\( \mathcal{PT} \) symmetry as a generalization of Hermiticity

Qing-hai Wang\(^1\), Song-zhi Chia\(^2\) and Jie-hong Zhang\(^2\)

\(^1\) Department of Physics, National University of Singapore, Singapore 117542
\(^2\) NUS High School of Mathematics and Science, Singapore 129957

E-mail: phyqw@nus.edu.sg

Received 19 April 2010, in final form 25 May 2010
Published 21 June 2010
Online at stacks.iop.org/JPhysA/43/295301

Abstract
The Hilbert space in \( \mathcal{PT} \)-symmetric quantum mechanics is formulated as a linear vector space with a dynamic inner product. The most general \( \mathcal{PT} \)-symmetric matrix Hamiltonians are constructed for the \( 2 \times 2 \) and \( 3 \times 3 \) cases. In the former case, the \( \mathcal{PT} \)-symmetric Hamiltonian represents the most general matrix Hamiltonian with a real spectrum. In both cases, Hermitian matrices are shown to be special cases of \( \mathcal{PT} \)-symmetric matrices. This finding confirms and strengthens the early belief that the \( \mathcal{PT} \)-symmetric quantum mechanics is a generalization of the conventional Hermitian quantum mechanics.

PACS numbers: 03.65.-w, 11.30.Er

1. Introduction

The seminal paper by Bender and Boettcher in 1998 has lead to an alternative formulation of quantum mechanics (QM): non-Hermitian \( \mathcal{PT} \)-symmetric QM [1]. Although the Hamiltonians involved do not appear to be Hermitian (\( H \neq H^\dagger \)), they yield only real spectra and the time evolution is unitary when the \( \mathcal{PT} \) symmetry is not broken [1–4].

Since the introduction of \( \mathcal{PT} \)-symmetric QM, there has been a debate about whether \( \mathcal{PT} \)-symmetric QM is more general than the conventional QM. In the first paper about the \( \mathcal{PT} \) symmetry, Bender and Boettcher stressed that the \( \mathcal{PT} \) symmetry is a weaker condition than Hermiticity and a \( \mathcal{PT} \)-symmetric theory can be considered as a complex extension of a conventional Hermitian theory [1]. In 2002, Bender \textit{et al} constructed a positive-definite norm of \( \mathcal{PT} \)-symmetric QM using the newly discovered \( C \) operator [2]. The claim that the \( \mathcal{PT} \) symmetry is more general than Hermiticity was restated in the title of the paper ‘\textit{Complex Extension of Quantum Mechanics}.’ Interestingly, in the same year, Mostafazadeh pointed out that all pseudo-Hermitian Hamiltonians are Hermitian (self-adjoint) with respect to a positive-semidefinite inner product [5]. As such a \( \mathcal{PT} \)-symmetric Hamiltonian can be considered as a special case of a pseudo-Hermitian Hamiltonian with a real spectrum. In 2003, Mostafazadeh...
showed that diagonalizable pseudo-Hermitian Hamiltonians are extensions of \( PT \)- or \( CPT \)-symmetric Hamiltonians [6]. A less general result was obtained independently by Bender et al in [7]. But they took a different point of view which can be seen from the title of the paper: ‘All Hermitian Hamiltonians Have Parity’.

The study of finite-dimensional matrix Hamiltonians may shed some light on the debate. The original \( 2 \times 2 \) \( PT \)-symmetric matrix Hamiltonian introduced in [2] has three real parameters. In 2003, Bender et al extended it to a four-parameter class and to higher dimensions [8]. From their results, they identified \( PT \)-symmetric Hamiltonians and Hermitian Hamiltonians as two distinct extensions of real-symmetric Hamiltonians. For matrix dimension higher than two, \( PT \)-symmetric Hamiltonians have less real parameters than Hermitian Hamiltonians in the same dimension. This view was challenged immediately by Mostafazadeh in a paper titled ‘Exact \( PT \)-Symmetry Is Equivalent to Hermiticity’ [9]. In this paper, the author constructed a \( 2 \times 2 \) \( PT \)-symmetric Hamiltonian with five real parameters. In 2006, Mostafazadeh and Özçelik explicitly constructed the most general \( 2 \times 2 \) quasi-Hermitian Hamiltonian with six real parameters [10].

In this paper, we are trying to settle the debate by constructing the most general \( PT \)-symmetric matrix Hamiltonians. Part of the reason for the debate is the different usage of the terminology. To avoid further confusion, we restrict the term ‘Hermitian conjugate’ or ‘\( \dagger \)’ in the Dirac sense: complex conjugate and transpose. In the present paper, we formulate \( PT \)-symmetric QM slightly different from the literature in two aspects. First, we define the time reversal operator as the Dirac conjugation rather than just the complex conjugation used in [1, 2, 8]. Second, we do not introduce any biorthonormal basis as in [5, 9]. We link the \( CPT \)-inner product to the general inner product in a linear vector space with a weight function. The latter is the standard notation which can be found in modern quantum mechanics textbooks such as [11].

With this formulation, we solve for the general \( \mathcal{P} \) operator and present the solutions explicitly in the case of \( 2 \times 2 \) and \( 3 \times 3 \). Using the general \( \mathcal{P} \) operators, we construct the general \( PT \)-symmetric matrix Hamiltonians. We confirm that the most general \( 2 \times 2 \) \( PT \)-symmetric Hamiltonian has six real parameters as shown in [10]. We find that the general \( 3 \times 3 \) \( PT \)-symmetric Hamiltonian has 13 real parameters. In the case of \( 2 \times 2 \), the general \( PT \)-symmetric Hamiltonian represents the most general matrix Hamiltonian with a real spectrum. Interestingly, this is not true in the case of \( 3 \times 3 \). In both cases, we show clearly that all Hermitian Hamiltonians are just special cases of \( PT \)-symmetric Hamiltonians. From these finite-dimensional results, we conjecture that \( PT \) symmetry is a generalization of Hermiticity in general.

