Non-Hermitian quantum Hamiltonians with $\mathcal{PT}$ symmetry

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We formulate quantum mechanics for non-Hermitian Hamiltonians that are invariant under $\mathcal{PT}$, where $\mathcal{P}$ is the parity and $\mathcal{T}$ denotes time reversal, for the case that time-reversal symmetry is odd ($\mathcal{T}^2 = -1$), generalizing prior work for the even case ($\mathcal{T}^2 = 1$). We discover an analog of Kramer's theorem for $\mathcal{PT}$ quantum mechanics, present a prototypical example of a $\mathcal{PT}$ quantum system with odd time reversal, and discuss potential applications of the formalism.

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I. INTRODUCTION

The basic structure of quantum mechanics was delineated in the early days of the theory [1] and it has not been modified since. Still it is desirable to ask whether the structure can be altered and generalized. For example, Weinberg showed that it is possible to formulate a nonlinear generalization of quantum mechanics and to thereby subject the linearity of quantum mechanics to a quantitative test [2]. A fruitful generalization of the canonical principles was the discovery that particles can have fractional statistics that interpolate between Bose and Fermi, albeit only in two spatial dimensions [3]. More recently, the principle that the Hamiltonian and other observables should be represented by Hermitian operators has been re-examined [4]. A non-Hermitian formulation of quantum mechanics promises to enlarge the set of possible Hamiltonians that physicists could deploy to describe fundamental physics beyond the standard model or for the effective description of condensed-matter phenomena.

Bender and co-workers have shown that the assumption of hermiticity can be relaxed under the circumstance that the Hamiltonian is invariant under the combined symmetry $\mathcal{PT}$, where $\mathcal{P}$ denotes the parity and $\mathcal{T}$ denotes time reversal, provided that in addition the eigenvalues of the Hamiltonian are real and the appropriately defined left and right eigenvectors coincide. By now many examples of $\mathcal{PT}$ quantum mechanics have been presented in the literature [4].

In all work on $\mathcal{PT}$ quantum mechanics to date it has been implicitly assumed that time reversal is even, $\mathcal{T}^2 = 1$. However, in quantum theory this is only true of bosonic systems with integer spin. For fermionic systems, with half-integer spin, time reversal is odd, $\mathcal{T}^2 = -1$. Quarks and leptons in particle physics, approximately half of all nuclei and atoms, and a plethora of condensed-matter problems including magnetic spin models and solid-state electronic matter fall into this category. Thus, it is important to generalize the construction of $\mathcal{PT}$ quantum mechanics to the case that $\mathcal{T}$ is odd; that is our purpose here.

The outline of this paper is as follows. In Sec. II we develop the principles of $\mathcal{PT}$ quantum mechanics for systems with odd time-reversal symmetry and contrast them with the established principles for systems with even time-reversal symmetry [4]. In Sec. III we illustrate the principles by giving the simplest two-level example of $\mathcal{PT}$ quantum mechanics with odd time-reversal symmetry and comparing it to its even counterpart. The discussion throughout is self-contained and should be accessible to readers with no prior familiarity with $\mathcal{PT}$ quantum mechanics.

In more detail, the contents of Sec. II are as follows. In Secs. II A and II B we discuss time reversal and parity, the two symmetry transformations that play a fundamental role in the formulation of $\mathcal{PT}$ quantum mechanics. We prove that time-reversal symmetry comes in two classes, even and odd, and we show that one can always find a basis in which time-reversal and parity operators have a simple canonical form. In Sec. II C we introduce the $\mathcal{PT}$ inner product, which is integral to the development of the theory. In Sec. II D we enunciate the criteria that a Hamiltonian must satisfy in $\mathcal{PT}$ quantum mechanics in lieu of the criterion of hermiticity. Among the key results in this section are the finding that $\mathcal{PT}$ quantum Hamiltonians with odd time reversal have a degeneracy analogous to Kramer's degeneracy for Hamiltonians with time-reversal symmetry in conventional Hermitian quantum mechanics. We also generalize a theorem of Ref. [5] regarding the spectrum of operators that commute with an even antilinear symmetry to operators that commute with an odd antilinear symmetry. A principal novelty of $\mathcal{PT}$ quantum mechanics is that the inner product on the Hilbert space of states is determined by the Hamiltonian. This "dynamically determined" inner product is called the $\mathcal{CPT}$ inner product and is the subject of Sec. II E. Finally, we conclude our discussion of the principles of $\mathcal{PT}$ quantum mechanics by discussing the conditions that must be satisfied by operators corresponding to observables other than the Hamiltonian in Sec. II F.

II. PRINCIPLES

A. Time reversal

First let us demonstrate that there are two classes of behavior under time reversal. For simplicity we assume that the Hilbert space of states has finite dimension so that the state of the system may be specified by a column vector with complex components $\psi(n)$, with $n = 1,2,3,\ldots,N$ in the even case and $n = 1,2,3,\ldots,2N$ in the odd case. We see below that for the case of odd time-reversal symmetry it will be required that the dimensionality of the Hilbert space is even.

Following Wigner [6], we now assume that time reversal is an antilinear operation. Thus, $\mathcal{T}\psi = L\psi^*$, where L is a linear operator. Next we assume that $\mathcal{T}^2$ leaves all states unchanged up to a phase $e^{i\phi}$. It follows that $LL^* = e^{i\phi}$.

This implies $L^{-1} = L^* e^{-i\phi}$. But by conjugation $L^* L = e^{-i\phi}$, which implies $L^{-1} = e^{i\phi} L^*$. Together these expressions for L^{-1} imply $e^{i\phi} = e^{-i\phi}$ or $e^{i\phi} = \pm 1$. Thus, we have established the proposition that there are two kinds of time reversal, with $\mathcal{T}^2 = 1$ and $\mathcal{T}^2 = -1$, respectively. In textbook Hermitian quantum mechanics it is assumed that we are working in an orthonormal basis and that L is unitary (see, for example, Ref. [7]). The proof here does not make that assumption and hence appropriately generalizes the proposition to the case of non-Hermitian quantum mechanics.

