

Quantum Mechanics Based on Non-Hermitian Hamiltonians

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Abstract

A physical theory of quantum mechanics can be based on a complex Hamiltonian that is not Hermitian but instead satisfies the physical condition of space-time reflection symmetry ($\mathcal{PT}$ symmetry). Thus, there are infinitely many new Hamiltonians that one can construct that might explain experimental data. One would think that a non-Hermitian Hamiltonian would give a quantum theory that violates unitarity. However, if $\mathcal{PT}$ symmetry is not broken, it is possible to use a physical symmetry of the Hamiltonian to construct an inner product whose associated norm is positive definite. This construction is general and works for any $\mathcal{PT}$ -symmetric Hamiltonian. The dynamics is governed by unitary time evolution. This formulation does not conflict with the requirements of conventional quantum mechanics. There are many possible observable and experimental consequences of extending quantum mechanics into the complex domain, both in particle physics and in solid state physics.

1 Introduction

In this paper we discuss an alternative a standard axiom of quantum mechanics; namely, that the Hamiltonian H , which incorporates the symmetries and specifies the dynamics of a quantum theory, must be Hermitian: $H = H^\dagger$. (The symbol $\dagger$ represents Dirac Hermitian conjugation; that is, transpose and complex conjugate.) It is commonly believed that the Hamiltonian must be Hermitian in order to ensure that the energy spectrum (the eigenvalues of the Hamiltonian) is real and that the time evolution of the theory is unitary (probability is conserved in time). This axiom is sufficient to guarantee these desired properties, but we argue that it is not necessary. We believe that the condition of Hermiticity is a mathematical requirement whose physical basis is somewhat obscure. We demonstrate that the more physical alternative axiom of space-time reflection symmetry ($\mathcal{PT}$ symmetry), $H = H^{\mathcal{PT}}$, allows for the possibility of non-Hermitian and complex Hamiltonians but still leads to a consistent theory of quantum mechanics.

We also show that because $\mathcal{PT}$ symmetry is an alternative to Hermiticity it is now possible to construct infinitely many new Hamiltonians that would have been rejected in the past because they are not Hermitian. An example of such a Hamiltonian is $H = p^2 + ix^3$. It should be emphasized that we do not regard Hermiticity as wrong. Rather, $\mathcal{PT}$ symmetry offers the possibility of studying new and interesting quantum theories.

Let us recall the properties of the space reflection (parity) operator $\mathcal{P}$ and the time-reflection operator $\mathcal{T}$. The parity operator $\mathcal{P}$ is *linear* and has the effect $p \rightarrow -p$ and $x \rightarrow -x$. The time-reversal operator $\mathcal{T}$ is *antilinear* and has the effect $p \rightarrow -p$, $x \rightarrow x$, and $i \rightarrow -i$. Note that $\mathcal{T}$

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changes the sign of i because, like the parity operator, it preserves the fundamental commutation relation of quantum mechanics, $[x, p] = i$, known as the Heisenberg algebra.¹

It is easy to construct infinitely many Hamiltonians that are not Hermitian but do possess $\mathcal{PT}$ symmetry. For example, consider the one-parameter family of Hamiltonians

$$H = p^2 + x^2(ix)^\epsilon \quad (\epsilon \text{ real}). \quad (1)$$

While H in (1) is not symmetric under $\mathcal{P}$ or $\mathcal{T}$ separately, it is invariant under their combined operation. We say that such Hamiltonians possess space-time reflection symmetry. Other Hamiltonians having $\mathcal{PT}$ symmetry are $H = p^2 + x^4(ix)^\epsilon$, $H = p^2 + x^6(ix)^\epsilon$, and so on [2].²

The $\mathcal{PT}$ -symmetric Hamiltonians considered here, which for simplicity are also symmetric, is larger than and includes real symmetric Hermitians because any real symmetric Hamiltonian is automatically $\mathcal{PT}$ -symmetric. For example, consider the real symmetric Hamiltonian $H = p^2 + x^2 + 2x$. This Hamiltonian is time-reversal symmetric, but according to the usual definition of space reflection for which $x \rightarrow -x$, this Hamiltonian appears not to have $\mathcal{PT}$ symmetry. However, the parity operator is defined only up to unitary equivalence. In this example, the Hamiltonian has the form $H = p^2 + (x + 1)^2 - 1$ and it is evident that H is $\mathcal{PT}$ symmetric, provided that the parity operator performs a space reflection about the point $x = -1$ rather than $x = 0$. See Ref. [1] for the construction of the relevant parity operator.

In 1998 it was discovered that with properly defined boundary conditions the spectrum of the Hamiltonian H in (1) is *real and positive* when $\epsilon \geq 0$ [3]. The spectrum is partly real and partly complex when $\epsilon < 0$. The eigenvalues have been computed numerically to very high precision, and the real eigenvalues are plotted as functions of ϵ in Fig. 1.

We say that the $\mathcal{PT}$ symmetry of a Hamiltonian H is *unbroken* if all of the eigenfunctions of H are simultaneously eigenfunctions of $\mathcal{PT}$.³ It is easy to show that if the $\mathcal{PT}$ symmetry of a Hamiltonian H is unbroken, then the spectrum of H is real. The proof is short and goes as follows: Assume that a Hamiltonian H possesses $\mathcal{PT}$ symmetry (that is, that H commutes with the $\mathcal{PT}$ operator), and that if ϕ is an eigenstate of H with eigenvalue E , then it is simultaneously an eigenstate of $\mathcal{PT}$ with eigenvalue λ :

$$H\phi = E\phi \quad \text{and} \quad \mathcal{PT}\phi = \lambda\phi. \quad (2)$$

We begin by showing that the eigenvalue λ is a pure phase. Multiplying $\mathcal{PT}\phi = \lambda\phi$ on the left by $\mathcal{PT}$ and using the fact that $\mathcal{P}$ and $\mathcal{T}$ commute and that $\mathcal{P}^2 = \mathcal{T}^2 = 1$ we conclude that $\phi = \lambda^*\lambda\phi$ and thus $\lambda = e^{i\alpha}$ for some real α . Next, we introduce the convention that is used throughout this paper. Without loss of generality we replace the eigenstate ϕ by $e^{-i\alpha/2}\phi$ so that its eigenvalue under the operator $\mathcal{PT}$ is unity:

$$\mathcal{PT}\phi = \phi. \quad (3)$$

¹The Heisenberg-Weyl algebra is a real three-dimensional Lie algebra whose generators satisfy the commutation relations $[e_1, e_2] = e_3$, $[e_1, e_3] = [e_2, e_3] = 0$. To recover the Heisenberg commutation relations we set $e_1 = i(\hbar)^{-1/2}p$, $e_2 = i(\hbar)^{-1/2}x$, and $e_3 = i$.

