequivalent notions of time-evolution in $\mathcal{H}$.

\(^{18}\)The converse of this statement is clearly true.

\(^{19}\)As $h$ is a diagonalizable operator with a real spectrum, one may appeal to the results of [20] to argue for the existence of an inner product with respect to which $h$ is Hermitian. This inner product will necessarily be $t$-dependent and hence ill-defined. Moreover, because of the $t$-dependence of such an inner product, the Hermiticity of $h$ is not sufficient for the unitarity of the dynamics it generates [5]. One can also attempt to construct an inner product with respect to which the dynamics generated by $h$ is unitary, but this inner product will also be necessarily $t$-dependent and consequently ill-defined.
5.3 Formulating the quantum mechanics of a nonstationary Klein-Gordon-type field using the Hilbert space $\mathcal{H}_*$

Let $A_0, A_0, \eta_0^+, \rho_0 : \tilde{\mathcal{H}} \otimes \mathbb{C}^2 \to \tilde{\mathcal{H}} \otimes \mathbb{C}^2$, be the values of the operators (32), (87), (29), and (79) at $t = t_0$, respectively, i.e.,

$$A_0 := A(t_0), \quad A_0 := A(t_0), \quad \eta_0^+ = \eta_+(t_0), \quad \rho_0 := \rho(t_0), \quad (120)$$

so that

$$\tilde{\eta}_0 = A_0^\dagger \eta_0^+ A_0, \quad (121)$$

$$\eta_0^+ = \rho_0^2, \quad (122)$$

Suppose that $\mathcal{W}, U'_2 : \tilde{\mathcal{H}} \otimes \mathbb{C}^2 \to \tilde{\mathcal{H}} \otimes \mathbb{C}^2$ are linear operators such that $\mathcal{W}$ is $\tilde{\eta}_0$-pseudo-unitary ($\mathcal{W} \in G_{\tilde{\eta}_0}$):

$$\mathcal{W}^\dagger \tilde{\eta}_0 \mathcal{W} = \tilde{\eta}_0, \quad (123)$$

and $U'_2$ is defined by

$$U'_2 := \rho_0 A_0 \mathcal{W} U(t, t_0)^{-1}. \quad (124)$$

Then a simple calculation shows that, for all $\xi, \zeta \in \tilde{\mathcal{H}} \otimes \mathbb{C}^2$,

$$\langle \langle \xi | \zeta \rangle \rangle_{\eta(t)} = \langle \xi, U(t, t_0)^{-1} \tilde{\eta}_0 U(t, t_0)^{-1} \zeta \rangle = \langle \xi, U(t, t_0)^{-1} \mathcal{W}^\dagger \tilde{\eta}_0 \mathcal{W} U(t, t_0)^{-1} \zeta \rangle = \langle \xi, U(t, t_0)^{-1} \mathcal{W}^\dagger A_0^\dagger \eta_0^+ A_0 \mathcal{W} U(t, t_0)^{-1} \zeta \rangle = \langle \xi, U'_2 \tilde{U}'_2 \zeta \rangle = \langle U'_2 \xi, U'_2 \zeta \rangle.$$

Therefore, $U'_2$ is a unitary operator mapping the Hilbert space $\mathcal{H}_{L_0\pm}$ to the Hilbert space $\mathcal{H}_*$, and the quantum mechanics $Q_{L_0\pm}$ and subsequently $q_{L_0\pm}$ with all possible choices for $L_{0\pm}$ are equivalent to $Q_*$. The following diagram shows the unitary mappings relating $\mathcal{H}, \mathcal{H}_{L_0\pm}$, and $\mathcal{H}_*$.

$$\mathcal{H} \xrightarrow{U'_1} \mathcal{H}_{L_0\pm} \xrightarrow{U'_2} \mathcal{H}_*.$$

We can also use $U'^{\dagger}_2$ to induce a Hamiltonian $H'_* \mathcal{H}_*$ from the Hamiltonian $H$ on $\mathcal{H}_{L_0\pm}$. Again because $U'_2$ depends on $t$, $H'_* := U'_2 H U'^{\dagger}_2 + i \hbar \tilde{U}'_2 U'^{\dagger}_2$. Substituting (124) in this equation, we find

$$H'_* = \rho_0 A_0 \mathcal{W} A_0^{-1} \rho_0^{-1} = \rho_0 W \rho_0^{-1}, \quad (125)$$

where

$$W := i \hbar \tilde{\mathcal{W}} \mathcal{W}^{-1}, \quad W_+ := A_0 W A_0^{-1}. \quad (126)$$
The $\tilde{\eta}_0$-pseudo-unitarity of $W$ implies that $W$ is an $\tilde{\eta}_0$-pseudo-Hermitian operator, i.e.,

$$W^\dagger = \tilde{\eta}_0 W \tilde{\eta}_0^{-1}. \quad (127)$$

Because $U_2' : \mathcal{H}_{L_0} \to \mathcal{H}_*$ and $H : \mathcal{H}_{L_0} \to \mathcal{H}_{L_0}$ are respectively unitary and Hermitian operators, $H_*$ is a Hermitian operator acting in the Hilbert space $\mathcal{H}_*$. We can also compute $H_*^\dagger$ directly. To do this, first we use (127) and (121) to show that $W_+$ is $\eta_0+$-pseudo-Hermitian, i.e., $W_+^\dagger = \eta_0+W_+ \eta_0^{-1}$. In view of this relation and (122) and (125), we then have

$$H_*^\dagger = (\rho_0 W_+ \rho_0^{-1})^\dagger = \rho_0^{-1} W_+^\dagger \rho_0 = \rho_0 W_+ \rho_0^{-1} = H_*'.$$

Hence $H_*'$ is indeed a Hermitian operator acting in $\mathcal{H}_*$. As seen from (125) it is determined by the choice of an $\eta_0+$-pseudo-Hermitian operator $W_+ \in G_{\tilde{\eta}_0}$. By construction, the unitary operator $U' : \mathcal{H} \to \mathcal{H}_*$ defined by

$$U' := U_2' U_1' \quad (128)$$

maps the Hamiltonian $h'$ of the quantum system $s_{L_0}^\prime$ to the Hamiltonian $H_*'$. Therefore, $s'_{L_0}$ is equivalent to the quantum system $S_*'$ defined by the Hilbert space $\mathcal{H}_*$ and the Hamiltonian $H_*'$.

For a stationary Klein-Gordon-type field where $D$ does not depend on $t$ and $U(t,t_0) \in G_{\tilde{\eta}_0}$, we can set $W = U(t,t_0)$ and $W = H$. Now using (83) and (125) and the fact that in this case $A_0$ commutes with $H$, we see that $H_*' = H_*$ and the quantum system $S_*'$ reduces to $S_*$.

### 5.4 Quantum observables for a nonstationary Klein-Gordon-type field

The construction of the observables for stationary Klein-Gordon-type fields as reported in Section 4.4 generalizes to nonstationary Klein-Gordon type fields. Again one uses the unitary operator $U' : \mathcal{H} \to \mathcal{H}_*$ to express the observables $o$ of $q_{L_0}$ in terms of the observables $O_*$ of $Q_*$ according to

$$o = U'^{-1} O_* U'. \quad (129)$$

Here $O_*$ has the general form (93) and $U'$ is the unitary operator (128).

Substituting (109) and (124) in (128), we find

$$U' = \rho_0 A_0 X U_1, \quad X := \mathcal{W} V. \quad (130)$$

As seen from this equation $U'$ is determined by the choice of an element $X$ of the group $G_{\tilde{\eta}_0}$. We start our derivation of the general form of the observables $o$ by showing that we can absorb
the arbitrariness in $X$ in the form of the observables $O_\star$. Using the $\tilde{\eta}_0$-pseudo-unitarity of $X$, i.e.,

$$X^\dagger = \tilde{\eta}_0 X^{-1} \tilde{\eta}_0,$$  \hspace{1cm} (131)

and (121), we can establish the identity

$$(A_0 X)^{-1} = \tilde{\eta}_0^{-1} (A_0 X)^\dagger \eta_0.$$  \hspace{1cm} (132)

Furthermore, we introduce a linear operator $R : \mathcal{H}_\star \to \mathcal{H}_\star$ given by

$$R := \rho_0 A_0 X,$$  \hspace{1cm} (133)

and let for each observable $O_\star$ of $Q_\star$,

$$O'_\star := R^\dagger O_\star R.$$  \hspace{1cm} (134)

Now, inserting (130) in (129) and using (132), (122), (133), and (134), we have

$$o = U^{-1}_1 (A_0 X)^{-1} \rho_0^{-1} O_\star \rho_0 A_0 X U_1$$

$$= U^{-1}_1 \tilde{\eta}_0^{-1} (A_0 X)^\dagger \eta_0 + \rho_0^{-1} O_\star \rho_0 A_0 X U_1$$

$$= U^{-1}_1 \tilde{\eta}_0^{-1} (A_0 X)^\dagger \rho_0 O_\star \rho_0 A_0 X U_1$$

$$= U^{-1}_1 \tilde{\eta}_0^{-1} R^\dagger O_\star R U_1$$

$$= U^{-1}_1 \tilde{\eta}_0^{-1} O'_\star U_1.$$  \hspace{1cm} (135)

Because $R$ is an invertible operator acting in $\mathcal{H}_\star$, we can express any Hermitian operator acting in $\mathcal{H}_\star$ in the form $R^\dagger O_\star R$ for some Hermitian operator $O_\star$. This means that in order to obtain the general form of the observables $o$ we can adopt the general form (133) for the operator $O'_\star$ in (135).

