Complex Extension of Quantum Mechanics

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Requiring that a Hamiltonian be Hermitian is overly restrictive. A consistent physical theory of quantum mechanics can be built on a complex Hamiltonian that is not Hermitian but satisfies the less restrictive and more physical condition of space-time reflection symmetry ($\mathcal{PT}$ symmetry). One might expect a non-Hermitian Hamiltonian to lead to a violation of unitarity. However, if $\mathcal{PT}$ symmetry is not spontaneously broken, it is possible to construct a previously unnoticed symmetry C of the Hamiltonian. Using C, an inner product whose associated norm is positive definite can be constructed. The procedure is general and works for any $\mathcal{PT}$-symmetric Hamiltonian. Observables exhibit $C\mathcal{PT}$ symmetry, and the dynamics is governed by unitary time evolution. This work is not in conflict with conventional quantum mechanics but is rather a complex generalization of it.

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Four years ago it was noted that with properly defined boundary conditions the spectrum of the Hamiltonian

$$H = p^2 + x^2(ix)^\nu \qquad (\nu \geq 0) \tag{1}$$

is *real and positive* [1]. The reality of the spectrum of H is a consequence of its unbroken $\mathcal{PT}$ symmetry. We say that $\mathcal{PT}$ symmetry is not spontaneously broken if eigenfunctions of H are simultaneously eigenfunctions of $\mathcal{PT}$. The linear parity operator $\mathcal{P}$ performs spatial reflection and has the effect $p \to -p$ and $x \to -x$, whereas the antilinear time-reversal operator $\mathcal{T}$ has the effect $p \to -p$, $x \to x$, and $i \to -i$. 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 examples [2] of complex Hamiltonians having unbroken $\mathcal{PT}$ symmetry and thus real, positive spectra are $H = p^2 + x^4(ix)^\nu$ $(\nu > 0)$, $H = p^2 + x^6(ix)^\nu$ $(\nu > 0)$, and so on.

Recently, Dorey *et al.* proved rigorously that the spectrum of H in (1) is indeed real and positive [3]. Many other $\mathcal{PT}$-symmetric Hamiltonians for which space-time reflection symmetry is not spontaneously broken have been investigated, and the spectra of these Hamiltonians have also been shown to be real and positive [4].

Nevertheless, if we attempt to develop a consistent quantum theory for these Hamiltonians, we encounter the severe difficulty of dealing with Hilbert spaces endowed with indefinite metrics [5]. The purpose of the present Letter is to identify a new symmetry, denoted C, inherent in all $\mathcal{PT}$-symmetric Hamiltonians that possess an unbroken $\mathcal{PT}$ symmetry. This allows us to introduce an inner-product structure associated with $C\mathcal{PT}$ conjugation for which the norms of quantum states are positive definite. In particular, $C\mathcal{PT}$ symmetry is shown to generalize the conventional Hermiticity requirement by replacing it with a dynamically determined inner product (one that is defined by the Hamiltonian itself). As a result, we can extend the Hamiltonian and its eigenstates into the complex domain so that the associated eigenvalues are real and the underlying dynamics is unitary.

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

$$-\phi_n''(x) + x^2(ix)^\nu \phi_n(x) = E_n \phi_n(x) \tag{2}$$

associated with the Hamiltonian H in (1). First, we emphasize that the differential Eq. (2) must be imposed on an infinite contour C in the complex-x plane. For large $|x|$ the contour C lies in wedges that are placed symmetrically with respect to the imaginary-x axis. These wedges are described in Ref. [1]. The boundary conditions on the eigenfunctions are that $\phi(x) \to 0$ exponentially rapidly as $|x| \to \infty$ on C. For $0 \leq \nu < 2$, the contour C may be taken to be the real axis.

Second, the eigenfunctions $\phi_n(x)$ are simultaneously eigenstates of the $\mathcal{PT}$ operator: $\mathcal{PT}\phi_n(x) = \lambda_n \phi_n(x)$. Because $(\mathcal{PT})^2 = 1$ and $\mathcal{PT}$ involves complex conjugation, it follows that $|\lambda_n| = 1$. Thus, $\lambda_n = e^{i\omega_n}$ is a pure phase. Without loss of generality for each n this phase can be absorbed into ϕ_n by the multiplicative rescaling $\phi_n \to e^{-i\omega_n/2}\phi_n$, so that the new eigenvalue is unity:

$$\mathcal{PT}\phi_n(x) = \phi_n^*(-x) = \phi_n(x). \tag{3}$$

Third, the eigenfunctions are complete. The statement of completeness (for real x and y) is

$$\sum_n (-1)^n \phi_n(x)\phi_n(y) = \delta(x-y). \tag{4}$$

This is a nontrivial result that has been verified numerically to extremely high accuracy [6].

