\( \mathcal{PT} \) symmetry and necessary and sufficient conditions for the reality of energy eigenvalues

Carl M. Bender\textsuperscript{1} and Philip D. Mannheim\textsuperscript{2}

\textsuperscript{1}Physics Department  
Washington University  
St. Louis, MO 63130, USA  
electronic address: cmb@wustl.edu

\textsuperscript{2}Department of Physics 
University of Connecticut  
Storrs, CT 06269, USA  
electronic address: philip.mannheim@uconn.edu

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Abstract

Despite its common use in quantum theory, the mathematical requirement of Dirac Hermiticity of a Hamiltonian is sufficient to guarantee the reality of energy eigenvalues but not necessary. By establishing three theorems, this paper gives physical conditions that are both necessary and sufficient. First, it is shown that if the secular equation is real, the Hamiltonian is necessarily \( \mathcal{PT} \) symmetric. Second, if a linear operator \( \mathcal{C} \) that obeys the two equations \([\mathcal{C}, H] = 0\) and \(\mathcal{C}^2 = 1\) is introduced, then the energy eigenvalues of a \( \mathcal{PT} \)-symmetric Hamiltonian that is diagonalizable are real only if this \( \mathcal{C} \) operator commutes with \( \mathcal{PT} \). Third, the energy eigenvalues of \( \mathcal{PT} \)-symmetric Hamiltonians having a nondiagonalizable, Jordan-block form are real. These theorems hold for matrix Hamiltonians of any dimensionality.
I. INTRODUCTION

In quantum mechanics physical observables must have real eigenvalues. Thus, it is conventional, and even axiomatic, to associate such observables with Dirac-Hermitian operators. (A Dirac-Hermitian operator is invariant under combined matrix transposition and complex conjugation. The Dirac adjoint of $A$ is written $A^\dagger$.) However, while a Dirac-Hermitian operator has real eigenvalues, there is nothing that prevents a non-Dirac-Hermitian operator from also having real eigenvalues. Thus, Dirac Hermiticity is sufficient to ensure the reality of eigenvalues but it is not necessary. In this paper we provide conditions that are both necessary and sufficient to guarantee real eigenvalues.

Interest in non-Dirac-Hermitian operators having real eigenvalues was triggered by the discovery that the energy eigenvalues of Hamiltonians such as $H = p^2 + ix^3$ are all real [1, 2, 3]. Because the parity operator $\mathcal{P}$ transforms $x^3$ into $-x^3$ and the time reversal operator $\mathcal{T}$ transforms $i$ into $-i$, the reality of the energy eigenvalues of $H = p^2 + ix^3$ was traced in Ref. [2] to the facts that the Hamiltonian is $\mathcal{PT}$ invariant and that its eigenstates are also eigenstates of the $\mathcal{PT}$ operator. Specifically, for an energy eigenstate, which satisfies $H|\psi\rangle = E|\psi\rangle$, the vanishing of the $[H, \mathcal{PT}]$ commutator and the antilinearity of the $\mathcal{T}$ operator imply that $\mathcal{PT}H|\psi\rangle = E^*\mathcal{PT}|\psi\rangle = H\mathcal{PT}|\psi\rangle$. Since $\mathcal{PT}|\psi\rangle$ is equal (apart from an irrelevant phase) to $|\psi\rangle$, one concludes that $E = E^*$. The Hamiltonian $H = p^2 + ix^3$ thus emerges as a non-Dirac-Hermitian operator whose eigenvalues are all real.

However, even if $H$ and $\mathcal{PT}$ commute, there is no guarantee that the eigenvalues of $H$ are real because the eigenstates of $H$ need not be eigenstates of the $\mathcal{PT}$ operator; $\mathcal{PT}$-symmetric Hamiltonians that are not Dirac Hermitian may possess complex as well ad real eigenvalues. (The familiar theorem that one can simultaneously diagonalize any two commuting operators does not hold when antilinear operators are involved.) Nonetheless, $\mathcal{PT}$ symmetry is still a powerful condition because it implies that the secular equation $\det(H - EI) = 0$, which determines the eigenvalues of the Hamiltonian, is real [4].