Incidentally, recall that we can reproduce the results obtained for the stationary Klein-Gordon-type fields by taking $V = U(t, t_0)^{-1}$ and $W = U(t, t_0)$. This in particular means that we can recover the results of Section 4.4 by setting $X = 1$ in the expressions (135) for $o$. Doing so, we find that for a stationary field

$$o_{\text{stat.}} = U^{-1}_1 \tilde{\eta}_0^{-1} A_0^\dagger \rho_0 O_\star \rho_0 A_0 U_1.$$  \hspace{1cm} (136)

We can also express the observables (135) for the nonstationary case in this form provided that we introduce

$$O''_\star := (\rho_0 A_0)^{-1 \dagger} O'_\star (\rho_0 A_0)^{-1}.$$  \hspace{1cm} (137)

Substituting this equation in (135) and recalling that $\rho_0^\dagger = \rho_0$ we find

$$o = U^{-1}_1 \tilde{\eta}_0^{-1} A_0^\dagger \rho_0 O''_\star U_1 \rho_0 A_0 U_1.$$  \hspace{1cm} (138)
Again because $\rho_0, A_0 : \mathcal{H}_r \to \mathcal{H}_r$ are invertible operators, every Hermitian operator acting in $\mathcal{H}_r$ may be expressed in the form (137). This together with (136) and (138) imply that the general form of the observables $o$ for a nonstationary Klein-Gordon-type field is given by the corresponding expressions, namely (101) and (102), for the stationary case provided that we let $O''_0$ have the general form (93) and identify the operators $A_\pm$ appearing in (103) with their value at $t_0$. This yields the initial values of the field $o\psi$ for a given $\psi \in \mathcal{H}$. Obviously, one can no longer obtain an analog of (104) for a nonstationary field. However, the matrix elements $(\psi, o\phi)_{t_0}$ are still given by the right-hand side of (105) provided that we set $D = D_0$ in this equation and identify the operators $A_\pm$ with their value at $t_0$ in (106).

Finally we wish to point out that because the choice of the operators $V, W \in G_{\tilde{\eta}_0}$ is arbitrary, one can always choose $V = W^{-1}$. In this case, $\mathcal{X} = 1$ and the unitary operator $U'$ is independent of $t$. This choice simplifies the construction of the Hamiltonians $\tilde{h}$ for the quantum systems $q_{L_0 \pm}$ from the Hamiltonians $\tilde{H}_r$ for $Q_r$. Clearly, for a $t$-independent $U'$, the Hamiltonians $\tilde{h}$ and $\tilde{H}_r$ are related according to the same formula that relates the observables $o$ and $O''_0$.

6 Quantum Mechanics on the Space of Classical Harmonic Oscillators

Consider the equation of motion for a classical harmonic oscillator with a possibly nonstationary frequency $\omega = \omega(t) \in \mathbb{R}^+$. This is clearly an example of a Klein-Gordon-type equation (11). In particular if we consider an isotropic harmonic oscillator in two real (one complex) dimensions, then we can identify its equation of motion with the Klein-Gordon-type equation (11) corresponding to the choice:

$$\tilde{H} = \mathbb{C} \text{ equipped with the Euclidean inner product, } D = \omega^2. \quad (139)$$

The space $\mathcal{H}$ of solutions of such an oscillator is, as a vector space, isomorphic to $\mathbb{C}^2$. In fact, because in this case the Hilbert space $\mathcal{H}_r$ is identical with the Euclidean space $\mathbb{C}^2$, $\mathcal{H}$ is also isomorphic to the Euclidean space $\mathbb{C}^2$ as a Hilbert space. Therefore, the classical oscillators (139) are simple nontrivial systems to which we can apply the results of Sections 4 and 5 and study their implications.

Besides being a useful toy model, the classical harmonic oscillators (139) have some application in quantum cosmology. For instance, the choice

$$\omega = \sqrt{\Lambda} e^{3t} \quad (140)$$

corresponds to the Wheeler-DeWitt equation for a flat FRW model with a positive cosmological...
constant \( \Lambda \), where \( t \) is to be identified with the logarithm of the scale factor, \[27, 28\]. Therefore, studying the quantum mechanics of time-dependent oscillators \[139\] sheds light on some of the basic problems of quantum cosmology. Specifically, we can use the results of Section 5 to construct the Hilbert space and the observables for this model, i.e., solve the Hilbert space problem \[3\].

An interesting outcome of our analysis, which generalizes to other cosmological models, is that one does not need to obtain solutions of the Wheeler-DeWitt equation to assess the kinematical structure of the corresponding quantum cosmological model. The states and the observables may be formulated in terms of the initial data of the defining Wheeler-DeWitt equation. The dynamics too may be expressed in terms of the initial data. However one must first choose an appropriate Hamiltonian operator. In view of the analogy with nonrelativistic quantum mechanics, this seems to require Dirac’s canonical quantization of the corresponding classical system (if there is any) which would assign physical meaning to the quantum observables and determine (up to factor-ordering ambiguities) the form of the Hamiltonian. Such a scheme should naturally be supported by an appropriate correspondence principle. As we have already imposed the quantum constraint (the Wheeler-DeWitt equation), the above-mentioned quantization scheme should be performed on the classical system obtained by imposing the classical constraint. The flat FRW model with a cosmological constant is too restricted to allow for a nontrivial classical internal dynamics. Therefore, we defer a discussion of the above quantization scheme to the next section where we consider FRW models coupled to a real scalar field.

In the following, we study the quantum mechanics of general classical oscillators \[139\] with an arbitrary possibly \( t \)-dependent frequency \( \omega \).

For the oscillators \[139\], the inner product \[107\] takes the form

\[
(\psi_1, \psi_2)_{t_0} = \frac{1}{2} \left\{ L_{0+} [\psi_1^*(t_0)\psi_2(t_0) + \omega_0^{-2}\dot{\psi}_1^*(t_0)\dot{\psi}_2(t_0)] + i\omega_0^{-1}L_{0-}[\psi_1^*(t_0)\dot{\psi}_2(t_0) - \dot{\psi}_1^*(t_0)\psi_2(t_0)] \right\},
\]

(141)

where \( t_0 \) is an initial value of \( t \), \( L_{0\pm} \) are a pair of real numbers such that \( L_{0+} \pm L_{0-} \) are positive, and \( \omega_0 := \omega(t_0) \). Note that if we choose \( L_{0-} = 0 \) and set \( L_{0+} = m\omega_0^2 \) where \( m \) is the mass of the oscillator, \[141\] yields the total energy of the oscillator at \( t_0 \). This shows that for a stationary oscillator the inner products \[141\] include the energy inner product \[29\] as a special case.

The observables \( o \) of \( q_{L_{0\pm}} \) may be constructed as linear combinations (with real coefficients) of a set of four basic observables \( o_\mu \). These are related via the unitary operator \( U' \) to the basic observables \( \sigma_\mu \) of \( Q_* \), where \( \mu \in \{0, 1, 2, 3\} \), \( \sigma_0 \) is the \( 2 \times 2 \) identity matrix and \( \sigma_\mu \) with \( \alpha \neq 0 \) are the Pauli matrices \[35\]. Letting \( O'_{\alpha} \) of \[137\] be equal to \( \sigma_\mu \), computing the corresponding

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\[20\]This is also true with a slightly more general expression for \( \omega \) for open FRW models.
values for $J_\pm$ and $K_\pm$ of (103), and using (102), we find, for all $\psi \in \mathcal{H}$, the following expressions for the initial values of $\phi_\mu := o_\mu \psi$.

$$
\begin{align*}
\phi_0(t_0) &= \psi_0, & \dot{\phi}_0(t_0) &= \dot{\psi}_0; \\
\phi_1(t_0) &= \frac{1}{2}(s_+ \psi_0 + i s_- \omega_0^{-1} \dot{\psi}_0), & \dot{\phi}_1(t_0) &= \frac{1}{2}(i \omega_0 s_- \psi_0 - s_+ \dot{\psi}_0), \\
\phi_2(t_0) &= \frac{1}{2}(i s_- \psi_0 - s_+ \omega_0^{-1} \dot{\psi}_0), & \dot{\phi}_2(t_0) &= \frac{1}{2}(-s_+ \omega_0 \psi_0 - i s_- \dot{\psi}_0), \\
\phi_3(t_0) &= i \omega_0^{-1} \dot{\psi}_0, & \dot{\phi}_3(t_0) &= -\omega_0 \dot{\psi}_0,
\end{align*}
$$

where

$$
\begin{align*}
s_\pm &:= \frac{A_{0+}}{A_{0-}} \pm \frac{A_{0-}}{A_{0+}} = \left(\frac{L_{0+} + L_{0-}}{L_{0+} - L_{0-}}\right) e^{i(\theta_+ - \theta_-)} \pm \left(\frac{L_{0+} - L_{0-}}{L_{0+} + L_{0-}}\right) e^{-i(\theta_+ - \theta_-)},
\end{align*}
$$

with $A_{0\pm} = A_\pm(t_0)$, and $\theta_\pm \in \mathbb{R}$ are arbitrary. As we explain in the Appendix, we can redefine the basic observables $\sigma_\mu$ in such a way that the phase angles $\theta_\pm$ disappear from (142) – (145). Therefore, the observables $o_\mu$ with $s_\pm$ given by (146) and $\theta_\pm = 0$ provide a set of basic observables for $q_{L_{0\pm}}$.

