$\mathcal{PT}$ symmetry in relativistic quantum mechanics

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In nonrelativistic quantum mechanics and in relativistic quantum field theory, the time coordinate t is a parameter and thus the time-reversal operator $\mathcal{T}$ does not actually reverse the sign of t. In contrast, in the five-dimensional approach to relativistic quantum mechanics introduced by Feynman, time t is a quantum-mechanical operator. In this paper it is shown how one can use this five-dimensional approach to extend $\mathcal{T}$ and $\mathcal{PT}$ symmetry from nonrelativistic to relativistic quantum mechanics and implement time-reversal as an operation that effects $\mathcal{T} t \mathcal{T} = -t$ just as $\mathcal{P}$ effects $\mathcal{P} x \mathcal{P} = -x$, with $\mathcal{PT}$ thus effecting $\mathcal{PT} x_\mu \mathcal{PT} = -x_\mu$. Some illustrative relativistic quantum-mechanical models are constructed whose associated Hamiltonians are non-Hermitian but $\mathcal{PT}$ symmetric, and it is shown that for each such Hamiltonian the energy eigenvalues are all real.

I. INTRODUCTION

In nonrelativistic quantum mechanics the position $\mathbf{x}(t)$ is taken to be an operator while the time t is only a c-number parameter. To make quantum mechanics relativistic our approach here is to treat time and space on an equivalent footing. There are two possibilities: one can either demote the spatial coordinates to parameters or promote the time coordinate to an operator. The former prescription is used in quantum field theory, where the field operators are treated as functions of the spacetime parameters $\mathbf{x}$ and t, but one can also construct sensible quantum-mechanical theories via the latter approach, which was introduced by Feynman [1] and Nambu [2]. In such theories a new parameter is needed to parameterize evolution, and thus one introduces a fifth coordinate τ that is an $SO(3, 1)$ Lorentz scalar. In this five-dimensional formalism the space and time coordinates $x^\mu(\tau)$ become operator functions of τ and one obtains an $SO(3, 1)$-invariant relativistic first-quantized generalization of the nonrelativistic Heisenberg algebra $[x_j, p_k] = i\delta_{j,k}$:

$$[x^\mu(\tau), p^\nu(\tau)] = i\eta^{\mu\nu}, \qquad [x^\mu(\tau), p_\nu(\tau)] = i\delta_\nu^\mu, \quad (1)$$

where $\eta^{\mu\nu}$ is the $SO(3, 1)$ Minkowski metric.

The dynamics in this formalism is $SO(3, 1)$ invariant in the four operators x^μ, but is nonrelativistic in the fifth coordinate τ [because the dynamics is not $SO(4, 1)$ or $SO(3, 2)$ invariant], and propagation is forward in τ. However, just as the nonrelativistic quantum-mechanical operator $\mathbf{x}(t)$ can propagate forward and backward with respect to its time parameter t, in relativistic quantum mechanics all four components of $x^\mu(\tau)$ can propagate forward and backward in τ [3]. The five-dimensional formalism of [1,2] readily incorporates forward and backward

time propagation, so one can introduce antiparticles with first quantization alone without requiring the second-quantization techniques of quantum field theory.

When the five-dimensional Hamiltonian operator $\hat{H}$ is Hermitian and its eigenfunctions have the separable form $\psi_n(x^\mu, \tau) = \phi_n(x^\mu)e^{-iE_n\tau}$ and when its states obey the standard Dirac completeness relation

$$\sum |n\rangle\langle n| = I, \qquad (2)$$

the five-space forward propagator takes the form

$$G_5(x_f^\mu, \tau; x_i^\mu, 0) = -i\theta(\tau)\langle x_f^\mu|e^{-i\hat{H}\tau}|x_i^\mu\rangle$$
$$= -i\theta(\tau)\sum \phi_n(x_f^\mu)\phi_n^*(x_i^\mu)e^{-iE_n\tau}. \quad (3)$$

This propagator obeys a Schrödinger equation that is first order in τ:

$$(i\partial_\tau + \hat{H})G_5(x^\mu, \tau; 0, 0) = \delta(\tau)\delta^4(x^\mu). \qquad (4)$$

The four-dimensional propagators in the five-dimensional formalism are constructed by integrating out the fifth coordinate. Given (3), the associated four-dimensional propagator is then defined as

$$G_4(x_f^\mu; x_i^\mu) = N \int_{-\infty}^{\infty} d\tau G_5(x_f^\mu, \tau; x_i^\mu, 0), \qquad (5)$$

where N is a normalization constant. Using the integral representation

$$\theta(\tau) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\nu \frac{e^{-i\nu\tau}}{\nu + i\epsilon}, \qquad (6)$$

one then obtains

$$G_4(x_f^\mu; x_i^\mu) = N \sum \frac{\phi_n(x_f^\mu)\phi_n^*(x_i^\mu)}{-E_n + i\epsilon}. \qquad (7)$$

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Finally, since the wave functions are eigenfunctions of $\hat{H}$, $G_4(x_f^\mu; x_i^\mu)$ obeys

$$-\hat{H}G_4(x^\mu, 0) = N\delta^4(x^\mu). \qquad (8)$$

The primary objective in using the approach of [1,2] is to choose a five-dimensional $\hat{H}$ so that $G_4(x^\mu, 0)$ obeys a differential wave equation of the form

$$D_4 G_4(x^\mu, 0) = \delta^4(x^\mu), \qquad (9)$$

where D_4 is one of the familiar wave operators that appear in quantum field theory (such wave operators are typically higher than first derivative in time). [Normalizing $G_4(x^\mu, 0)$ according to (9) would fix the constant N.] Thus, in the simple case where the five-dimensional Hamiltonian has the form $\hat{H} = \hat{\vec{p}}^2 - (\hat{p}^0)^2 + m^2$, (7) is the Fourier transform of the standard four-dimensional scalar field Feynman propagator $D_4 = \partial_\mu \partial^\mu$. Because forward propagation in τ gives the correct $i\epsilon$ prescription for the causal Feynman contour in four dimensions, $D_4 = \partial_\mu \partial^\mu$ is the usual four-dimensional Klein-Gordon operator. Using the five-dimensional formalism, one can solve for a one-body quantum-mechanical Schrödinger-type propagator in five-space, and from it one can construct a many-body quantum-field-theoretic propagator in four-space. The five-space formalism also permits one to choose five-space Hamiltonians for which the resulting four-space propagator does not obey an equation of the form (9) with a familiar D_4. In this paper we construct some simple models that lead to a propagator equation with a familiar D_4 and some that have a more general structure.