The paper is organized as follows. In section 2, we give our formulation of \( PT \)-symmetric QM. In section 3, we illustrate our ideas in the case of \( 2 \times 2 \). All relevant operators or matrices are calculated explicitly. Special cases discussed in the literature are analyzed. In section 4, we construct the \( \mathcal{P} \) operator and the \( PT \)-symmetric Hamiltonian in the case of \( 3 \times 3 \). Finally, in section 5, we give some concluding remarks.

2. **\( PT \)-symmetric quantum mechanics**

In this section, we formulate \( PT \)-symmetric QM. We start with a brief summary on the inner product in QM. We adopt the notation used in [11].

2.1. **Inner product**

In quantum mechanics, the Hilbert space can be considered as a linear vector space associated with an inner product. The inner product between two quantum states, denoted \((\cdot, \cdot)\), must
satisfy the following conditions [11]:

1. \((\psi, \phi)\) is a complex number;
2. \((\psi, \phi) = (\phi, \psi)^\ast\), where \(\ast\) denotes complex conjugate;
3. \((\psi, c_1\phi_1 + c_2\phi_2) = c_1(\psi, \phi_1) + c_2(\psi, \phi_2)\), where \(c_1\) and \(c_2\) are complex numbers and
4. \((\phi, \phi) \geq 0\), with equality holding if and only if \(\phi = 0\).

In general, we may define the inner product as

\[
(\psi, \phi) \equiv (\psi|W|\phi),
\]

where \(W\) is the weight function and the bra state is defined as the Hermitian conjugate of the ket state \(\langle \cdot | \equiv | \cdot \rangle^\dagger\) [11].

From equation (2.1) and the first three properties of the inner product, it can be easily shown that \(W\) must be a Hermitian operator: \(W = W^\dagger\). From the fourth property of the inner product, \(W\) has to be positive definite. That is, all the eigenvalues of \(W\) are positive.

In the Hilbert space defined above, a self-adjoint operator, such as the Hamiltonian \(H\), satisfies

\[
(\psi, H\phi) = (H\psi, \phi)
\]

for the arbitrary states \(\phi\) and \(\psi\). All eigenvalues of a self-adjoint operator are real. And the eigenstates corresponding to different eigenvalues are orthogonal [11].

Plugging the self-adjoint condition (2.2) into the definition of the inner product in (2.1), we obtain

\[
WH = H^\dagger W.
\]

We may consider this equation as the definition of the weight function \(W\) for a given Hamiltonian \(H\). Thus, the inner product is dynamic (Hamiltonian dependent) in general.

In conventional QM, the weight function can be chosen as the identity operator. In this case, the self-adjoint condition in (2.3) reduces to the Hermiticity condition: \(H = H^\dagger\). Since the identity operator is independent of Hamiltonians, the inner product is no longer dynamic.

2.2. \(\mathcal{P}\mathcal{T}\) symmetry

We define the time reversal operator \(T\) as a Dirac conjugate. That is, for an operator \(A\),

\[
TAT = A^\dagger.
\]

It follows that \(T^2 = \mathbb{1}\); here \(\mathbb{1}\) is the identity matrix. Note that our definition of the \(T\) operator differs from \([1, 2, 8]\). This definition allows us to have a more general parity operator.

For the parity operator \(\mathcal{P}\), we demand it to commute with the time reversal operator and to be an involution. That is,

1. \([\mathcal{P}, T] = 0\), or equivalently, \(\mathcal{P} = \mathcal{P}^\dagger\);
2. \(\mathcal{P}^2 = \mathbb{1}\).

There are obviously two trivial solutions to these constraints,

\[
\mathcal{P}_0 = \pm \mathbb{1}.
\]

We will discuss the non-trivial \(2 \times 2\) solutions of \(\mathcal{P}\) in section 3 and \(3 \times 3\) in section 4.

A \(\mathcal{P}\mathcal{T}\)-symmetric Hamiltonian commutes with the combination operator \(\mathcal{P}\mathcal{T}\):

\[
[H, \mathcal{P}\mathcal{T}] = 0 \iff \mathcal{P}H^\dagger\mathcal{P} = H.
\]

Using the trivial solutions of \(\mathcal{P}_0\) in (2.5), we get that a \(\mathcal{P}_0\mathcal{T}\)-symmetric Hamiltonian is Hermitian:

\[
[H, \mathcal{P}_0\mathcal{T}] = 0 \iff H = H^\dagger.
\]
In this sense, a Hermitian Hamiltonian is $\mathcal{PT}$-symmetric with $\mathcal{P}_0$ to be the plus or minus identity matrix.

In general, the eigenstates of a $\mathcal{PT}$-symmetric Hamiltonian with different eigenvalues are not orthogonal with respect to the Dirac inner product. To solve this problem, one may define a $\mathcal{PT}$ inner product as

$$\langle \psi, \phi \rangle_{\mathcal{PT}} \equiv \langle \psi | \mathcal{P} | \phi \rangle.$$  \hspace{1cm} (2.8)

From the commutation relation between $H$ and $\mathcal{P}$, it can be shown that the eigenstates of $H$ with different eigenvalues are orthogonal with respect to the $\mathcal{PT}$ inner product $[1, 3]$.

However, the norm with respect to the $\mathcal{PT}$ inner product is not positive definite. This is simply because $\mathcal{P}$ has negative eigenvalues. One has to normalize the eigenstates to $\pm 1$.

