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Finite-dimensional \mathcal{PT} -symmetric Hamiltonians

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Abstract

This paper investigates finite-dimensional \mathcal{PT} -symmetric Hamiltonians. In doing so, it clarifies some of the claims made in earlier papers on \mathcal{PT} -symmetric quantum mechanics. In particular, it is shown here that there are two ways to extend real symmetric Hamiltonians into the complex domain: (i) the usual approach is to generalize such Hamiltonians to include complex Hermitian Hamiltonians. (ii) Alternatively, one can generalize real symmetric Hamiltonians to include complex \mathcal{PT} -symmetric Hamiltonians. In the first approach, the spectrum remains real, while in the second approach the spectrum remains real if the \mathcal{PT} symmetry is not broken. Both generalizations give a consistent theory of quantum mechanics, but if D > 2, a D-dimensional Hermitian matrix Hamiltonian has more arbitrary parameters than a D-dimensional \mathcal{PT} -symmetric matrix Hamiltonian.

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1. Introduction

It has been observed that non-Hermitian Hamiltonians that exhibit \mathcal{PT} symmetry can have real spectra. For example, the class of non-Hermitian Hamiltonians

 $H = p^2 + x^2 (ix)^{\nu}$

has positive real discrete spectra so long as v > 0 and appropriate boundary conditions are specified [1–3]. The domain v > 0 is the region of *unbroken* \mathcal{PT} symmetry, while v < 0 is the region of *broken* \mathcal{PT} symmetry. The distinction between these two regions is as follows: when v > 0, the eigenstates of H are also eigenstates of \mathcal{PT} , but when v < 0, the eigenstates of H are not eigenstates of \mathcal{PT} . In the unbroken region the eigenvalues of H are all real and in the broken region some eigenvalues of H may be real, but the rest appear as complex-conjugate pairs.

In a recent paper it was shown that in the region of unbroken \mathcal{PT} symmetry, a \mathcal{PT} -symmetric Hamiltonian possesses an additional symmetry represented by the complex linear operator \mathcal{C} [4]. The operator \mathcal{C} commutes with H and with \mathcal{PT} and can be used to construct an inner product whose associated norm is positive. The theory defined by the complex

(1)



Figure 1. Venn diagram showing that the intersection between the classes of Hermitian and \mathcal{PT} -symmetric matrix Hamiltonians is the class of real symmetric matrix Hamiltonians.

non-Hermitian Hamiltonian (1) with $\nu > 0$ is a fully consistent and unitary theory of quantum mechanics [4].

One might conjecture that \mathcal{PT} symmetry is a generalization of Hermiticity. However, as we will argue in this paper, this view is not quite precise. Rather, we will argue that the appropriate way to construct complex Hamiltonians is to begin with a real symmetric Hamiltonian and to extend the matrix elements into the complex domain in such a way that certain constraints are satisfied. There are two distinct ways to perform this construction. First, one can generalize real symmetric Hamiltonians to the case of Hermitian Hamiltonians and second, one can generalize real symmetric Hamiltonians to the case of \mathcal{PT} -symmetric Hamiltonian is maintained but the matrix elements are allowed to become complex with the condition that the \mathcal{PT} operator commutes with H.

Many of the Hermitian Hamiltonians commonly studied in quantum mechanics are actually real and symmetric. For example, this is the case of the Hamiltonian $H = p^2 + V(x)$ representing a particle in a real potential V(x); this Hamiltonian is real [5]. To show that it is symmetric we display it as a continuous matrix in coordinate space:

$$H(x, y) = -\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}y}\delta(x - y) + V\left(\frac{x + y}{2}\right)\delta(x - y). \tag{2}$$

This matrix is explicitly symmetric under the interchange of x and y. The \mathcal{PT} -symmetric Hamiltonian in (1) is also symmetric in coordinate space; however, it is complex for all $\nu > 0$.¹

In this paper we investigate the case of finite-dimensional matrix Hamiltonians. We show that Hermitian matrix Hamiltonians and \mathcal{PT} -symmetric matrix Hamiltonians are both acceptable generalizations of real symmetric matrix Hamiltonians. Furthermore, they define consistent theories of quantum mechanics. We also demonstrate that for the case of *D*-dimensional matrices, the class of Hermitian matrix Hamiltonians is larger than that of \mathcal{PT} -symmetric matrix Hamiltonians. Specifically, for large *D* the number of real parameters in a real symmetric matrix is asymptotically $\frac{1}{2}D^2$ and the number of real parameters in a Hermitian matrix Hamiltonian is asymptotically $\frac{3}{4}D^2$. The overlap between the classes of Hermitian and \mathcal{PT} -symmetric matrix Hamiltonians is only the class of real symmetric matrices. A Venn diagram showing the relationships between the classes of Hermitian, \mathcal{PT} -symmetric and real symmetric matrix Hamiltonians is given in figure 1.