Under a change of basis $\psi' = V\psi$, it is easy to see that the matrix L changes to $L' = V L V^{-1*}$. It is shown in the Appendix A that for the case of even time reversal one can always find a basis in which the matrix L is the identity and the operation of time reversal consists simply of complex conjugation. For the case of odd time reversal one can always find a basis in which the matrix L has a particular canonical form denoted Z (defined below). The proof of this proposition given in the Appendix A also reveals that for the odd case the Hilbert space must be even dimensional; thus, Z is a $2N \times 2N$ matrix. That the operation of time reversal can be brought to these canonical forms is a standard proposition of Hermitian quantum mechanics [7]. The proof given in the Appendix A is a generalization of the standard proposition because we do not assume that we are working in an orthonormal basis or that L is unitary.

In describing Z, and in much of the following discussion, it is convenient to refer to 2×2 matrices as quaternions. Any quaternion can be expanded as $q = q_0\sigma_0 + i q_1 \sigma_1 + i q_2 \sigma_2 + i q_3 \sigma_3$, where σ_0 is the 2×2 identity matrix and σ_1, σ_2, and σ_3 are the Pauli matrices. The coefficients q_0, q_1, q_2, and q_3 are complex in general. In the case that they are real, the quaternion is said to be real. It is important to realize that if a quaternion is real that does not mean that the elements of the corresponding 2×2 matrix are real. By suitably partitioning a $2N \times 2N$ matrix into 2×2 blocks, one can view it as an $N \times N$ matrix of quaternions. Such a matrix is said to be quaternion real if it is composed of real quaternions. Some additional useful results regarding quaternions are compiled and proved in Appendix B.

In particular, the matrix Z is an $N \times N$ quaternion matrix with every diagonal term equal to $i\sigma_2$ and every off-diagonal term equal to zero. Thus,

$$Z = \begin{pmatrix} e_2 & & \\ & \ddots & \\ & & e_2 \end{pmatrix}, \quad \text{where} \quad e_2 = i\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{1}$$

A basis in which the matrix L is the identity is hereafter called a canonical basis in the even case. In such a basis the operation of time reversal consists of just conjugation. Similarly, in the odd case a basis in which L is Z is called a canonical basis. In such a basis, time reversal consists of conjugation followed by multiplication by Z.

From the transformation law $L' = V L V^{-1*}$, we see that in the even case if $V V^{-1*} = 1$ and if the initial basis is canonical, the final basis will also be canonical. Equivalently, we may write the condition as $V = V^*$. In other words, for the even case, canonical bases are linked by real transformation matrices. Similarly, in the odd case we see that if $V Z V^{-1*} = Z$ then if the initial basis is canonical so too is the final basis. Equivalently, we may write the condition as $VZ = ZV^*$. The latter condition implies that the matrix V is quaternion real (see Appendix B). In other words, for the odd case, canonical bases are linked by transformation matrices that are quaternion real, an elegant generalization of the corresponding even result.

B. Parity

The second symmetry operation that plays a fundamental role in $\mathcal{PT}$ quantum mechanics is parity. We make the following assumptions about parity: (i) Parity is a linear operator and hence it may be represented by a matrix we denote S; thus, $\mathcal{P}\psi = S\psi$. (ii) Parity applied twice is the identity operator and hence $S^2 = 1$. (iii) We assume that parity commutes with time reversal: $\mathcal{PT} = \mathcal{TP}$. In a basis where time reversal has a canonical form this implies that $S = S^*$ in the even case and $SZ = ZS^*$ in the odd case. In other words, in a canonical basis S is real in the even case and S is quaternion real in the odd case.

It follows from assumption (ii) that the eigenvalues of S are all ± 1. For the odd case, in addition, the eigenvalues of S come in degenerate pairs since S is quaternion real and its eigenvalues are all real (see discussion of Kramer's theorem in Appendix B).

For the even case, since S is real in a canonical basis and since its eigenvalues are real, being equal to ± 1, it follows that the eigenvectors of S can be chosen real and the eigenmatrix of vectors that diagonalize S can also be chosen real. Thus, we can always find a basis in which parity is diagonal and time reversal is canonical in the even case. Similarly for the odd case, since S is quaternion real in a canonical basis it follows that the eigenmatrix that diagonalizes S can be chosen quaternion real (see Appendix B). Thus, we can always find a basis in which parity is diagonal and time reversal is canonical in the odd case also.

Although it is not essential to do so, for illustrative purposes we sometimes assume in the following that the number of states with positive parity equals the number with negative parity. Then in a basis where time reversal has a canonical form and parity is diagonal, the matrix S has the form

$$S = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \tag{2}$$

where $\mathbb{I}$ denotes the $(N/2)$-dimensional identity matrix in the even case and the N-dimensional identity matrix in the odd case.

C. $\mathcal{PT}$ inner product

Conventionally in quantum mechanics we assume that the inner product of two states is given by $(\phi, \psi) = \phi^\dagger \psi = \sum_{n=1}^{N} \phi^*(n)\psi(n)$. Implicit in this formula is the assumption that we are working in an orthonormal basis. However, in $\mathcal{PT}$ quantum mechanics we do not assume that the conventional inner product applies or that we are working in an orthonormal basis. Instead a different inner product is used, one that is determined by the Hamiltonian. This "dynamically determined" inner product is formulated below. As a prelude, however, it is useful to first introduce the $\mathcal{PT}$ inner product.

The purpose of this subsection is to generalize the definition of the $\mathcal{PT}$ inner product used in the even case [4] to the case of odd time-reversal symmetry.

For the even case the $\mathcal{PT}$ inner product is defined by

$$(\phi,\psi)_{\mathcal{PT}} = (\mathcal{PT}\phi)^{\mathcal{T}}\psi = \phi^{\dagger}S\psi. \tag{3}$$

The definition given here assumes we are in a basis where time reversal has the canonical form and parity is diagonal. For the odd case we define the $\mathcal{PT}$ inner product as

$$(\phi,\psi)_{\mathcal{PT}} = (\mathcal{PT}\phi)^{\mathcal{T}}Z\psi = \phi^{\dagger}S\psi; \tag{4}$$

note the crucial insertion of Z. Again we assume that we are in a basis where time reversal has the canonical form and parity is diagonal.[1]

It is clear from Eqs. (3) and (4) that the norm of any state $(\phi,\phi)_{\mathcal{PT}}$ is real but of indefinite sign. Thus, the $\mathcal{PT}$ inner product is not a viable inner product to use in quantum mechanics. In the odd case we also see that the states ϕ and $\psi = \mathcal{PT}\phi$ are orthogonal to each other and have the same norm; in other words, $(\phi,\psi)_{\mathcal{PT}} = 0$ and $(\phi,\phi)_{\mathcal{PT}} = (\psi,\psi)_{\mathcal{PT}}$.