To overcome this difficulty, one needs to find a positive-definite norm by introducing the $\mathcal{C}$ operator $[2]$. Here, we define the $\mathcal{C}$ operator as

$$\mathcal{C} \equiv \sum_i |E_i\rangle\langle E_i| \mathcal{P},$$  \hspace{1cm} (2.9)

where $|E_i\rangle$ are the eigenstates of $H$ with the $\mathcal{PT}$-norm $+1$ or $-1$.

Our definition of the $\mathcal{C}$ operator has the same properties as the one constructed in $[2]$. From the orthogonality and the (non-positive-definite) normalization of the $\mathcal{PT}$ inner product, it can be shown that $|E_i\rangle$ are the eigenstates of $\mathcal{C}$ with the eigenvalue equal to the $\mathcal{PT}$-norm:

$$\mathcal{C}|E_i\rangle = \langle E_i|\mathcal{P}|E_i\rangle |E_i\rangle.$$  \hspace{1cm} (2.10)

Thus, $\mathcal{C}$ commutes with $H$. The $\mathcal{C}$ operator also commutes with $\mathcal{PT}$: $[\mathcal{C}, \mathcal{PT}] = 0$. This fact can be verified by using $\mathcal{P}\mathcal{C}^\dagger \mathcal{P} = \mathcal{C}$. Because the eigenvalues of $\mathcal{C}^2$ are all unity, the $\mathcal{C}$ operator is an involution just like the $\mathcal{P}$ operator.

Note that we do not require $|E_i\rangle$ to be the simultaneous eigenstates of $\mathcal{PT}$ and of $H$. In fact, this can only be achieved in the special cases of symmetric matrices, such as Hamiltonians constructed in $[2, 8]$. We will discuss more details about these two examples in section 3.

Equipped with the $\mathcal{C}$ operator, we construct an inner product with the positive-definite norm. We define the $\mathcal{CPT}$ inner product as

$$\langle \psi, \phi \rangle_{\mathcal{CPT}} \equiv \langle \psi | \mathcal{P}\mathcal{C} | \phi \rangle.$$  \hspace{1cm} (2.11)

Comparing to the general inner product in (2.1), we recognize that the weight function for the $\mathcal{CPT}$-inner product is

$$W = \mathcal{P}\mathcal{C}.$$  \hspace{1cm} (2.12)

Since the weight function is positive definite, we may find its square root $W = \eta^2$, where $\eta$ is Hermitian, $\eta^\dagger = \eta$. Using the operator $\eta$, we may define a Hermitian Hamiltonian $h$, which has same spectrum as a $\mathcal{PT}$-symmetric Hamiltonian $H$ $[9]$,

$$h \equiv \eta H \eta^{-1}, \quad \text{where} \quad h = h^\dagger.$$  \hspace{1cm} (2.13)

We would like to emphasize that the transformation $\eta$ is Hermitian rather than unitary; hence, the above relation is not unitary equivalence in the usual sense.

### 3. 2 × 2 case

In this section, we illustrate the ideas presented in the previous section by using $2 \times 2$ matrices. We find that any $2 \times 2$ Hermitian matrix is a special case of the general $\mathcal{PT}$-symmetric matrices. Furthermore, it is found that the most general matrix with a real spectrum must coincide with the general $\mathcal{PT}$-symmetric matrix we constructed.
Since the \( \mathcal{P} \) operator is an involution, it is a square root of the identity matrix. In \( 2 \times 2 \) matrices, other than the trivial roots in (2.5), there is a non-trivial root with the form

\[
\mathcal{P} = \begin{pmatrix}
\cos \theta & \sin \theta e^{-i \varphi} \\
\sin \theta e^{i \varphi} & -\cos \theta
\end{pmatrix},
\]

(3.1)

where \( \theta \) and \( \varphi \) are the two real parameters. In terms of the Pauli matrices, the \( \mathcal{P} \) operator can be written as \( \mathcal{P} = \mathbf{n}' \cdot \mathbf{\sigma} \), where \( \mathbf{n}' \equiv (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \) is a unit vector.

To find the general \( \mathcal{P} \mathcal{T} \)-symmetric Hamiltonian, we use the following ansatz:

\[
\mathcal{H} = \varepsilon \mathbb{1} + \alpha \cdot \mathbf{\sigma},
\]

(3.2)

where \( \varepsilon \) and \( \alpha \equiv (\alpha_x, \alpha_y, \alpha_z) \) are complex numbers. Plugging the above ansatz into (2.6), we get the equations satisfied by \( \varepsilon \) and \( \alpha \):

\[
\varepsilon = \varepsilon^*, \quad \alpha + \alpha^* = 2(\alpha^* \cdot \mathbf{n}')\mathbf{n}'.
\]

(3.3)

The first equation simply says that \( \varepsilon \) is real. The second equation can be written as

\[
\sum_i M_{ki} \alpha_i = \alpha_k^* \quad \text{with} \quad M_{ki} \equiv -\delta_{ki} + 2n'_i n'_k.
\]

(3.4)

In this form, the searching for a \( \mathcal{P} \mathcal{T} \)-symmetric Hamiltonian becomes an eigenvalue problem. If we separate the real part and the imaginary part as \( \alpha = \mathbf{A} + i \mathbf{B} \), then \( \mathbf{A} \) and \( \mathbf{B} \) can be considered as the eigenvectors of the matrix \( M \) with eigenvalues +1 and −1, respectively. The matrix \( M \) always has one eigenvector with eigenvalue +1, and two eigenvectors with eigenvalue −1. It is easy to show that the eigenvector with a positive eigenvalue is parallel to \( \mathbf{n}' \), and the eigenvectors with a negative eigenvalue are perpendicular to \( \mathbf{n}' \). Thus, the solutions to the eigenvalue problem are

\[
\mathbf{A} = \gamma \mathbf{n}', \quad \mathbf{B} = \mu \mathbf{n}^0 + v \mathbf{n}^v,
\]

(3.5)

where \( \gamma, \mu \) and \( v \) are the real parameters, and \( \mathbf{n}^0 \equiv (\cos \theta \cos \varphi, \cos \theta \sin \varphi, -\sin \theta) \) and \( \mathbf{n}^v \equiv (-\sin \varphi, \cos \varphi, 0) \) are the two unit vectors.