²These classes of Hamiltonians are all *different*. For example, the Hamiltonian obtained by continuing H in (1) along the path $\epsilon : 0 \rightarrow 8$ has a different spectrum from the Hamiltonian obtained by continuing $H = p^2 + x^6(ix)^\epsilon$ along the path $\epsilon : 0 \rightarrow 4$. This is because the boundary conditions on the eigenfunctions are different.

³If an equation possesses a discrete symmetry, the solution to this equation need not exhibit that symmetry. For example, the differential equation $\ddot{y}(t) = y(t)$ is symmetric under the discrete time-reversal symmetry $t \rightarrow -t$. The solutions $y(t) = e^t$ and $y(t) = e^{-t}$ do not exhibit this time-reversal symmetry while the solution $y(t) = \cosh(t)$ is time-reversal symmetric. The same is true of a system whose Hamiltonian is $\mathcal{PT}$ symmetric. Even if the Schrödinger equation and the corresponding boundary conditions are $\mathcal{PT}$ symmetric, the wave function that solves the Schrödinger equation boundary value problem may not be symmetric under space-time reflection. When the solution exhibits $\mathcal{PT}$ symmetry, we say that the $\mathcal{PT}$ symmetry is *unbroken* and if the solution does not possess $\mathcal{PT}$ symmetry, we say that the $\mathcal{PT}$ symmetry is *broken*.

Next, we multiply the eigenvalue equation $H\phi = E\phi$ on the left by $\mathcal{PT}$ and use the fact that $[\mathcal{PT}, H] = 0$ to obtain $E\phi = E^*\phi$. Hence, $E = E^*$ and the eigenvalue E is real.

The crucial assumption in this argument is that ϕ is simultaneously an eigenstate of H and $\mathcal{PT}$. In quantum mechanics if a linear operator X commutes with the Hamiltonian H , then the eigenstates of H are also eigenstates of X . However, we emphasize that the operator $\mathcal{PT}$ is not linear (it is antilinear) and thus we must make the extra assumption that the $\mathcal{PT}$ symmetry of H is unbroken; that is, that ϕ is simultaneously an eigenstate of H and $\mathcal{PT}$. This extra assumption is nontrivial because it is not easy to determine *a priori* whether the $\mathcal{PT}$ symmetry of a particular Hamiltonian H is broken or unbroken. For the Hamiltonian H in (1) the $\mathcal{PT}$ symmetry is unbroken when $\epsilon \geq 0$ and it is broken when $\epsilon < 0$. The conventional Hermitian Hamiltonian for the quantum mechanical harmonic oscillator lies at the boundary of the unbroken and the broken regimes. Dorey *et al.* proved rigorously that the spectrum of H in (1) is real and positive [4] in the region $\epsilon \geq 0$. Many other $\mathcal{PT}$ -symmetric Hamiltonians for which space-time reflection symmetry is not broken have been investigated, and the spectra of these Hamiltonians have also been shown to be real and positive [5].

It is useful to show that a given non-Hermitian $\mathcal{PT}$ -symmetric Hamiltonian operator has a positive real spectrum, but the urgent question that must be answered is whether such a Hamiltonian defines a physical theory of quantum mechanics. By a *physical theory* we mean that there is a Hilbert space of state vectors and that this Hilbert space has an inner product

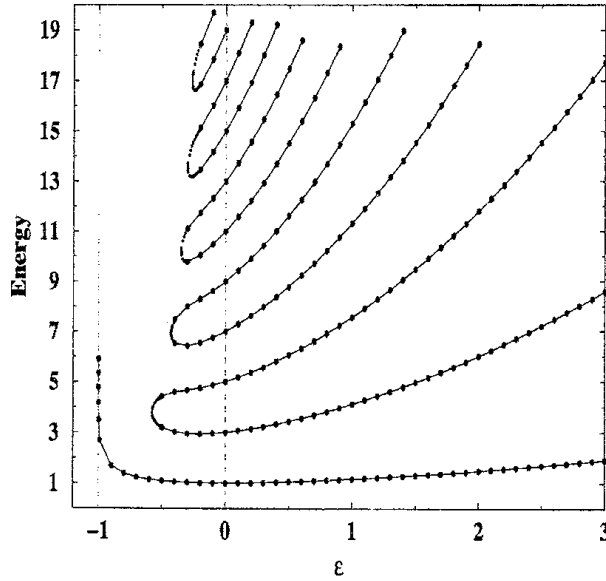


Figure 1: Energy levels of the Hamiltonian $H = p^2 + x^2(ix)^\epsilon$ as a function of the parameter ϵ . There are three regions: When $\epsilon \geq 0$, the spectrum is real and positive and the energy levels rise with increasing ϵ . The lower bound of this region, $\epsilon = 0$, corresponds to the harmonic oscillator, whose energy levels are $E_n = 2n + 1$. When $-1 < \epsilon < 0$, there are a finite number of real positive eigenvalues and an infinite number of complex conjugate pairs of eigenvalues. As ϵ decreases from 0 to -1 , the number of real eigenvalues decreases; when $\epsilon \leq -0.57793$, the only real eigenvalue is the ground-state energy. As ϵ approaches -1^+ , the ground-state energy diverges. For $\epsilon \leq -1$ there are no real eigenvalues.

with a positive norm. In the theory of quantum mechanics we interpret the norm of a state as a probability and this probability must be positive. Furthermore, we must show that the time evolution of the theory is unitary. This means that as a state vector evolves in time the probability does not leak away.