Next, we construct a Hamiltonian operator $\hat{h}$ acting in $\mathcal{H}$. Following the prescription described in the last paragraph of Section 5.4, $\hat{h}$ may be obtained from a Hamiltonian $\hat{H}_*$ acting in $\mathcal{H}_*$ by the same unitary transformation $U'$ that is used to construct the basic observables $o_\mu$. This in turn means that $\hat{h}$ will be a linear combination of $o_\mu$ with real coefficients.

If the oscillator is stationary, i.e., $\omega$ does not depend on $t$, we have the canonical Hamiltonian $h$ that is obtained via the unitary transformation $U$ of (85) from the Hamiltonian $H_*$ of (83). The latter has the simple form

$$
H_* = \hbar \omega \sigma_3.
$$

As we discussed in section 4.3, the Hamiltonian $h$ identifies the parameter $t$ with time. In view of (147), $H_*$ and consequently $h$ describe the interaction of a spin-half particle with a constant magnetic field [26].

For a nonstationary oscillator, where $\omega$ depends on $t$, we can still choose

$$
\hat{H}_* = H_*.
$$

But the corresponding Hamiltonian $\hat{h}$ does not generate $t$-translations in $\mathcal{H}$. Instead, it defines its own time-parameter $\bar{t} \in \mathbb{R}$. Clearly, in this case, $\bar{h} = \hbar \omega \sigma_3$. Therefore, the eigenvectors of $\bar{h}$ do not depend on $\bar{t}$ and its evolution operator is readily obtained as [26]

$$
\bar{v}(\bar{t}, \bar{t}_0) = e^{-i\Omega(\bar{t}, \bar{t}_0) \sigma_3},
$$

where

$$
\Omega(\bar{t}, \bar{t}_0) = \int_{\bar{t}_0}^{\bar{t}} \omega(s) ds.
$$

36
where

\[ \Omega(\tilde{t}, \tilde{t}_0) := \int_{\tilde{t}_0}^{\tilde{t}} \omega(t) dt, \] (150)

and \( \tilde{t}_0 \) is an initial time. Moreover, because \( \tilde{h} \) is related to \( \tilde{H}_\star \) via the unitary operator \( U' \), \( \tilde{v}(\tilde{t}, \tilde{t}_0) \) may be obtained from the time-evolution operator for \( \tilde{H}_\star \), namely

\[ \tilde{U}_\star(\tilde{t}, \tilde{t}_0) = e^{-i\Omega(\tilde{t}, \tilde{t}_0) \sigma_3} = \cos[\Omega(\tilde{t}, \tilde{t}_0)] \sigma_0 - i \sin[\Omega(\tilde{t}, \tilde{t}_0)] \sigma_3. \]

This yields

\[ \tilde{v}(\tilde{t}, \tilde{t}_0) = \cos[\Omega(\tilde{t}, \tilde{t}_0)] o_0 - i \sin[\Omega(\tilde{t}, \tilde{t}_0)] o_3. \] (151)

Now, let \( \psi_\tilde{t} \in \mathcal{H} \) be an evolving state vector with initial condition \( \phi \in \mathcal{H} \), i.e.,

\[ \psi_\tilde{t} = \tilde{v}(\tilde{t}, \tilde{t}_0) \phi. \] (152)

Then, in view of (142), (145) and (151), the initial data \((\psi_\tilde{t}(t_0), \dot{\psi}_\tilde{t}(t_0))\) for \( \psi_\tilde{t} \) are related to the initial data \((\phi(t_0), \dot{\phi}(t_0))\) for \( \phi \) according to

\[ \psi_\tilde{t}(t_0) = \cos[\Omega(\tilde{t}, \tilde{t}_0)] \phi(t_0) + \omega_0^{-1} \sin[\Omega(\tilde{t}, \tilde{t}_0)] \dot{\phi}(t_0), \] (153)

\[ \dot{\psi}_\tilde{t}(t_0) = i \omega_0 \sin[\Omega(\tilde{t}, \tilde{t}_0)] \phi(t_0) + \cos[\Omega(\tilde{t}, \tilde{t}_0)] \dot{\phi}(t_0). \] (154)

Clearly, the time-evolution generated by the Hamiltonian (148) corresponds to ‘rotations’ of the state vectors in \( \mathcal{H} \). The time-parameter \( \tilde{t} \) of this Hamiltonian cannot be identified with the parameter \( t \) of the defining classical oscillator.

The description of the dynamics generated by the Hamiltonian (148) in terms of rotations in \( \mathcal{H} \) generalizes to arbitrary choices for the Hamiltonian \( \tilde{h} \). This is because any Hamiltonian \( \tilde{H}_\star \) belongs to the Lie algebra \( u(2) \). As the dynamics of the states take place in the projective Hilbert space \( \mathbb{C}P^1 \), which in this case has the structure of \( \mathbb{C}P^1 \), it is the traceless part of \( \tilde{H}_\star \) that is physically significant. This belongs to the Lie algebra \( su(2) \). Hence the group \( SU(2) \) serves as the dynamical Lie group for the quantum systems of \( Q_\star \) and consequently \( q_{lo\pm} \). In particular, the evolution operator for any Hamiltonian \( \tilde{h} \) corresponds to a \( (SU(2)-) \) rotation of the states in the Schrödinger-picture (respectively of observables in the Heisenberg-picture).

7 Quantum Mechanics of a FRW Model Coupled to a Real Scalar Field

It is well-known that the canonical quantization of an FRW model coupled to a real scalar field \( \varphi \) yields a single quantum constraint \( \hat{K} \psi = 0 \):

\[ \hat{K} \psi = 0, \] (155)
where \( \hat{K} \) is obtained by quantizing the classical Hamiltonian constraint \[ K := -\pi_\alpha^2 + \pi_\varphi^2 - \kappa e^{4\alpha} + e^{6\alpha} V(\varphi) = 0, \] (156)

\( \pi_\alpha \) and \( \pi_\varphi \) are respectively the momenta associated with the logarithm \( \alpha \) of the scale factor \( a \) and the scalar field \( \varphi \), \( V = V(\varphi) \) is a real-valued potential for the field \( \varphi \), \( \kappa = -1, 0, 1 \) determines whether the universe is open, flat, or closed, respectively, and we have used the natural system of units as discussed in [10].

The above-mentioned quantization of the classical constraint (156) means the canonical quantization \( \Xi \) that respectively associates to the classical unconstrained phase-space variables \( \alpha, \varphi, \pi_\alpha, \) and \( \pi_\varphi \) the operators \( \Xi(\alpha), \Xi(\varphi), \Xi(\pi_\alpha), \) and \( \Xi(\pi_\varphi) \) that act in the auxiliary (kinematic) Hilbert space \( \mathcal{H}' = L^2(\mathbb{R}^2) \), where \( \mathbb{R}^2 \) is the configuration space parameterized by \( (\alpha, \varphi) \). Specifically, one treats \( \vec{X} := (\Xi(\alpha), \Xi(\varphi)) \) as the position operator and \( \vec{P} := (\Xi(\pi_\alpha), \Xi(\pi_\varphi)) \) as the momentum operator acting in \( L^2(\mathbb{R}^2) \) and uses the position kets \( |\vec{x}\rangle := |\alpha, \varphi\rangle \) to express the quantum constraint (155) in terms of the wave functions

\[ \psi(\alpha, \varphi) := \langle \alpha, \varphi|\psi\rangle, \] (157)

where \( \langle \cdot | \cdot \rangle \) stands for the inner product in \( \mathcal{H}' = L^2(\mathbb{R}^2) \). In view of the identities

\[ \langle \alpha, \varphi|\Xi(\alpha) = \alpha \langle \alpha, \varphi|, \quad \langle \alpha, \varphi|\Xi(\varphi) = \varphi \langle \alpha, \varphi|, \]

\[ \langle \alpha, \varphi|\Xi(\pi_\alpha) = -i \frac{\partial}{\partial \alpha} \langle \alpha, \varphi|, \quad \langle \alpha, \varphi|\Xi(\pi_\varphi) = -i \frac{\partial}{\partial \varphi} \langle \alpha, \varphi|, \]

the quantum constraint (155) — written in the form \( \langle \alpha, \varphi|\hat{K}\psi\rangle = 0 \) — yields the Wheeler-DeWitt equation (3):

\[ \left[ -\frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \varphi^2} + \kappa e^{4\alpha} - e^{6\alpha} V(\varphi) \right] \psi(\alpha, \varphi) = 0. \] (158)

Here and in what follows we set \( \hbar = 1 \), but recover \( \hbar \) where appropriate.