Thereafter, plugging \( \alpha = \gamma \mathbf{n}' + i \mu \mathbf{n}^0 + i v \mathbf{n}^v \) into the ansatz in (3.2), we get the general \( \mathcal{P} \mathcal{T} \)-symmetric \( 2 \times 2 \) Hamiltonian matrix

\[
\mathcal{H} = \varepsilon \mathbb{1} + (\gamma \mathbf{n}' + i \mu \mathbf{n}^0 + i v \mathbf{n}^v) \cdot \mathbf{\sigma}
\]

\[
= \begin{pmatrix}
\varepsilon + \gamma \cos \theta - i \mu \sin \theta & (\gamma \sin \theta + i \mu \cos \theta + v) e^{-i \varphi} \\
(\gamma \sin \theta + i \mu \cos \theta - v) e^{i \varphi} & \varepsilon - \gamma \cos \theta + i \mu \sin \theta
\end{pmatrix}.
\]

(3.6)

This Hamiltonian has six real parameters: \( \varepsilon, \gamma, \mu, \nu, \theta \) and \( \varphi \). All \( 2 \times 2 \) Hermitian matrices can be recovered as special cases with \( \mu = \nu = 0 \). In other words, the \( \mathcal{P} \mathcal{T} \) symmetry is a generalization of Hermiticity.

The eigenvalues of the Hamiltonian \( \mathcal{H} \) are

\[
E_{\pm} = \varepsilon \pm \sqrt{\gamma^2 - \mu^2 - \nu^2}.
\]

(3.7)

For eigenvalues to be real, it requires \( \gamma^2 \geq \mu^2 + \nu^2 \). For simplicity, we consider only the non-degenerated case with \( \gamma^2 > \mu^2 + \nu^2 \) in this paper. The corresponding eigenstates are

\[
\langle E_{\pm} \rangle = \frac{u}{\sqrt{2}} \begin{pmatrix}
\frac{e^{i \kappa_0 - i \varphi}}{\sqrt{1 + \frac{1}{\gamma} \sin \theta}} \\
\frac{e^{i \kappa_\pm}}{\sqrt{1 - \frac{1}{\gamma} \sin \theta}}
\end{pmatrix} \begin{pmatrix} 1 + \frac{1}{\gamma} \sin \theta \pm \frac{1}{\gamma} \sqrt{\gamma^2 - \mu^2 - \nu^2} \cos \theta \end{pmatrix},
\]

(3.8)

where we have defined three angles and a normalization constant as

\[
\kappa_0 \equiv \arg (\gamma \sin \theta + \nu + i \mu \cos \theta),
\]

\[
\kappa_\pm \equiv \arg (-\gamma \cos \theta \pm \sqrt{\gamma^2 - \mu^2 - \nu^2} + i \mu \sin \theta),
\]

(3.9)

\[
u \equiv \sqrt{\frac{\gamma^2}{\gamma^2 - \mu^2 - \nu^2}}.
\]
The normalization is chosen such that
\[ \langle E_\pm | P | E_\pm \rangle = \pm \text{sign}(\gamma). \] (3.10)

The six-parameter class of the matrix in (3.6) with the condition \( \gamma^2 \geq \mu^2 + \nu^2 \) coincides with the most general 2 \( \times \) 2 matrix with only real eigenvalues. Qualitatively, this can be seen from parameter counting. A general complex 2 \( \times \) 2 matrix has eight real parameters. The reality of all eigenvalues puts two constraints on the matrix. Therefore, the most general 2 \( \times \) 2 matrix with only real eigenvalues should consist of six real parameters.

This coincidence can also be proved rigorously. By direct computation, the eigenvalues of an arbitrary 2 \( \times \) 2 matrix with the form of the ansatz in (3.2) are \( E_\pm = \epsilon \pm \sqrt{\alpha \cdot \alpha} \). Imposing reality condition on the eigenvalues leads to
\[ \epsilon = \epsilon^*, \quad \alpha \cdot \alpha \geq 0. \] (3.11)

The first condition is the same constraint on the parameter \( \epsilon \) as in the \( PT \)-symmetric Hamiltonian in (3.6). The second condition in (3.11) implies that the real part and the imaginary part of \( \alpha \) are perpendicular to each other, \( A \cdot B = 0 \), and that the real part vector is not shorter than the imaginary part vector, \( A \cdot A \geq B \cdot B \). Without loss of generality, we may parametrize the real part vector as \( A = \gamma n_r \). Then the above conditions lead to a unique solution for the imaginary part vector which can be parametrized as \( B = \mu n_\theta + \nu n_\phi \). Since \( A \) is not shorter than \( B \), we have \( \gamma^2 \geq \mu^2 + \nu^2 \). Clearly then, the \( PT \)-symmetric Hamiltonian in (3.6) represents the most general 2 \( \times \) 2 matrices with only real eigenvalues.

