Giving up the ghost

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Abstract

The Pais–Uhlenbeck model is a quantum theory described by a higher-derivative field equation. It has been believed for many years that this model possesses ghost states (quantum states of negative norm) and therefore that this model is a physically unacceptable quantum theory. The existence of such ghost states was believed to be attributable to the field equation having more than two derivatives. This paper shows that the Pais–Uhlenbeck model does not possess any ghost states at all and that it is a perfectly acceptable quantum theory. The supposed ghost states in this model arise if the Hamiltonian of the model is (incorrectly) treated as being Dirac Hermitian (invariant under combined matrix transposition and complex conjugation). However, the Hamiltonian is *not* Dirac Hermitian, but rather it is $\mathcal{PT}$ symmetric. When it is quantized correctly according to the rules of $\mathcal{PT}$ quantum mechanics, the energy spectrum is real and bounded below and all of the quantum states have positive norm.

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1. Introduction

Ghost states are quantum states having negative norm. If a quantum theory has ghost states, it is fundamentally unacceptable because the norm of a quantum state is interpreted as a probability, and a negative probability is forbidden on physical grounds.

One can present a simple and apparently compelling argument that if the field equation of a quantum theory is a differential equation of higher than second order in the time derivative, the theory must have ghost states. However, as we will show in this paper, this argument is incorrect.

The argument goes as follows: suppose, for example, that a field equation is fourth order in the time derivative. If we take the Fourier transform of this equation, we obtain

the corresponding propagator $G(E)$ whose denominator is a fourth-order polynomial in the energy E. In a factored form such a propagator in Euclidean space would have the form

$$G(E) = \frac{1}{\left(E^2 + m_1^2\right)\left(E^2 + m_2^2\right)}. \tag{1}$$

Observe that $G(E)$ describes the propagation of two kinds of states, one of mass m_1 and the other of mass m_2. Assuming without loss of generality that $m_2 > m_1$, we can rewrite this propagator in the form of a partial fraction

$$G(E) = \frac{1}{m_2^2 - m_1^2} \left(\frac{1}{E^2 + m_1^2} - \frac{1}{E^2 + m_2^2} \right). \tag{2}$$

Evidently, m_2 is a state of *negative* probability because its residue contribution to the propagator is negative. This appears to contradict the well-known form of the Lehmann representation: recall that when the two-point Green function is expressed in the Lehmann representation, the condition that all quantum states have positive norm implies that the residues of all intermediate propagating states must be strictly positive [1].

However, this argument is *incorrect* because it contains an implicit assumption; namely, that the inner product for the Hilbert space of quantum states is the Dirac inner product. The Dirac adjoint, which is indicated by the notation †, consists of combined matrix transposition and complex conjugation. If another inner product is used, such as the inner product that arises in $\mathcal{PT}$ quantum mechanics [2], then the negative sign in the coefficient of the $1/\left(E^2 + m_2^2\right)$ term in (2) does not necessarily indicate the presence of a ghost state.

In $\mathcal{PT}$ quantum mechanics the Hamiltonian H is not Dirac Hermitian, $H \neq H^\dagger$, but is instead invariant under the more physical discrete symmetry of spacetime reflection $H = H^{\mathcal{PT}}$ [2–4]. Here, parity $\mathcal{P}$ is a linear operator that performs space reflection and $\mathcal{T}$ is an antilinear operator that performs time reversal. If the energy spectrum of H is real and positive, then the $\mathcal{PT}$ symmetry of H is unbroken, and it can be shown that H possesses a hidden reflection symmetry represented by the linear operator $\mathcal{C}$. Because $\mathcal{C}$ is a reflection symmetry, it satisfies $\mathcal{C}^2 = 1$. The $\mathcal{C}$ operator commutes with the Hamiltonian, $[H, \mathcal{C}] = 0$, and also with the $\mathcal{PT}$ operator, $[\mathcal{C}, \mathcal{PT}] = 0$ [5]. In terms of $\mathcal{C}$ one can then construct a new inner product for which the adjoint is the combined $\mathcal{CPT}$ operation: $\langle | \equiv |\rangle^{\mathcal{CPT}}$. Using this new inner product, the norm of a state is strictly positive [5–7]. Thus, given a $\mathcal{PT}$-symmetric Hamiltonian that is not Hermitian in the Dirac sense, one is not free to choose the inner product *ab initio* because the inner product is dynamically determined by the Hamiltonian itself. Time evolution in $\mathcal{PT}$ quantum mechanics is unitary because $\mathcal{CPT}$ commutes with H in the time-evolution operator $\mathrm{e}^{-\mathrm{i}Ht}$.