For later reference it is useful to define the adjoint of an operator under the $\mathcal{PT}$ inner product. Let us denote the adjoint of A under the $\mathcal{PT}$ inner product as A_D. A_D is then defined by the condition that $(A_D\phi,\psi)_{\mathcal{PT}} = (\phi,A\psi)_{\mathcal{PT}}$. This condition should be met for all pairs of states ϕ and ψ. One can show explicitly that

$$A_D = SA^{\dagger}S \tag{5}$$

by making use of the formula $(\phi,\psi)_{\mathcal{PT}} = \phi^{\dagger}S\psi$ [cf. Eqs. (3) and (4)]. In the case that A commutes with $\mathcal{PT}$, with a little work the following alternative expressions for the $\mathcal{PT}$ adjoint may be derived:

$$\begin{aligned} A_D &= A^T \quad \text{(even)},\\ &= Z^T A^T Z \quad \text{(odd)}. \end{aligned} \tag{6}$$

D. Hamiltonian conditions

The principal new feature of $\mathcal{PT}$ quantum mechanics is that it is now acceptable for the Hamiltonian H to be non-Hermitian. We no longer impose the condition of hermiticity, $H = H^{\dagger}$. Instead, in $\mathcal{PT}$ quantum mechanics the Hamiltonian is required to meet the following three criteria:

(i) It is invariant under $\mathcal{PT}$, $[H,\mathcal{PT}] = 0$.
(ii) $\mathcal{PT}$ symmetry is unbroken.
(iii) H is self-adjoint under the $\mathcal{PT}$ inner product.

These conditions were originally formulated for the case of even time reversal [4] and need generalization to the case of odd time reversal. We discuss that generalization in this section. Most notably, we find that the modification of condition (ii) leads to a $\mathcal{PT}$ analog of the phenomenon of Kramer's degeneracy in textbook quantum mechanics.

Motivated by $\mathcal{PT}$ quantum mechanics, Bender, Berry, and Mandilara [5] studied Hamiltonians that commute with an arbitrary antiunitary symmetry $\mathcal{A}$ that satisfies $\mathcal{A}^{2k} = 1$, where k is an odd integer. They found that such a Hamiltonian has eigenvalues that come in conjugate pairs and that in a suitable basis such a Hamiltonian would be real. We have generalized their findings to the case of an odd antiunitary symmetry $\mathcal{A}$ that satisfies $\mathcal{A}^{2k} = -1$, where k is an odd integer. For this case, too, we find that the eigenvalues come in conjugate pairs and that in a suitable basis the Hamiltonian is quaternion real. This result is a straightforward extension of our analysis of condition (i) and is therefore presented in Appendix C. We now turn to a detailed discussion of each of the conditions.

(i) Invariance under $\mathcal{PT}$. The first condition imposed on the Hamiltonian is that it must be invariant under $\mathcal{PT}$ (i.e., it must commute with $\mathcal{PT}$). It is easy to verify that invariance under $\mathcal{PT}$ implies that the eigenvalues of H come in conjugate pairs for if ϕ is an eigenvector with eigenvalue λ then $\mathcal{PT}\phi$ is an eigenvector with eigenvalue λ^*. Evidently, this is true for both even and odd time reversal. Suppose that time reversal is even and that we are working in a canonical basis where time reversal consists of conjugation and parity has the form of Eq. (2). Invariance under $\mathcal{PT}$ then forces the Hamiltonian to have the following block structure:

$$H = \begin{pmatrix} A & iB \\ iC & D \end{pmatrix}, \tag{7}$$

where A, B, C, and D are real matrices. Now suppose that time reversal is odd. In that case, invariance under $\mathcal{PT}$ forces the Hamiltonian to have the same block structure but with A, B, C, and D now quaternion real matrices.

(ii) Unbroken $\mathcal{PT}$ symmetry. For the case of even time reversal that has been discussed in the literature, a key role is played by states that are invariant under $\mathcal{PT}$ in the formulation of the condition of unbroken $\mathcal{PT}$ symmetry. An immediate problem in generalizing this condition to the odd case is that one can prove rigorously that there are no states that are invariant under $\mathcal{PT}$. Before we surmount this obstacle, let us first review the condition of unbroken $\mathcal{PT}$ symmetry for the even case.

In the even case, $\mathcal{PT}$ is said to be unbroken if we can find a complete set of eigenvectors of H, ψ_i, that are invariant under $\mathcal{PT}$; that is, each eigenvector satisfies $\mathcal{PT}\psi_i = \psi_i$. In practice, the task of verifying that H is invariant under $\mathcal{PT}$ is generally straightforward, whereas proving that $\mathcal{PT}$ is unbroken for a given H can pose formidable difficulties.

The condition of unbroken $\mathcal{PT}$ ensures that the eigenvalues of H are real in the even case:

Proof. Invariance under $\mathcal{PT}$ implies that if ψ is an eigenvector with eigenvalue λ, then $\mathcal{PT}\psi$ is an eigenvector with eigenvalue λ^*. If $\mathcal{PT}$ is unbroken, $\psi = \mathcal{PT}\psi$, implying $\lambda = \lambda^*$; that is, the eigenvalues are real. Conversely, if the eigenvalues of H are real, one can show that $\mathcal{PT}$ is unbroken.

Suppose, for illustration, that we are working in a canonical basis where time reversal consists of conjugation and parity has the form given in Eq. (2). Then it is easy to see that a state that is invariant under $\mathcal{PT}$ has the form

$$\psi = \begin{pmatrix} \xi \\ i\eta \end{pmatrix}, \tag{8}$$

[1]More generally the definitions of Eqs. (3) and (4) apply in a basis in which time reversal has a canonical form and the parity matrix is Hermitian, $S = S^{\dagger}$.

where ξ and η are real column vectors with $N/2$ components each.