It is not obvious whether a Hamiltonian such as H in (1) gives rise to a consistent quantum theory. Indeed, while early investigations of this Hamiltonian have shown that the spectrum is entirely real and positive when $\epsilon \geq 0$, it appeared that one inevitably encountered the severe problem of dealing with Hilbert spaces endowed with indefinite metrics [6]. We will identify here a new symmetry that all $\mathcal{PT}$ -symmetric Hamiltonians having an unbroken $\mathcal{PT}$ -symmetry possess. We denote the operator representing this symmetry by $\mathcal{C}$ because the properties of this operator resemble those of the charge conjugation operator in particle physics. This will allow us to introduce an inner product structure associated with $\mathcal{CPT}$ conjugation for which the norms of quantum states are positive definite. We will see that $\mathcal{CPT}$ symmetry is an alternative to the conventional Hermiticity requirement; it introduces the new concept of a *dynamically determined* inner product (one that is defined by the Hamiltonian itself). As a consequence, we will extend the Hamiltonian and its eigenstates into the complex domain so that the associated eigenvalues are real and the underlying dynamics is unitary.

2 Construction of the $\mathcal{C}$ Operator

We begin by summarizing the mathematical properties of the solution to the Sturm-Liouville differential equation eigenvalue problem

$$-\phi_n''(x) + x^2(ix)^\epsilon \phi_n(x) = E_n \phi_n(x) \quad (4)$$

associated with the Hamiltonian H in (1). The differential equation (4) must be imposed on an infinite contour in the complex- x plane. For large $|x|$ this contour lies in wedges that are placed symmetrically with respect to the imaginary- x axis [3]. The boundary conditions on the eigenfunctions are that $\phi(x) \rightarrow 0$ exponentially rapidly as $|x| \rightarrow \infty$ on the contour. For $0 \leq \epsilon < 2$, the contour may be taken to be the real axis.

When $\epsilon \geq 0$, the Hamiltonian has an unbroken $\mathcal{PT}$ symmetry. Thus, the eigenfunctions $\phi_n(x)$ are simultaneously eigenstates of the $\mathcal{PT}$ operator: $\mathcal{PT}\phi_n(x) = \lambda_n \phi_n(x)$. As we argued above, λ_n is a pure phase and, without loss of generality, for each n this phase can be absorbed into $\phi_n(x)$ by a multiplicative rescaling so that the new eigenvalue is unity:

$$\mathcal{PT}\phi_n(x) = \phi_n^*(-x) = \phi_n(x). \quad (5)$$

There is strong evidence that, when properly normalized, the eigenfunctions $\phi_n(x)$ are complete. The coordinate-space statement of completeness (for real x and y) reads

$$\sum_n (-1)^n \phi_n(x) \phi_n(y) = \delta(x - y). \quad (6)$$

This is a nontrivial result that has been verified numerically to extremely high accuracy (twenty decimal places) [7, 8]. The unusual factor of $(-1)^n$ in the sum does not appear in conventional quantum mechanics. The presence of this factor is explained in the following discussion of orthonormality [see (8)].

A problem associated with non-Hermitian $\mathcal{PT}$ -symmetric Hamiltonians arises because there seems to be a natural way to define the inner product of two functions $f(x)$ and $g(x)$:

$$(f, g) \equiv \int dx [\mathcal{PT}f(x)]g(x), \quad (7)$$

where $\mathcal{PT}f(x) = [f(-x)]^*$ and the integral is taken over the contour described above in the complex- x plane. The apparent advantage of this inner product is that the associated norm (f, f) is independent of the overall phase of $f(x)$ and is conserved in time. Phase independence is desired because in quantum mechanics one uses a space of rays to represent quantum mechanical states. With respect to this inner product the eigenfunctions $\phi_m(x)$ and $\phi_n(x)$ of H in (1) are orthogonal for $n \neq m$. However, when $m = n$ the norm is *not positive*:

$$(\phi_m, \phi_n) = (-1)^n \delta_{mn}. \quad (8)$$

This result is apparently true for all values of ϵ in (4) and it has been verified numerically to extremely high precision. Because the norms of the eigenfunctions alternate in sign, the Hilbert space metric associated with the $\mathcal{PT}$ inner product $(\cdot, \cdot)$ is indefinite. This split signature (sign alternation) is a *generic* feature of the $\mathcal{PT}$ inner product. Extensive numerical calculations verify that the formula in (8) holds for all $\epsilon \geq 0$.

Despite the nonpositivity of the inner product, we proceed with the usual analysis that one would perform for any Sturm-Liouville problem of the form $H\phi_n = E_n\phi_n$. First, we use (8) to verify that (6) is the representation of the unity operator. That is, we verify that

$$\int dy \delta(x-y)\delta(y-z) = \delta(x-z). \quad (9)$$

Second, we reconstruct the parity operator $\mathcal{P}$ in terms of the eigenstates. The parity operator in position space is $\mathcal{P}(x, y) = \delta(x+y)$, so from (6) we get

$$\mathcal{P}(x, y) = \sum_n (-1)^n \phi_n(x) \phi_n(-y). \quad (10)$$

By virtue of (8) the square of the parity operator is unity: $\mathcal{P}^2 = 1$.

Third, we reconstruct the Hamiltonian H in coordinate space:

$$H(x, y) = \sum_n (-1)^n E_n \phi_n(x) \phi_n(y). \quad (11)$$

Using (6) - (8) it is easy to see that this Hamiltonian satisfies $H\phi_n(x) = E_n\phi_n(x)$. Fourth, we construct the coordinate-space Green's function $G(x, y)$:

$$G(x, y) = \sum_n (-1)^n \frac{1}{E_n} \phi_n(x) \phi_n(y). \quad (12)$$

The Green's function is the functional inverse of the Hamiltonian; that is, G satisfies

$$\int dy H(x, y)G(y, z) = \left[-\frac{d^2}{dx^2} + x^2(ix)^\epsilon \right] G(x, z) = \delta(x-z). \quad (13)$$