To establish the reality of the secular equation of a $\mathcal{PT}$-symmetric Hamiltonian, one can use standard properties of determinants: $\det(H - EI) = \det(\mathcal{PT}HT^{-1}\mathcal{P}^{-1} - EI) = \det(THT^{-1} - EI)$. Then, writing the time-reversal operator as $\mathcal{T} = LK$ and $T^{-1} = KL^{-1}$, where $L$ is a linear operator and $K$ performs complex conjugation, one obtains $\det(H - EI) = \det(H^* - EI)$. Thus, $H$ and $H^*$ have the same set of eigenvalues and $H$ has a real secular
equation. Note that this conclusion holds for any choice of linear operators $P$ and $L$. Thus, we can interpret the condition of $PT$ symmetry in the generalized sense, where $P$ is any linear operator and $T$ is any antilinear operator. These generalized operators $P$ and $T$ need not even commute with one another.

There is an even shorter proof that the secular equation is real. The secular equation is a polynomial in the eigenvalue $E$ of the form $\sum_n a_n E^n = 0$. The Hamiltonian matrix itself solves this equation: $\sum_n a_n H^n = 0$. If the Hamiltonian commutes with any antilinear operator $\kappa$, $[H, \kappa] = 0$, then $H$ also obeys $\sum_n a_n^* H^n = 0$. Thus, the secular equation is real. Establishing the reality of the secular equation does not require that $\kappa^2 = 1$.

The $PT$ symmetry of a Hamiltonian thus requires that any energy eigenvalue must either be real or belong to a complex-conjugate pair. If the eigenvalue is real, the associated eigenstate is also an eigenstate of the $PT$ operator. If the energy is a member of a complex conjugate pair, the $PT$ operator maps its eigenstate into the eigenstate associated with the complex-conjugate energy eigenvalue.

From the discussion above we see that $PT$ symmetry alone is not powerful enough to force the energy eigenvalues of a Hamiltonian to be real. Moreover, while $PT$ symmetry implies a real secular equation, it does not follow that $PT$ symmetry is the only way to produce a real secular equation; $PT$ symmetry is sufficient but not necessary to give a real secular equation.

In this paper we prove three theorems: (i) If the secular equation is real, the Hamiltonian is necessarily $PT$ symmetric. Thus, $PT$ symmetry is both necessary and sufficient for the reality of the secular equation, and it is not possible for a Hamiltonian that is not $PT$-symmetric to possess an entirely real set of energy eigenvalues. (ii) Introduce the $C$ operator, which is linear and obeys $[C, H] = 0$ and $C^2 = 1$ \cite{5, 6}. Then, the energy eigenvalues of a $PT$-symmetric Hamiltonian that is diagonalizable are real only if this $C$ operator commutes with $PT$. (iii) The energy eigenvalues of $PT$-symmetric Hamiltonians having a nondiagonalizable, Jordan-block form are real. These theorems hold for Hamiltonians of any dimensionality, but because a pair of complex-conjugate eigenvalues span a two-dimensional space, one can derive these results by considering two-dimensional Hamiltonians.

In Sec. II the properties of two-dimensional $PT$-symmetric matrices are discussed. The $C$ operator is introduced in Sec. III nondiagonalizable Jordan-block matrices are examined in Sec. IV and the $CP = e^Q$ operator of $PT$ quantum mechanics is studied in Sec. VI.
II. TWO-DIMENSIONAL MATRICES

The Pauli matrices form a basis of $2 \times 2$ matrices, so in a $2 \times 2$ space we can take general Hamiltonian, parity, and time-reversal operators to have the form

$$ H = \sigma_0 h^0 + \sigma \cdot h, \quad \mathcal{P} = \sigma_0 p^0 + \sigma \cdot p, \quad T = K \sigma_2 (\sigma_0 t^0 + \sigma \cdot t). \quad (1) $$