When Lorentz invariance was introduced in classical mechanics, it described the invariance properties of the line element $ds^2 = dt^2 - d\mathbf{x}^2$. In addition to invariance under the continuous orthochronous Lorentz transformations, the line element also possesses a set of discrete invariances, namely, space reflection $\mathcal{P}: \mathbf{x} \to -\mathbf{x}, t \to t$, time-reversal $\mathcal{T}: \mathbf{x} \to \mathbf{x}, t \to -t$, and their product spacetime reflection $\mathcal{PT}: \mathbf{x} \to -\mathbf{x}, t \to -t$. However, when time-reversal was introduced into quantum mechanics by Wigner, the time reflection of the $i\partial/\partial t$ operator was achieved not by replacing t by $-t$ but rather by taking $\mathcal{T}$ to be an antiunitary operator that transforms i into $-i$ ($\mathcal{T}: i \to -i$); time t was treated as a c-number parameter that is not affected by $\mathcal{T}$. In relativistic quantum field theory time-reversal is also not implemented by making the direct replacement $t \to -t$ even though the line element $ds^2 = dt^2 - d\mathbf{x}^2$ possesses this time-reversal invariance. As noted above, in the five-dimensional relativistic quantum-mechanical approach used here, we treat time as an operator and thus we can implement a time-reversal operation that acts directly on the time. We can also implement $\mathcal{PT}$ transformations directly on the time operator.

The ability to implement a $\mathcal{PT}$ transformation on the time operator is appealing because of the implications of $\mathcal{PT}$ invariance for Hamiltonians that are not Hermitian. In the last few years it has been recognized [4–7] that a quantum-mechanical Hamiltonian that is not Hermitian may still have an entirely real set of energy eigenvalues. In the cases that were explicitly considered in [4–7], the reality of the eigenvalues was traced to the existence of an underlying invariance of the Hamiltonian with respect to a combined $\mathcal{PT}$ reflection. Thus, while Dirac Hermiticity of the Hamiltonian is sufficient for reality of eigenvalues, it is not necessary. (Of course, Hamiltonians with entirely real eigenvalues can be both $\mathcal{PT}$ invariant and Dirac-Hermitian.) However, recently it has been shown [8] that a Hamiltonian that is not $\mathcal{PT}$ invariant cannot have an entirely real set of energy eigenvalues. This means that $\mathcal{PT}$ invariance, in contrast to Dirac Hermiticity, is necessary for the reality of energy eigenvalues [9]. (If one knows only that a Hamiltonian is not Dirac-Hermitian, one can say nothing about the reality of the eigenvalues.) Thus, $\mathcal{PT}$ invariance of a Hamiltonian is a broader requirement than Dirac Hermiticity.

In the non-Hermitian $\mathcal{PT}$-invariant context we apply the five-dimensional formalism described above. To do this we recall [9] that when a Hamiltonian is $\mathcal{PT}$ invariant, its eigenvalues are either real or they come in complex-conjugate pairs. Consequently, both $\hat{H}$ and its Dirac-Hermitian conjugate $\hat{H}^\dagger$ have the same eigenspectrum, and they are related by some similarity transform V [10]

$$V\hat{H}V^{-1} = \hat{H}^\dagger. \qquad (10)$$

In this case, if $|n\rangle$ is a right eigenvector $|R\rangle$ of $\hat{H}$, then $\langle n|V$ rather then $\langle n|$ is a left eigenvector $\langle L|$ of $\hat{H}$. Consequently, the energy-eigenstate-completeness relation (2) is replaced by

$$\sum |R\rangle\langle L| = \sum |n\rangle\langle n|V = I, \qquad (11)$$

and (3) and (7) are replaced by

$$G_5(x_f^\mu, \tau; x_i^\mu, 0) = -i\theta(\tau)\langle x_f^\mu|e^{-i\hat{H}\tau}|x_i^\mu\rangle$$
$$= -i\theta(\tau)\sum\langle x_f^\mu|n\rangle e^{-iE_n\tau}\langle n|V|x_i^\mu\rangle, \quad (12)$$

$$G_4(x_f^\mu; x_i^\mu) = N\sum\frac{\langle x_f^\mu|n\rangle\langle n|V|x_i^\mu\rangle}{-E_n + i\epsilon}. \qquad (13)$$

The propagator (13) is the relevant one in the $\mathcal{PT}$ case, and with its $\mathcal{PT}$-symmetric $\hat{H}$, it also obeys (8).

Invariance under $\mathcal{PT}$ reflection is a more physical requirement than Hermiticity because the proper orthochronous Lorentz group has a complex $\mathcal{PT}$ extension. Until now, this aspect of the Lorentz group has not been utilized because transformations that reverse the sign of the time have not been considered. In the present paper we consider such transformations and explicitly extend $\mathcal{PT}$ symmetry to the relativistic quantum-mechanical domain.

In particular, we study some simple non-Hermitian but $\mathcal{PT}$-symmetric $SO(3, 1)$-invariant model Hamiltonians using the five-dimensional formalism and for each Hamiltonian we show that all of the energy eigenvalues are real.

II. A SIMPLE FIVE-DIMENSIONAL $\mathcal{PT}$-SYMMETRIC HAMILTONIAN

The generic five-dimensional action has the form $I = \int_0^\tau d\tau' L(\tau')$, where τ is the end point of integration. We begin with a simple example that illustrates the five-dimensional formalism. Specifically, we take a Lagrangian of the form

$$L = \frac{m}{2}\dot{x}_\mu \dot{x}^\mu - \frac{m\omega^2}{2}(x_\mu x^\mu - 2ia_\mu x^\mu - a_\mu a^\mu), \quad (14)$$

where $\mu = (0, 1, 2, 3)$, the dot denotes differentiation with respect to τ, and a^μ is a real, external, τ-independent four-vector operator that commutes with x^μ. As constructed, the action is a relativistic $SO(3, 1)$ scalar function of the four x^μ coordinates, but it is nonrelativistic in the fifth coordinate τ. We define a canonical momentum

$$p_\mu \equiv \frac{\delta I}{\delta \dot{x}^\mu} = m\dot{x}_\mu, \quad (15)$$

and then eliminate $\dot{x}^\mu$ to obtain a canonical Hamiltonian

$$\begin{aligned} H &= p_\mu \dot{x}^\mu - L \\ &= \frac{1}{2m}p_\mu p^\mu + \frac{m\omega^2}{2}(x_\mu x^\mu - 2ia_\mu x^\mu - a_\mu a^\mu). \end{aligned} \quad (16)$$

The Hamiltonian (16) is not Dirac-Hermitian because of the $ia_\mu x^\mu$ term.