¹ This Hamiltonian is complex even when ν is a positive even integer because the boundary conditions associated with the eigenvalue problem $H\phi = E\phi$ are complex (see [1]).

2. Construction of \mathcal{PT} -symmetric matrix Hamiltonians

To construct a finite-dimensional \mathcal{PT} -symmetric matrix Hamiltonian, we begin by defining the operators that represent time reversal \mathcal{T} and parity \mathcal{P} . Both of these operators represent discrete reflection symmetries and thus we must have $\mathcal{T}^2 = \mathcal{P}^2 = 1$. Furthermore, we assume \mathcal{T} and \mathcal{P} are independent operators, so that they commute: $[\mathcal{P}, \mathcal{T}] = 0$. Let us define the time reversal operator as complex conjugation. One can also define \mathcal{T} to be Hermitian conjugation (complex conjugation and transpose), but we will see that because all of the relevant matrices in the theory are symmetric, it makes no difference whether \mathcal{T} performs a transpose. It is also possible to choose a more complicated definition for \mathcal{T} . For example, \mathcal{T} could be the combined action of complex conjugation and multiplication by some complex matrix. Such alternative definitions for \mathcal{T} will be considered later and we will argue that without any loss of generality we may define \mathcal{T} to be just complex conjugation.

Next, we consider the operator \mathcal{P} representing parity. Since \mathcal{P} commutes with \mathcal{T} , the entries in the matrix representing \mathcal{P} are all real. Furthermore, we will see that \mathcal{P} must be symmetric. (If it is not symmetric, then we will find that the \mathcal{C} matrix that we will ultimately construct will not commute with the Hamiltonian H. As a result, the quantum theory will violate unitarity. We will return to this point later on.)

Because $\mathcal{P}^2 = 1$ all the eigenvalues of \mathcal{P} are either +1 or -1. To construct the most general *D*-dimensional matrix \mathcal{P} , let us suppose that there are m_+ positive eigenvalues and m_- negative eigenvalues, where $m_+ + m_- = D$. That is, if \mathcal{P} is diagonalized, then it has the form

$$\mathcal{P}_0 = \text{diag}\{1, 1, \dots, 1, -1, -1, \dots, -1\}.$$
(3)

The most general parity matrix can be expressed as

$$\mathcal{P} = R\mathcal{P}_0 R^{-1} \tag{4}$$

where *R* is the most general *D*-dimensional rotation (orthogonal) matrix [6]. One might try to take the matrix *R* to be more general than orthogonal by choosing it to be unitary. However, in this case the parity operator \mathcal{P} will be complex and will not commute with \mathcal{T} .

There are $\frac{1}{2}D(D-1)$ arbitrary parameters in the matrix R. However, there are fewer than this number of parameters in the matrix \mathcal{P} in (4). Indeed, if $m_{-} = 0$ so that \mathcal{P}_{0} is the identity matrix, then there are no arbitrary parameters in \mathcal{P} . The exact number of arbitrary parameters in \mathcal{P} is given by the formula

$$\frac{1}{2}D(D-1) - \frac{1}{2}m_{+}(m_{+}-1) - \frac{1}{2}m_{-}(m_{-}-1).$$
(5)

Clearly, when *D* is even, \mathcal{P} has the greatest number of arbitrary parameters if $m_+ = m_- = \frac{1}{2}D$. When *D* is odd, the number of parameters is maximized if we choose $m_+ - m_- = 1$; that is, $m_+ = \frac{1}{2}(D+1)$ and $m_- = \frac{1}{2}(D-1)$. Thus, for all *D*, the greatest number of parameters in \mathcal{P} is given by the formula

$$\frac{1}{4}D^2 - \frac{1}{8}[1 - (-1)^D].$$
(6)