While the time-independent Schrödinger equation (4) cannot be solved analytically, the differential equation for $G(x, z)$ in (13) *can* be solved exactly and in closed form [8]. The technique is to consider the case $0 < \epsilon < 2$ so that we may treat x as real and then to decompose the x axis into two regions, $x > z$ and $x < z$. We can solve the differential equation in each of these regions in terms of Bessel functions. Then, using this coordinate-space representation of the Green's function, we construct an exact closed-form expression for the *spectral zeta function* (sum of the

inverses of the energy eigenvalues). To do so we set $y = x$ in $G(x, y)$ and use (8) to integrate over x . For all $\epsilon > 0$ we obtain [8]

$$\sum_n \frac{1}{E_n} = \left[1 + \frac{\cos\left(\frac{3\epsilon\pi}{2\epsilon+8}\right) \sin\left(\frac{\pi}{4+\epsilon}\right)}{\cos\left(\frac{\epsilon\pi}{4+2\epsilon}\right) \sin\left(\frac{3\pi}{4+\epsilon}\right)} \right] \frac{\Gamma\left(\frac{1}{4+\epsilon}\right) \Gamma\left(\frac{2}{4+\epsilon}\right) \Gamma\left(\frac{\epsilon}{4+\epsilon}\right)}{(4+\epsilon)^{\frac{4+2\epsilon}{4+\epsilon}} \Gamma\left(\frac{1+\epsilon}{4+\epsilon}\right) \Gamma\left(\frac{2+\epsilon}{4+\epsilon}\right)}. \quad (14)$$

Having presented these general Sturm-Liouville constructions, we discuss the question of whether a $\mathcal{PT}$ -symmetric Hamiltonian defines a physically viable quantum mechanics or whether it merely provides an intriguing Sturm-Liouville eigenvalue problem. The apparent difficulty with formulating a quantum theory is that the vector space of quantum states is spanned by energy eigenstates, of which half have norm $+1$ and half have norm -1 . Because the norm of the states carries a probabilistic interpretation in standard quantum theory, the existence of an indefinite metric in (8) seems to be a serious obstacle.

The situation here in which half of the energy eigenstates have positive norm and half have negative norm is analogous to the problem that Dirac encountered in formulating the spinor wave equation in relativistic quantum theory [9]. Following Dirac's approach, we attack the problem of an indefinite norm by finding a physical interpretation for the negative norm states. We claim that in *any* theory having an unbroken $\mathcal{PT}$ symmetry there exists a symmetry of the Hamiltonian connected with the fact that there are equal numbers of positive-norm and negative-norm states. To describe this symmetry we construct a linear operator denoted by $\mathcal{C}$ and represented in position space as a sum over the energy eigenstates of the Hamiltonian [10]:

$$\mathcal{C}(x, y) = \sum_n \phi_n(x) \phi_n(y). \quad (15)$$

As stated earlier, the properties of this new operator $\mathcal{C}$ are nearly identical to those of the charge conjugation operator in quantum field theory. For example, we can use equations (6) - (8) to verify that the square of $\mathcal{C}$ is unity ($\mathcal{C}^2 = 1$):

$$\int dy \mathcal{C}(x, y) \mathcal{C}(y, z) = \delta(x - z). \quad (16)$$

Thus, the eigenvalues of $\mathcal{C}$ are ± 1 . Also, $\mathcal{C}$ commutes with the Hamiltonian H . Therefore, since $\mathcal{C}$ is linear, the eigenstates of H have definite values of $\mathcal{C}$. Specifically, if the energy eigenstates satisfy (8), then we have $\mathcal{C}\phi_n = (-1)^n \phi_n$ because

$$\mathcal{C}\phi_n(x) = \int dy \mathcal{C}(x, y) \phi_n(y) = \sum_m \phi_m(x) \int dy \phi_m(y) \phi_n(y).$$

We then use $\int dy \phi_m(y) \phi_n(y) = (\phi_m, \phi_n)$ according to our convention. We conclude that $\mathcal{C}$ is the operator that represents the measurement of the signature of the $\mathcal{PT}$ norm of a state.

The operators $\mathcal{P}$ and $\mathcal{C}$ are distinct square roots of the unity operator $\delta(x - y)$. That is, while $\mathcal{P}^2 = 1$ and $\mathcal{C}^2 = 1$, $\mathcal{P}$ and $\mathcal{C}$ are not identical. Indeed, the parity operator $\mathcal{P}$ is real, while $\mathcal{C}$ is complex.⁴ Furthermore, these two operators do not commute:

$$(\mathcal{C}\mathcal{P})(x, y) = \sum_n \phi_n(x) \phi_n(-y) \quad \text{but} \quad (\mathcal{P}\mathcal{C})(x, y) = \sum_n \phi_n(-x) \phi_n(y), \quad (17)$$

⁴The parity operator in coordinate space is explicitly real $\mathcal{P}(x, y) = \delta(x + y)$; the operator $\mathcal{C}(x, y)$ is complex because it is a sum of products of complex functions, as we see in (15). The complexity of the $\mathcal{C}$ operator can be seen explicitly in perturbative calculations of $\mathcal{C}(x, y)$ [11].

which shows that $\mathcal{CP} = (\mathcal{PC})^*$. However, $\mathcal{C}$ does commute with $\mathcal{PT}$.

Finally, having obtained the operator $\mathcal{C}$ we define a new inner product structure having *positive definite* signature by

$$\langle f|g \rangle \equiv \int_C dx [\mathcal{CPT} f(x)]g(x). \quad (18)$$

Like the $\mathcal{PT}$ inner product (7), this inner product is phase independent and conserved in time. This is because the time evolution operator, just as in ordinary quantum mechanics, is e^{iHt} . The fact that H commutes with the $\mathcal{PT}$ and the $\mathcal{CPT}$ operators implies that both inner products, (7) and (18), remain time independent as the states evolve in time. However, unlike (7), the inner product (18) is positive definite because $\mathcal{C}$ contributes -1 when it acts on states with negative $\mathcal{PT}$ norm. In terms of the $\mathcal{CPT}$ conjugate, the completeness condition (4) reads

$$\sum_n \phi_n(x) [\mathcal{CPT} \phi_n(y)] = \delta(x - y). \quad (19)$$

Unlike the inner product of conventional quantum mechanics, the $\mathcal{CPT}$ inner product (19) is *dynamically determined*; it depends implicitly on the choice of Hamiltonian.