For the \( PT \)-symmetric Hamiltonian \( H \) in (3.6), the \( C \) operator can be calculated directly from its definition in (2.9). It is also straightforward to construct it from the relation in (2.10). Either way, the \( C \) operator is found to be
\[ C = \frac{u}{\gamma} \alpha \cdot \sigma. \] (3.12)

The form of the \( C \) operator is not a surprise because it is defined as an involution. Therefore, it must be a square root of the identity matrix just like the \( P \) operator. This fact can be easily verified by observing that \((u/\gamma)\alpha\) is a unit vector.

Because the \( C \) operator has the eigenvalues \( C |E_\pm\rangle = \pm \text{sign}(\gamma) |E_\pm\rangle \), the eigenstates in (3.8) are normalized to unity with respect to the \( CPT \)-inner product. Thus, we have a set of orthonormal eigenstates,
\[ \langle E_i | PC | E_j \rangle = \delta_{ij}, \quad i, j = \pm. \] (3.13)

The weight function has the form
\[ W = PC = u (\mathbb{1} + \beta \cdot \sigma), \quad \text{where} \quad \beta \equiv \frac{\nu}{\gamma} \mathbb{n}_\theta - \frac{\mu}{\gamma} \mathbb{n}_\phi. \] (3.14)

Note that \( \beta \) is a unit vector, and it is perpendicular to \( \alpha \). Interestingly, the square root of \( W \) has the form
\[ \eta_\pm = \frac{1}{\sqrt{2(u \pm 1)}} (W \pm \mathbb{1}). \] (3.15)

There are two solutions for \( \eta \), which is not because of the arbitrary overall sign in the square root. Rather, it is corresponding to the two choices of mapping the eigenstates during the similarity transformation in (2.13). In the Hermitian limit, \( W \to \mathbb{1} \), \( \eta \) is once again a square root of the identity matrix. The ‘+’ sign in (3.15) has the limit \( \eta_+ \to \mathbb{1} \) and the ‘−’ sign has the limit \( \eta_- \to n_3 \cdot \sigma \), where \( n_3 \) is the unit vector in the direction of \( \beta \).

Using the operator \( \eta \), we find the Hermitian equivalence of the \( PT \)-symmetric Hamiltonian \( H \) in (3.6):
\[ h = \epsilon \mathbb{1} \pm \frac{\gamma}{u} n_r \cdot \sigma. \] (3.16)
Now let us consider some special cases. We show that both Hermitian Hamiltonians and several \( P T \)-symmetric 2 \( \times \) 2 Hamiltonians studied in the literature can be reduced from our general \( P T \)-symmetric Hamiltonian in (3.6).

3.1. Special case 1: Hermiticity

If we set \( \mu = \nu = 0 \), \( H \) becomes Hermitian, \( H = H^\dagger \),

\[
H_{\text{Hermitian}} = \left( \begin{array}{cc} \varepsilon & \gamma \\
\gamma & \varepsilon \end{array} \right),
\]

This matrix Hamiltonian has four real parameters, and it includes all 2 \( \times \) 2 Hermitian matrices.

In this case, the weight function reduces to the identity matrix and the \( C \) operator coincides with the parity operator:

\[
W_{\text{Hermitian}} = 1, \quad C_{\text{Hermitian}} = P.
\]

All these observations are consistent with the conventional QM. We may say that the Hermitian Hamiltonian is a special case of the \( P T \)-symmetric Hamiltonian with \( C = P \). Or, equivalently, \( P T \) symmetry is a generalization of Hermiticity.

3.2. Special case 2: Bender–Brody–Jones Hamiltonian

In [2], Bender et al studied a \( P T \)-symmetric Hamiltonian with real and symmetric off-diagonal matrix elements. Their choice of the parity operator is \( P_{\text{BBJ}} = \sigma_x \). This case can be reduced from our general case by setting \( \nu = \phi = 0 \) and \( \theta = \pi/2 \). In particular, we have

\[
H_{\text{BBJ}} = \left( \begin{array}{cc} \varepsilon - \mu \gamma & \gamma \\
\gamma & \varepsilon + \mu \gamma \end{array} \right), \quad C_{\text{BBJ}} = \sqrt{\frac{\gamma^2 - \mu^2}{\gamma^2}} \left( \begin{array}{cc} -i & 1 \\
1 & i \end{array} \right).
\]

These expressions are equivalent to those in [2] by mapping our parameters \( \varepsilon, \mu \) and \( \gamma \) to \( r \cos \theta, -r \sin \theta \) and \( s \) therein.

3.3. Special case 3: Bender–Meisinger–Wang Hamiltonian

In [8], Bender et al generalized the Hamiltonian matrix in [2] by choosing a one-parameter class of parity operator,

\[
P_{\text{BMW}} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & -\cos \theta \end{pmatrix}.
\]

This can be recovered by setting \( \varphi = 0 \) in (3.1). If we consider only symmetric Hamiltonian as in [8], we can further set \( \nu = 0 \) in (3.6). With this choice of parameters, we have

\[
H_{\text{BMW}} = \left( \begin{array}{cc} \varepsilon + \gamma \cos \theta - i \mu \sin \theta & \gamma \sin \theta + i \mu \cos \theta \\
\gamma \sin \theta + i \mu \cos \theta & \varepsilon - \gamma \cos \theta - i \mu \sin \theta \end{array} \right),
\quad C_{\text{BMW}} = \sqrt{\frac{\gamma^2 - \mu^2}{\gamma^2}} \left( \begin{array}{cc} \cos \theta - i \mu \sin \theta & \sin \theta + i \mu \gamma \\
\sin \theta + i \mu \gamma & -\cos \theta + i \mu \sin \theta \end{array} \right).
\]

Once again, these are the same formulas as in [8] by properly mapping the parameters.