Now let us generalize to the odd case. It is impossible to find a state that is invariant under $\mathcal{PT}$ in the case of odd time reversal. This is most readily seen by working in a basis where time reversal has the canonical form and parity is diagonal. It is then easy to verify that imposing the condition $\phi = \mathcal{PT}\phi$ implies $\phi = 0$. However, one can assemble the two column vectors ϕ and $-\mathcal{PT}\phi$ into a $\mathcal{PT}$ doublet,

$$\begin{pmatrix} | & | \\ \phi & -\mathcal{PT}\phi \\ | & | \end{pmatrix}. \tag{9}$$

The doublet is a $2N \times 2$ matrix that can equivalently be viewed as a single N-component column of quaternions. It is easy to see that the $\mathcal{PT}$ doublet has the form shown in Eq. (8) where ξ and η now both represent real columns of real quaternions (see the parallel discussion of the Kramer's doublet in Appendix B). Under the application of $\mathcal{PT}$, the $\mathcal{PT}$ doublet gets postmultiplied by a single Pauli matrix $i\sigma_y$.

We are now ready to formulate the condition of unbroken $\mathcal{PT}$ in the odd case. We say that $\mathcal{PT}$ is unbroken for a Hamiltonian H if for every eigenvector ϕ we find that the pair of states ϕ and $\mathcal{PT}\phi$ are degenerate eigenvectors of H.

Clearly this condition ensures that the eigenvalues must be real. We have already demonstrated that the eigenvalues of ϕ and $\mathcal{PT}\phi$ are a conjugate pair λ and λ^*. If the states are degenerate, then $\lambda = \lambda^*$; that is, the eigenvalues are real. Conversely, if the eigenvalues are real then clearly ϕ and $\mathcal{PT}\phi$ are degenerate and therefore $\mathcal{PT}$ is unbroken.

In odd $\mathcal{PT}$ quantum mechanics the condition of unbroken $\mathcal{PT}$ not only ensures that the eigenvalues of H are real, it also ensures they come in degenerate pairs. This is analogous to Kramer's theorem for a Hamiltonian invariant under odd time reversal in conventional quantum mechanics.

(iii) $\mathcal{PT}$ self-adjoincy. The motivation for this third criterion is that we want the eigenvectors of all observables to be orthogonal to each other under the dynamical $\mathcal{CPT}$ inner product. As a stepping stone toward this goal, we require that the Hamiltonian be self-adjoint under the $\mathcal{PT}$ inner product. In other words, we impose $H = H_D$. Making use of Eq. (6), we may express this condition as

$$\begin{aligned} H &= H^T \text{ (even)}, \\ &= Z^T H^T Z \text{ (odd)}. \end{aligned} \tag{10}$$

As explained below, this requirement ensures that the eigenvectors of $\mathcal{H}$ are appropriately orthogonal to each other under the $\mathcal{PT}$ inner product.

Suppose for illustration that we are working in a basis where time reversal has the canonical form and parity is given by Eq. (2). Then if the Hamiltonian is invariant under $\mathcal{PT}$ and also $\mathcal{PT}$ self-adjoint, it has the following block structure:

$$H = \begin{pmatrix} A & iB \\ iB^\dagger & D \end{pmatrix}. \tag{11}$$

Here B is a real matrix and A and D are real and symmetric in the case that time reversal is even. For odd time reversal, A, B, and D are all quaternion real and A and D are Hermitian in addition. It is instructive to compare Eq. (11) to Eq. (7), which corresponds to a Hamiltonian invariant under $\mathcal{PT}$ but not necessarily $\mathcal{PT}$ self-adjoint.

Now we address the orthogonality theorem. Let us suppose that H satisfies all three conditions of $\mathcal{PT}$ quantum mechanics. Let ψ_i denote an eigenstate of H with eigenvalue λ_i. It follows that

$$\begin{aligned} (\psi_i, H\psi_j)_{\mathcal{PT}} &= (H\psi_i, \psi_j)_{\mathcal{PT}} \\ \Rightarrow (\psi_i, \lambda_j\psi_j)_{\mathcal{PT}} &= (\lambda_i\psi_i, \psi_j)_{\mathcal{PT}} \\ \Rightarrow (\lambda_j - \lambda_i)(\psi_i, \psi_j)_{\mathcal{PT}} &= 0. \end{aligned} \tag{12}$$

In other words, eigenstates of H with distinct eigenvalues must be orthogonal under the $\mathcal{PT}$ inner product, provided H satisfies the three conditions. Note that we used $\mathcal{PT}$ self-adjoincy in the first line of Eq. (12) and the reality of the eigenvalues, which follows from the conditions of $\mathcal{PT}$ invariance and unbroken $\mathcal{PT}$, in going from the second line to the third.

To summarize this section, invariance under $\mathcal{PT}$ ensures that the eigenvalues of H come in conjugate pairs; unbroken $\mathcal{PT}$ ensures that the eigenvalues are real (and twofold degenerate in the odd case); and self-adjoincy of H under the $\mathcal{PT}$ inner product ensures that the eigenvectors of H are orthonormal under the $\mathcal{PT}$ inner product as well as under the dynamically generated and physically relevant $\mathcal{CPT}$ inner product to be discussed below. In this manner the three conditions of $\mathcal{PT}$ quantum mechanics endow the Hamiltonian H with all the desirable qualities normally obtained by imposing hermiticity.