The operator $\mathcal{C}$ does not exist as a distinct entity in conventional quantum mechanics. Indeed, if we allow the parameter ϵ in (1) to tend to zero, the operator $\mathcal{C}$ in this limit becomes identical to $\mathcal{P}$. Thus, in this limit the $\mathcal{CPT}$ operator becomes $\mathcal{T}$, which is just complex conjugation. As a consequence, the inner product (18) defined with respect to the $\mathcal{CPT}$ conjugation reduces to the complex conjugate inner product of conventional quantum mechanics when $\epsilon \rightarrow 0$. Similarly, in this limit (19) reduces to the usual statement of completeness $\sum_n \phi_n(x) \phi_n^*(y) = \delta(x - y)$.

The $\mathcal{CPT}$ inner-product (18) is independent of the choice of integration contour C so long as C lies inside the asymptotic wedges associated with the boundary conditions for the Sturm-Liouville problem (2). Path independence follows from Cauchy's theorem and the analyticity of the integrand. In conventional quantum mechanics, where the inner product is $\int dx f^*(x)g(x)$, the integral must be taken along the real axis and the path of the integration cannot be deformed into the complex plane because the integrand is not analytic.⁵ The $\mathcal{PT}$ inner product (7) shares with (18) the advantage of analyticity and path independence, but suffers from nonpositivity. We find it surprising that a positive-definite metric can be constructed using $\mathcal{CPT}$ conjugation without disturbing the path independence of the inner-product integral.

Finally, we explain why $\mathcal{PT}$ -symmetric theories are unitary. Time evolution is determined by the operator e^{-iHt} , whether the theory is expressed in terms of a $\mathcal{PT}$ -symmetric Hamiltonian or just an ordinary Hermitian Hamiltonian. To establish the global unitarity of a theory we must show that as a state vector evolves its norm does not change in time. If $\psi_0(x)$ is a prescribed initial wave function belonging to the Hilbert space spanned by the energy eigenstates, then it evolves into the state $\psi_t(x)$ at time t according to

$$\psi_t(x) = e^{-iHt} \psi_0(x).$$

With respect to the $\mathcal{CPT}$ inner product defined in (18), the norm of the vector $\psi_t(x)$ does not change in time,

$$\langle \psi_t | \psi_t \rangle = \langle \psi_0 | \psi_0 \rangle,$$

⁵Note that if a function satisfies a linear ordinary differential equation, then the function is analytic wherever the coefficient functions of the differential equation are analytic. The Schrödinger equation (4) is linear and its coefficients are analytic except for a branch cut at the origin; this branch cut can be taken to run up the imaginary axis. We choose the integration contour for the inner product (8) so that it does not cross the positive imaginary axis. Path independence occurs because the integrand of the inner product (8) is a product of analytic functions.

because the Hamiltonian H commutes with the $\mathcal{CPT}$ operator. Establishing unitarity at a local level is more difficult. Here, we must show that in coordinate space, there exists a local probability density that satisfies a continuity equation so that the probability does not leak away. This is a subtle result because the probability current flows about in the complex plane rather than along the real axis as in conventional Hermitian quantum mechanics. Preliminary numerical studies indeed indicate that the continuity equation is fulfilled [14].

3 Illustrative Example: A 2×2 Matrix Hamiltonian

We will now illustrate the above results concerning $\mathcal{PT}$ -symmetric quantum mechanics in a very simple context. To do so we will consider systems characterized by finite-dimensional matrix Hamiltonians. In finite-dimensional systems the $\mathcal{P}$, $\mathcal{T}$, and $\mathcal{C}$ operators appear, but there is no analogue of the boundary conditions associated with coordinate-space Schrödinger equations.

Let us consider the 2×2 matrix Hamiltonian

$$H = \begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix}, \quad (20)$$

where the three parameters r , s , and θ are real. This Hamiltonian is not Hermitian in the usual sense, but it is $\mathcal{PT}$ symmetric, where the parity operator is given by [15]

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (21)$$

and $\mathcal{T}$ performs complex conjugation.

There are two parametric regions for this Hamiltonian. When $s^2 < r^2 \sin^2 \theta$, the energy eigenvalues form a complex conjugate pair. This is the region of broken $\mathcal{PT}$ symmetry. On the other hand, if $s^2 \geq r^2 \sin^2 \theta$, then the eigenvalues $\varepsilon_{\pm} = r \cos \theta \pm \sqrt{s^2 - r^2 \sin^2 \theta}$ are real. This is the region of unbroken $\mathcal{PT}$ symmetry. In the unbroken region the simultaneous eigenstates of the operators H and $\mathcal{PT}$ are given by

$$|\varepsilon_+\rangle = \frac{1}{\sqrt{2 \cos \alpha}} \begin{pmatrix} e^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix} \quad \text{and} \quad |\varepsilon_-\rangle = \frac{i}{\sqrt{2 \cos \alpha}} \begin{pmatrix} e^{-i\alpha/2} \\ -e^{i\alpha/2} \end{pmatrix}, \quad (22)$$

where we set $\sin \alpha = (r/s) \sin \theta$. It is easily verified that $(\varepsilon_{\pm}, \varepsilon_{\pm}) = \pm 1$ and that $(\varepsilon_{\pm}, \varepsilon_{\mp}) = 0$, recalling that $(u, v) = (\mathcal{PT}u) \cdot v$. Therefore, with respect to the $\mathcal{PT}$ inner product, the resulting vector space spanned by energy eigenstates has a metric of signature $(+, -)$. The condition $s^2 > r^2 \sin^2 \theta$ ensures that $\mathcal{PT}$ symmetry is not broken. If this condition is violated, the states (22) are no longer eigenstates of $\mathcal{PT}$ because α becomes imaginary.⁶

Next, we construct the operator $\mathcal{C}$:

$$\mathcal{C} = \frac{1}{\cos \alpha} \begin{pmatrix} i \sin \alpha & 1 \\ 1 & -i \sin \alpha \end{pmatrix}. \quad (23)$$

Note that $\mathcal{C}$ is distinct from H and $\mathcal{P}$ and has the key property that

$$\mathcal{C}|\varepsilon_{\pm}\rangle = \pm|\varepsilon_{\pm}\rangle. \quad (24)$$

The operator $\mathcal{C}$ commutes with H and satisfies $\mathcal{C}^2 = 1$. The eigenvalues of $\mathcal{C}$ are precisely the signs of the $\mathcal{PT}$ norms of the corresponding eigenstates.

⁶When $\mathcal{PT}$ symmetry is broken, we find that the $\mathcal{PT}$ norm of the energy eigenstate vanishes.