The symmetric Hamiltonian, \( H \) in (3.6) with \( \nu = \varphi = 0 \), has additional properties. In this case, the eigenstates of \( H \) are also the eigenstates of \( PT \). By choosing a proper phase, the eigenvalue of \( PT \) can be set to unity:

\[
PT |E_{\pm}\rangle = P|E_{\pm}\rangle^* = |E_{\pm}\rangle.
\]
One may think that our definition of the $CPT$-inner product is slightly different from the one in the literature. In [2, 8] the $CPT$-inner product was defined as

$$(\psi, \phi)_{BBJ-BMW} = (CPT|\psi\rangle)^T |\phi\rangle = (\psi|P^TC^T|\phi\rangle),$$

where $T$ denotes the matrix transpose. This definition leads to a weight function $W_{BBJ-BMW} = P^TC^T$. Since both $P$ and $C$ are symmetric in this case, the two definitions of the inner product are actually the same.

### 3.4. Special case 4: Mostafazadeh Hamiltonian

In [9], Mostafazadeh introduced a five-parameter class of Hamiltonians with the form

$$H_{\text{Mostafazadeh}} = \begin{pmatrix}
 r + t \cos \phi - i s \sin \phi & t \sin \phi + i(s \cos \phi - u) \\
 t \sin \phi + i(s \cos \phi + u) & r - t \cos \phi + i s \sin \phi
\end{pmatrix}.$$  

(3.24)

This is a special case of our general Hamiltonian in (3.6) by the following parameter mapping:

$$\varepsilon \rightarrow r, \quad \gamma \rightarrow \sqrt{t^2 + u^2},$$

$$\mu \rightarrow \frac{s \sqrt{t^2 + u^2} \sin \phi}{\sqrt{t^2 \sin^2 \phi + u^2}}, \quad \nu \rightarrow -\frac{s u \cos \phi}{\sqrt{t^2 \sin^2 \phi + u^2}},$$

$$\cos \theta \rightarrow \frac{t \cos \phi}{\sqrt{t^2 + u^2}}, \quad \tan \varphi \rightarrow \frac{\mu}{t \sin \phi}.$$  

(3.25)

### 3.5. Special case 5: Mostafazadeh–Özçelik Hamiltonian

In [10], Mostafazadeh and Özçelik constructed a six-parameter class of Hamiltonians with a very elegant form

$$H_{\text{MO}} = \begin{pmatrix}
 \cos \Theta & e^{-i\Phi} \sin \Theta \\
e^{i\Phi} \sin \Theta & \cos \Theta
\end{pmatrix}.$$  

(3.26)

where $q$ and $E$ are real, and $\Theta$ and $\Phi$ are complex. In principle, this Hamiltonian is equivalent to our Hamiltonian in (3.6) by the following parameter mapping:

$$\varepsilon \rightarrow q, \quad \pm \sqrt{\gamma^2 - \mu^2 - \nu^2} \rightarrow E,$$

$$\gamma \cos \theta - i \mu \sin \theta \rightarrow E \cos \Theta, \quad \gamma \sin \theta + i \mu \cos \theta - \nu \rightarrow \frac{\gamma \sin \theta + i \mu \cos \theta + \nu}{\sqrt{\gamma^2 \sin^2 \Theta + \mu^2 \cos^2 \Theta + \nu^2}} e^{2i\Phi}.$$  

(3.27)

However, at the degenerate point, $E = 0$ in (3.26) or $\gamma^2 = \mu^2 + \nu^2$ in (3.6), these two parametrizations are no longer equivalent. At this special point, $H_{\text{MO}}$ is proportional to the identity matrix but $H$ in (3.6) is not.

### 4. 3 × 3 case

In this section, we reveal the general form of $\mathcal{PT}$-symmetric $3 \times 3$ matrix Hamiltonians. In this case, we use the Gell–Mann matrices, which are the generalization of the Pauli matrices in $3 \times 3$. Any $3 \times 3$ matrix can be written as a linear combination of the identity matrix and the eight Gell–Mann matrices. If a matrix is Hermitian, the expansion coefficients are all real.

There are two types of solutions for the $\mathcal{P}$ operator as well. The first type is the trivial solutions $\mathcal{P}_0 = \pm \mathbb{I}$. The second type is the non-trivial solutions. If we expand the non-trivial solutions of $\mathcal{P}$ as

$$\mathcal{P}_{3 \times 3} = \pm \left( \mathbb{I} + \sum_{i=1}^{8} P_i \lambda_i \right),$$  

(4.1)
where $\lambda_i$ are Gell–Mann matrices for $i = 1, \ldots, 8$, we find that
\[ P_0 = \frac{1}{3} \]
and that the coefficients $P_i$ depend on four independent parameters. We thus choose the parametrization as
\[
\begin{align*}
P_4 &= \sin 2\chi \sin \theta \cos \varphi, \\
P_5 &= \sin 2\chi \sin \theta \sin \varphi, \\
P_6 &= \sin 2\chi \cos \theta \cos \rho, \\
P_7 &= \sin 2\chi \cos \theta \sin \rho.
\end{align*}
\]
(4.3)

The other four components $P_1, P_2, P_3,$ and $P_8$ depend on the sign of $\cos 2\chi$. For the case of $\cos 2\chi \geq 0$, we have
\[
\begin{align*}
P_1 &= -\sin^2 \chi \sin 2\theta \cos(\rho - \varphi), \\
P_2 &= \sin^2 \chi \sin 2\theta \sin(\rho - \varphi), \\
P_3 &= \sin^2 \chi \cos 2\theta, \\
P_8 &= \frac{1}{2\sqrt{3}} (1 + 3 \cos 2\chi).
\end{align*}
\]
(4.4)