In this paper we demonstrate that the famous Pais–Uhlenbeck model [8], which has a higher-derivative field equation, is defined by a non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian. We show that the long-held belief that this model has ghost states is in fact not correct, and we do so by calculating the $\mathcal{C}$ operator exactly and in closed form, thereby identifying the inner product that is consistent with the Pais–Uhlenbeck Hamiltonian.

2. Pais–Uhlenbeck model

The Pais–Uhlenbeck oscillator model is defined by the higher-derivative, acceleration-dependent action

$$I = \frac{\gamma}{2} \int \mathrm{d}t \left[\ddot{z}^2 - \left(\omega_1^2 + \omega_2^2\right) \dot{z}^2 + \omega_1^2 \omega_2^2 z^2 \right], \tag{3}$$

where γ, ω_1 and ω_2 are all positive constants. We may assume without loss of generality that $\omega_1 \geqslant \omega_2$. If we vary the action, we obtain the *fourth-order* field equation

$$z''''(t) + (\omega_1^2 + \omega_2^2)z''(t) + \omega_1^2\omega_2^2 z(t) = 0. \tag{4}$$

One can construct the Pais–Uhlenbeck Hamiltonian by introducing a new dynamical variable x and obtaining a description of the theory using two degrees of freedom [9]:

$$H = \frac{p_x^2}{2\gamma} + p_z x + \frac{\gamma}{2}\left(\omega_1^2 + \omega_2^2\right)x^2 - \frac{\gamma}{2}\omega_1^2\omega_2^2 z^2. \tag{5}$$

In the Fock-space representation there are now two sets of creation and annihilation operators:

$$z = a_1 + a_1^\dagger + a_2 + a_2^\dagger, \qquad p_z = \mathrm{i}\gamma\omega_1\omega_2^2\left(a_1 - a_1^\dagger\right) + \mathrm{i}\gamma\omega_1^2\omega_2\left(a_2 - a_2^\dagger\right),$$
$$x = -\mathrm{i}\omega_1\left(a_1 - a_1^\dagger\right) - \mathrm{i}\omega_2\left(a_2 - a_2^\dagger\right), \qquad p_x = -\gamma\omega_1^2\left(a_1 + a_1^\dagger\right) - \gamma\omega_2^2\left(a_2 + a_2^\dagger\right). \tag{6}$$

These operators satisfy the usual set of commutation relations, with the nonzero commutator given by

$$\omega_1\left[a_1, a_1^\dagger\right] = -\omega_2\left[a_2, a_2^\dagger\right] = \frac{1}{2\gamma\left(\omega_1^2 - \omega_2^2\right)}. \tag{7}$$

In terms of these operators the Hamiltonian for the Pais–Uhlenbeck model is

$$H = 2\gamma\left(\omega_1^2 - \omega_2^2\right)\left(\omega_1^2 a_1^\dagger a_1 - \omega_2^2 a_2^\dagger a_2\right) + \tfrac{1}{2}(\omega_1 + \omega_2). \tag{8}$$

There appear to be only two possible realizations of the commutation relations in (7), and we enumerate these below:

(I) If a_1 and a_2 annihilate the 0-particle state $|\Omega\rangle$,

$$a_1|\Omega\rangle = 0, \qquad a_2|\Omega\rangle = 0, \tag{9}$$

then the energy spectrum is real and bounded below. The state $|\Omega\rangle$ is the ground state of the theory and it has zero-point energy $\frac{1}{2}(\omega_1 + \omega_2)$. The problem with this realization is that the excited state $a_2^\dagger|\Omega\rangle$, whose energy is ω_2 above the ground state, has a *negative Dirac norm* given by $\langle\Omega|a_2 a_2^\dagger|\Omega\rangle$.

(II) If a_1 and $a_2^\dagger$ annihilate the 0-particle state $|\Omega\rangle$,

$$a_1|\Omega\rangle = 0, \qquad a_2^\dagger|\Omega\rangle = 0, \tag{10}$$

then the theory is free of negative-norm states. However, this realization has a different and equally serious problem; namely, that the energy spectrum is unbounded below.

The two realizations (I) and (II) are clearly unacceptable physically and they characterize the generic problems that are thought to plague higher-derivative quantum-mechanical theories and quantum field theories. The Pais–Uhlenbeck model has been believed to be unphysical because there appear to be no other realizations for which both the energy spectra and the norms of the states are positive.

We emphasize that there may be many realizations of a given Hamiltonian depending on the boundary conditions that are imposed on the coordinate-space eigenfunctions. Let us consider two elementary examples:

2.1. Harmonic oscillator $H = p^2 + x^2$

This Hamiltonian seems to be positive-definite because it is a sum of squares, and one might therefore expect that the spectrum of this Hamiltonian would be positive. However, this is incorrect. There are actually two distinct possible realizations, that is, solutions to the Schrödinger equation eigenvalue problem

$$-\psi''(x) + x^2\psi(x) = E\psi(x),\tag{11}$$

and these realizations are distinguished by the boundary conditions that are imposed on the eigenfunction $\psi(x)$.

If we require that $\psi(x)$ vanish exponentially fast as $|x| \to \infty$ with arg$x$ inside two $90°$ Stokes wedges [11] centered about the positive- and negative-real axes, then the spectrum is strictly positive and the nth eigenvalue is given exactly by $E_n = 2n + 1$ ($n = 0, 1, 2, 3, \ldots$). On the other hand, if we require that $\psi(x)$ vanish exponentially fast as $|x| \to \infty$ with arg x inside two $90°$ Stokes wedges centered about the positive- and negative-*imaginary* axes, then the spectrum is strictly negative and the nth eigenvalue is given exactly by $E_n = -2n - 1$ ($n = 0, 1, 2, 3, \ldots$) [2].

2.2. Anharmonic oscillator $H = p^2 - x^4$ with an 'upside-down' potential

This oscillator has many possible realizations. For example, if we do not require that the solution to the Schrödinger equation

$$-\psi''(x) - x^4\psi(x) = E\psi(x)\tag{12}$$

satisfy any boundary conditions at all on the real-x axis, then the spectrum is continuous and unbounded below.

On the other hand, if we require that $\psi(x)$ vanish exponentially fast in a pair of $60°$ Stokes wedges centered about the rays arg$x = -30°$ and arg$x = -150°$, then the spectrum is real, discrete and strictly positive, and in fact the spectra of $H = p^2 - x^4$ and $\tilde{H} = p^2 + 4x^4 - 2\hbar x$, where $\hbar$ is Planck's constant, are exactly identical [10]. In $\tilde{H}$ the term proportional to $\hbar$ vanishes in the classical limit and is thus a quantum anomaly [10].

3. Pais–Uhlenbeck model as a $\mathcal{PT}$ quantum theory

To make sense of the Pais–Uhlenbeck model as a consistent and physical quantum theory, it is necessary to interpret the Pais–Uhlenbeck Hamiltonian (5) as a $\mathcal{PT}$ quantum theory. The detailed analysis is given in [12], and we summarize it here.