Let us illustrate these results. The most general one-dimensional parity matrix $\mathcal{P} = 1$ has no free parameters. The most general two-dimensional parity matrix has one parameter:

$$\mathcal{P} = \begin{pmatrix} \cos\phi & \sin\phi\\ \sin\phi & -\cos\phi \end{pmatrix}.$$
(7)

The most general three-dimensional parity matrix has two parameters:

$$\mathcal{P} = \begin{pmatrix} \cos^2 \phi - \sin^2 \phi \cos 2\theta & \sin 2\phi \cos \theta & -\sin^2 \phi \sin 2\theta \\ \sin 2\phi \cos \theta & -\cos 2\phi & \sin 2\phi \sin \theta \\ -\sin^2 \phi \sin 2\theta & \sin 2\phi \sin \theta & \cos^2 \phi + \sin^2 \phi \cos 2\theta \end{pmatrix}.$$
 (8)

Table 1. Number of arbitrary real parameters in the following most general $D \times D$ matrices: (i) real symmetric parity \mathcal{P} , (ii) $\mathcal{P}_0 \mathcal{T}$ -symmetric H_0 , (iii) $\mathcal{P}\mathcal{T}$ -symmetric H, (iv) Hermitian H and (v) real symmetric H.

Dimension D	1	2	3	4	5	6	Large D
Real symmetric \mathcal{P} : $\frac{1}{4}D^2 - \frac{1}{8}[1 - (-1)^D]$	0	1	2	4	6	9	$\sim \frac{1}{4}D^2$
$\mathcal{P}_0\mathcal{T}$ -symmetric $H_0: \frac{1}{2}D(D+1)$	1	3	6	10	15	21	$\sim \frac{1}{2}D^2$
\mathcal{PT} -symmetric H: $\frac{3}{4}D^2 + \frac{1}{2}D - \frac{1}{8}[1 - (-1)^D]$	1	4	8	14	21	30	$\sim \frac{3}{4}D^2$
Hermitian $H: D^2$	1	4	9	16	25	36	D^2
Real symmetric $H: \frac{1}{2}D(D+1)$	1	3	6	10	15	21	$\sim \frac{1}{2}D^2$

Now, let us construct the most general *D*-dimensional \mathcal{PT} -symmetric matrix Hamiltonian *H*, where by \mathcal{PT} -symmetric we mean that the operator \mathcal{PT} commutes with *H*. We will assume that the matrix *H* is symmetric. (If *H* were not symmetric, then the eigenvectors of *H* would not be orthogonal². We will consider the possibility of an asymmetric *H* later.) To count the number of parameters in *H*, we take the parity matrix to be in diagonal form \mathcal{P}_0 as in (3). If the operator $\mathcal{P}_0\mathcal{T}$ commutes with H_0 ,

$$\mathcal{P}_0 H_0^* = H_0 \mathcal{P}_0 \tag{9}$$

then H_0 has the 2 × 2 block form

$$H_0 = \begin{pmatrix} A & \mathrm{i}B\\ \mathrm{i}B^T & C \end{pmatrix} \tag{10}$$

where *A* is a real symmetric $m_+ \times m_+$ matrix, *C* is a real symmetric $m_- \times m_-$ matrix and *B* is a real $m_+ \times m_-$ matrix. Thus, the number of parameters in H_0 is $\frac{1}{2}D(D+1)$. We then transform \mathcal{P}_0 to \mathcal{P} using the rotation matrix *R*, and find that the number of arbitrary real parameters in the corresponding \mathcal{PT} -symmetric Hamiltonian $H = RH_0R^{-1}$ is given by the combined number $\frac{1}{2}D(D+1)$ of free parameters in H_0 and the number (6) of free parameters in \mathcal{P} . Since H_0 is not Hermitian (it is complex and symmetric) and *R* is orthogonal, as we have argued above, it follows that the Hamiltonian *H* is non-Hermitian and is not unitarily equivalent to any Hermitian matrix.

As an example, for the case D = 2 the most general \mathcal{PT} -symmetric Hamiltonian, where \mathcal{P} is given in (7), contains four free parameters and has the form³

$$H = \begin{pmatrix} r + t\cos\phi - is\sin\phi & is\cos\phi + t\sin\phi\\ is\cos\phi + t\sin\phi & r - t\cos\phi + is\sin\phi \end{pmatrix}.$$
 (11)

The most general $3 \times 3 \mathcal{PT}$ -symmetric Hamiltonian has eight free parameters.