Next, we assign $\mathcal{P}$ and $\mathcal{T}$ quantum numbers to the x^μ and p^μ operators, just as we do with the nonrelativistic $\mathbf{x}$ and $\mathbf{p} = d\mathbf{x}/dt$; to wit, we take the three spatial components x^k to be $\mathcal{P}$ odd $[\mathcal{P}x^k(\tau)\mathcal{P}^{-1} = -x^k(\tau)]$ and $\mathcal{T}$ even $[\mathcal{T}x^k(\tau)\mathcal{T}^{-1} = x^k(-\tau)]$, and take the three spatial components $p^k = dx^k/d\tau$ to be $\mathcal{P}$ odd $[\mathcal{P}p^k(\tau)\mathcal{P}^{-1} = -p^k(\tau)]$ and $\mathcal{T}$ odd $[\mathcal{T}p^k(\tau)\mathcal{T}^{-1} = -p^k(-\tau)]$. Similarly, we take the time component x^0 to be $\mathcal{P}$ even $[\mathcal{P}x^0(\tau)\mathcal{P}^{-1} = x^0(\tau)]$ and $\mathcal{T}$ odd $[\mathcal{T}x^0(\tau)\mathcal{T}^{-1} = -x^0(-\tau)]$ and take the time component $p^0 = dx^0/d\tau$ to be $\mathcal{P}$ even $[\mathcal{P}p^0(\tau)\mathcal{P}^{-1} = p^0(\tau)]$ and $\mathcal{T}$ even $[\mathcal{T}p^0(\tau)\mathcal{T}^{-1} = p^0(-\tau)]$. With these assignments the four x^μ are $\mathcal{PT}$ odd while the four p^μ are $\mathcal{PT}$ even. Because $\mathcal{T}$ also converts i to $-i$, these assignments are consistent with the commutation algebra in (1). We summarize these assignments as follows:

$$\begin{array}{c|cccc} & \mathbf{p} & p^0 & \mathbf{x} & x^0 \\ \hline \mathcal{P} & - & + & - & + \\ \mathcal{T} & - & + & + & - \\ \mathcal{PT} & + & + & - & - \end{array} \quad (17)$$

Finally, we take the four-vector a^μ to be $\mathcal{PT}$ even. For our purposes we will need $\mathbf{a}$ to be $\mathcal{P}$ even and thus $\mathcal{T}$ even, and a^0 to be $\mathcal{P}$ odd and thus $\mathcal{T}$ odd. In the five-space the Hamiltonian (16) is conjugate to τ and not to x^0. Neither $\mathcal{P}$ nor $\mathcal{T}$ affect τ because τ is only a parameter, so with $p_\mu \dot{x}^\mu = p_\mu p^\mu/m$ being $\mathcal{PT}$ even, the Hamiltonian is $\mathcal{PT}$ symmetric.

To determine the energy eigenvalues we take the space-time metric to be $\text{diag}(\eta_{\mu\nu}) = (-1, 1, 1, 1)$. Writing $x^\mu = (t, x, y, z)$, we obtain a wave-mechanics representation of the algebra (1) when $p_\mu = -i\partial/\partial x^\mu$; that is,

$$p_0 = -i\frac{\partial}{\partial t}, \qquad p_k = -i\frac{\partial}{\partial x^k}. \quad (18)$$

Consequently, in five-space the Schrödinger equation takes the form

$$\begin{aligned} i\frac{\partial \psi(\tau, x^\mu)}{\partial \tau} = &\left[-\frac{1}{2m}\eta^{\mu\nu}\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\nu} \right. \\ &\left. + \frac{m\omega^2}{2}(x_\mu - ia_\mu)(x^\mu - ia^\mu) \right]\psi(\tau, x^\mu). \end{aligned} \quad (19)$$

The substitution $y^\mu = x^\mu - ia^\mu$ brings (19) to the form

$$\begin{aligned} i\frac{\partial \psi(\tau, y^\mu)}{\partial \tau} = &\left[\frac{1}{2m}\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial \mathbf{y}^2}\right) \right. \\ &\left. + \frac{m\omega^2}{2}(\mathbf{y}^2 - t^2) \right]\psi(\tau, y^\mu), \end{aligned} \quad (20)$$

and reduces the Schrödinger equation to a four-dimensional harmonic oscillator with Minkowski signature. Noting that

$$\begin{aligned} &\left[\frac{1}{2m}\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial \mathbf{y}^2}\right) + \frac{m\omega^2}{2}(\mathbf{y}^2 - t^2) \right]e^{-m\omega(\mathbf{y}^2 - t^2)/2} \\ &= 2\omega e^{-m\omega(\mathbf{y}^2 - t^2)/2}, \end{aligned} \quad (21)$$

we see that the t-dependent sector contributes a positive zero-point energy equal to $\omega/2$ just as the $\mathbf{y}$-dependent sector does. Because all the eigenvalues of a harmonic oscillator are real, the five-space energy eigenvalues of (19) are given by

$$E_5 = (n_x + n_y + n_z + n_t + 2)\omega, \quad (22)$$

where each of n_x, n_y, n_z and n_t ranges over the positive integers. Thus, while the Hamiltonian (16) is not Hermitian, all of its energy eigenvalues are real.