Fourth, there appears to be a natural choice for an inner product of two functions $f(x)$ and $g(x)$ given by

$$(f, g) \equiv \int_C dx [\mathcal{PT} f(x)] g(x), \qquad (5)$$

where $\mathcal{PT} f(x) = [f(-x)]^*$. The 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 required because we wish to construct a space of rays to represent quantum mechanical states. With respect to this inner product the eigenfunctions of H in (1) for all $\nu \geq 0$ satisfy

$$(\phi_m, \phi_n) = (-1)^n \delta_{mn}. \qquad (6)$$

With this inner product it is easy to verify the position-space representation of the unity operator in (4). For example, one can verify that $\int dy\, \delta(x-y)\delta(y-z) = \delta(x-z)$ using (4) and (6). However, because the norms of the eigenfunctions alternate in sign, the Hilbert space metric associated with the $\mathcal{PT}$ inner product $(\cdot, \cdot)$ is indefinite.

Having reviewed these general properties, the crucial question that must be addressed is whether a $\mathcal{PT}$-symmetric Hamiltonian defines a physically viable quantum mechanics or whether it merely provides an intriguing Sturm-Liouville problem. The apparent difficulty with formulating a quantum theory is that the Hilbert space 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 immediately raises an obstacle.

With the above inner product $(\cdot, \cdot)$, the state space for a finite-dimensional $2n \times 2n$ matrix Hamiltonian that is symmetric under space-time reflection embodies the symmetry of $SU(n, n)$ rather than the conventional $SU(2n)$. The space-time reflection operator in finite dimensions is the product of a parity operator satisfying $\mathcal{P}^2 = 1$ and $\mathrm{tr}\mathcal{P} = 0$ and an antilinear Hermitian conjugation operator satisfying $\mathcal{T}^2 = 1$. Unlike the unitary group, $SU(n, n)$ is not simply connected, and consequently, the state space is partitioned into two disjoint halves, one associated with norm $+1$ and the other with norm -1.

One can try to formulate a quantum theory associated with $\mathcal{PT}$-symmetric Hamiltonians by insisting that physical states must have positive norm [7]. This leads to a quantum mechanics defined on a nonlinear state space. Such investigations are of interest, but the existence of negative-norm eigenstates still leaves open serious interpretational issues. In particular, one finds that expectation values of bounded observables are unbounded in such quantum theories. 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 wave equation in relativistic quantum theory [8].

We resolve the problem of an indefinite norm by finding a physical interpretation for the negative-norm states. We observe that in *any* theory having an unbroken $\mathcal{PT}$ symmetry there exists a previously unnoticed 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 that we denote by $\mathcal{C}$. We use the notation $\mathcal{C}$ because the properties of this operator are nearly identical to those of the charge-conjugation operator in quantum field theory. The operator $\mathcal{C}$ is the observable that represents the measurement of the signature of the $\mathcal{PT}$ norm of a state. We see that $\mathcal{C}$ commutes with both the Hamiltonian H and the operator $\mathcal{PT}$. Therefore, eigenstates of H have definite values of $\mathcal{C}$. We also see that $\mathcal{C}^2 = 1$, so the eigenvalues of $\mathcal{C}$ are ± 1.

We can construct the operator $\mathcal{C}$ explicitly in terms of the energy eigenstates of the Hamiltonian. The position-space representation of $\mathcal{C}$ is

$$\mathcal{C}(x, y) = \sum_n \phi_n(x)\phi_n(y). \qquad (7)$$

Note that $\mathcal{C}$ is a linear operator. From Eqs. (4) and (6) we can verify that the square of $\mathcal{C}$ is unity:

$$\int dy\, \mathcal{C}(x, y)\mathcal{C}(y, z) = \delta(x - z). \qquad (8)$$

We can also construct the parity operator $\mathcal{P}$ in terms of the energy eigenstates. In position space

$$\mathcal{P}(x, y) = \delta(x + y) = \sum_n (-1)^n \phi_n(x)\phi_n(-y). \qquad (9)$$

Like the operator $\mathcal{C}$, the square of the parity operator is also unity.