Here the factor $\sigma_2$ has been introduced in $T$ because of its convenient property $\sigma_2 \sigma_2 = -\sigma^*$. Since $h^0 = h_R^0 + i h_I^0$ and $h = h_R + i h_I$ are not required to be real, the Hamiltonian $H$ is not necessarily Dirac Hermitian. For $\mathcal{P}$ and $T$ to serve as the conventional parity and time-reversal operators they need to obey $\mathcal{P}^2 = 1$, $T^2 = 1$, $[\mathcal{P}, T] = 0$, with $\mathcal{P}$ being Dirac Hermitian and unitary and $T$ being expressible as $K$ times a unitary operator. These conditions can be satisfied if we take $p^0 = 0$, $p \cdot p = 1$, $p = p^*$, $t^0 = 0$, $t \cdot t = 1$, $t = t^*$, and require that $p \cdot t = 0$. The vectors $p$ and $t$ are thus real, orthogonal unit vectors.

For the Hamiltonian (1), the secular equation for the energy eigenvalues $E$ is

$$ E^2 - 2 i \sigma_0 h^0 + (h^0)^2 = h \cdot h = h_R \cdot h_R - h_I \cdot h_I + 2 i h_R \cdot h_I. \quad (2) $$

Furthermore, since $(\sigma \cdot A)(\sigma \cdot B)(\sigma \cdot A) = 2(\sigma \cdot A)(A \cdot B) - (\sigma \cdot B)(A \cdot A)$ for any two vectors $A$ and $B$, we obtain

$$ \mathcal{P} \mathcal{T} H T^{-1} \mathcal{P}^{-1} - H = -2 i \sigma_0 h_I^0 + 2 \sigma \cdot F - 2 i \sigma \cdot G, \quad (3) $$

where

$$ F = (h_R \cdot p)p + (h_R \cdot t)t - h_R, \quad G = (h_I \cdot p)p + (h_I \cdot t)t. \quad (4) $$

If we now assume that the Hamiltonian is $\mathcal{PT}$ invariant, then from (3) we obtain $h_I^0 = 0$, $F = 0$, $G = 0$. Since $p \cdot t = 0$, the vanishing of $G$ implies that both $h_I \cdot p$ and $h_I \cdot t$ vanish. Then, from the vanishing of $F$ we see that $h_R \cdot h_I = 0$. Consequently, the secular equation (2) is strictly real, and we recover the result of [4] for $\mathcal{PT}$-symmetric Hamiltonians.

On the other hand, suppose we start by assuming that the secular equation is real and set $h_I^0 = 0$ and $h_R \cdot h_I = 0$. The vanishing of $h_R \cdot h_I$ can be achieved in three ways: $h_I = 0$, $h_R = 0$, $h_I$ and $h_R$ orthogonal. If $h_I = 0$, and thus $G = 0$, the choice $p = h_R/(h_R \cdot h_R)^{1/2}$ then yields $h_R \cdot t = 0$ and thus $F = 0$. If $h_R = 0$, and thus $F = 0$, because $h_I$ is a 3-vector and $p \cdot t = 0$, for any $h_I$ we can pick an appropriate $p$ and $t$ so that $h_I$, $p$, and $t$ form an orthogonal triad. This then yields $G = 0$. If both $h_R$ and $h_I$ are nonzero, the choice
\[ p = h_R/(h_R \cdot h_R)^{1/2} \] then yields \( h_R \cdot t = 0 \) and \( F = 0 \). Moreover, this choice for \( p \) leads to \( h_I \cdot p = 0 \) because \( h_R \cdot h_I = 0 \), and thus to \( G = (h_I \cdot t)t \). With \( p \) being parallel to \( h_R \), the vectors \( t \) and \( h_I \) must lie in a plane that is normal to \( h_R \). For any choice of \( h_I \) in that plane we can always find a \( t \) that is orthogonal to it, and thus make \( G \) vanish. Hence, for any choice of \( h_I \) and \( h_R \), there will always be a choice of \( p \) and \( t \) for which \( H \) is \( PT \) symmetric. Therefore, \( PT \) invariance of \( H \) is both necessary and sufficient to ensure the reality of all the coefficients in its secular eigenvalue equation.