We begin by modifying H in (5) by making the substitution $y = -iz$ (and the corresponding substitution $q = ip_z$ to enforce $[y, q] = i$) to obtain the modified Hamiltonian

$$H = \frac{p^2}{2\gamma} - iqx + \frac{\gamma}{2}\left(\omega_1^2 + \omega_2^2\right)x^2 + \frac{\gamma}{2}\omega_1^2\omega_2^2 y^2.\tag{13}$$

Here, we have simplified the notation by replacing p_x by p. The operators p, x, q and y are now formally Hermitian, but because of the $-iqx$ term H has become explicitly complex and is manifestly not Dirac Hermitian. We stress that this non-Hermiticity property is not apparent in the original form of the Pais–Uhlenbeck Hamiltonian. This surprising and unexpected emergence of a non-Hermitian term in the Pais–Uhlenbeck Hamiltonian provides insight into the origin of the infamous ghost problem of the Pais–Uhlenbeck model.

Next, we make an unusual assignment for the properties of the dynamical variables under space and time reflection: we take p and x to transform like conventional coordinate

and momentum variables under $\mathcal{P}$ and $\mathcal{T}$ reflection, but we define q and y to transform *unconventionally* in a way not seen in previous studies of $\mathcal{PT}$ quantum mechanics [2]. (In the language of quantum field theory, q and y transform as parity *scalars* instead of *pseudoscalars*.) Note that q and y also have abnormal behavior under time reversal. We summarize the symmetry properties of these operators in the following table:

$$
\begin{array}{c|cccc}
 & p & x & q & y \\
\hline
\mathcal{P} & - & - & + & + \\
\mathcal{T} & - & + & + & - \\
\mathcal{PT} & + & - & + & -.
\end{array}
\tag{14}
$$

Under these definitions the Pais–Uhlenbeck Hamiltonian (13) is $\mathcal{PT}$ symmetric. Also, the spectrum in the realization (I) in section 2 is entirely real, so the $\mathcal{PT}$ symmetry of the Pais–Uhlenbeck Hamiltonian is unbroken.

The next step is to calculate the hidden symmetry operator $\mathcal{C}$. As discussed in section 1, the operator $\mathcal{C}$ satisfies a system of three algebraic equations:

$$
\mathcal{C}^2 = 1, \qquad [\mathcal{C}, \mathcal{PT}] = 0, \qquad [\mathcal{C}, H] = 0.
\tag{15}
$$

In previous investigations [13] it was found that $\mathcal{C}$ has the general form

$$
\mathcal{C} = e^{\mathcal{Q}}\mathcal{P},
\tag{16}
$$

where $\mathcal{Q}$ is a real function of dynamical variables and it is Hermitian in the Dirac sense. In past studies it was found that $\mathcal{Q}$ was odd in the momentum variables and even in coordinate variables. However, because of the abnormal behavior of the y and q operators in (14), the exact solution to the three simultaneous algebraic equations for $\mathcal{C}$ in (15) exhibits an unusual and previously unobserved structure for $\mathcal{Q}$:

$$
\mathcal{Q} = \alpha pq + \beta xy,
\tag{17}
$$

where

$$
\beta = \gamma^2 \omega_1^2 \omega_2^2 \alpha \qquad \text{and} \qquad \sinh(\sqrt{\alpha\beta}) = \frac{2\omega_1\omega_2}{\omega_1^2 - \omega_2^2}.
\tag{18}
$$