As we have noted in Section 1, the Wheeler-DeWitt equation (158) is another example of Klein-Gordon-type equations. We can write it in the form (1), if we identify \( \alpha \) with the variable \( t \) and let \( \mathcal{H} = L^2(\mathbb{R}) \) and

\[ D = -\frac{\partial^2}{\partial \varphi^2} + e^{6\alpha} V(\varphi) - \kappa e^{4\alpha}. \] (159)

Clearly \( D \) is a Hermitian operator acting in \( L^2(\mathbb{R}) \). However, depending on the form of \( V \) and the value of \( \kappa \) it may or may not be positive-definite. In what follows we shall only consider nonnegative confining potentials, i.e., suppose that for all \( \varphi \in \mathbb{R} \), \( V(\varphi) \geq 0 \) and \( \lim_{\varphi \to \pm \infty} V(\varphi) = +\infty \). In this case \( D \) has a nondegenerate discrete spectrum [30]. Moreover, for the open and flat models, \( D \) is a positive-definite operator.

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A typical choice for the potential \( V \) is

\[
V(\varphi) = m^2 \varphi^2
\]  

(160)

which corresponds to \( \varphi \) being a massive scalar field of mass \( m \). For such a field, the operator \( D \) is identical with the Hamiltonian operator of a time-dependent quantum harmonic oscillator. Therefore its eigenvalue problem can be easily solved \(31\). 

Before we apply the theory developed in the preceding sections to formulate a quantum cosmology based on the Wheeler-DeWitt equation \( \text{(158)} \), we wish to point out that the definition of the operator \( \hat{K} \) alternatively \( \text{(155)} \) suffers from a factor-ordering ambiguity. For example, one may quantize the term \( \pi^2 \alpha \) appearing in the classical constraint \( \text{(156)} \) according to \( \Xi(\pi^2 \alpha) = \Xi(\alpha)^p \Xi(\pi_\alpha) \Xi(\alpha)^{-2p} \Xi(\pi_\alpha) \Xi(\alpha)^p \) for any \( p \in \mathbb{R} \). This leads to additional terms in the left-hand side of the Wheeler-DeWitt equation \( \text{(158)} \). The factor-ordering problem is more transparent if one expresses the classical constraint in terms of the scale factor \( a \). Certainly it does not go away if one uses \( \alpha \).

The presence of \( \alpha \) in the expression for \( D \) indicates that the corresponding Wheeler-DeWitt equation is a nonstationary Klein-Gordon-type equation. We can apply the results of Sections 3 and 5 to obtain the most general Hilbert space structure on the physical space \( \mathcal{H} \) of solutions of the Wheeler-DeWitt equation, construct the observables, and perhaps more importantly reduce the problem of the identification of time to the issue of choosing a Hamiltonian operator acting in \( \mathcal{H} \) (equivalently acting in \( \mathcal{H}_a \)). Following the approach of Section 6, as a method of choosing a specific Hamiltonian, we propose to perform a canonical quantization of the classical system obtained after imposing the classical constraint.

According to the results of Section 3, all the choices for an inner product on the physical Hilbert space \( \mathcal{H} \) are physically equivalent. We can choose the inner product \( \text{(107)} \) with \( D_0 = D(\alpha_0) \) for any \( \alpha_0 \in \mathbb{R} \) for the flat and open FRW models. For a closed FRW model we may identify \( D_0 \) with \( D(\alpha_0) \) for any \( \alpha_0 \) that makes \( D(\alpha_0) \) positive-definite. For a positive confining potential \( V \) the smallest eigenvalue of \( D + \kappa e^{4\alpha} \) is necessarily positive. This together with the particular \( \alpha \)-dependence of \( D \) imply that there is always some \( \alpha_0 \in \mathbb{R} \) such that \( D(\alpha_0) \) is a positive-definite operator. In the following we shall choose such an \( \alpha_0 \) and endow \( \mathcal{H} \) with an inner product of the form \( \text{(107)} \).

In order to facilitate the application of the results of Section 5 and avoid potential ambiguities, we introduce for each real number \( \alpha \) and Wheeler-DeWitt field \( \psi \) the value \( \psi(\alpha) \) of \( \psi \). This is the function:

\[ \psi(\alpha)[\varphi] := \psi(\alpha, \varphi), \quad \forall \varphi \in \mathbb{R}. \]

We shall view \( \psi(\alpha) \) as an element of the Hilbert space \( \tilde{\mathcal{H}} = L^2(\mathbb{R}) \).\(^{21}\) In this way we can rewrite

\(^{21}\)This is a standard approach in dealing with hyperbolic partial differential equations. See for example \(32\).
the Wheeler-DeWitt equation \(^{(158)}\) in the standard form \(^{(11)}\) of a Klein-Gordon-type equation, namely

\[ \ddot{\psi}(\alpha) + D\psi(\alpha) = 0, \quad (161) \]

where a dot means an \(\alpha\)-derivative and the operator \(D\) is viewed as a linear operator acting in the abstract Hilbert space \(\tilde{\mathcal{H}} = L^2(\mathbb{R})\).

Because the inner product \(^{(107)}\) is positive-definite, unlike the Klein-Gordon inner product \(^{[3, 9]}\), it allows for a genuine probability interpretation for the Wheeler-DeWitt fields. Evidently such an interpretation is useful only if we also have a set of basic observables. As we discussed in detail in Section 5, the observables of the quantum mechanics \(q_{L0,\pm}\) having \(\mathcal{H}\) with inner product \(^{(107)}\) as its Hilbert space are obtained via the unitary transformations \(U'\) from the observables \(O''_\star\) of \(Q_\star\).

It is not difficult to see that any observable \(O''_\mu\) can be expressed in terms of the following basic observables:

\[ O_\mu := 1 \otimes \sigma_\mu, \quad \hat{Q} := \hat{q} \otimes \sigma_0, \quad \hat{P} := \hat{p} \otimes \sigma_0, \quad (162) \]

where 1 stands for the identity operator of \(\tilde{\mathcal{H}}\), \(\mu \in \{0, 1, 2, 3\}\), \(\sigma_0\) is the \(2 \times 2\) identity matrix, \(\sigma_\mu\) with \(\alpha \neq 0\) are the Pauli matrices \(^{(35)}\), and \(\hat{q}\) and \(\hat{p}\) respectively play the role of the position and momentum operators acting in \(\mathcal{H} = L^2(\mathbb{R})\). In particular, they satisfy the canonical commutation relations \(\left[\hat{q}, \hat{p}\right] = i\hbar\).

We can represent the elements of \(\tilde{\mathcal{H}}\) in the position basis. The position kets \(|q\rangle\), with \(q \in \mathbb{R}\), are defined by \(\hat{q}|q\rangle = q|q\rangle\). They satisfy

\[ \langle q|q'\rangle = \delta(q - q'), \quad \langle q|\hat{p} = -i\hbar \frac{d}{dq} \langle q| . \]

As seen from \(^{(162)}\), any linear combination of \(O_\mu\) commutes with both \(\hat{Q}\) and \(\hat{P}\). In particular \(\{O_3, \hat{Q}\}\) is a smallest set of commuting basic observables. Therefore, we may use their generalized eigenvectors\(^{22}\) to construct a complete basis of \(\mathcal{H}_\star\). They are given by \(\xi^{(q,\epsilon)} := |q\rangle \otimes e_\epsilon\) where \(\epsilon = \pm\) and

\[ e_+ := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e_- := \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \]

Clearly, the following orthonormality and completeness relations hold:

\[ \langle \xi^{(q,\epsilon)}, \xi^{(q',\epsilon')} \rangle = \delta_{\epsilon,\epsilon'}\delta(q - q'), \quad \sum_{\epsilon = \pm} \int_{-\infty}^{\infty} dq \ |\xi^{(q,\epsilon)}\rangle \langle \xi^{(q,\epsilon)}| = O_0. \quad (163) \]

\(^{22}\)Here ‘generalized eigenvector’ means a generalized eigenfunction (distribution) viewed as an abstract vector. It does not refer to the concept of a generalized eigenvector used in linear algebra.
As a result, any two-component state vector \( \xi \in \tilde{\mathcal{H}} \otimes \mathbb{C}^2 \) may be represented by the wave functions \( g(q, \epsilon) := \langle \xi(q, \epsilon), \xi \rangle \) according to

\[
\xi = \sum_{\epsilon = \pm} \int_{-\infty}^{\infty} dq \ g(q, \epsilon) \ \xi(q, \epsilon).
\]

In the following we will, without loss of generality, adopt \( \mathcal{X} = 1 \) in the expression (130) for the operator \( U' \). This choice identifies \( U' \) with the value of the operator \( U \) of (85) at \( t = t_0 = \alpha_0 \) and, as we explained in Section 5.4, simplifies the construction of the Hamiltonian operators acting in \( \mathcal{H} \).