We have shown that the reality of the secular equation implies the \( PT \) symmetry of the Hamiltonian in the two-dimensional case. To extend this result to higher-dimensional matrices we need only assume that the Hamiltonian can be diagonalized. (Remember that \( PT \)-symmetric Hamiltonians have real secular equations regardless of their dimensionality.) In its diagonal form a Hamiltonian whose secular equation is real consists of a set of real eigenvalues and a set of complex-conjugate pairs of eigenvalues \( E_R \pm iE_I \) on the diagonal. For the real eigenvalues \( PT \) symmetry is made manifest by simply taking \( P \) to be diagonal and \( T \) to be \( K \) in that sector of the Hamiltonian. In each two-dimensional block of complex-conjugate eigenvalues the Hamiltonian behaves as \( H^i = E^i_R \sigma_0 + iE^i_I \sigma_3 \) and it is thus \( PT \) invariant block-by-block under \( P = \sigma_1 \) and \( T = K \). [equivalent to taking \( p = (1,0,0), t = (0,1,0) \) in (1)]. Transforming back to the original, undiagonalized form of the Hamiltonian then yields a Hamiltonian that is symmetric under the transformed \( PT \) operator. The theorem on the secular equation thus holds for diagonalizable Hamiltonians of arbitrary dimensionality. To determine the conditions for which the roots of the now real secular equation are all real, we introduce the \( C \) operator.

### III. THE \( C \) OPERATOR

In previous studies a linear operator \( C \) was introduced that satisfied the three conditions

\[ [C, H] = 0, \quad C^2 = 1, \quad [C, PT] = 0. \quad (5) \]

The \( C \) operator was then used to construct a Hilbert-space inner product for \( PT \)-symmetric Hamiltonians whose energy eigenvalues were all real. The associated \( CPT \) norm \( \langle \psi | CPT | \psi \rangle \) was positive definite. For our purposes here we do not impose the third condition in (5) and
instead introduce a generalized linear $\mathcal{C}$ operator that obeys just the two conditions

$$[\mathcal{C}, H] = 0, \quad \mathcal{C}^2 = 1.$$  \hfill (6)

Unlike the $\mathcal{P}$ operator, the $\mathcal{C}$ operator is not required to be Dirac Hermitian.

To construct this generalized operator $\mathcal{C}$ in the two-dimensional case we set $\mathcal{C} = \sigma_0 c^0 + \sigma \cdot c$, and find that we need to impose the conditions

$$c^0 = 0, \quad c \cdot c = 1, \quad (c \cdot h)c - h = 0.$$  \hfill (7)

(We exclude the trivial solution $\mathcal{C} = 1$.) Equation (7) shows that $c = h/(h \cdot h)^{1/2}$ unless $h \cdot h$ happens to vanish. Because $[\mathcal{C}, H] = 0$ our analysis extends to diagonalizable Hamiltonians of arbitrary dimensionality and establishes that apart from the special case $h \cdot h = 0$, a nontrivial $\mathcal{C}$ operator satisfying $[\mathcal{C}, H] = 0, \mathcal{C}^2 = 1$ exists [8].

For the special case in which $h \cdot h$ vanishes, the conditions required by (7) cannot be realized because a nonzero $h$ would require a nonzero $c \cdot h$, while a vanishing $h \cdot h$ would require a vanishing $(c \cdot h)^2$. Thus, when $h \cdot h = 0$, $\mathcal{C}$ is undefined. (We defer further discussion of the $h \cdot h = 0$ case to Sec. [IV]. Unlike $\mathcal{C}$, both $\mathcal{P}$ and $\mathcal{T}$ remain well-defined at $h \cdot h = 0$.)