Using the operator $\mathcal{C}$ we construct the new inner product structure

$$\langle u|v\rangle = (\mathcal{CPT}u) \cdot v. \quad (25)$$

This inner product is positive definite because $\langle \varepsilon_{\pm}|\varepsilon_{\pm}\rangle = 1$. Thus, the two-dimensional Hilbert space spanned by $|\varepsilon_{\pm}\rangle$, with inner product $\langle \cdot | \cdot \rangle$, has a Hermitian structure with signature $(+, +)$.

Let us demonstrate that the $\mathcal{CPT}$ norm of any vector is positive. We choose the arbitrary vector $\psi = \begin{pmatrix} a \\ b \end{pmatrix}$, where a and b are any complex numbers. Then $\mathcal{T}\psi = \begin{pmatrix} a^* \\ b^* \end{pmatrix}$, $\mathcal{PT}\psi = \begin{pmatrix} b^* \\ a^* \end{pmatrix}$, and $\mathcal{CPT}\psi = \frac{1}{\cos \alpha} \begin{pmatrix} a^* + ib^* \sin \alpha \\ b^* - ia^* \sin \alpha \end{pmatrix}$. Thus, $\langle \psi|\psi\rangle = (\mathcal{CPT}\psi) \cdot \psi = \frac{1}{\cos \alpha} [a^*a + b^*b + i(b^*b - a^*a) \sin \alpha]$. Now let $a = x + iy$ and $b = u + iv$, where x, y, u , and v are real. Then

$$\langle \psi|\psi\rangle = \frac{1}{\cos \alpha} (x^2 + v^2 + 2xv \sin \alpha + y^2 + u^2 - 2yu \sin \alpha), \quad (26)$$

which is explicitly positive and vanishes only if $x = y = u = v = 0$.

Recalling that $\langle u|$ denotes the $\mathcal{CPT}$ -conjugate of $|u\rangle$, the completeness condition reads

$$|\varepsilon_+\rangle\langle\varepsilon_+| + |\varepsilon_-\rangle\langle\varepsilon_-| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (27)$$

Furthermore, using the $\mathcal{CPT}$ conjugate $\langle\varepsilon_{\pm}|$, we can express $\mathcal{C}$ in the form $\mathcal{C} = |\varepsilon_+\rangle\langle\varepsilon_+| - |\varepsilon_-\rangle\langle\varepsilon_-|$, as opposed to the representation in (15), which uses the $\mathcal{PT}$ conjugate.

An observable in this theory is represented by a linear operator A that satisfies the equation $\mathcal{CPT}A\mathcal{CPT} = A^T$, where A^T is the transpose of A . If $\mathcal{CPT}$ symmetry is unbroken, the eigenvalues of A are real. The operator $\mathcal{C}$ satisfies this requirement, and hence it is an observable. For the two-state system, if we set $\theta = 0$, then the Hamiltonian (20) becomes Hermitian. However, the operator $\mathcal{C}$ then reduces to the parity operator $\mathcal{P}$. As a consequence, the above condition satisfied by an operator reduces to the standard condition of Hermiticity, namely, that $H = H^*$. This is why the hidden symmetry $\mathcal{C}$ was not noticed previously. The operator $\mathcal{C}$ emerges only when we extend a real symmetric Hamiltonian into the complex domain.

We have calculated the $\mathcal{C}$ operator in many kinds of quantum mechanical and quantum field theoretic models. For an $x^2 + ix^3$ potential, $\mathcal{C}$ can be obtained from the summation in (15) using perturbative methods [11]. For an $x^2 - x^4$ potential, $\mathcal{C}$ can be calculated using nonperturbative WKB methods [12]. Quantum field theoretic calculations of $\mathcal{C}$ are reported in Ref. [13].

4 Applications and Possible Observable Consequences

We have described here an alternative to the axiom of Hermiticity in quantum mechanics. In quantum field theory, Hermiticity, Lorentz invariance, and a positive spectrum are crucial for establishing $\mathcal{CPT}$ invariance [16]. Here, we have established the converse of the $\mathcal{CPT}$ theorem in the following limited sense: We assume that the Hamiltonian possesses space-time reflection symmetry, and that this symmetry is not broken. From these assumptions, we know that the spectrum is real and positive and we construct an operator $\mathcal{C}$ that is like the charge conjugation operator. Quantum states in this theory have positive norms with respect to $\mathcal{CPT}$ conjugation. In effect, we replace the mathematical condition of Hermiticity by the physical condition of space-time and charge-conjugation symmetry. These symmetries ensure the reality of the spectrum of the Hamiltonian in complex quantum theories.

Could non-Hermitian, $\mathcal{PT}$ -symmetric Hamiltonians be used to describe experimentally observable phenomena? Non-Hermitian Hamiltonians have *already* been used to describe interacting systems. For example in 1959, Wu showed that the ground state of a Bose system of

hard spheres is described by a non-Hermitian Hamiltonian [17]. Wu found that the ground-state energy of this system is real and conjectured that all of the energy levels were real. In 1992, Hollowood showed that even though the Hamiltonian of a complex Toda lattice is non-Hermitian, the energy levels are real [18]. Non-Hermitian Hamiltonians of the form $H = p^2 + ix^3$ arise in various Reggeon field theory models that exhibit real positive spectra [19]. These cubic Hamiltonians also arise in the study of the Lee-Yang edge singularity [20]. In each of these cases the fact that a non-Hermitian Hamiltonian had a real spectrum appeared mysterious at the time, but now the explanation is simple: In each of these cases the non-Hermitian Hamiltonian is $\mathcal{PT}$ -symmetric. That is, the Hamiltonian in each case is constructed so that the position operator x or the field operator ϕ is always multiplied by i .

An experimental signal of a complex Hamiltonian might be found in the context of condensed matter physics. Consider the complex crystal lattice whose potential is given by $V(x) = i \sin x$. While the Hamiltonian $H = p^2 + i \sin x$ is not Hermitian, it is $\mathcal{PT}$ -symmetric, and all of the energy bands are *real*. However, at the edge of the bands the wave function of a particle in such a lattice is always bosonic (2π -periodic) and, unlike the case of ordinary crystal lattices, the wave function is never fermionic (4π -periodic) [21]. Direct observation of such a band structure would give unambiguous evidence of a $\mathcal{PT}$ -symmetric Hamiltonian.