For this model the five-space propagator obeys

$$\begin{aligned} &\left[i\frac{\partial}{\partial \tau} + \frac{1}{2m}\frac{\partial}{\partial x_\mu}\frac{\partial}{\partial x^\mu} - \frac{m\omega^2}{2} \right. \\ &\left. \times (x_\mu - ia_\mu)(x^\mu - ia^\mu) \right]G_5(x^\mu, \tau; 0, 0) \\ &= \delta(\tau)\delta^4(x^\mu) \end{aligned} \quad (23)$$

and we show in Appendix A that

$$G_5(x^\mu, \tau; 0, 0)$$
$$= \theta(\tau) \frac{1}{(\sin\omega\tau)^2} \exp\left[\frac{im\omega \cos\omega\tau(x_\mu - ia_\mu)(x^\mu - ia^\mu)}{2\sin\omega\tau}\right]. \tag{24}$$

The propagator of the associated four-dimensional theory is then obtained via (5), and it obeys (8) with the $\mathcal{PT}$-symmetric $\hat{H} = -\partial_\mu \partial^\mu/2m + m\omega^2(x_\mu - ia_\mu) \times (x^\mu - ia^\mu)/2$.

Using the $\mathcal{PT}$-theory techniques described in [6], one can demonstrate the reality of the eigenvalues algebraically without actually solving the Schrödinger equation. To do so, one must construct an operator $e^\mathcal{Q}$ that possesses four key properties: (i) a similarity transformation using $e^\mathcal{Q}$ preserves the commutation relations; (ii) $\mathcal{Q}$ is a Hermitian operator (so that $e^\mathcal{Q}$ is not unitary); (iii) like V in (10), $e^\mathcal{Q}$ effects the transformation

$$e^{-\mathcal{Q}}He^\mathcal{Q} = H^\dagger; \tag{25}$$

(iv) the operator

$$\tilde{H} = e^{-\mathcal{Q}/2}He^{\mathcal{Q}/2} \tag{26}$$

obeys $\tilde{H}^\dagger = \tilde{H}$. The existence of such a $\mathcal{Q}$ operator implies that the energy eigenvalues of H are all real.

We now construct the $\mathcal{Q}$ operator for our simple five-dimensional model. Note that the momentum operator will effect the transformation

$$e^{-b^\nu p_\nu}x^\mu e^{b^\rho p_\rho} = x^\mu + ib^\mu, \tag{27}$$

and leave the commutation relations (1) untouched for any four-vector b^μ that commutes with both x^μ and p^μ. Given (27), we identify $\mathcal{Q}$ as the Hermitian operator $2a^\nu p_\nu$ because

$$e^{-2a^\nu p_\nu}He^{2a^\rho p_\rho}$$
$$= \frac{1}{2m}p_\mu p^\mu + \frac{m\omega^2}{2}(x_\mu x^\mu + 2ia_\mu x^\mu - a_\mu a^\mu) = H^\dagger. \tag{28}$$

Similarly, the transformation

$$e^{-a^\nu p_\nu}He^{a^\rho p_\rho} = \frac{1}{2m}p_\mu p^\mu + \frac{m\omega^2}{2}x_\mu x^\mu = \tilde{H} \tag{29}$$

generates an equivalent Hamiltonian $\tilde{H}$ that is manifestly Hermitian.

In $\mathcal{PT}$ quantum mechanics one introduces an operator $\mathcal{C}$ that is required to obey

$$[\mathcal{C}, H] = 0, \qquad \mathcal{C}^2 = I. \tag{30}$$

One constructs this operator by making the *ansatz* $\mathcal{C} = e^\mathcal{Q}\mathcal{P}$, where the operator $\mathcal{P}$ obeys $\mathcal{P}^2 = I$. In this form the operator $\mathcal{C}$ fulfills the condition $\mathcal{C}^2 = I$ provided that $\mathcal{Q}$

satisfies $\mathcal{PQP} = -\mathcal{Q}$. With $e^{-\mathcal{Q}}$ generating $e^{-\mathcal{Q}}He^\mathcal{Q} = H^\dagger$, the operator $\mathcal{C}$ obeys $\mathcal{C}^{-1}H\mathcal{C} = H$ if $\mathcal{P}$ generates $\mathcal{PHP} = H^\dagger$. For the $\mathcal{Q}$ and H of interest here, both $\mathcal{PQP} = -\mathcal{Q}$ and $\mathcal{PHP} = H^\dagger$ hold provided that a^0 is $\mathcal{P}$ odd and $\mathbf{a}$ is $\mathcal{P}$ even. With this choice for the parity of a^μ, we then identify $\mathcal{C} = e^\mathcal{Q}\mathcal{P}$. (Previously, we had required that a^μ be $\mathcal{PT}$ even.) Then, if both a^μ and p^μ are $\mathcal{PT}$ even, the operator $\mathcal{Q}$ is $\mathcal{PT}$ even. As constructed, $\mathcal{C}$ thus obeys $[\mathcal{C}, \mathcal{PT}] = 0$, as expected [8,9] when all energy eigenvalues are real [11].

III. FIVE-DIMENSIONAL PAIS-UHLENBECK OSCILLATOR

In 1950 Pais and Uhlenbeck [12] explored the question of whether the Pauli-Villars regulator associated with the fourth-order equation of motion

$$(\partial_t^2 - \nabla^2 + M_1^2)(\partial_t^2 - \nabla^2 + M_2^2)\phi(\mathbf{x}, t) = 0 \tag{31}$$

and propagator

$$D(k^2) = \frac{1}{(k^2 + M_1^2)(k^2 + M_2^2)}$$
$$= \frac{1}{M_2^2 - M_1^2}\left(\frac{1}{k^2 + M_1^2} - \frac{1}{k^2 + M_2^2}\right), \tag{32}$$

where $k^2 = -(k^0)^2 + \mathbf{k}^2$, could be physically viable, or whether it was merely a mathematical technique to regulate Feynman integrals. To this end they replaced the scalar field $\phi(\mathbf{x}, t)$ by a single coordinate $z(t)$ and examined single momentum modes $\omega_1^2 = \mathbf{k}^2 + M_1^2$ and $\omega_2^2 = \mathbf{k}^2 + M_2^2$. The resulting nonrelativistic quantum-mechanical limit of the equation of motion (31) and the propagator (32),

$$(\partial_t^2 + \omega_1^2)(\partial_t^2 + \omega_2^2)z(t) = 0,$$
$$G(E) = \frac{1}{\omega_1^2 - \omega_2^2}\left(\frac{1}{E^2 - \omega_1^2} - \frac{1}{E^2 - \omega_2^2}\right), \tag{33}$$

is known as the PU oscillator.