To explore the implications of (7) it is convenient to set $c \cdot h = X + iY$, where

$$c_R \cdot h_R - c_I \cdot h_I = X, \quad c_R \cdot h_I + c_I \cdot h_R = Y.$$  \hfill (8)

Since the condition $(c \cdot h)c - h = 0$ forbids the vanishing of $c \cdot h$ once $h$ is nonzero, at least one of the parameters $X$ and $Y$ must be nonzero. From (7) we obtain

$$c_R \cdot c_R - c_I \cdot c_I = 1, \quad c_R \cdot c_I = 0, \quad Xc_R - Yc_I = h_R, \quad Yc_R + Xc_I = h_I,$$  \hfill (9)

and because $X^2 + Y^2$ cannot be zero we get $c = (X - iY)h/(X^2 + Y^2)$. From (9) we obtain

$$h_R \cdot h_I = XY, \quad h_R \cdot h_R - h_I \cdot h_I = X^2 - Y^2.$$  \hfill (10)

When the Hamiltonian is $\mathcal{PT}$ symmetric, $h_R \cdot h_I$ is required to vanish, and we see that the $XY$ product also vanishes. Thus, either $X$ and $Y$, but not both, must vanish. Since the solutions to the eigenvalue equation (2) have the form $E = h^0 \pm (h_R \cdot h_R - h_I \cdot h_I)^{1/2}$ when $h_R \cdot h_I = 0$, for $\mathcal{PT}$-symmetric Hamiltonians (where $h_I^0 = 0$) the energy eigenvalues will both be real if we realize the condition $XY = 0$ via $Y = 0$, and they will form a complex-conjugate pair if we set $X = 0$. Thus, to complete the proof we must relate the vanishing of $Y$ or $X$ to the vanishing or nonvanishing of the $[\mathcal{C}, \mathcal{PT}]$ commutator.
We evaluate the $[\mathcal{C}, \mathcal{PT}]$ commutator in the two cases and obtain
\[
\mathcal{PTCT}^{-1}\mathcal{P}^{-1} - \mathcal{C} = \frac{2(X + iY)}{X^2 + Y^2} \sigma \cdot (\mathcal{F} - i\mathcal{G}) + \frac{2iY}{X^2 + Y^2} \sigma \cdot \mathcal{h}.
\] (11)

Since $\mathcal{F}$ and $\mathcal{G}$ vanish when $H$ is $\mathcal{PT}$ symmetric, $\mathcal{PTCT}^{-1}\mathcal{P}^{-1} - \mathcal{C}$ vanishes only if $Y = 0$. We thus establish that when $\mathcal{PT}$ commutes with $H$ and $\mathcal{C}$, all energy eigenvalues are real.

It is of interest to evaluate the $\{\mathcal{C}, \mathcal{PT}\}$ anticommutator as well, and it has the form
\[
\mathcal{PTCT}^{-1}\mathcal{P}^{-1} + \mathcal{C} = \frac{2(X + iY)}{X^2 + Y^2} \sigma \cdot (\mathcal{F} - i\mathcal{G}) + \frac{2X}{X^2 + Y^2} \sigma \cdot \mathcal{h}.
\] (12)

Thus, when $H$ is $\mathcal{PT}$ symmetric, $\mathcal{PTCT}^{-1}\mathcal{P}^{-1} + \mathcal{C}$ vanishes only if $X = 0$. Therefore, when $X = 0$, $\mathcal{C}$ and $\mathcal{PT}$ anticommute rather than commute. Hence, when $\mathcal{PT}$ commutes with $H$ but not with $\mathcal{C}$, the energy eigenvalues appear in complex-conjugate pairs.

Finally, since $\mathcal{C}$ and $H$ commute, our result immediately generalizes to diagonalizable Hamiltonians of arbitrary dimensionality. Specifically, one first constructs the appropriate $\mathcal{C}$ operator in the basis in which both $\mathcal{C}$ and $H$ are diagonal, and then one transforms back to the original nondiagonal basis. Thus, except when the Hamiltonian is not diagonalizable, we have shown that energy eigenvalues are real only if $[H, \mathcal{PT}] = 0$ and $[\mathcal{C}, \mathcal{PT}] = 0$. We turn next to the case of nondiagonalizable Hamiltonians.