E. $\mathcal{CPT}$ inner product

Having specified the kinds of Hamiltonians that are permissible in $\mathcal{PT}$ quantum mechanics, we now return to the formulation of the appropriate inner product. It is instructive to first recall the formulation for the even case [4]. In this case, eigenvectors of H fall into two classes under the $\mathcal{PT}$ inner product: namely, those for which $(\psi_i, \psi_i)_{\mathcal{PT}}$ is positive and those for which $(\psi_i, \psi_i)_{\mathcal{PT}}$ is negative.[2] We now introduce a linear operator denoted $\mathcal{C}$ which has the property $\mathcal{C}\psi_i = s_i\psi_i$, where ψ_i are eigenvectors of H and s_i is the sign of the $\mathcal{PT}$ norm of the eigenvector, $(\psi_i, \psi_i)_{\mathcal{PT}}$. We have defined $\mathcal{C}$ by its action on the eigenvectors of H but since it is a linear operator it must be represented by some matrix in the standard basis; we denote this matrix K (i.e., $\mathcal{C}\psi = K\psi$). Evidently the operator $\mathcal{C}$ commutes with the combination $\mathcal{PT}$ (although it may not commute with either $\mathcal{P}$ or $\mathcal{T}$ separately). Thus, $KS = SK^*$. Furthermore, $\mathcal{C}^2 = 1$. It is evident from the definition given here that the Hamiltonian plays a crucial role in determining the operator $\mathcal{C}$.

The $\mathcal{CPT}$ inner product is now defined as $(\phi, \psi)_{\mathcal{CPT}} \equiv (\mathcal{CPT}\phi)^T\psi = \phi^\dagger K^T S\psi$. This is the inner product used in $\mathcal{PT}$ quantum mechanics in lieu of the standard inner product. Evidently all states have a positive norm with this inner product; this is most easily seen by expanding in the eigenbasis

[2]The case $(\psi_i, \psi_i)_{\mathcal{PT}} = 0$ is a catastrophe. In the absence of degeneracies, it then becomes impossible to formulate $\mathcal{PT}$ quantum mechanics for the Hamiltonian under consideration.

of the Hamiltonian. Furthermore, the $\mathcal{CPT}$ norm of any state is preserved under time evolution via Schrödinger's equation $i\partial\psi/\partial t = H\psi$. Thus, it is possible to consistently formulate quantum mechanics using the $\mathcal{CPT}$ inner product, notwithstanding the non-Hermitian Hamiltonian.

We now turn to the generalization to the odd case. $\mathcal{PT}$ doublets $(\phi, -\mathcal{PT}\phi)$ fall into two classes under the $\mathcal{PT}$ inner product: those for which $(\phi_i,\phi_i)_{\mathcal{PT}}$ is positive and those for which it is negative. As in the even case, we introduce a linear operator $\mathcal{C}$ with a corresponding matrix K which has the defining property that $\mathcal{C}\psi_i = s_i\psi_i$, where ψ_i denotes an eigenvector of H and s_i is the sign of the $\mathcal{PT}$ norm of that eigenvector, $(\psi_i,\psi_i)_{\mathcal{PT}}$. $\mathcal{C}$ commutes with $\mathcal{PT}$ corresponding to the statement $KSZ = SZK^*$. As in the even case, $\mathcal{C}^2 = 1$.

The $\mathcal{CPT}$ inner product is defined for the odd case as $(\phi,\psi)_{\mathcal{CPT}} \equiv (\mathcal{CPT}\phi)^{\mathcal{T}} Z\psi = \phi^\dagger K^T S\psi$. As in the even case, all states have a positive norm with this inner product; moreover, the norm of any state is preserved under Schrödinger time evolution. Thus, it is possible to consistently formulate quantum mechanics using the $\mathcal{CPT}$ inner product as defined here for the case of systems that are odd under time reversal.

F. Observables

Finally, in $\mathcal{PT}$ quantum mechanics it is no longer required that observables be Hermitian. Rather we define the $\mathcal{CPT}$ adjoint $A^\star$ of an operator A by imposing the condition that $(\phi,A\psi)_{\mathcal{CPT}} = (A^\star\phi,\psi)_{\mathcal{CPT}}$ for all states ϕ and ψ. Observables are then required to be $\mathcal{CPT}$ self-adjoint, $A = A^\star$. This is sufficient to ensure that the eigenvalues of A are real and that the usual principles of quantum measurement and uncertainty relations [8] may be applied even though the observables are no longer Hermitian in the usual sense.

This concludes our formulation of $\mathcal{PT}$ quantum mechanics for the case of odd time reversal. Although for simplicity we have only discussed finite-dimensional Hilbert spaces, the extension to the infinite-dimensional case is straightforward.

III. TWO-LEVEL EXAMPLES

We now consider the simplest nontrivial examples of $\mathcal{PT}$ quantum mechanics corresponding to $N = 2$ for the even case and $2N = 4$ for the odd case; the two-level model for the even case has been discussed before in Ref. [5]. We note that in conventional quantum mechanics a variety of complicated quantum-mechanical problems can be truncated to a two-level model [9]. Thus, the two- and four-level models presented here should be regarded not merely as toy models but as effective Hamiltonians that can be used to investigate the quantum dynamics of $\mathcal{PT}$ quantum systems.

For the even case the most general Hamiltonian matrix that meets all the conditions of $\mathcal{PT}$ quantum mechanics is

$$H = \begin{pmatrix} a & ib \\ ib & -a \end{pmatrix}. \tag{13}$$

Here a and b are real numbers and we have imposed the additional condition that H is traceless for simplicity. Note that for $b \neq 0$ this matrix is explicitly non-Hermitian. It is instructive to compare Eq. (13) to the most general two-level Hermitian Hamiltonian that is invariant under even time reversal. That Hamiltonian is obtained from Eq. (13) by replacing the pure imaginary off-diagonal terms with pure real ones (i.e., $ib \to b$). The eigenvalues of H are $\pm\sqrt{a^2 - b^2}$. Thus, $\mathcal{PT}$ is unbroken only for $a^2 > b^2$. So long as this condition is satisfied, the Hamiltonian H may be parametrized as $a = \rho\cosh(\chi)$ and $b = \rho\sinh\chi$, where $\rho > 0$ and $-\infty < \chi < \infty$. This parametrization applies for $a > 0$, which we assume hereafter. The case $a < 0$ can be parametrized and analyzed in exactly the same way. The eigenmatrix is

$$U = \begin{pmatrix} q\cosh\chi/2 & q\sinh\chi/2 \\ iqp\sinh\chi/2 & iqp\cosh\chi/2 \end{pmatrix}, \tag{14}$$

where for the moment we set $q = p = 1$. Here the first column corresponds to the eigenvector with positive eigenvalue ρ and the second to the negative eigenvalue $-\rho$; note that the eigenvectors have the $\mathcal{PT}$ invariant form in Eq. (8). It is easy to verify that the positive eigenvector also has positive $\mathcal{PT}$ norm; the negative has negative norm. Thus, the operator $\mathcal{C}$ is simply the normalized Hamiltonian (i.e., H divided by the magnitude of the eigenvalues $\sqrt{a^2 - b^2}$). Finally, the most general operator A that corresponds to an observable by virtue of being $\mathcal{CPT}$ self-adjoint is

$$A = \begin{pmatrix} A_0 + A_3 - iA_1\tanh\chi & A_1 - iA_2 + iA_3\tanh\chi \\ A_1 + iA_2 + iA_3\tanh\chi & A_0 - A_3 + iA_1\tanh\chi \end{pmatrix}. \tag{15}$$