Pais and Uhlenbeck found that if the theory were quantized with a standard positive-metric Hilbert space, the energy spectrum would not be bounded below. One can evade this negative-energy problem by quantizing the theory in a negative-metric Hilbert space, but as the relative minus sign in (33) indicates, the disadvantage of doing so is that one obtains states of negative Dirac norm and evidently loses unitarity.

The PU oscillator was revisited in 2008 [13,14] and a new realization of the theory was found in which the Hilbert space has neither negative-energy nor negative-norm states. In this realization the Hamiltonian is not Dirac-Hermitian but is instead $\mathcal{PT}$ invariant. The norm is given by $\langle L|R\rangle = \langle n|V|n\rangle$, rather than by the Dirac norm $\langle n|n\rangle$, and the completeness relation is given by (11) rather than by (2). In analogy with (13), the relative minus signs in (32) and (33) are generated by the presence of the V

operator in the propagator and not by quantizing with an indefinite metric. This realization took a long time (more than half a century) to discover because the Hamiltonian of the theory appeared to be Dirac-Hermitian even though it is not. (In Refs. [13,14] the nonrelativistic $\mathcal{PT}$ realization of the PU oscillator is studied, and in Ref. [14] the relativistic scalar field theory is examined.)

For the case of the nonrelativistic PU oscillator, the equation of motion (33) for the coordinate $z(t)$ can be derived by a stationary variation of the PU oscillator action

$$I_{PU} = \frac{\gamma}{2} \int dt [\ddot{z}^2 - (\omega_1^2 + \omega_2^2)\dot{z}^2 + \omega_1^2\omega_2^2 z^2], \quad (34)$$

where γ, ω_1 and ω_2 are positive constants. Since $\dot{z}$ serves as the conjugate of both z and $\ddot{z}$, the action is constrained. One thus replaces $\dot{z}$ by a new variable x, and using the method of Dirac constraints, one obtains [15,16] the Hamiltonian

$$H_{PU} = \frac{p_x^2}{2\gamma} + p_z x + \frac{\gamma}{2}(\omega_1^2 + \omega_2^2)x^2 - \frac{\gamma}{2}\omega_1^2\omega_2^2 z^2 \quad (35)$$

with two canonical pairs that obey $[x, p_x] = i$ and $[z, p_z] = i$.

In the realization of the theory for which the energy eigenvalues are bounded below, H_{PU} appears to be Hermitian but it is not. Specifically, one solves the Schrödinger equation for the ground state of the system with energy $E_0 = (\omega_1 + \omega_2)/2$. The eigenfunction is

$$\psi_0(z, x) = \exp\left[\frac{\gamma}{2}(\omega_1 + \omega_2)\omega_1\omega_2 z^2 + i\gamma\omega_1\omega_2 zx \right.$$
$$\left. - \frac{\gamma}{2}(\omega_1 + \omega_2)x^2\right]. \quad (36)$$

This eigenfunction diverges exponentially for large z, so integration by parts generates surface terms that cannot be discarded. Thus, one cannot represent the operator p_z by $-i\partial_z$. However, one can replace z by iz (this is equivalent to working in a Stokes wedge in the complex-z plane that includes the imaginary z axis but not the real one [13]), and represent p_z by $-i\partial_{iz} = -\partial_z$. The eigenfunction then vanishes exponentially as z becomes large. The highly unusual implication of the structure of (36) (and the reason it took so long to find) is that while both conjugate pairs of coordinates are obtained from the same Lagrangian, the commutator $[x, p_x] = i$ is realized by Hermitian operators, while the commutator $[z, p_z] = i$ is realized by anti-Hermitian operators. As a result, the $p_z x$ cross-term in (35) is not Hermitian, and the Hamiltonian H_{PU} is also not Hermitian.

Rather than using non-Hermitian operators, we make the similarity transformation

$$y = e^{\pi p_z z/2} z e^{-\pi p_z z/2} = -iz,$$
$$q = e^{\pi p_z z/2} p_z e^{-\pi p_z z/2} = ip_z, \quad (37)$$

to construct Hermitian operators y and q that obey $[y, q] = i$. In terms of y and q the Hamiltonian now takes the form

$$H_{PU} = \frac{p^2}{2\gamma} - iqx + \frac{\gamma}{2}(\omega_1^2 + \omega_2^2)x^2 + \frac{\gamma}{2}\omega_1^2\omega_2^2 y^2, \quad (38)$$

where for notational simplicity we have replaced p_x by p. The Hamiltonian H_{PU} is now manifestly non-Hermitian.

While H_{PU} is not Hermitian, the $\mathcal{P}$ and $\mathcal{T}$ quantum-number assignments

$$
\begin{array}{c|cccc}
 & p & x & q & y \\
\hline
\mathcal{P} & - & - & + & + \\
\mathcal{T} & - & + & + & - \\
\mathcal{PT} & + & - & + & -
\end{array}
\quad (39)
$$

make H_{PU} symmetric under $\mathcal{PT}$ reflection. Introducing the operator

$$\mathcal{Q} = \alpha pq + \beta xy,$$
$$\alpha = \frac{1}{\gamma\omega_1\omega_2}\log\left(\frac{\omega_1 + \omega_2}{\omega_1 - \omega_2}\right), \quad (40)$$
$$\beta = \alpha\gamma^2\omega_1^2\omega_2^2,$$

we then find that [13,14] the similarity-transformed PU Hamiltonian

$$\tilde{H}_{PU} = e^{-\mathcal{Q}/2} H_{PU} e^{\mathcal{Q}/2}$$
$$= \frac{p^2}{2\gamma} + \frac{q^2}{2\gamma\omega_1^2} + \frac{\gamma}{2}\omega_1^2 x^2 + \frac{\gamma}{2}\omega_1^2\omega_2^2 y^2 \quad (41)$$

represents two uncoupled harmonic oscillators. The transformed Hamiltonian $\tilde{H}_{PU}$ in (41) is both Hermitian and manifestly positive definite. This realization of the quantum theory, which is associated with the non-Hermitian H_{PU}, has no negative-norm or negative-energy eigenstates [17].