Once the $\mathcal{Q}$ operator is known, we can use it to find a Hamiltonian $\tilde{H}$ that is Hermitian in the Dirac sense by means of the similarity transformation [14]

$$
\tilde{H} = e^{-\mathcal{Q}/2} H\, e^{\mathcal{Q}/2}.
\tag{19}
$$

When we perform this transformation using the operator $\mathcal{Q}$ in (17), we find that

$$
\tilde{H} = e^{-\mathcal{Q}/2} H\, e^{\mathcal{Q}/2} = \frac{p^2}{2\gamma} + \frac{q^2}{2\gamma\omega_1^2} + \frac{\gamma}{2}\omega_1^2 x^2 + \frac{\gamma}{2}\omega_1^2\omega_2^2 y^2.
\tag{20}
$$

Observe that the spectrum of $\tilde{H}$ is manifestly real because this Hamiltonian is the sum of two harmonic-oscillator Hamiltonians. Furthermore, the spectrum is positive because the transformations we have used to obtain $\tilde{H}$ ensure that its eigenfunctions vanish in wedges containing the real axis. But $\tilde{H}$ is related to the original Pais–Uhlenbeck Hamiltonian by the isospectral similarity transformation in (19). Thus, despite the $-iqx$ term in (13), the positivity of the Pais–Uhlenbeck Hamiltonian is proved.

To see why there are no ghosts and that the norm associated with the Pais–Uhlenbeck model is strictly positive, we note that the eigenstates $|\tilde{n}\rangle$ of $\tilde{H}$ have a positive inner product and they are normalized in the standard Dirac way using the inner product $\langle\tilde{n}|\tilde{n}\rangle = 1$, where the bra vector is the Dirac–Hermitian adjoint † of the ket vector. Equivalently, for the eigenstates

$|n\rangle$ of the Hamiltonian H, because the vectors are mapped by $|\tilde{n}\rangle = e^{-Q/2}|n\rangle$, the eigenstates of H are normalized as

$$\langle n|e^{-Q}|m\rangle = \delta(m,n) \qquad \text{with} \quad \sum |n\rangle\langle n|e^{-Q} = 1. \qquad (21)$$

The norm in (21) is relevant for the Pais–Uhlenbeck model, with $\langle n|e^{-Q}$ rather than $\langle n|$ being the appropriate conjugate for $|n\rangle$. Since the norm in (21) is positive and because $[H, \mathcal{CPT}] = 0$, the Pais–Uhlenbeck Hamiltonian H generates unitary time evolution.

4. Discussion

The Pais–Uhlenbeck model is not the first instance for which it can be shown that what was previously thought to be a ghost is actually a conventional quantum state having a positive norm. The first model that was discovered to have a false ghost state was the Lee model. The Lee model was proposed in 1954 as a quantum field theory in which mass, wavefunction and charge renormalization could be performed exactly and in closed form [15]. However, in 1955 Källén and Pauli showed that when the renormalized coupling constant is larger than a critical value, the Hamiltonian becomes non-Hermitian (in the Dirac sense) and a ghost state appears [16]. The appearance of the ghost was assumed to be a fundamental defect of the Lee model. However, the non-Hermitian Lee model Hamiltonian is $\mathcal{PT}$ symmetric. When the norms of the states of this model are determined using the $\mathcal{C}$ operator, which, as in the Pais–Uhlenbeck model, can be calculated in closed form, the ghost state is seen to be an ordinary physical state having a positive norm [17]. Thus, the following words by Barton [1] are *not true*: 'A non-Hermitian Hamiltonian is unacceptable partly because it may lead to complex energy eigenvalues, but chiefly because it implies a non-unitary S matrix, which fails to conserve probability and makes a hash of the physical interpretation'.

Thus, there are now *two* independent models in which one can show that what was believed to be a ghost state is actually an ordinary state having a positive norm. This suggests that there may be many more examples of quantum theories that have been abandoned as being unphysical and that can be repaired by using the methods of $\mathcal{PT}$ quantum mechanics. The problem of ghosts arises in quantizing gravity, and we hope that the methods of $\mathcal{PT}$ quantum mechanics will be able to establish that the classical theory of gravity can be consistently quantized without the appearance of ghosts.

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