We can use the operator \( U' \) to define a set of basic observables for \( q_{L_0} \). These are given by substituting the observables (162) for \( O''_\mu \) in (138). We will denote the observables of \( q_{L_0} \) obtained in this way from \( O_{\mu}, \hat{Q} \) and \( \hat{P} \) by \( \hat{o}_\mu, \hat{q} \) and \( \hat{p} \), respectively. In order to determine the latter we express the former in the matrix form (93), i.e., find the corresponding operators \( \tilde{O}_1, \tilde{O}_2 \) and \( \tilde{\mathcal{O}} \), and use (101) – (103) with \( D \) and \( A_\pm \) replaced with their value at \( \alpha_0 \).

The action of \( \hat{o}_\mu, \hat{q} \) and \( \hat{p} \) on an arbitrary solution \( \psi \) of the Wheeler-DeWitt equation is described as follows. \( \phi_\mu := o_\mu \psi \) is determined by the initial conditions given by (142) – (145). \( \phi_\hat{q} := \hat{q} \psi \) is determined by the initial conditions

\[
\phi_\hat{q}(\alpha_0) = \hat{q} \ \psi_0, \quad \dot{\phi}_\hat{q}(\alpha_0) = \hat{q} \ \dot{\psi}_0.
\]

Similarly, \( \phi_\hat{p} := \hat{p} \psi \) is determined by the initial conditions:

\[
\phi_\hat{p}(\alpha_0) = \hat{p} \ \psi_0, \quad \dot{\phi}_\hat{p}(\alpha_0) = \hat{p} \ \dot{\psi}_0.
\]

Obviously, the eigenvectors

\[
\psi(\varphi, \epsilon) := U'^{-1} \xi(\varphi, \epsilon)
\]

of the commuting observables \( o_3 \) and \( \hat{q} \) form a complete orthonormal basis for \( \mathcal{H} \):

\[
\langle \psi(q, \epsilon), \psi(q', \epsilon') \rangle_{\alpha_0} = \delta_{\epsilon, \epsilon'} \delta(q - q'), \quad \sum_{\epsilon = \pm} \int_{-\infty}^{\infty} dq \ |\psi(q, \epsilon)|^2 = I,
\]

where for all \( \psi, \phi \in \mathcal{H} \) the operator \( |\psi\rangle \langle \phi| \) is defined by

\[
|\psi\rangle \langle \phi| := \langle \phi, \varrho \rangle_{\alpha_0} \psi,
\]

\( \varrho \in \mathcal{H} \) is an arbitrary state vector, and \( I \) denotes the identity operator for \( \mathcal{H} \). Clearly, the generalized eigenvectors \( \psi(\varphi, \epsilon) \) represent a complete set of localized states of the corresponding FRW universe.
Furthermore, any solution $\psi \in \mathcal{H}$ of the Wheeler-DeWitt equation (158) may be expressed as

$$
\psi = \sum_{\epsilon = \pm} \int_{-\infty}^{\infty} dq \, f(q, \epsilon) \, \psi^{(q,\epsilon)}.
$$

where

$$
f(q, \epsilon) := \langle (\psi^{(q,\epsilon)}, \psi) \rangle_{\alpha_0} = \langle \xi^{(q,\epsilon)}, U' \psi \rangle = \frac{1}{2} \left[ \langle q | \mathcal{A}_{0\epsilon} \psi_0 \rangle + \epsilon i \langle q | \mathcal{A}_{0\epsilon} D_0^{-1/2} \psi_0 \rangle \right].
$$

In the derivation of this expression we have made use of (92) which yields the operator $U'$ upon evaluating its right-hand side at $\alpha_0$. We also recall that $\mathcal{A}_{0\pm}$ appearing in (169) are arbitrary invertible operators commuting with $D_0$. They reflect the freedom of the choice of the operators $L_{0\pm}$ in the expression for the inner product (107) on $\mathcal{H}$. For instance, we can set, without loss of generality, $L_{0+} = \ell D_0, L_{0-} = 0$, and (107) turns into an energy inner product [29].

Having obtained position- and momentum-like operators acting in $\mathcal{H}$, we can also define a set of coherent states. The latter will be represented by the eigenvectors of the annihilation operator $\hat{a} := \sqrt{k/2\hbar}(\hat{q} + i\hat{p}/k)$, where $k \in \mathbb{R}^+$ is a constant.²³

By construction, the wave function (169), which maps $\mathbb{R} \times \{-1, 1\}$ into $\mathbb{C}$, determines the solution $\psi$ of the Wheeler-DeWitt equation uniquely. In terms of the wave functions (169), the inner product of a pair of Wheeler-DeWitt fields $\psi_1, \psi_2 \in \mathcal{H}$ takes the form

$$
\langle (\psi_1, \psi_2) \rangle_{\alpha_0} = \langle U' \psi_1, U' \psi_2 \rangle = \sum_{\epsilon = \pm} \int_{-\infty}^{\infty} dq \, f_1(q, \epsilon)^* f_2(q, \epsilon),
$$

where $f_i$ denotes the wave function (169) associated with $\psi_i$.

The observables $o$ of $q_{L_{0\pm}}$ are also uniquely specified in terms of their representation in the basis $\{\psi^{(q,\epsilon)}\}$; for all $\psi \in \mathcal{H}$

$$
o \psi = \sum_{\epsilon = \pm} \int_{-\infty}^{\infty} dq \, [\hat{o} f(q, \epsilon)] \, \psi^{(q,\epsilon)},
$$

where

$$
\hat{o} f(q, \epsilon) = \sum_{\epsilon' = \pm} \int_{-\infty}^{\infty} dq' \, o(q, \epsilon; q', \epsilon') \, f(q', \epsilon'),
$$

$$
o(q, \epsilon; q', \epsilon') := \langle (\psi^{(q,\epsilon)}, o \psi^{(q',\epsilon')}) \rangle_{\alpha_0}.\quad (173)
$$

²³We may also consider ‘directed coherent states’ where the corresponding state vectors are the eigenvectors of the ‘directed annihilation operators’ $\hat{a}_{\vec{n}} := \sqrt{k/2\hbar}(\hat{q} + i\hat{p}/k) \sum_{i=1}^{3} n_i a_i$, where $\vec{n} = (n_1, n_2, n_3) \in \mathbb{R}^3$ is a unit vector.
If we let $O := U' o U'^{-1}$, then we can express the matrix elements $o(q, \epsilon; q', \epsilon')$ of the operator $o$ in the form

$$o(q, \epsilon; q', \epsilon') = \langle \xi(q, \epsilon), O \xi(q', \epsilon') \rangle = \langle q| O_{\epsilon, \epsilon'} |q' \rangle, \tag{174}$$

where $O_{\epsilon, \epsilon'} := e_\epsilon^\dagger O e_{\epsilon'}$. Similarly we have, for any pair of Wheeler-DeWitt fields $\psi_1$ and $\psi_2$, with wave functions $f_1$ and $f_2$, and observables $o : \mathcal{H} \to \mathcal{H}$,

$$\langle (\psi_1, o\psi_2) \rangle_{\alpha_0} = \sum_{\epsilon = \pm} \int_{-\infty}^{\infty} dq f_1(q, \epsilon)^* \hat{o} f_2(q, \epsilon), \tag{175}$$

In particular, we can compute the expectation values of the observable $o$ using the wave functions $f$.

The above discussion shows that we can formulate the quantum cosmology of any FRW model coupled to a real scalar field in terms of the wave functions (169). The latter belong to the Hilbert space $L^2(\mathbb{R} \times \{-1, 1\})$ which is isomorphic to $L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) = \mathcal{H}_s$. The observables $o$ (including any Hamiltonian operator) are specified by the kernels (174) according to (171) and (172) or alternatively by the operators $\hat{o}$ that act on the wave functions. For instance, for the basic observables $o_3$, $\hat{q}$ and $\hat{p}$, we have

$$\hat{o}_3 f(q, \epsilon) = \epsilon f(q, \epsilon), \quad \hat{q} f(q, \epsilon) = q f(q, \epsilon), \quad \hat{p} f(q, \epsilon) = -i\hbar \frac{\partial}{\partial q} f(q, \epsilon). \tag{176}$$

In view of the above description of the wave functions $f(q, \epsilon)$, the name ‘wave function of the universe’ seems more appropriate for $f(q, \epsilon)$ than the wave functions $\psi(\alpha, \varphi)$ of (157), provided that we assign a physical meaning for the variables $q$ and $\epsilon$.