Because the transformation with $e^{\mathcal{Q}/2}$ is not unitary, the propagator

$$D(H_{PU}) = \langle x', y'|e^{-iH_{PU}t}|x, y\rangle$$
$$= \langle x', y'|e^{\mathcal{Q}/2} e^{-i\tilde{H}_{PU}t} e^{-\mathcal{Q}/2}|x, y\rangle \quad (42)$$

associated with H_{PU} does not transform into the propagator

$$D(\tilde{H}_{PU}) = \langle x', y'|e^{-i\tilde{H}_{PU}t}|x, y\rangle \quad (43)$$

that one would ordinarily associate with a two-uncoupled-oscillator system. The state $\langle x, y|e^{\mathcal{Q}/2}$ is not the conjugate of $e^{-\mathcal{Q}/2}|x, y\rangle$, and the propagators in (42) and (43) are not equivalent; for this realization of the PU Hamiltonian we must use (42) and not (43). The dependence on the operator $V = e^{-\mathcal{Q}}$ is crucial because it generates the relative minus sign in (33).

We now illustrate $\mathcal{PT}$ invariance in relativistic quantum mechanics by applying the five-dimensional formalism to the PU oscillator. We will see that a straightforward covariant generalization of the PU oscillator does not lead back to (32). Consequently, in the next section we provide an alternate five-dimensional formalism that does.

To generalize the PU oscillator to relativistic quantum mechanics we replace (34) by

$$I = \frac{\gamma}{2} \int_0^\tau d\tau [\ddot{z}_\mu \ddot{z}^\mu - (M_1^2 + M_2^2)\dot{z}_\mu \dot{z}^\mu + M_1^2 M_2^2 z_\mu z^\mu], \tag{44}$$

where the dot denotes differentiation with respect to τ. Because of constraints associated with this action, the Hamiltonian has the form

$$H = \frac{(p_x)_\mu (p_x)^\mu}{2\gamma} + (p_z)_\mu x^\mu + \frac{\gamma}{2}(M_1^2 + M_2^2)x_\mu x^\mu$$
$$- \frac{\gamma}{2} M_1^2 M_2^2 z_\mu z^\mu. \tag{45}$$

Recalling the transformation in (37), we let $y^\mu = -iz^\mu$ and $q^\mu = i(p_z)^\mu$. On setting $(p_x)^\mu = p^\mu$ we obtain two canonical pairs of operators that obey

$$[x^\mu(\tau), p^\nu(\tau)] = i\eta^{\mu\nu}, \qquad [q^\mu(\tau), y^\nu(\tau)] = i\eta^{\mu\nu}, \tag{46}$$

and a Hamiltonian of the form

$$H = \frac{p_\mu p^\mu}{2\gamma} - iq_\mu x^\mu + \frac{\gamma}{2}(M_1^2 + M_2^2)x_\mu x^\mu$$
$$+ \frac{\gamma}{2} M_1^2 M_2^2 y_\mu y^\mu. \tag{47}$$

The assignments

$$\begin{array}{c|cccccccc}
 & \mathbf{p} & p^0 & \mathbf{x} & x^0 & \mathbf{q} & q^0 & \mathbf{y} & y^0 \\
\hline
\mathcal{P} & - & + & - & + & + & - & + & - \\
\mathcal{T} & - & + & + & - & + & - & - & + \\
\mathcal{PT} & + & + & - & - & + & + & - & -
\end{array} \tag{48}$$

in which x^0 changes sign under $\mathcal{T}$, then establish that H_{PU} is $\mathcal{PT}$ symmetric.

Next, we introduce the operator

$$\mathcal{Q} = \alpha p_\mu q^\mu + \beta x_\mu y^\mu,$$
$$\alpha = \frac{1}{\gamma M_1 M_2} \log\left(\frac{M_1 + M_2}{M_1 - M_2}\right), \tag{49}$$
$$\beta = \alpha \gamma^2 M_1^2 M_2^2,$$

and find that

$$\tilde{H} = e^{-\mathcal{Q}/2} H e^{\mathcal{Q}/2}$$
$$= \frac{p_\mu p^\mu}{2\gamma} + \frac{q_\mu q^\mu}{2\gamma M_1^2} + \frac{\gamma}{2} M_1^2 x_\mu x^\mu + \frac{\gamma}{2} M_1^2 M_2^2 y_\mu y^\mu. \tag{50}$$

Thus, the energy eigenvalues of the $\mathcal{PT}$-symmetric Hamiltonian H are all real.

We show in Appendix A that if we set $M_1 = M$ and $M_2 = 0$, the five-space propagator is

$$G_5(x^\mu, y^\mu, \tau; 0, 0, 0) = \theta(\tau)\frac{e^{iB/A}}{A^2}, \tag{51}$$

where

$$2B/\gamma = Mx_\mu x^\mu(\sin M\tau - M\tau \cos M\tau) - M^3 y_\mu y^\mu \sin M\tau$$
$$+ 2iM^2 x_\mu y^\mu (1 - \cos M\tau),$$
$$A = 2 - 2\cos M\tau - M\tau \sin M\tau. \tag{52}$$

The propagator of the associated four-dimensional theory may now be obtained by performing the integral in (5), and the resulting propagator will obey (8) with $\hat{H} = -(1/2\gamma)\partial/\partial x_\mu \partial/\partial x^\mu - x^\mu \partial/\partial y^\mu + \gamma M^2 x_\mu x^\mu/2$. While of interest in itself, this propagator is not of the generic Pauli-Villars form given in (32). Thus, in Sec. IV we provide an alternate choice for the five-dimensional Hamiltonian that will lead to (32).

IV. ALTERNATE FORMULATION OF THE FIVE-SPACE PU OSCILLATOR

Given the structure of (31) we take the five-space $\hat{H}$ to have the operator form

$$\hat{H} = -[-(\hat{p}^0)^2 + \hat{\vec{p}}^2 + M_1^2][-(\hat{p}^0)^2 + \hat{\vec{p}}^2 + M_2^2]. \tag{53}$$

For this Hamiltonian the five-dimensional energies are given by

$$E_5 = -[-(p^0)^2 + \vec{p}^2 + M_1^2][-(p^0)^2 + \vec{p}^2 + M_2^2], \tag{54}$$

where the momenta in (54) are the eigenvalues of the operators in (53). Inserting these energies into (7), we obtain the Pauli-Villars propagator in (32), with (9) being satisfied.