Plugging $P_0$ and $P_i$ into (4.1), we get the non-trivial four-parameter solutions of the $P$ operator with the form
\[
P_{3\times 3} = \pm \begin{pmatrix} 
\cos 2\chi \sin^2 \theta + \cos^2 \theta & -\sin^2 \chi \sin 2\theta \ e^{i(\rho - \varphi)} & \sin 2\chi \sin \theta \ e^{-i\varphi} \\
-\sin^2 \chi \sin 2\theta \ e^{-i(\rho - \varphi)} & \cos 2\chi \cos^2 \theta + \sin^2 \theta & \sin 2\chi \cos \theta \ e^{-i\varphi} \\
\sin 2\chi \sin \theta \ e^{i\varphi} & \sin 2\chi \cos \theta \ e^{i\varphi} & -\cos 2\chi
\end{pmatrix}.
\]
(4.5)

For the case of $\cos 2\chi < 0$, the correct results are obtained by replacing $\cos 2\chi$ by $-\cos 2\chi$ in (4.4) and (4.5).

Just like in the $2\times 2$ case, $\mathcal{PT}$-symmetric Hamiltonians can be found by solving an eigenvalue problem. If we use the ansatz of the Hamiltonian as
\[
H_{3\times 3} = \varepsilon \mathbf{1} + \sum_{i=1}^{8} \alpha_i \lambda_i,
\]
(4.6)
the $\mathcal{PT}$ symmetry leads to the conditions of $\varepsilon = \varepsilon^*$ and that $\alpha_i$ satisfy the eigenvalue equation
\[
\sum_{i=1}^{8} M_{ki} \alpha_i = \alpha_k^*,
\]
(4.7)
where
\[
M_{ki} = P_0^2 \delta_{ki} + 2P_0 \sum_j P_j d^{i|j} + \frac{2}{3} P_0 P_7 + \sum_{jml} P_j P_m (d^{i|j} d^{m|l} + f^{i|j} f^{m|l})
\]
(4.8)
with $d^{i|j}$ and $f^{i|j}$ being the symmetric and antisymmetric structure constants respectively of the SU(3) group.

Once again, the real part of $\alpha_i$ forms the eigenvectors of $M$ with eigenvalue $+1$, and the imaginary part of $\alpha_i$ forms eigenvectors with eigenvalue $-1$. There are always four eigenvectors with eigenvalue $+1$ and four eigenvectors with eigenvalue $-1$.

It is straightforward to show that the vector $P_i$ with components defined in (4.3) and (4.4) is an eigenvector of $M$ with eigenvalue $+1$. All other eigenvectors can be constructed by the derivatives of $P_i$. The set of all four first-order derivatives, $\{ \partial_x P_i, \partial_y P_i, \partial_y P_i, \partial_y P_i \}$, forms a subspace with eigenvalue $-1$. The remaining three eigenvectors with eigenvalue $+1$ can be
constructed from the second derivatives. Below is a choice of orthonormal set of eigenvectors with eigenvalue +1:

\[
A_i^{(1)} = \frac{\sqrt{3}}{2} P_i = \frac{\sqrt{3}}{2} \left( -\sin^2 \chi \sin 2\theta \cos(\rho - \varphi), \sin^2 \chi \sin 2\theta \sin(\rho - \varphi), \sin^2 \chi \cos 2\theta, \\
\sin 2\chi \sin \theta \cos \varphi, \sin 2\chi \sin \theta \sin \varphi, \sin 2\chi \sin \theta \cos \rho, \sin 2\chi \sin \theta \sin \rho, \frac{1 + 3 \cos 2\chi}{2\sqrt{3}} \right),
\]

\[
A_i^{(2)} = \frac{1}{2} \partial \chi P_i + \frac{3}{2} P_i = \frac{1}{2} \left( -3 + \cos 2\chi \cos 2\theta, \frac{3 + \cos 2\chi}{2} \sin 2\theta \sin(\rho - \varphi), \frac{3 + \cos 2\chi}{2} \cos 2\theta, \\
-\sin 2\chi \sin \theta \cos \varphi, -\sin 2\chi \sin \theta \sin \varphi, -\sin 2\chi \cos \theta \cos \rho, -\sin 2\chi \cos \theta \sin \rho, \sqrt{3} \sin^2 \chi \right),
\]

\[
A_i^{(3)} = \left( -\cos \chi \cos 2\theta \sin(\rho - \varphi), \cos \chi \cos 2\theta \cos(\rho - \varphi), -\cos \chi \sin 2\theta, \\
-\sin \chi \cos \theta \cos \varphi, -\sin \chi \cos \theta \sin \varphi, \sin \chi \sin \theta \cos \rho, \sin \chi \sin \theta \sin \rho, 0 \right),
\]

\[
A_i^{(4)} = \left( \cos \chi \sin(\rho - \varphi), \cos \chi \cos(\rho - \varphi), 0, -\sin \chi \cos \theta \sin \varphi, \sin \chi \cos \theta \cos \varphi, \\
\sin \chi \sin \theta \sin \rho, -\sin \chi \sin \theta \cos \rho, 0 \right).
\] 