Note that, in the limit $\chi \to 0$, the most general observable is simply a Hermitian matrix; in the same limit, the Hamiltonian H becomes Hermitian as well.

Finally, let us consider the simplest nontrivial example of $\mathcal{PT}$ quantum mechanics for the case of odd time-reversal symmetry with $2N = 4$. The most general traceless Hamiltonian matrix that meets the criteria of being invariant and self-adjoint under $\mathcal{PT}$ is given by

$$H = \begin{pmatrix} a & ib \\ ib^\dagger & -a \end{pmatrix}, \tag{16}$$

where $b = b_0\sigma_0 + ib_1\sigma_1 + ib_2\sigma_2 + ib_3\sigma_3$ is a real quaternion, and $a = a_0\sigma_0$ is a real quaternion proportional to the identity. It is instructive to compare this Hamiltonian to the most general four-level Hermitian Hamiltonian that is invariant under odd time reversal; the latter is obtained by replacing the pure imaginary off-diagonal quaternions with pure real quaternions, $ib,ib^\dagger \to b,b^\dagger$. It is also instructive to compare Eq. (16) to its counterpart in the even case, Eq. (13), obtained by replacing the real quaternions a and b with real numbers. The eigenvalues of the $\mathcal{PT}$ invariant Hamiltonian are $\pm\sqrt{a^2 - b^2}$, where $a^2 = a_0^2$ and $b^2 = b_0^2 + b_1^2 + b_2^2 + b_3^2$ denote the magnitudes of the quaternions a and b. Note that the eigenvalues are twofold degenerate in accordance with the general analysis above. $\mathcal{PT}$ is unbroken only for $a^2 > b^2$. So long as this condition is met (and $a_0 > 0$; the case $a_0 < 0$ can be analyzed similarly), we can parametrize the $\mathcal{PT}$ Hamiltonian by writing $a_0 = \cosh\chi$ and adopting polar coordinates $(\sinh\chi,\varphi,\theta,\phi)$ in the four-dimensional space of the components of b so that $b_0 = \sinh\chi\cos\varphi$, $b_3 = \sinh\chi\sin\varphi\cos\theta$, $b_1 = \sinh\chi\sin\varphi\sin\theta\cos\phi$, and $b_2 = \sinh\chi\sin\varphi\sin\theta\sin\phi$. In terms of this parametrization, the eigenmatrix has the form

(14) where q is the real quaternion corresponding to a rotation about the $n_x = \sin\phi, n_y = -\cos\phi, n_z = 0$ axis by an angle of θ; and $p = \exp(-i\varphi\sigma_z)$, a rotation about the z axis by an angle 2φ. The first two columns correspond to the positive-energy $\mathcal{PT}$ doublet; the second two correspond to the negative-energy doublet. It is easy to verify that the positive doublet also has positive $\mathcal{PT}$ norm; the negative has negative norm. Thus, the operator $\mathcal{C}$ coincides with the normalized Hamiltonian (i.e., H divided by $\sqrt{a^2 - b^2}$). Finally, the most general operator B that corresponds to an observable by virtue of being $\mathcal{CPT}$ self-adjoint is

$$B = \begin{pmatrix} q & 0 \\ 0 & qp \end{pmatrix} A \begin{pmatrix} q^\dagger & 0 \\ 0 & p^\dagger q^\dagger \end{pmatrix}, \tag{17}$$

where A is given by Eq. (15) with A_0, A_1, A_2, and A_3 now interpreted as arbitrary 2×2 Hermitian matrices.

IV. CONCLUSION

In summary, we have generalized the construction of $\mathcal{PT}$ quantum mechanics to the case that time-reversal symmetry is odd. We hope this generalization will further stimulate the search for natural phenomena that are described by $\mathcal{PT}$ quantum mechanics. The most important model in fundamental physics that is odd under time reversal is the Dirac equation. It is natural to ask whether the formulation of $\mathcal{PT}$ quantum mechanics presented here may lead to a different form of Dirac equation. The results of that investigation are reported elsewhere [10].

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APPENDIX A: CONSTRUCTION OF CANONICAL BASIS

Let us start in a basis wherein time reversal has the form $\mathcal{T}\psi = L\psi^*$, where L is a linear operator. Under a change of basis $\psi' = V\psi$, the matrix L transforms to $L' = VLV^{-1*}$. The purpose of this Appendix is to show that we can always find a basis in which the matrix L has a canonical form, namely $L = 1$ for even time reversal and $L = Z$ for odd time reversal. We focus on the case of odd time reversal here. The analysis for the even case is a straightforward extension and is omitted for the sake of brevity. For the odd case, $\mathcal{T}^2 = -1$, implying $LL^* = -1$.