Equation (53) leads directly to (32), but its use here is nonstandard because it does not have a simple Lagrangian counterpart. In the previous examples and in the derivation of the Klein-Gordon propagator, one can start with a five-dimensional action (of the form $\int_0^\tau d\tau \dot{x}_\mu \dot{x}^\mu$ for the specific Klein-Gordon case) and by a canonical procedure derive a Hamiltonian from it. The Lagrangians in these examples are quadratic functions of the coordinates, so the procedure is straightforward and yields Hamiltonians that are also quadratic. However, the Hamiltonian (53) is not quadratic; it is quartic because the wave operator in (31) is a fourth-order derivative operator [18]. Since the Lagrangian is given by $L(\dot{x}^\mu) = p_\mu \dot{x}^\mu - H(p_\mu p^\mu)$ and since $p_\mu = \partial L/\partial \dot{x}^\mu$, one can in principle construct $L(\dot{x}^\mu)$ if one knows $H(p_\mu p^\mu)$. Doing so for (53) is difficult, so we start directly with $H(p_\mu p^\mu)$. Once we have $H(p_\mu p^\mu)$, we can then use the representation in (7) without needing to know the structure of the Lagrangian.

We can recover the four-dimensional Pauli-Villars propagator, but at first it appears that the Hamiltonian in (53) is Hermitian. Moreover, in the second-order Klein-Gordon case with $\hat{H} = -(p^0)^2 + \bar{p}^2 + M_1^2$ and real E_5 the Hamiltonian is Hermitian. However, in the fourth-order case, we note that $(p^0)^2$ is given as

$$(p^0)^2 = \frac{1}{2}(E_1^2 + E_2^2 \pm [(E_1^2 - E_2^2)^2 - 4E_5]^{1/2}), \quad (55)$$

where $E_i^2 = \bar{p}^2 + M_i^2$. Thus, now there can be real values of E_5 for which $(p^0)^2$ is complex and for which the operator $(\hat{p}^0)^2$, and thus $\hat{H}$, is not Hermitian. (Note that with E_5 being real, the Hamiltonian must be $\mathcal{PT}$ invariant.)

In addition, we note that for general M_1 and M_2, if we take E_5 to be zero, the eigenfunctions associated with the operator $\hat{H}$ in (53) will have the form $\psi_1 = e^{-iE_1t+i\bar{p}\cdot\bar{x}}$ and $\psi_2 = e^{-iE_2t+i\bar{p}\cdot\bar{x}}$. However, if we then set $M_1 = 0$ and $M_2 = 0$, there will be eigenfunctions of the form $\psi_a = e^{-ipt+i\bar{p}\cdot\bar{x}}$ and $\psi_b = n_\mu x^\mu e^{-ipt+i\bar{p}\cdot\bar{x}}$, where n^μ is the unit timelike vector $n^\mu = (1, 0, 0, 0)$. Of the two ψ_a and ψ_b eigenfunctions, only ψ_a is stationary; ψ_b grows linearly in the time coordinate, which indicates that the Hamiltonian has Jordan-block form and that it has an incomplete set of eigenvectors. Consequently, the Hamiltonian $\hat{H}$ in (53) cannot be diagonalized and is not Hermitian. Since $\hat{H}$ is not Hermitian when $E_5 = M_1 = M_2 = 0$, it must also not be Hermitian for a range of values of these parameters. In Ref. [14] it was found that in the equal-frequency limit $\omega_1 = \omega_2$ of the PU oscillator, the Hamiltonian in (38) is also nondiagonalizable and non-Hermitian.

The solutions to (55) thus break up into two sectors. In one sector the Hamiltonian is Hermitian and the energy eigenvalues are unbounded below ($4E_5 < (M_1^2 - M_2^2)^2$). In the other sector the Hamiltonian is not Hermitian and the energies are bounded below ($4E_5 > (M_1^2 - M_2^2)^2$), just as in the case of the nonrelativistic PU oscillator. If E_5 is real, the Hamiltonian is $\mathcal{PT}$ invariant in both cases. In the sector where $\hat{H}$ is Hermitian the four-space propagator is given by (7). In the non-Hermitian sector the four-space propagator is given by (13) and as before, the V operator then generates the relative minus sign in the Pauli-Villars propagator [19]. Our five-space treatment of the Pauli-Villars propagator based on (53) recovers the key features of the analyses of Refs. [13,14]. We see that one can extend $\mathcal{PT}$ symmetry to the five-dimensional formalism, and while we have not directly studied the time-reversal and $\mathcal{PT}$ properties of the time operator in the Pauli-Villars case, those properties follow directly from the commutation relations (1) depending on how they are explicitly specified for $(\hat{p})^0$.

V. SUMMARY

Using a number of elementary models, we have shown in this paper that the standard techniques of $\mathcal{PT}$ quantum mechanics extend and apply to relativistic quantum mechanics, where the time-reversal operator $\mathcal{T}$ reverses the sign of the time operator x^0. We conclude that relativistic $\mathcal{PT}$-symmetric quantum mechanics is physically viable.

ACKNOWLEDGMENTS

APPENDIX A: CONSTRUCTION OF FIVE-SPACE PROPAGATORS

To construct propagators that obey the five-dimensional equation $(i\partial_\tau + \hat{H})G_5(x^\mu, \tau; 0, 0) = \delta(\tau)\delta^4(x^\mu)$, we first recall how a propagator is constructed when the eigenmodes of $\hat{H}$ are plane waves. For the nonrelativistic quantum-mechanical free particle in one space dimension there is a plane-wave basis and the propagator is given by

$$G_1(x, t; 0, 0) = -\frac{i\theta(t)}{2\pi} \int dp e^{-ipx - ip^2t/m}. \quad (A1)$$

When $i\partial_t$ acts on $-i\theta(t)$, we generate the $\delta(t)\delta(x)$ term, while if we omit the $\theta(t)$ function, the rest of the propagator obeys

$$\left[i\frac{\partial}{\partial t} + \frac{1}{2m}\frac{\partial^2}{\partial x^2}\right]R_1(x, t; 0, 0) = 0, \quad (A2)$$

where $G_1(x, t; 0, 0) = \theta(t)R_1(x, t; 0, 0)$. The Fourier transform in (A1) can be performed analytically and yields

$$G_1(x, t; 0, 0) = \theta(t)\left(\frac{m}{2\pi it}\right)^{1/2} e^{imx^2/2t}. \quad (A3)$$

The term $I_{STAT} = mx^2/2t$ in the exponent is the value of the classical action $I = (m/2) \int_0^t dt\dot{x}^2$ for the stationary path $\ddot{x} = 0$ between the end points ($x = 0, t = 0$) and (x, t).