### IV. NONDIAGONALIZABLE HAMILTONIANS

Dirac-Hermitian Hamiltonians can always be diagonalized by means of a unitary transformation, but a Hamiltonian that is not Dirac Hermitian may not be diagonalizable. Jordan showed that via a sequence of similarity transformations any $N$-dimensional square matrix can be brought to either a diagonal form or a triangular Jordan-block form in which all of the elements on one side of the diagonal are zero. Since the nonzero elements on the other side of the diagonal of a Jordan-block matrix do not contribute to the secular equation, the $N$ elements on its diagonal are the $N$ eigenvalues of the matrix. Because Jordan-block matrices cannot be brought to a diagonal form by a similarity transform, they possess fewer than $N$ eigenvectors (even though they possess a full set of $N$ eigenvalues). Thus, the eigenvectors of a Jordan-block matrix do not form a complete basis.

A Jordan-block matrix has fewer solutions to the eigenvector equation $H\psi = E\psi$ than there are to the determinantal condition $\text{det}(H - EI) = 0$. For diagonalizable Hamiltonians
the eigenvalue equation $H\psi = E\psi$ yields $N$ eigenvalues, and so one does not need to
distinguish between eigenvalue solutions to $H\psi = E\psi$ and eigenvalue solutions to $\det(H - EI) = 0$. However, for nondiagonalizable Hamiltonians one does need to make a distinction, and we shall thus refer to $H\psi = E\psi$ as the eigenvector equation and to $\det(H - EI) = 0$ as the eigenvalue or secular equation.

A typical two-dimensional example of a Jordan-block matrix is

$$M = \begin{pmatrix} a & b \\ 0 & a \end{pmatrix}.$$  \hfill (13)

This matrix possesses two eigenvalues, both equal to $a$, but has only one eigenvector because the eigenvector condition

$$\begin{pmatrix} a & b \\ 0 & a \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} ac + bd \\ ad \end{pmatrix} = \begin{pmatrix} ac \\ ad \end{pmatrix}$$

(14)

only has one solution, namely, that with $d = 0$. When the parameter $a$ is real, (13) provides a simple example of a non-Hermitian matrix whose eigenvalues are all real.

Jordan-block matrices must have degenerate eigenvalues. Note that if we replace the matrix $M$ of (13) by the non-Jordan-block matrix

$$M(\epsilon) = \begin{pmatrix} a & b \\ 0 & a + \epsilon \end{pmatrix},$$

(15)

we find two eigenvalues $a$ and $a + \epsilon$ and two independent eigenvectors:

$$\psi(a) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi(a + \epsilon) = \begin{pmatrix} 1 \\ \epsilon/b \end{pmatrix}.$$  \hfill (16)

However, in the limit $\epsilon \to 0$ the two eigenvectors merge and one eigenvector is lost [10].

The theorem requiring the secular equation to be real if $[H, \mathcal{PT}] = 0$ is not sensitive to Jordan-block structures. This theorem follows from the determinant condition $\det(H - EI) = 0$ on the eigenvalues and does not refer to the solutions to the eigenvector equation $H\psi = E\psi$. Thus, $\mathcal{PT}$-invariant Hamiltonians that have Jordan-block structure still have a real secular equation. Such secular equations could have complex-conjugate pairs of solutions. However, such pairs would not be degenerate. Since Jordan-block Hamiltonians cannot have nondegenerate eigenvalues, the eigenvalues of $\mathcal{PT}$-invariant Jordan-block Hamiltonians have no choice but to be real. This establishes the reality of the energy eigenvalues of $\mathcal{PT}$-symmetric Jordan-block Hamiltonians in the Jordan-block sector(s).
As one varies the parameters in a Hamiltonian such as that in (1) to transit from real to complex eigenvalues, one passes through a point where the two energy eigenvalues become degenerate. Since there is such a transition at that point, the energy spectrum has a square-root-branch-point singularity at $\mathbf{h} \cdot \mathbf{h} = 0$; because of this singularity, the $C$ operator must also be discontinuous and become undefined. At the transition two things can occur: Either the two degenerate eigenvalues can have independent eigenvectors, or the two eigenvectors can merge. By adjusting the parameters in (1) accordingly, one can achieve either of these two outcomes [11]. The special points at which the transitions occur are thus points at which all energy eigenvalues are real. At such points there is no need to find a criterion that would force the eigenvalues of a $\mathcal{PT}$-symmetric Hamiltonian to be real since they already are. Thus, at such transition points the reality of the eigenvalues of a $\mathcal{PT}$-symmetric Hamiltonian is guaranteed. At points other than these special points, the reality or complexity of eigenvalues is fixed by the vanishing or nonvanishing of the $[C,\mathcal{PT}]$ commutator [12].