It is worthy of noting that the physical meaning of the variables $\alpha$ and $\varphi$ of the wave functions $\psi(\alpha, \varphi)$ is not clear. By definition, these variables are respectively the eigenvalues of the position-like operators $\Xi(\alpha)$ and $\Xi(\varphi)$. Because these operators act in the non-physical auxiliary (kinematic) Hilbert space and do not commute with the operator $\hat{K}$, they cannot be restricted to the physical Hilbert space $\mathcal{H}$. This in turn means that they do not represent physical observables, and their eigenvalues have nothing to do with the results of any physical measurement. Therefore, a priori one does not have a good reason for identifying the independent variables $\alpha$ and $\varphi$ of the wave functions $\psi(\alpha, \varphi)$ with the classical counterparts of $\Xi(\alpha)$ and $\Xi(\varphi)$ — which are nevertheless denoted by the same symbols. To the author’s best knowledge the only way of relating these variables to the classical observables is by restricting to the approximate WKB solutions of the Wheeler-DeWitt equation [1, 33, 10]. The main purpose of the present study is to formulate a quantum theory of cosmology that avoids this and similar restrictions. Hence we hold that at a fundamental level, the variables $\alpha$ and $\varphi$ appearing in $\psi(\alpha, \varphi)$ and therefore the wave functions $\psi(\alpha, \varphi)$ lack a clear physical interpretation. As we shall see below, the same
is not the case for the variables \( q \) and \( \epsilon \) and the wave functions \( f(q, \epsilon) \). It turns out that the physical meaning of the latter is intertwined with the dynamical aspects of the theory.

Consider a linear operator \( \hat{h}' \) acting in the space \( L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \) of the wave functions \(^{(169)}\) and corresponding to a Hamiltonian operator \( h' \) acting on the Wheeler-DeWitt fields \( \psi \) of \(^{(158)}\). It is not difficult to check that because \( h' : \mathcal{H} \rightarrow \mathcal{H} \) is a Hermitian operator, so is \( \hat{h}' : L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \). Moreover, every evolving Wheeler-DeWitt field \( \psi \) satisfying the Schrödinger equation

\[
i\hbar \frac{d}{dt} \psi = h' \psi_i,
\]

may be specified in terms of its wave function \( f(q, \epsilon) = f(q, \epsilon; \tilde{t}) \) that fulfills the Schrödinger equation

\[
i\hbar \frac{\partial}{\partial \tilde{t}} f(q, \epsilon; \tilde{t}) = \hat{h}' f(q, \epsilon; \tilde{t}).
\]

This reduces the study of the dynamical aspects of the quantum FRW models with a real scalar field to the formulation of a canonical quantization of an appropriate classical system that would assign physical meaning to the operators \( \hat{q} \) and \( \hat{\epsilon} \) (and consequently to the variables \( q \) and \( \epsilon \) and the operators \( \hat{q} \) and \( \hat{\epsilon} \)) and leads to a choice of a Hermitian operator \( \hat{h}' \) acting in the Hilbert space \( L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \).

Before presenting further details of the dynamical structure of the theory, we wish to comment on the factor-ordering ambiguity associated with the definition of the Wheeler-DeWitt equation. As we explained above, we can formulate the whole theory in terms of the wave functions \(^{(169)}\). These are the coefficients of the Wheeler-DeWitt fields in the position-basis \(^{(166)}\). If one chooses another factor-ordering prescription for the operator corresponding to the Hamiltonian constraint, one obtains a Wheeler-DeWitt equation which differs from \(^{(158)}\). However, the latter will be a linear hyperbolic partial differential equation with the same highest order terms; the corresponding differential operators have identical leading symbol \(^{[34]}\). This in turn implies that although a different factor-ordering leads to a different form of the solutions for a given initial data, the space of solutions will have the same vector space structure. In particular, the position-basis vectors \(^{(166)}\) will be different, but one will have the same set of wave functions \(^{(169)}\). As the Hilbert space \( \mathcal{H} \) is uniquely determined (up to unitary-equivalence) by the vector space structure of the space of solutions, the factor-ordering problem is not relevant to the kinematical structure of the quantum theory. This argument relies on two basic assumptions:

1. It is the space of solutions of the Wheeler-DeWitt equation that serves as the Hilbert space of the quantum theory.
2. The Hilbert space is separable and therefore its Hilbert space structure is unique \[13\].

The irrelevance of the factor-ordering problem for the kinematics of the quantum theory holds generally for any quantum gravitational model that does not violate these assumptions.

Next, we wish to explore the dynamical aspects of the quantum FRW model defined by the Wheeler-DeWitt equation (158) that has the classical theory defined by the classical Hamiltonian constraint (156) as its ‘classical limit.’ The first step in this direction is to identify the physical meaning of the configuration variables \(q\) and \(\epsilon\) as well as the time variable \(\hat{t}\) appearing as the argument of an evolving wave function \(f(q, \epsilon; \hat{t})\).

Using the prescription provided by Dirac’s canonical quantization, \(q\) and \(\epsilon\) are to be identified with the coordinates of the classical configuration space. The fact that the wave functions determine the solutions of the Wheeler-DeWitt equation (i.e., the quantum constraint) suggests that \(q\) must be chosen among the configuration variables of the classical system \(C_0\) obtained after imposing the classical constraint. The same applies to the \(\epsilon\) degree of freedom whose interpretation is slightly more subtle.

In light of analogy with nonrelativistic quantum mechanics, we propose to identify the time parameter \(\hat{t}\) with a classical time parameter for \(C_0\). One has the well-known set of choices corresponding to the internal and external classical time variables \[3\]. For example if we identify \(\hat{t}\) with the variable \(\alpha\) appearing in the classical Hamiltonian constraint (156), we obtain the corresponding classical Hamiltonian as outlined in Ref. \[8\]: We first solve (156) for \(\pi\) and substitute the result in the expression for the first-order Lagrangian

\[
\mathcal{L} := \pi_\alpha \dot{\alpha} + \pi_\varphi \dot{\varphi} + NK,
\]

(179)

where \(N\) is the lapse function. Employing \(\alpha = \hat{t}\) and imposing the classical constraint \(K = 0\), we then find

\[
\mathcal{L} = \pi_\varphi \dot{\varphi} \pm \sqrt{\pi_\varphi^2 - \kappa e^{4\alpha} + e^{6\alpha} V(\varphi)}.
\]

(180)

We may also describe the classical dynamics of the resulting system using a Hamiltonian formulation based on the classical Hamiltonian

\[
\mathcal{K}_0 := \pm \sqrt{\pi_\varphi^2 - \kappa e^{4\alpha} + e^{6\alpha} V(\varphi)}.
\]

(181)

The expression (180) suggests the natural identification of \(q\) with \(\varphi\). The undetermined sign in (180) and (181) is usually fixed by demanding that the Hamiltonian (181) be positive \[8\]. This sign may be viewed as a suitable candidate for the classical analog of the sign \(\epsilon\) appearing as one of the arguments of the wave functions (169). As it multiplies the Hamiltonian, it may be connected to whether one takes \(\alpha\) or \(-\alpha\) as a time-variable. Both these choices are necessary whenever the dynamics of the classical universe involves a recollapse. The quantum description
of the model seems to include this phenomenon whether the classical universe recollapses or not.

Incorporating the $\epsilon$ degree of freedom as the sign of the rate of change of $\alpha$ (with respect to any classical physical time $\tau$) in the above choice of an internal time is equivalent to setting

$$\tilde{t} = \epsilon \alpha,$$  \hspace{1cm} (182)

where $\epsilon := \text{sign}(d\alpha(\tau)/d\tau)$, $\text{sign}(0) := 1$, and $\text{sign}(x) := x/|x|$ for $x \neq 0$. Repeating the above derivation of the Lagrangian (180) and the Hamiltonian (181) with the choice (182) for time and requiring that the resulting Hamiltonian be positive yield

$$\mathcal{L} = \pi_\varphi \dot{\varphi} + \sqrt{\pi_\varphi^2 - \kappa e^{4\tilde{t}} + e^{6\tilde{t}} V(\varphi)},$$  \hspace{1cm} (183)

$$\mathcal{K}_0 := \sqrt{\pi_\varphi^2 - \kappa e^{4\tilde{t}} + e^{6\tilde{t}} V(\varphi)}.$$  \hspace{1cm} (184)

The above discussion shows that the structure of the classical system $C_0$ provides the physical meaning of the variables $q, \epsilon$ and $\tilde{t}$. The next step is to perform a canonical quantization of the system $C_0$ to clarify the physical interpretation of the operators $\hat{q}$ and $\hat{o}_3$ (respectively $\hat{q}$ and $\hat{p}_3$) and construct the Hamiltonian $\hat{h}'$ (respectively $h'$).

It is important to note the difference between the quantum operators $\Xi(\varphi) \equiv \varphi$ and $\Xi(\pi_\varphi) \equiv -i\partial/\partial \varphi$ that appear in the Wheeler-DeWitt equation (158) and $\hat{\varphi}$ and $\hat{\pi}_\varphi$ of (176). The former are obtained by quantizing $\varphi$ and $\pi_\varphi$ viewed as classical observables of the system before imposing the classical constraint. This unconstrained system does not define a specific physical theory capable of describing a cosmological model, as the constraint is the only nontrivial consequence of Einstein’s equation. It is the constrained system $C_0$ that has physical significance. The operators $\hat{\varphi}$ and $\hat{\pi}_\varphi$ (alternatively $\hat{\varphi}$ and $\hat{\pi}$) are obtained by quantizing the same variables $\varphi$ and $\pi_\varphi$ but with a different physical meaning, namely as the classical observables of the physical system $C_0$. Therefore, it is these operators that are to be identified with the physical observables of the corresponding quantum system.