The two 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. Furthermore, these two operators do not commute; specifically, in the position representation

$$(\mathcal{CP})(x, y) = \sum_n \phi_n(x)\phi_n(-y), \qquad (10)$$

whereas

$$(\mathcal{PC})(x, y) = \sum_n \phi_n(-x)\phi_n(y), \qquad (11)$$

which shows by (3) that $\mathcal{CP} = (\mathcal{PC})^*$. Evidently, $\mathcal{C}$ does commute with $\mathcal{PT}$.

The operator $\mathcal{C}$ does not exist as a distinct entity in conventional Hermitian quantum mechanics. Indeed, if we allow the parameter ν 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 $\mathcal{T}$. In short, in standard quantum mechanics the requirements of $\mathcal{CPT}$

symmetry and conventional Hermiticity coincide. Therefore, $\mathcal{CPT}$ invariance can be viewed as the natural complex extension of the Hermiticity condition, which ensures the reality of observables and the unitarity of the dynamics when the Hamiltonian becomes complex.

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

$$\langle f \mid g \rangle \equiv \int_C dx [\mathcal{CPT} f(x)] g(x). \tag{12}$$

Like the $\mathcal{PT}$ inner product (5), this inner product is also phase independent and conserved in time. The inner product (12) 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) now reads

$$\sum_n \phi_n(x)[\mathcal{CPT}\phi_n(y)] = \delta(x-y). \tag{13}$$

Unlike the case of conventional quantum mechanics, the $\mathcal{CPT}$ inner product is dynamically determined; it implicitly depends on the choice of Hamiltonian. When H is Hermitian, (13) reduces to the conventional completeness condition of quantum mechanics because $\mathcal{T}$ performs Hermitian conjugation.

We remark that the $\mathcal{CPT}$ inner product (12) defined above 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 is a consequence of Cauchy's theorem and the analyticity of the integrand. In the case of standard quantum mechanics, where the positive-definite inner product has the form $\int dx\, f^*(x)g(x)$, 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. The $\mathcal{PT}$ inner product (5) shares with (12) the advantage of analyticity and path independence, but suffers from the lack of positivity. We find it surprising that a positive-definite metric structure can be constructed using $\mathcal{CPT}$ conjugation without disturbing the path independence of the inner-product integral.

Let us illustrate these results for a 2×2 Hamiltonian (see, also, Ref. [9]). In this case we may choose the parity operator to be

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{14}$$

without loss of generality, because in finite dimensions the parity operator $\mathcal{P}$ is defined uniquely up to unitary transformations [7]. Consequently, the most general form of a $\mathcal{PT}$-invariant Hamiltonian satisfying $\mathcal{P}H^\dagger\mathcal{P} = H$, where $H^\dagger$ is the Hermitian conjugate of H, can be expressed as a four-parameter family of matrices

$$H = \begin{pmatrix} re^{i\theta} & s \\ t & re^{-i\theta} \end{pmatrix}, \tag{15}$$

where r, s, t, and θ are real. Note that this Hamiltonian is not Hermitian in the conventional sense. Nevertheless, the eigenvalues $\varepsilon_\pm = r\cos\theta \pm \sqrt{st - r^2\sin^2\theta}$ are real, provided that

$$st > r^2 \sin^2\theta. \tag{16}$$

The simultaneous eigenstates of the operators H and $\mathcal{PT}$ are given by

$$|\varepsilon_+\rangle = \frac{1}{\sqrt{2\cos\alpha}} \begin{pmatrix} e^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix} \tag{17}$$

and

$$|\varepsilon_-\rangle = \frac{i}{\sqrt{2\cos\alpha}} \begin{pmatrix} e^{-i\alpha/2} \\ -e^{i\alpha/2} \end{pmatrix}, \tag{18}$$

where we set $\sin\alpha = (r/\sqrt{st})\sin\theta$. It is easy to verify 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 Hilbert space has a metric structure of signature $(+, -)$. The condition (16) ensures that $\mathcal{PT}$ symmetry is not spontaneously broken. If this condition is violated, the states (17) and (18) are no longer eigenstates of $\mathcal{PT}$ because α becomes imaginary.