V. THE GENERALIZED $Q$ OPERATOR

In $\mathcal{PT}$ studies some special cases have been found (see [6] and references therein) in which all energies are real and one can set $\mathcal{P}^{-1}H\mathcal{P} = H^\dagger$ and thus $\mathcal{P}^{-1}C^{-1}H\mathcal{C}\mathcal{P} = H^\dagger$ (because $[H,C] = 0$). In some of those cases the operator product $C\mathcal{P}$ can be written as $C\mathcal{P} = e^Q$, where $Q$ is Dirac Hermitian [7]. In these instances, the similarity-transformed Hamiltonian $e^{-Q/2}He^{Q/2}$ is Dirac Hermitian. However, no rule has been given that would determine the circumstances under which these properties might hold or how they might generalize.

The energies of $\mathcal{PT}$-symmetric Hamiltonians are real or appear in complex-conjugate pairs. For such Hamiltonians $H$ and $H^\dagger$ have the same energy eigenspectra and must be related by a similarity transformation. The requisite similarity transform generalizes the relation $\mathcal{P}^{-1}H\mathcal{P} = H^\dagger$, even when there are complex energies. To find the appropriate generalization, we note that in the $2 \times 2$ case the operator $A = (\sigma_1h_1 + \sigma_3h_3)/(h_1^2 + h_3^2)^{1/2}$ with inverse $A^{-1} = A$ performs transposition according to $A^{-1}\sigma \cdot \mathbf{h}A = \sigma^T \cdot \mathbf{h}$. With the $T$ operator having the form $T = K\sigma_2\sigma \cdot \mathbf{t}$, we introduce an operator $B^{-1} = A^*\sigma^* \cdot \mathbf{t}\sigma_2^*$ and get $B^{-1}T = KA$ and thus $B^{-1}\mathcal{T}\mathcal{H}T^{-1}B = H^\dagger$. For $2 \times 2 \mathcal{PT}$-symmetric Hamiltonians, we obtain $B^{-1}\mathcal{P}^{-1}H\mathcal{P}B = H^\dagger$. Therefore, the requisite similarity transform is given by $\mathcal{P}B$.

To generalize this derivation to $N$-dimensional matrices, we must find an $N$-dimensional
transposition operator. To this end we introduce the $N^2$ generators $\lambda_i$ of $U(N)$ as written
in the $N$-dimensional fundamental representation and set $H = \sum_{n=1}^{N^2} \lambda_n h_n$. Of the $U(N)$ 
generators, $N(N+1)/2$ are symmetric and real while $N(N-1)/2$ are antisymmetric and imaginary. The anticommutator 
of any symmetric $SU(N)$ generator with any antisymmetric generator vanishes. Therefore, an operator of the form $A = (\sum_i \lambda_i h_i)/J$ as summed 
over the symmetric $SU(N)$ $\lambda_i$ generators only with $J$ being an appropriate normalization factor will effect 
$A^{-1}(\sum_n \lambda_n h_n)A = \sum_n \lambda_n^T h_n$. This gives the transposition operator.

To express the operator $\mathcal{CP}$ in the form $e^Q$ with Dirac-Hermitian $Q$, it is necessary that $\mathcal{CP}$ be Hermitian and that it be a positive operator (that is, all of its eigenvalues are positive).