If we quantize the Hamiltonian (181) according to

$$\epsilon \rightarrow \hat{o}_3, \quad \varphi = q \rightarrow \hat{q}; \quad \pi_\varphi = \pi_q \rightarrow \hat{p},$$  \hspace{1cm} (185)

we find the quantum Hamiltonian operator

$$\hat{h}' = \sqrt{\hat{\varphi}^2 - \kappa e^{4\hat{\tilde{t}}} + e^6 \hat{\tilde{t}} V(\hat{\varphi})},$$  \hspace{1cm} (186)

that yields the dynamics of the evolving Wheeler-DeWitt fields $\psi_{\tilde{t}}$ in terms of their wave functions $f(q, \epsilon; \tilde{t})$. Using (176) and (186) and rescaling $\tilde{t} \rightarrow \epsilon \tilde{t}$ for fixed $\epsilon$, we can express the
Schrödinger equation (178) in the form

\[ i\hbar \frac{\partial}{\partial \tilde{t}} f(q, \epsilon; \epsilon \tilde{t}) = \epsilon \left[ -\hbar^2 \frac{\partial^2}{\partial q^2} - \kappa e^{4t} + e^{6t} V(q) \right]^{1/2} f(q, \epsilon; \epsilon \tilde{t}). \]  

(187)

We can also express the dynamics of \( \psi_\tilde{t} \) by identifying the form of the Hamiltonian \( h' \) appearing in the Schrödinger equation (177). In view of the correspondence between \( \hat{q}, \hat{p}, o_3 \) and \( \hat{\hat{q}}, \hat{\hat{p}}, \hat{o}_3 \), we have

\[ h' = \sqrt{\hat{p}^2 - \kappa e^{4o_3} + e^{6o_3} V(\hat{q})}. \]  

(188)

As we discussed in great detail in Section 5, \( h' \) does not generate \( \alpha \)-translations in the physical Hilbert space \( \mathcal{H} \) of the solutions of the Wheeler-DeWitt equation, and one cannot identify the \( \alpha \) appearing in the Wheeler-DeWitt equation (158) with a time variable (unless one relaxes the condition that evolution must be unitary with respect to some inner product on \( \mathcal{H} \)).

The above discussion of the dynamics uses the Schrödinger-picture of quantum mechanics. Having obtained the basic observables \( o_3, \hat{q}, \hat{p} \) and the Hamiltonian \( h' \), we can also study the quantum dynamics in the Heisenberg-picture. In particular, one has the Heisenberg equations

\[ i\hbar \frac{d}{d \tilde{t}} \hat{q}_H(\tilde{t}) = [\hat{q}_H(\tilde{t}), h'_H(\tilde{t})], \quad i\hbar \frac{d}{d \tilde{t}} \hat{p}_H(\tilde{t}) = [\hat{p}_H(\tilde{t}), h'_H(\tilde{t})], \]  

(189)

where the subscript \( H \) denotes the corresponding Heisenberg-picture observables. Note however that because the Schrödinger-picture Hamiltonian \( h' \) is explicitly time-dependent, it differs from the Heisenberg-picture Hamiltonian \( h'_H \),

\[ h'_H = \sqrt{\hat{p}_H^2 - \kappa e^{4o_3} + e^{6o_3} V(\hat{q}_H)} \neq h'. \]

Here we use the fact that \( o_3 \) commutes with \( h' \), hence the corresponding Heisenberg-picture operator coincides with \( o_3 \).

An alternative way of formulating the dynamics is to pursue a path-integral quantization of the classical system \( C_0 \). This amounts to selecting a classical action functional \( S \) and postulating the following expression for the propagator of the theory

\[ \psi(q, \epsilon, \tilde{t}; q', \epsilon', \tilde{t}') = \int_{\gamma} Dq(\tilde{t}) \ e^{iS[q(\tilde{t})] + i(\epsilon - \epsilon'(\tilde{t}))} \]

where \( \gamma \) stands for the paths in the configuration space \( \mathbb{R} \times \{-1, 1\} \) joining the points \((q, \epsilon)\) to \((q', \epsilon')\), \( Dq \) denotes the ‘measure’ for the path-integral, and \( S \) is a classical action functional for the system \( C_0 \). Then the dynamics of the Wheeler-DeWitt fields is given in terms of their wave functions (169) according to

\[ f(q, \epsilon; \tilde{t}) = \sum_{\epsilon' = \pm} \int_{-\infty}^{\infty} dq' \psi(q, \epsilon, \tilde{t}; q', \epsilon', \tilde{t}_0) f(q', \epsilon'; \tilde{t}_0), \]

(169)
where \( t_0 \) is the initial time.

Path-integral quantization of minisuperspace models based on quantization after imposing the classical constraint has been studied in the literature, see for example Ref. [28]. Our formulation may be viewed as providing the missing link between these studies and the more tradition canonical approach (like ours) that is based on the Wheeler-DeWitt equation.

8 Discussion and Conclusion

If we follow Dirac’s prescription [35] to quantize a constrained system with a single first-class constraint \( K \), then the physical Hilbert space is determined by the quantum constraint \( \hat{K}\psi = 0 \). For a system with a finite number of continuous degrees of freedom, this is equivalent to a linear partial differential equation involving the independent variables that may be interpreted as the dynamical variables of the unconstrained (nonphysical) classical system. The Hilbert space defining the quantum mechanics of the constrained (physical) system is the solution space \( \mathcal{H} \) of this equation. Therefore the quantum constraint only determines the vector space structure of the physical Hilbert space \( \mathcal{H} \). It does not endow this space with a specific positive-definite inner product. In this article, we obtained the most general positive-definite inner product on \( \mathcal{H} \) for a class of constraint equations called the Klein-Gordon-type equations. We also constructed explicit unitary maps that related various choices for the inner product on \( \mathcal{H} \).

Our analysis is based on a simple observation that the states of a quantum system having \( \mathcal{H} \) as its Hilbert space are not uniquely determined by the value \( \psi(t) \) of a solution \( \psi \) of the corresponding Klein-Gordon-type equation at a given value of the time-like parameter \( t \). The latter requires the knowledge of a pair of elements of \( \tilde{\mathcal{H}} \), namely \( \psi(t) \) and \( \dot{\psi}(t) \). This rather trivial observation together with the demand that the corresponding quantum theory admits a probabilistic interpretation (which translates into the mathematical requirement that \( \mathcal{H} \) is to be equipped with a positive-definite inner product) lead to an explicit construction of the unique Hilbert space structure on \( \mathcal{H} \).

The developments reported in this paper differ from the traditional approaches to quantum cosmology [1, 3, 4] as summarized by the following remarks.

1. It is based solely on the postulates of quantum mechanics and adheres to Dirac’s treatment of quantizing systems with first class constraints. It relies on the Wheeler-DeWitt equation, but, in contrast with the conventional approaches based on the Klein-Gordon inner product or conditional probabilities, it admits a genuine probabilistic interpretation and a unitary Schrödinger time-evolution.
2. It does not rely on the properties of the auxiliary (kinematic) Hilbert space of the unconstrained system. Neither does it involve a gauge-fixing or group averaging scheme. Yet it leads to a class of inner products on the physical Hilbert space that up to unitary-equivalence includes all possible positive-definite inner products, i.e., it yields the unique Hilbert space structure on $\mathcal{H}$.

3. It does not involve selecting a time-parameter before clarifying the kinematic structure of the theory. In a sense, it decouples the Hilbert space problem from the problem of time. It further provides invaluable insight as to how one should approach the problem of selecting a time parameter. It identifies the latter with the issue of determining a Hamiltonian operator. This restricts the choice of the possible time-variables. Specifically, the variable $t$ appearing in the definition of a nonstationary Klein-Gordon-type equation, in general, and the variable $\alpha$ appearing in the Wheeler-DeWitt equation, in particular, cannot be identified with a time-parameter.

4. It does not identify the solutions of the Wheeler-DeWitt equation with the wave functions of the universe. It treats the former as abstract vectors in the physical Hilbert space and employs the usual definition of a wave function to identify the wave functions of the universe with the coefficients of the former in an appropriate position-like basis of the physical Hilbert space. The quantum theory may be formulated in terms of these wave functions that are not sensitive to the choice of the factor-ordering prescription used to specify the Wheeler-DeWitt equation. This leads to a resolution of the factor-ordering problem in the kinematic level that seems to apply generally.

5. The fact that it involves using a particular choice for a time-like parameter in the construction of an inner product on the Hilbert space may be viewed as an indication that it suffers from a multiple-choice problem already in the kinematic level. This is actually not true, because any other choice would give rise to the same Hilbert space structure on $\mathcal{H}$. This is manifestly seen in the formulation of the theory based on the wave functions. What is essential is the existence of a time-like variable among the independent variables appearing in the Wheeler-DeWitt equation which is guaranteed by the Lorentzian signature of the DeWitt supermetric on the minisuperspace.