Next, we construct the operator $\mathcal{C}$. For the parity operator $\mathcal{P}$ in (14), the corresponding operator $\mathcal{C}$ is

$$\mathcal{C} = \frac{1}{\cos\alpha} \begin{pmatrix} i\sin\alpha & 1 \\ 1 & -i\sin\alpha \end{pmatrix}. \tag{19}$$

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

$$\mathcal{C}|\varepsilon_\pm\rangle = \pm|\varepsilon_\pm\rangle. \tag{20}$$

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

With the aid of the operator $\mathcal{C}$ we construct the new inner-product structure having positive signature by

$$\langle u \mid v \rangle = (\mathcal{CPT}u)\cdot v. \tag{21}$$

This inner product is positive definite. In particular, we have $\langle \varepsilon_\pm \mid \varepsilon_\pm \rangle = 1$. It follows that the two-dimensional Hilbert space spanned by $|\varepsilon_\pm\rangle$, with inner product $\langle \cdot \mid \cdot \rangle$, has a Hermitian structure with signature $(+, +)$. Recalling that $\langle u|$ denotes the $\mathcal{CPT}$ conjugate of $|u\rangle$, the completeness condition is

$$|\varepsilon_+\rangle\langle\varepsilon_+| + |\varepsilon_-\rangle\langle\varepsilon_-| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{22}$$

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 (7), which uses the $\mathcal{PT}$ conjugate.

In general, an observable in this theory is represented by a $\mathcal{CPT}$ invariant operator; that is, one that commutes with $\mathcal{CPT}$. Thus, if $\mathcal{CPT}$ symmetry is not spontaneously broken, the eigenvalues of the observable are real. The operator $\mathcal{C}$ satisfies this requirement and, hence, is an observable. For the two-state system, if we set $\theta = 0$, then the Hamiltonian in (15) becomes Hermitian in the conventional sense. However, the operator $\mathcal{C}$ then reduces to the parity operator $\mathcal{P}$. As a consequence, the requirement of $\mathcal{CPT}$ invariance reduces to the standard condition of Hermiticity. It is for this reason that the hidden symmetry $\mathcal{C}$ was not noticed previously. The operator $\mathcal{C}$ surfaces only when we extend the Hamiltonian of conventional quantum mechanics into the complex domain.

In summary, we have generalized the condition of Hermiticity in quantum mechanics to the statement of $\mathcal{CPT}$ invariance. In quantum field theory, the conditions of Hermiticity, Lorentz invariance, and positive spectrum are crucial for establishing $\mathcal{CPT}$ invariance [10]. In this Letter, we establish 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 spontaneously 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 and show that quantum states in this theory have positive norms with respect to $\mathcal{CPT}$ conjugation. In effect, we replace the mathematical condition of Hermiticity, whose physical content is somewhat remote and obscure, 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.

In the real formulation of conventional quantum theory, the dimensionality of the Hilbert space must be even. This is necessary in order to introduce a complex structure in the underlying real Hilbert space [11]. In the present theory, we must introduce the parity operator $\mathcal{P}$, which can be defined only on an even-dimensional complex Hilbert space. Hence, the dimensionality of the underlying real space is a multiple of four. This is related to the fact that for each quantum state there is a corresponding partner state, and these two states are always formed pairwise in the sense that when $\mathcal{PT}$ symmetry is spontaneously broken, the corresponding pairs of eigenvalues become complex conjugates of one another. This is because the secular equation for a $\mathcal{PT}$-symmetric Hamiltonian is real [9].

In a conventional Hermitian quantum field theory, the operators $\mathcal{C}$ and $\mathcal{P}$ satisfy the commutation relation $\mathcal{CP} = (-1)^N \mathcal{PC}$, where N is the fermion number of the state on which these operators act. In a $\mathcal{PT}$-symmetric quantum field theory, the commutation relations are as follows: If we write $\mathcal{C} = \mathcal{C}_R + i\mathcal{C}_I$ where $\mathcal{C}_R$ and $\mathcal{C}_I$ are real, then it follows from (10) and (11) that $\mathcal{C}_R\mathcal{P} = \mathcal{P}\mathcal{C}_R$ and $\mathcal{C}_I\mathcal{P} = -\mathcal{P}\mathcal{C}_I$. As a consequence, it may not necessarily be true that particles and their partners (for example, antiparticles) have the same energy eigenvalues. We recall that space-time reflection symmetry is weaker than the condition of Hermiticity, and therefore it is possible to consider new kinds of quantum field theories, whose self-interaction potentials are, for example, $-ig\varphi^3$ or $-g\varphi^4$, that have previously been thought to be unacceptable. A plausible signal of one of these new theories would be the observation of a particle and its corresponding partner having different masses.

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