There are many opportunities for the use of non-Hermitian Hamiltonians in the study of quantum field theory. For example, a scalar quantum field theory with a cubic self-interaction described by the Lagrangian $\mathcal{L} = \frac{1}{2}(\nabla\varphi)^2 + \frac{1}{2}m^2\varphi^2 + g\varphi^3$ is physically unacceptable because the energy spectrum is not bounded below. However, the cubic scalar quantum field theory that corresponds to H in (1) with $\epsilon = 1$ is given by the Lagrangian density $\mathcal{L} = \frac{1}{2}(\nabla\varphi)^2 + \frac{1}{2}m^2\varphi^2 + ig\varphi^3$. This is a new, physically acceptable quantum field theory. Moreover, the theory that corresponds to H in (1) with $\epsilon = 2$ is described by the Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\nabla\varphi)^2 + \frac{1}{2}m^2\varphi^2 - \frac{1}{4}g\varphi^4. \quad (28)$$

What is remarkable about this “wrong-sign” field theory is that, in addition to the energy spectrum being real and positive, the one-point Green’s function (the vacuum expectation value of the field φ) is *nonzero* [22]. Furthermore, the field theory is renormalizable, and in four dimensions is asymptotically free (and thus nontrivial) [23]. Based on these features of the theory, we believe that the theory may provide a useful setting to describe the dynamics of the Higgs sector in the standard model.

Other field theory models whose Hamiltonians are non-Hermitian and $\mathcal{PT}$ -symmetric have also been studied. For example, $\mathcal{PT}$ -symmetric electrodynamics is particularly interesting because it is asymptotically free (unlike ordinary electrodynamics) and because the direction of the Casimir force is the negative of that in ordinary electrodynamics [24]. This theory is remarkable because it can determine its own coupling constant. Supersymmetric $\mathcal{PT}$ -symmetric quantum field theories have also been studied [25].

These $\mathcal{PT}$ -symmetric quantum theories exhibit unexpected phenomena. For example, when g is sufficiently small, the $-g\varphi^4$ theory described by the Lagrangian (28) possesses bound states (the conventional $g\varphi^4$ theory does not because the potential is repulsive). Bound states occur for all dimensions $0 \leq D < 3$ [26], but for purposes of illustration we describe the bound states in the context of one-dimensional quantum field theory (quantum mechanics). For the conventional anharmonic oscillator, which is described by the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}m^2x^2 + \frac{1}{4}gx^4 \quad (g > 0), \quad (29)$$

the small- g Rayleigh-Schrödinger perturbation series for the k th energy level E_k is

$$E_k \sim m \left[k + \frac{1}{2} + \frac{3}{4}(2k^2 + 2k + 1)\nu + O(\nu^2) \right] \quad (\nu \rightarrow 0^+), \quad (30)$$

where $\nu = g/(4m^3)$. The *renormalized mass* M is defined as the first excitation above the ground state: $M \equiv E_1 - E_0 \sim m[1 + 3\nu + O(\nu^2)]$ as $\nu \rightarrow 0^+$.

To determine if the two-particle state is bound, we examine the second excitation above the ground state using (30). We define

$$B_2 \equiv E_2 - E_0 \sim m[2 + 9\nu + O(\nu^2)] \quad (\nu \rightarrow 0^+). \quad (31)$$

If $B_2 < 2M$, then a two-particle bound state exists and the (negative) binding energy is $B_2 - 2M$. If $B_2 > 2M$, then the second excitation above the vacuum is interpreted as an unbound two-particle state. We see from (31) that in the small-coupling region, where perturbation theory is valid, the conventional anharmonic oscillator does not possess a bound state. Indeed, using WKB, variational methods, or numerical calculations, one can show that there is no two-particle bound state for any value of $g > 0$. Because there is no bound state the gx^4 interaction may be considered to represent a repulsive force.⁷

We obtain the perturbation series for the non-Hermitian, $\mathcal{PT}$ -symmetric Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}m^2x^2 - \frac{1}{4}gx^4 \quad (g > 0), \quad (32)$$

from the perturbation series for the conventional anharmonic oscillator by replacing ν with $-\nu$. While the conventional anharmonic oscillator does not possess a two-particle bound state, the $\mathcal{PT}$ -symmetric oscillator does possess such a state. We measure the binding energy of this state in units of the renormalized mass M and we define the *dimensionless* binding energy Δ_2 by

$$\Delta_2 \equiv \frac{B_2 - 2M}{M} \sim -3\nu + O(\nu^2) \quad (\nu \rightarrow 0^+). \quad (33)$$

This bound state disappears when ν increases beyond $\nu = 0.0465 \dots$. As ν continues to increase, Δ_2 reaches a maximum of 0.427 at $\nu = 0.13$ and then approaches the value 0.28 as $\nu \rightarrow \infty$.

In the $\mathcal{PT}$ -symmetric anharmonic oscillator, there are not only two-particle bound states for small coupling constant but also k -particle bound states for all $k \geq 2$. The dimensionless binding energies are

$$\Delta_k \equiv (B_k - kM)/M \sim -3k(k-1)\nu/2 + O(\nu^2) \quad (\nu \rightarrow 0^+). \quad (34)$$

The key feature of this equation is that the coefficient of ν is negative. Since the dimensionless binding energy becomes negative as ν increases from 0, there is a k -particle bound state. The higher multiparticle bound states cease to be bound for smaller values of ν ; starting with the three-particle bound state, the binding energy of these states becomes positive as ν increases past 0.039, 0.034, 0.030, and 0.027.

For any value of ν there are always a finite number of bound states and an infinite number of unbound states. The number of bound states decreases with increasing ν until there are no bound states at all. There is a range of ν for which there are only two- and three-particle bound states. This situation is analogous to the physical world in which one observes only states of two and three bound quarks. In this range of ν if one has an initial state containing a number of particles (renormalized masses), these particles will clump together into bound states, releasing

⁷In general, a repulsive force in a quantum field theory is represented by an energy dependence in which the energy of a two-particle state decreases with separation. The conventional anharmonic oscillator Hamiltonian corresponds to a field theory in one space-time dimension, where there cannot be any spatial dependence. In this case the repulsive nature of the force is understood to mean that the energy B_2 needed to create two particles at a given time is more than twice the energy M needed to create one particle.

energy in the process. Depending on ν , the final state will consist either of two- or of three-particle bound states, whichever is energetically favored. Also, there is a special value of ν for which two- and three-particle bound states can exist in thermodynamic equilibrium.