If one were to calculate this propagator as a path integral $\int[dx]e^{iI}$ over a complete basis of paths between the end points, one would obtain the same $e^{iI_{STAT}}$ phase, but one would not know the multiplicative prefactor. This prefactor is determined by requiring that the propagator obey (A2). (If one does not have a plane-wave basis, one can evaluate the propagator via a path integral and then use the Schrödinger equation to determine the prefactor.)

For the one-dimensional harmonic oscillator (where the basis is not plane waves), the path integral again has the form $e^{iI_{STAT}}$, where I_{STAT} is the value of $I = (m/2) \times \int_0^T dt[\dot{x}^2 - \omega^2 x^2]$ as evaluated in the stationary path $\ddot{x} + \omega^2 x = 0$ between the end points ($x = 0, t = 0$) and ($x = x_f, t = T$). Noting that $\dot{x}^2 - \omega^2 x^2 = d(x\dot{x})/dt - x\ddot{x} - \omega^2 x^2$, we obtain $I_{STAT} = mx_f\dot{x}_f/2$. The solution to the equation of motion is $x(t) = x_f \sin\omega t/\sin\omega T$, $\dot{x}(t) = \omega x_f \cos\omega t/\sin\omega T$, so we obtain $I_{STAT} = m\omega x_f^2 \cos\omega T/2\sin\omega T$. With this form for I_{STAT}, the prefactor evaluates to $(\sin\omega T)^{-1/2}$ and the propagator is

$$G_1(x, T; 0, 0) = \theta(T)\left(\frac{1}{\sin\omega T}\right)^{1/2} \exp\left(\frac{im\omega x^2 \cos\omega T}{2\sin\omega T}\right).$$
(A4)

The propagator (24) is the shifted covariant generalization of this result.

The propagator associated with the PU oscillator action given in (34) has already been reported in the literature [20], and because the action is quadratic, the $\int d[z]$ path integral between end points with fixed z and $\dot{z}$ has the form $\exp(iI_{\text{STAT}})$ with the appropriate I_{STAT}. Here, we present a simplified version of the propagator in which we set $\omega_1 = \omega$, $\omega_2 = 0$. In this case the classical action reduces to

$$I_{\text{PU}} = \frac{\gamma}{2}\int dt(\ddot{z}^2 - \omega^2\dot{z}^2),$$
(A5)

and the stationary classical equation of motion is given by

$$\partial_t^2(\ddot{z} + \omega^2 z) = 0.$$
(A6)

Noting that

$$\partial_t(\dot{z}\,\ddot{z} - z\partial_t^3 z - \omega^2 z\dot{z}) = \ddot{z}^2 - \omega^2\dot{z}^2 - z\partial_t^2(\ddot{z} + \omega^2 z),$$
(A7)

on evaluating I_{STAT} between $z = 0$, $\dot{z} = 0$ at $t = 0$, and $z(T)$, $\dot{z}(T)$ at $t = T$, we obtain

$$I_{\text{STAT}} = (\gamma/2)(\dot{z}(T)\ddot{z}(T) - z(T)\partial_t^3 z(T) - \omega^2 z(T)\dot{z}(T)).$$
(A8)

Hence, introducing

$$\omega\alpha A(T) = \dot{z}(T)(\omega T - \sin\omega T) - \omega z(T)(1 - \cos\omega T),$$
$$\beta A(T) = \dot{z}(T)(1 - \cos\omega T) - z(T)\omega\sin\omega T,$$
(A9)
$$A(T) = 2 - 2\cos\omega T - \omega T\sin\omega T,$$

we find that the solution to (A6) that satisfies the boundary conditions takes the form

$$z(t) = -\alpha(1 - \cos\omega t) - (\beta/\omega)\sin\omega t + \beta t,$$
$$\dot{z}(t) = -\alpha\omega\sin\omega t - \beta\cos\omega t + \beta,$$
$$\ddot{z}(t) = -\alpha\omega^2\cos\omega t + \beta\omega\sin\omega t,$$
(A10)
$$\partial_t^3 z(t) = \alpha\omega^3\sin\omega t + \beta\omega^2\cos\omega t.$$

In this solution I_{STAT} obeys

$$\frac{2A(T)}{\gamma}I_{\text{STAT}} = \omega\dot{z}^2(T)(\sin\omega T - \omega T\cos\omega T)$$
$$- 2\omega^2 z(T)\dot{z}(T)(1 - \cos\omega T)$$
$$+ \omega^3 z^2(T)\sin\omega T.$$
(A11)

Finally, we verify that this function is a solution to the Schrödinger equation associated with (35) and identify the prefactor as $A^{-1/2}(T)$. The propagator is thus $A^{-1/2}(T)e^{iI_{\text{STAT}}}$. Its covariant generalization, obtained by using (37), is given in (51).

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[18] One can either represent the fourth-order derivative theory as a quadratic theory based on two sets of conjugate position and momentum pairs or as a quartic theory based on one conjugate pair alone. Both representations yield the same energy eigenvalues.

[19] A relative minus sign can appear in (32) in the Hermitian Hamiltonian case where there are no states with negative-norm because as noted in [14], in this case the contour for the p^0 integration is not the standard Feynman one. Specifically, in the generic form $1/(A + i\epsilon_a) - 1/(B + i\epsilon_b) = (B - A)/(AB + i\epsilon)$, where $\epsilon = B\epsilon_a + A\epsilon_b$ the sense of the contours depends on the values of A and B.

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