Likewise, a set of eigenvectors with eigenvalue −1 can be chosen as

\[
B_i^{(1)} = \frac{1}{2} \partial \chi P_i = \frac{1}{2} \left( -\sin 2\chi \sin 2\theta \cos(\rho - \varphi), \sin 2\chi \sin 2\theta \sin(\rho - \varphi), \\
\sin 2\chi \cos 2\theta, 2 \cos 2\chi \sin \theta \cos \varphi, \\
2 \cos 2\chi \sin \theta \sin \varphi, 2 \cos 2\chi \cos \theta \cos \rho, 2 \cos 2\chi \cos \theta \sin \rho, -\sqrt{3} \sin 2\chi \right),
\]

\[
B_i^{(2)} = \frac{1}{2 \sin \chi} \partial \theta P_i = \frac{1}{2 \sin \chi} \left( -\sin \chi \cos 2\theta \cos(\rho - \varphi), \sin \chi \cos 2\theta \sin(\rho - \varphi), -\sin \chi \sin 2\theta, \\
\cos \chi \cos \theta \cos \varphi, \cos \chi \cos \theta \sin \varphi, -\cos \chi \sin \theta \cos \rho, -\cos \chi \sin \theta \sin \rho, 0 \right),
\]

\[
B_i^{(3)} = \frac{\partial \phi P_i + \partial \varphi P_i}{\sin 2\chi} = \left( 0, 0, -\sin \theta \sin \varphi, \sin \theta \cos \varphi, -\cos \theta \sin \rho, \cos \theta \cos \rho, 0 \right),
\]

\[
B_i^{(4)} = \left( \sin \chi \sin(\rho - \varphi), \sin \chi \cos(\rho - \varphi), 0, \cos \chi \cos \theta \sin \varphi, \\
-\cos \chi \cos \theta \cos \varphi, -\cos \chi \sin \theta \sin \rho, \cos \chi \sin \theta \cos \rho, 0 \right).
\] 

(4.9)
With the solution of $\alpha_i = A_i + iB_i$, we can construct the general $3 \times 3$ $\mathcal{PT}$-symmetric Hamiltonian by plugging the above results into the ansatz in (4.6):

$$H_{3 \times 3} = \varepsilon \mathbb{I} + \sum_{i=1}^{8} \left[ \gamma_1 A_1^{(i)} + \gamma_2 A_2^{(i)} + \gamma_3 A_3^{(i)} + \gamma_4 A_4^{(i)} + i(\mu_1 B_1^{(i)} + \mu_2 B_2^{(i)} + \mu_3 B_3^{(i)} + \mu_4 B_4^{(i)}) \right] \lambda_i.$$

This construction has 13 real parameters, four in $\mathcal{P}$, four $\gamma$’s, four $\mu$’s and one $\varepsilon$. Any $3 \times 3$ Hermitian Hamiltonian can be considered as a special case with all $\mu$’s vanishing, which also has the correct number of parameters: nine. Unlike the $2 \times 2$ case, the general $\mathcal{PT}$-symmetric matrix Hamiltonian in (4.11) does not present all $3 \times 3$ matrices with all real eigenvalues. This can be seen by a simple parameter counting. A $3 \times 3$ matrix with all real eigenvalues should have 15 real parameters, but $H_{3 \times 3}$ in (4.11) only has 13 parameters.

5. Conclusion

In this paper, we find the general $\mathcal{P}$ operator and construct the general $\mathcal{PT}$-symmetric matrix Hamiltonians in $2 \times 2$ and $3 \times 3$. In both cases, the $\mathcal{PT}$ symmetry can be considered as a generalization of Hermiticity. We conjecture that this statement is true in general.

We convert the searching for a general $\mathcal{PT}$-symmetric Hamiltonian problem to an eigenvalue problem. This method also applies to higher dimensions. For example, the definition for the matrix $M_{ki}$ in (4.8) can be easily generalized to $N$ dimensions by replacing 3 by $N$.

Acknowledgments

QW is very grateful to Professor Carl M Bender for helpful comments and correspondence. QW would also like to thank Dr Jiangbin Gong for many useful discussions and some help on writing this paper.

References

[1] Bender C M and Boettcher S 1998 Real spectra in non-Hermitian Hamiltonians having $\mathcal{PT}$ symmetry Phys. Rev. Lett. 80 5243–6
[2] Bender C M, Brody D C and Jones H F 2002 Complex extension of quantum mechanics Phys. Rev. Lett. 89 270401
[3] Bender C M 2007 Making sense of non-Hermitian Hamiltonians Rep. Prog. Phys. 70 947–1018 (arXiv:hep-th/0703096)
[4] Mostafazadeh A 2008 Pseudo Hermitian Quantum Mechanics arXiv:0810.5643
[5] Mostafazadeh A 2002 Pseudo Hermiticity for a class of nondiagonalizable Hamiltonians J. Math. Phys. 43 6343–52
[6] Mostafazadeh A 2003 J. Math. Phys. 44 943 (erratum)
[7] Mostafazadeh A 2003 Pseudo Hermiticity and generalized $\mathcal{PT}$- and $\mathcal{CPT}$-symmetries J. Math. Phys. 44 974–89
[8] Bender C M, Meisinger P N and Wang Q 2003 All Hermitian Hamiltonians have parity J. Phys. A: Math. Gen. 36 1029–31 (arXiv:quant-ph/0211123)
[9] Bender C M, Meisinger P N and Wang Q 2003 Finite-dimensional $\mathcal{PT}$-symmetric Hamiltonians J. Phys. A: Math. Gen. 36 6791–7 (arXiv:quant-ph/0303174)
[10] Mostafazadeh A 2003 Exact $\mathcal{PT}$-symmetry is equivalent to Hermiticity J. Phys. A: Math. Gen. 36 7081–92 (arXiv:quant-ph/0304080)
[11] Mostafazadeh A and Özçelik S 2006 Explicit realization of pseudo Hermitian and quasi-Hermitian quantum mechanics for two-level systems Turk. J. Phys. 30 437–43 (arXiv:quant-ph/0607120)
[12] Ballentine L E 1998 Quantum Mechanics: A Modern Development (Singapore: World Scientific)