We start by observing that the eigenvectors of L come in pairs: if ψ is an eigenvector of L with eigenvalue λ, then ψ^* is an eigenvector with eigenvalue $-1/\lambda^*$. This follows from conjugating the relation $L\psi = \lambda\psi$ and noting that for odd time reversal $L^* = -L^{-1}$. It follows that the eigenmatrix of L has the form

$$U = \begin{pmatrix} | & | & & | & | \\ \psi_1 & \psi_1^* & \cdots & \psi_N & \psi_N^* \\ | & | & & | & | \end{pmatrix}. \tag{A1}$$

Since the eigenvectors of L come in pairs, the Hilbert space it inhabits must necessarily have even dimensionality, which we take to be $2N$ here. For later convenience, we write the eigenvalues of L as $\lambda_1 = e^{\alpha_1}e^{i\phi_1}, \ldots, \lambda_N = e^{\alpha_N}e^{i\phi_N}$. We now define the matrix

$$D = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & & 0 & 0 \\ 1 & i & & 0 & 0 \\ & & \cdots & & \\ 0 & 0 & & 1 & -i \\ 0 & 0 & & 1 & i \end{pmatrix}. \tag{A2}$$

It is easy to see that $R^{-1} = UD$ is then a real matrix. Under a change of basis via R, L therefore transforms to $L' = RLR^{-1*} = D^{-1}U^{-1}LUD$. Explicitly, L' is a block-diagonal matrix

$$L' = \begin{pmatrix} \ell_1 & & \\ & \cdots & \\ & & \ell_N \end{pmatrix}, \tag{A3}$$

where the ith block ℓ_i is given by

$$\ell_i = e^{i\phi_i} \begin{pmatrix} \sinh\alpha_i & -i\cosh\alpha_i \\ i\cosh\alpha_i & \sinh\alpha_i \end{pmatrix}. \tag{A4}$$

We now construct the block-diagonal matrix

$$M = \begin{pmatrix} \mu_1 & & \\ & \cdots & \\ & & \mu_N \end{pmatrix}, \tag{A5}$$

where the ith block μ_i is given by

$$\mu_i = \exp\left(i\frac{\pi}{4}\right)\exp\left(i\frac{\phi_i}{2}\right)\begin{pmatrix} \cosh\frac{1}{2}\alpha_i & i\sinh\frac{1}{2}\alpha_i \\ -i\sinh\frac{1}{2}\alpha_i & \cosh\frac{1}{2}\alpha_i \end{pmatrix}. \tag{A6}$$

Straightforward matrix multiplication reveals that under the transformation M the matrix L' transforms as $ML'M^{-1*} = Z$. This establishes the desired result.

APPENDIX B: QUATERNIONS AND KRAMER'S THEOREM

It is helpful to first prove the following proposition: If an $N \times N$ quaternion matrix A satisfies

$$AZ = ZA^* \tag{B1}$$

then A is quaternion real (i.e., composed of real quaternions). Conversely, if A is quaternion real, it satisfies the condition Eq. (B1). Evidently, it follows that if A is quaternion real then so is A^{-1}. (*Proof:* Rewrite Eq. (B1) as $A^{-1}Z = ZA^{-1*}$.)

The proof of this proposition is as follows. Equation (B1) implies that each quaternion matrix element of A satisfies

$$ae_2 = e_2a^*, \tag{B2}$$

where a denotes any quaternion element of A. By using the explicit formula for $e_2 = i\sigma_y$, it is not difficult to show that Eq. (B2) restricts a to be of the form

$$a = \begin{pmatrix} q_0 + iq_2 & iq_1 + q_2 \\ iq_1 - q_2 & q_0 - iq_3 \end{pmatrix} = q_0 + i\mathbf{q}\cdot\boldsymbol{\sigma}. \tag{B3}$$

In other words, a is a real quaternion and hence A is quaternion real. In Eq. (B3), q_0, q_1, q_2, and q_3 are real numbers.

Next let us consider the invariance of states under time reversal. Working in a canonical basis, for even time reversal evidently $\psi = \mathcal{T}\psi$ if the vector ψ is real. For the odd case, on the other hand, it is impossible to find a nontrivial state that is invariant under time reversal, $\psi = \mathcal{T}\psi$. This is evident from consideration of a $2N$-component column vector of complex numbers, ψ, and its time-reversed counterpart $\mathcal{T}\psi$:

$$\psi = \begin{bmatrix} a(1) \\ b(1) \\ \cdots \\ a(N) \\ b(N) \end{bmatrix}, \qquad \mathcal{T}\psi = Z\psi^* = \begin{bmatrix} b(1)^* \\ -a(1)^* \\ \cdots \\ b(N)^* \\ -a(N)^* \end{bmatrix}. \tag{B4}$$

Using the explicit form in Eq. (B4), one can show indeed that ψ and $\mathcal{T}\psi$ are linearly independent.

It is instructive to assemble ψ and $-\mathcal{T}\psi$ into a pair of columns called a "Kramer doublet." We may regard the doublet as a $2N \times 2$ complex matrix or as a single column of N quaternions. Writing the complex components in terms of their real and imaginary parts as $a(1) = q_0(1) + iq_3(1)$, $b(1) = -q_2(1) + iq_1(1)$, and so on reveals that a Kramer doublet is composed of real quaternions:

$$\begin{bmatrix} | & | \\ \psi & -\mathcal{T}\psi \\ | & | \end{bmatrix} = \begin{bmatrix} a(1) & -b(1)^* \\ b(1) & a(1)^* \\ \cdots & \cdots \\ a(N) & -b(N)^* \\ b(N) & a(N)^* \end{bmatrix}$$
$$= \begin{bmatrix} q_0(1)+iq_3(1) & q_2(1)+iq_1(1) \\ -q_2(1)+iq_1(1) & q_0(1)-iq_3(1) \\ \cdots & \cdots \\ q_0(N)+iq_3(N) & q_2(N)+iq_1(N) \\ -q_2(N)+iq_1(N) & q_0(N)-iq_3(N) \end{bmatrix}. \tag{B5}$$

We now turn to Kramer's theorem, the main proposition of this section. Suppose that A is an $N \times N$ quaternion matrix that is quaternion real. Furthermore, let us suppose that the eigenvalues of A are known to be real. Then (i) the eigenvalues of A come in degenerate pairs (Kramer's degeneracy) and (ii) the eigenmatrix that diagonalizes A (in the sense that $U^{-1}AU$ is diagonal with the eigenvalues of A along the diagonal) can be chosen to be quaternion real.