How does a $g\varphi^3$ theory compare with a $g\varphi^4$ theory? A $g\varphi^3$ theory has an attractive force. The bound states that arise as a consequence of this force can be found by using the Bethe-Salpeter equation. However, the $g\varphi^3$ field theory is unacceptable because the spectrum is not bounded below. If we replace g by ig , the spectrum becomes real and positive, but now the force becomes repulsive and there are no bound states. The same is true for a two-scalar theory with interaction of the form $ig\varphi^2\chi$. This latter theory is an acceptable model of scalar electrodynamics, but has no analog of positronium.

5 Concluding Remarks

We have argued in this paper that there is an alternative to the axiom of standard quantum mechanics that the Hamiltonian must be Hermitian. We have shown that the axiom of Hermiticity may be replaced by the more physical condition of $\mathcal{PT}$ (space-time reflection) symmetry. Space-time reflection symmetry is distinct from the condition of Hermiticity, so it is possible to consider new kinds of quantum theories, such as quantum field theories whose self-interaction potentials are $ig\varphi^3$ or $-g\varphi^4$. Such theories have previously been thought to be mathematically and physically unacceptable because the spectrum might not be real and because the time evolution might not be unitary.

These new kinds of theories can be thought of as extensions of ordinary quantum mechanics into the complex plane; that is, continuations of real symmetric Hamiltonians to complex Hamiltonians. The idea of analytically continuing a Hamiltonian was first discussed in 1952 by Dyson, who argued heuristically that perturbation theory for quantum electrodynamics is divergent [27]. Dyson's argument involves rotating the electric charge e into the complex plane $e \rightarrow ie$. Applied to the quantum anharmonic oscillator, whose Hamiltonian is given in (29), Dyson's argument would go as follows: If the coupling constant g is continued in the complex- g plane to $-g$, then the potential is no longer bounded below, so the resulting theory has no ground state. Thus, the ground-state energy $E_0(g)$ has an abrupt transition at $g = 0$. If we represent $E_0(g)$ as a series in powers of g , this series must have a zero radius of convergence because $E_0(g)$ has a singularity at $g = 0$ in the complex-coupling-constant plane. Hence, the perturbation series must diverge for all $g \neq 0$. While the perturbation series does indeed diverge, this heuristic argument is flawed because the spectrum of the Hamiltonian (32) that is obtained remains ambiguous until the boundary conditions that the wave functions must satisfy are specified. The spectrum depends crucially on how this Hamiltonian with a negative coupling constant is obtained.

There are two ways to obtain the Hamiltonian (32). First, one can substitute $g = |g|e^{i\theta}$ into the Hamiltonian (29) and rotate from $\theta = 0$ to $\theta = \pi$. Under this rotation, the ground-state energy $E_0(g)$ becomes complex. Evidently, $E_0(g)$ is real and positive when $g > 0$ and complex when $g < 0$ ⁸. Second, one can obtain (32) as a limit of the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}m^2x^2 + \frac{1}{4}gx^2(ix)^\epsilon \quad (g > 0) \quad (35)$$

as $\epsilon : 0 \rightarrow 2$. The spectrum of this Hamiltonian is real, positive, and discrete. The spectrum of the limiting Hamiltonian (32) obtained in this manner is similar in structure to that of the Hamiltonian in (29).

⁸Rotating from $\theta = 0$ to $\theta = -\pi$, we obtain the same Hamiltonian as in (32) but the spectrum is the complex conjugate of the spectrum obtained when we rotate from $\theta = 0$ to $\theta = \pi$.

How can the Hamiltonian (32) possess two different spectra? The answer lies in the boundary conditions satisfied by the wave functions $\phi_n(x)$. In the first case, in which $\theta = \arg g$ is rotated in the complex- g plane from 0 to π , $\psi_n(x)$ vanishes in the complex- x plane as $|x| \rightarrow \infty$ inside the wedges $-\pi/3 < \arg x < 0$ and $-4\pi/3 < \arg x < -\pi$. In the second case, in which the exponent ϵ ranges from 0 to 2, $\phi_n(x)$ vanishes in the complex- x plane as $|x| \rightarrow \infty$ inside the wedges $-\pi/3 < \arg x < 0$ and $-\pi < \arg x < -2\pi/3$. In this second case the boundary conditions hold in wedges that are symmetric with respect to the imaginary axis; these boundary conditions enforce the $\mathcal{PT}$ symmetry of H and are responsible for the reality of the energy spectrum.

Apart from the spectra, there is another striking difference between the two theories corresponding to H in (32). The one-point Green's function $G_1(g)$ is defined as the expectation value of the operator x in the ground-state wave function $\phi_0(x)$,

$$G_1(g) = \langle 0|x|0 \rangle / \langle 0|0 \rangle \equiv \int_C dx x \psi_0^2(x) / \int_C dx \psi_0^2(x), \quad (36)$$

where C is a contour that lies in the asymptotic wedges described above. The value of $G_1(g)$ for H in (32) depends on the limiting process by which we obtain H . If we substitute $g = g_0 e^{i\theta}$ into the Hamiltonian (29) and rotate from $\theta = 0$ to $\theta = \pi$, we find that $G_1(g) = 0$ for all g on the semicircle in the complex- g plane. Thus, this rotation in the g plane preserves parity symmetry ($x \rightarrow -x$). However, if we define H in (32) by using the Hamiltonian in (35) and by allowing ϵ to go from 0 to 2, we find that $G_1(g) \neq 0$. Indeed, $G_1(g) \neq 0$ for *all* values of $\epsilon > 0$. Thus, in this theory $\mathcal{PT}$ symmetry (reflection about the imaginary axis, $x \rightarrow -x^*$) is preserved, but parity symmetry is permanently broken. This means that one might be able to describe the dynamics of the Higgs sector by using a $-g\varphi^4$ quantum field theory.

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