The solutions of the Wheeler-DeWitt equation are the abstract state vectors in the Hilbert space. Constructing a complete set of explicit solutions of this equation provides a specific realization of the Hilbert space. Because the physical content of the quantum theory is independent of the choice of a realization, the explicit form of the solutions does not have any
physical significance unless the formulation of the dynamics (the determination of an appropriate Hamiltonian operator and the associated time variable) is linked with the particular form of the Wheeler-DeWitt equation or its solutions.

In this article we explored the basic kinematical structure of the theory trying to use as small number of physical assumptions as possible. This leads to a fairly simple description of the general kinematic structure of the quantum theory of FRW models coupled to a real scalar field. It is not difficult to see that a similar treatment applies to more complicated (spatially homogeneous) minisuperspace models [6]. Our treatment of the kinematical aspects of the theory also provides clues for elucidating its dynamical structure.

We have also outlined a proposal for formulating the dynamics that involves identifying the time and the physical observables respectively with a classical time variable and Hermitian operators obtained by canonically quantizing the observables of the constrained classical system. This proposal applies to more general minisuperspace models provided that they admit a Hamiltonian formulation [38]. Its main disadvantage is that it suffers from the well-known problems of quantization after imposing the classical constraint(s) [3]. In particular, the multiple-choice problem arises and one must face the nonlocal character of the resulting quantum Hamiltonian operator (188) and the fact that for a closed universe there is a range of the time-variable \( \tilde{t} \) for which this operator fails to be Hermitian.

Among the main advantages of this proposal are that it provides a link between the two widely used approaches to quantum cosmology namely quantization before and after imposing the constraints and that it clarifies the conceptual basis of the path-integral approaches to quantum cosmology that are based on a Schrödinger description of dynamics such as the one used in Ref. [28]. The investigation of the classical limit of the theory is similar to the one in ordinary nonrelativistic quantum mechanics. One can in principle employ the WKB approximation, the mode expansion, or time-dependent perturbation theory and use these methods to extract the physical implications of the theory. However, the issue of the initial condition for the wave function of the universe requires additional input.

The quantum mechanics of Klein-Gordon-type fields developed in this article has other areas of application. An obvious example is relativistic quantum mechanics of (non-self-interacting) massive scalar fields. We can formulate the quantum mechanics of such fields by identifying the space of the corresponding Klein-Gordon fields with the Hilbert space of the theory. As we show in Ref. [5], the class of inner products (12) for Klein-Gordon field (2) includes a subclass of Lorentz invariant inner products (These are the inner products studied in the Appendix.) In fact, the analysis of Section 3 shows that requiring relativistic invariance is actually not as significant as one might imagine: All the positive-definite inner products, including the energy inner product (29), the relativistically invariant inner product originally constructed by
Woodard [36] using the gauge-fixing method and rediscovered by Von Zuben [39]), and the inner products [12] that include the preceding two as special cases are all physically equivalent.²⁴  

The main advantage of the application of our method to Klein-Gordon fields is that it allows for a straightforward representation of the quantum mechanics of a Klein-Gordon field based on the Hilbert space \( \mathcal{H}_* = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \). In this representation the Hamiltonian \( H_* \) of (83) coincides with the Foldy’s Hamiltonian [17]. In a sense, our method may be viewed as a way of explicitly performing a Foldy-Wouthuysen transformation in the Schrödinger-picture of the first-quantized scalar field theory [17]. The Hamiltonian \( h \) that is induced from \( H_* \) by the unitary operator \( U \) of (85) is precisely the generator of the Poincaré group (in its spin-zero representation) corresponding to time-translations. Our approach is especially suitable for addressing the problem of constructing a relativistic position operator and the associated localized [41] and coherent states [42]. We leave a more detailed treatment of these issues for a future publication.

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Appendix

In Ref. [5], we identified a class of positive-definite inner products on the solution space of a Klein-Gordon field in a Minkowski space that were invariant under Lorentz transformations. Here we shall consider a generalization of these inner products for a general stationary Klein-Gordon-type field and present a derivation of the general form of the corresponding observables. The results are directly relevant to the issue of constructing and exploring relativistic position operators and localized states.

Consider the two-parameter family of the operators:

\[
L_\pm = \frac{1}{2} (c_+^2 \pm c_-^2) D^{1/2},
\]

(190)

where \( c_\pm \) are positive real numbers having the dimension of \( \sqrt{7} \). Comparing this equation with (37), we see that (190) corresponds to the following choice for the coefficients \( a_{\pm,n} \):

\[
a_{\pm,n} = c_\pm e^{i\theta_{\pm,n}} \sqrt{\omega_n},
\]

(191)

²⁴For an earlier related work see [40].
where \( \theta_{\pm,n} \in [0, 2\pi) \) are still arbitrary. In view of (191), the operators \( A_\pm \) of (88) have the form
\[
A_\pm = c_\pm u_\pm D^{1/4},
\]
where \( u_\pm : \mathcal{H} \rightarrow \tilde{\mathcal{H}} \) are unitary operators
\[
u_\pm = \sum_n e^{i \theta_{\pm,n}} |\phi_n\rangle \langle \phi_n| \tag{193}
\]
that commute with \( D \). In effect, (190) is equivalent to requiring that \( A_\pm \) have the form (192) for a pair of unitary operators \( u_\pm \) commuting with \( D \).

The observables (104) of \( q_{L_\pm} \) corresponding to the choice (190) are determined by substituting (192) in (103). This yields
\[
J_\pm = \frac{1}{2} D^{-1/4} \left[ O_1 \pm \left( \frac{c_+}{c_-} \right) \mathcal{O} \right] D^{1/4}, \quad K_\pm = \frac{1}{2} D^{-1/4} \left[ \left( \frac{c_-}{c_+} \right) \mathcal{O}^\dagger + O_2 \right] D^{1/4}, \tag{194}
\]
where
\[
O_1 := u_+^\dagger \tilde{O}_1 u_+, \quad O_2 := u_-^\dagger \tilde{O}_2 u_-, \quad \mathcal{O} := u_+^\dagger \tilde{\mathcal{O}} u_-. \tag{195}
\]
As seen from these equations, the effect of the operators \( u_\pm \) is a simple redefinition of the observables \( O_\ast \) of \( Q_\ast \) which corresponds to changing \( \tilde{O}_1 \rightarrow O_1, \tilde{O}_2 \rightarrow O_2, \) and \( \tilde{\mathcal{O}} \rightarrow \mathcal{O} \). This means that for the cases that \( L_\pm \) are given by (190), the observables \( o \) of \( q_{L_\pm} \) have the general form (104) where \( J_\pm \) and \( K_\pm \) are determined (according to (194)) by three operators \( O_1, O_2, \mathcal{O} : \tilde{\mathcal{H}} \rightarrow \tilde{\mathcal{H}} \) with \( O_1 \) and \( O_2 \) being Hermitian. Similarly, we can show that the matrix elements (\( \langle \psi, o \phi \rangle \)) of \( o \) are given by (105) with
\[
J_\pm = \frac{c_\pm^2}{2} D^{1/4} \left[ O_1 \pm \left( \frac{c_-}{c_+} \right) \mathcal{O} \right] D^{1/4}, \quad K_\pm = \frac{c_\pm^2}{2} D^{1/4} \left[ \left( \frac{c_-}{c_+} \right) \mathcal{O}^\dagger + O_2 \right] D^{1/4}. \tag{196}
\]
Inserting these equation in (105) leads to
\[
\langle \psi, o \phi \rangle = \frac{c_\pm^2}{4} \left\{ \langle \psi_0 | D^{1/4} \left[ O_1 + r (\mathcal{O} + \mathcal{O}^\dagger) + r^2 O_2 \right] D^{1/4} \phi_0 \rangle + \langle \psi_0 | D^{-1/4} \left[ O_1 - r (\mathcal{O} + \mathcal{O}^\dagger) + r^2 O_2 \right] D^{-1/4} \phi_0 \rangle \right. + \left. i \left( \langle \psi_0 | D^{1/4} \left[ O_1 - r (\mathcal{O} - \mathcal{O}^\dagger) - r^2 O_2 \right] D^{1/4} \phi_0 \rangle + \langle \psi_0 | D^{-1/4} \left[ -O_1 - r (\mathcal{O} - \mathcal{O}^\dagger) + r^2 O_2 \right] D^{-1/4} \phi_0 \rangle \right) \right\}, \tag{197}
\]
where \( r := c_- / c_+ \).

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25If some or all the eigenvalues \( \omega^2_n \) of \( D \) are degenerate, the operators \( u_\pm \) will have the form \( \sum_n \sum_{a,b=1}^{d_n} (u_{\pm,n})_{ab} |\phi_{n,a}\rangle \langle \phi_{n,b}| \) where \( d_n \) is the multiplicity of \( \omega^2_n \), \( a, b \) are degeneracy labels, and \( (u_{\pm,n})_{ab} \) are the entries of an arbitrary unitary \( d_n \times d_n \) matrix \( u_{\pm,n} \).
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