In the two-dimensional case the determinants of both $\mathcal{C}$ and $\mathcal{P}$ are equal to $-1$. Hence, the determinant of $\mathcal{CP}$ is $+1$. Thus, if we could show that $\mathcal{CP}$ is Hermitian and that its trace is positive, we could show that it is a positive operator. Let us evaluate

$$\mathcal{CP} - (\mathcal{CP})^\dagger = c \cdot p + i \sigma \cdot c \times p - c^* \cdot p + i \sigma \cdot c^* \times p = 2ic_1 \cdot p + 2i\sigma \cdot c_R \times p.$$  (17)

Since we can set $c = h/X$ when $Y = 0$, since $h_R \cdot h_I = 0$, and since $p$ can be chosen so that $h_R$ is parallel to $p$ when the secular equation is real, we see that $\mathcal{CP} - (\mathcal{CP})^\dagger$ is zero when $Y = 0$. If all energies are real, then $\mathcal{CP}$ is Hermitian. (When $X = 0$, one can show that $\mathcal{CP} + (\mathcal{CP})^\dagger = 0$, with all eigenvalues of $\mathcal{CP}$ being pure imaginary.) In the real-energy sector we find that $\text{Tr}(\mathcal{CP}) = 2c_R \cdot p + 2ic_1 \cdot p$ is always real and positive. Thus, in the real-energy sector $\mathcal{CP}$ is always a positive operator $[13]$. 

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[8] As such, this result is a generalization to non-Hermitian Hamiltonians of the result of C. M. Bender, P. N. Meisinger, and Q. Wang, J. Phys. A: Math. Gen. 36, 1029 (2003) that all Hermitian Hamiltonians have a generalized parity invariance.

[9] Because $\det(C) = -1$, one eigenstate of $H$ has $C$ eigenvalue $\eta = 1$ while the other has $\eta = -1$. Since the $\eta$ are real, for any energy eigenstate $|\alpha\rangle$ we obtain $(C\mathcal{P}C \mp \mathcal{PT})|\alpha\rangle = \eta_\alpha(C\mathcal{P}T|\alpha\rangle \mp \eta_\alpha\mathcal{PT}|\alpha\rangle)$. If $\mathcal{PT}|\alpha\rangle = |\alpha\rangle$ then $(C\mathcal{P}T - \mathcal{PT})|\alpha\rangle = 0$, while if $\mathcal{PT}|\alpha\rangle = |\beta\rangle$ where $|\beta\rangle$ has $\eta_\beta = -\eta_\alpha$ we obtain $(C\mathcal{P}TC + \mathcal{PT})|\alpha\rangle = 0$. Thus, as noted in Sec. II if $\mathcal{PT}|\alpha\rangle = |\alpha\rangle$, for each energy eigenstate the energies are real; if $\mathcal{PT}|\alpha\rangle = |\beta\rangle$, the energies are complex.

[10] The Hamiltonian of the equal-frequency fourth-order derivative Pais-Uhlenbeck oscillator model [A. Pais and G. E. Uhlenbeck, Phys. Rev. 79, 145 (1950)] is $\mathcal{PT}$ symmetric [C. M. Bender and P. D. Mannheim, Phys. Rev. Lett. 100, 110402 (2008)] but nondiagonalizable [C. M. Bender and P. D. Mannheim, Phys. Rev. D 78, 025022 (2008)]. The missing eigenvectors reemerge as nonstationary solutions of the associated time-dependent Schrödinger equation. The set of stationary and nonstationary solutions is complete and time evolution is unitary even though the Hamiltonian is neither Dirac Hermitian nor diagonalizable.

[11] The only way a two-dimensional matrix with two equal eigenvalues can avoid being Jordan block is the special case in which it has no nondiagonal terms at all.

[12] Although it is beyond the scope of this paper, $\mathcal{PT}$ symmetry provides a natural framework for treating decays, with a continuous change in parameters converting stable states into unstable ones. Thus, $\mathcal{PT}$-symmetric Hamiltonians may be of relevance to open quantum systems.

[13] Since $\mathcal{CP}$ does not commute with $H$, one cannot introduce a diagonal basis to try to generalize any two-dimensional $\mathcal{CP}$ result to the general $N$-dimensional case. Rather one must work with the full $U(N)$ operators given above. We do not pursue this question here.