Eigenvalues of A. Let ψ be an eigenvector of A with the real eigenvalue λ. Then

$$\begin{aligned} A\psi &= \lambda\psi \\ \Rightarrow ZA^*\psi^* &= \lambda Z\psi^* \\ \Rightarrow A(Z\psi^*) &= \lambda(Z\psi^*). \end{aligned} \tag{B6}$$

The second line follows from complex conjugating the first and premultiplying by Z; the second by using quaternion reality, $ZA^* = AZ$. In other words, ψ and $Z\psi^* = \mathcal{T}\psi$ are both eigenvectors of A with the same eigenvalue λ. This proves proposition (i).

Eigenmatrix of A. The eigenmatrix of any matrix is constructed by assembling its eigenvectors into columns. By the analysis above, if ψ is an eigenvector of A the $-Z\psi^*$ is another independent eigenvector with the same eigenvalue. Thus, the eigenmatrix of A has the form

$$U = \begin{pmatrix} | & | & & | & | \\ \psi_1 & -Z\psi_1^* & \cdots & \psi_N & -Z\psi_N^* \\ | & | & & | & | \end{pmatrix}. \tag{B7}$$

Thus, U is a stack of N Kramer doublets. Regarded as an $N \times N$ quaternion matrix, U is therefore quaternion real. Moreover if U is quaternion real, then so is U^{-1} as discussed above. This proves proposition (ii) above.

Parenthetically, we note that the textbook Kramer theorem [6,7] applies to a Hermitian Hamiltonian H that commutes with an odd time-reversal operator $\mathcal{T}$. In a canonical basis, commutation with time reversal, $H\mathcal{T} = \mathcal{T}H$, implies H is quaternion real, $HZ = ZH^*$. The hermiticity of H ensures its eigenvalues are real. Thus, H meets the conditions of the theorem formulated here.

APPENDIX C: GENERALIZATION OF BENDER, BERRY, AND MANDILARA THEOREM

According to Bender, Berry, and Mandilara [5], if $\mathcal{A}$ is an antilinear operator that commutes with H and satisfies $\mathcal{A}^{2k} = 1$ (where k is a positive odd integer) then (i) the eigenvalues of H come in conjugate pairs and (ii) in some basis the Hamiltonian matrix H is real. We first give a proof of this theorem that is conducive to the odd generalization of the theorem that we seek.

That the eigenvalues of H come in conjugate pairs follows simply from the fact that H and $\mathcal{A}$ commute and $\mathcal{A}$ is antilinear. The argument is as follows. Let ψ be an eigenvector of H with eigenvalue λ, $H\psi = \lambda\psi$. Then $H(\mathcal{A}\psi) = \mathcal{A}(H\psi) = \mathcal{A}(\lambda\psi) = \lambda^*\psi$. In other words, if ψ is an eigenvector with eigenvalue λ then $\mathcal{A}\psi$ is an eigenvector with eigenvalue λ^*; the eigenvalues come in conjugate pairs. Note that no use was made in this argument of the fact that $\mathcal{A}^{2k} = 1$.

Next let us show that H is real in a suitable basis. First let us prove this in the case that $k = 1$ so that $\mathcal{A}$ satisfies $\mathcal{A}^2 = 1$. Then by the analysis of Appendix A we can always find a basis in which $\mathcal{A}$ consists of conjugation, $\mathcal{A}\psi = \psi^*$. In this basis, $H\mathcal{A} = \mathcal{A}H$ implies $H = H^*$. In other words, H is real in this basis.

Now let us consider the case that $k = 3$ so that $\mathcal{A}$ satisfies $\mathcal{A}^6 = 1$. In this case our strategy is to show that there is an antilinear operator $\mathcal{B}$ that commutes with H and satisfies $\mathcal{B}^2 = 1$. This reduces the problem to the case already proved, namely $k = 1$. To implement this strategy all we need to do is construct an antilinear operator $\mathcal{B}$ with the desired properties. To this end, suppose that $\mathcal{A}$ has the form $\mathcal{A}\psi = \alpha\psi^*$. We define $\mathcal{B}\psi = \beta\psi^*$, where $\beta = \alpha\alpha^*\alpha$ is a linear operator. It is easy to verify that $\mathcal{A}^6 = 1$ implies that $\alpha\alpha^*\alpha\alpha^*\alpha\alpha^* = 1$. Comparing the definition of β, this implies $\beta\beta^* = 1$ and hence $\mathcal{B}^2 = 1$. That H commutes with $\mathcal{A}$ implies that $H\alpha = \alpha H^*$. By repeated use of this relation and its complex conjugate, we can show that $\alpha\alpha^*\alpha H^* = H\alpha\alpha^*\alpha$, implying that H commutes with $\mathcal{B}$. Thus, we have indeed succeeded in constructing an antilinear operator $\mathcal{B}$ with the desired properties. The extension of this proof to higher k should be evident at this point.

We now turn to the odd generalization of the theorem of Bender, Berry, and Mandilara. We claim that if $\mathcal{A}$ is an antilinear operator that commutes with H and satisfies $\mathcal{A}^{2k} = -1$ (where k is a positive odd integer) then (i) the eigenvalues of H come in conjugate pairs and (ii) in some basis the Hamiltonian matrix is quaternion real. The proof follows by close analogy to the even counterpart.

The proof that the eigenvalues come in conjugate pairs is identical to the even case above. To show that H is quaternion real in some basis, first let us consider the case that $k = 1$ so that $\mathcal{A}^2 = -1$. Then by the analysis in Appendix A we can always find a basis in which $\mathcal{A}$ has the canonical form $\mathcal{A}\psi = Z\psi^*$. In this basis, $H\mathcal{A} = \mathcal{A}H$ implies that $HZ = ZH^*$. In other words, H is quaternion real in this basis. Next consider the case $k = 3$ so that $\mathcal{A}$ satisfies $\mathcal{A}^6 = -1$. In this case we can construct another antilinear operator $\mathcal{B}$ that commutes with H and satisfies $\mathcal{B}^2 = -1$ and thereby reduce the problem to the case already proved, namely $k = 1$. The construction of $\mathcal{B}$ and the proof that the constructed operator $\mathcal{B}$ has the desired properties is identical to the even case above. Thus, we have proved the proposition for the case $k = 2$ as well. The extension to higher values of k may be carried out similarly.

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