For arbitrary D there are

$$\frac{3}{4}D^2 + \frac{1}{2}D - \frac{1}{8}[1 - (-1)^D]$$
(12)

real parameters in the most general \mathcal{PT} -symmetric matrix Hamiltonian. For purposes of comparison, in table 1 we give formulae for the number of free parameters in the most general real symmetric $D \times D$ parity matrix, the most general matrix H_0 that commutes with $\mathcal{P}_0\mathcal{T}$, the most general \mathcal{PT} -symmetric matrix H, the most general Hermitian matrix Hamiltonian and finally, the most general real symmetric matrix Hamiltonian.

² The inner product here is just the ordinary dot product, $\mathbf{v} \cdot \mathbf{v} \equiv \mathbf{v}^T \mathbf{v}$, where *T* means matrix transpose.

 $^{^{3}}$ A normal matrix is one that commutes with its Hermitian adjoint. Normal matrices are the largest class of matrices that can be diagonalized by unitary matrices. Note that H is not normal.

Once we have found the most general \mathcal{PT} -symmetric matrix Hamiltonian, we proceed according to the recipe described in [4]. First, we find the energy eigenvalues. The eigenvalues for *H* in (11) are

$$\varepsilon_{\pm} = r \pm t \cos \alpha \tag{13}$$

where $\sin \alpha = s/t$ and the unbroken \mathcal{PT} -symmetric region is $s^2 \leq t^2$. Next, we find the corresponding eigenstates:

 $1 \qquad (\sin\alpha\cos\frac{\phi}{2} - i(1 \pm \cos\alpha)\sin\frac{\phi}{2})$

$$|\varepsilon_{\pm}\rangle = \frac{1}{\sqrt{2(1 \mp \cos\alpha)\cos\alpha}} \left(\frac{\sin\alpha\cos\frac{1}{2} - i(1 \mp \cos\alpha)\sin\frac{1}{2}}{\sin\alpha\sin\frac{\phi}{2} + i(1 \mp \cos\alpha)\cos\frac{\phi}{2}} \right).$$
(14)

Because we are in the *unbroken* \mathcal{PT} -symmetric region, these states are also eigenstates of the \mathcal{PT} operator. We have chosen the phase in (14) so that the eigenvalue under the \mathcal{PT} operator is unity:

$$\mathcal{PT}|\varepsilon_{+}\rangle = |\varepsilon_{+}\rangle \qquad \mathcal{PT}|\varepsilon_{-}\rangle = |\varepsilon_{-}\rangle.$$
 (15)

It seems appropriate now to define an inner product with respect to the \mathcal{PT} operator. To do so, we define the \mathcal{PT} conjugate (\cdot | of the state $|\cdot$) as follows:

$$\left(\cdot\right) \equiv \left[\mathcal{PT}\right]^{T} \tag{16}$$

where T is matrix transpose. The \mathcal{PT} inner product of two states $|a\rangle$ and $|b\rangle$ is now defined as the dot product of the \mathcal{PT} conjugate of $|a\rangle$ and $|b\rangle$:

$$(a|b) \equiv \left[\mathcal{PT}|a\right]^{I} \cdot |b\rangle. \tag{17}$$

This inner product has the symmetry property $(a|b)^* = (b|a)$.

By virtue of (15), for the eigenstates of the Hamiltonian the state (ε_{\pm} | is just the transpose of $|\varepsilon_{\pm}$). The states in (14) are normalized so that their \mathcal{PT} norms are

$$(\varepsilon_+|\varepsilon_+) = 1 \qquad (\varepsilon_-|\varepsilon_-) = -1. \tag{18}$$

Also, the matrix Hamiltonian is symmetric, so these states are orthogonal with respect to the \mathcal{PT} inner product:

$$(\varepsilon_+|\varepsilon_-) = (\varepsilon_-|\varepsilon_+) = 0. \tag{19}$$

Finally, we construct the C operator as outlined in [4]:

$$\mathcal{C} = |\varepsilon_{+}\rangle(\varepsilon_{+}| + |\varepsilon_{-}\rangle(\varepsilon_{-}|) = \frac{1}{\cos\alpha} \begin{pmatrix} \cos\phi - i\sin\alpha\sin\phi & \sin\phi + i\sin\alpha\cos\phi \\ \sin\phi + i\sin\alpha\cos\phi & -\cos\phi + i\sin\alpha\sin\phi \end{pmatrix}.$$
 (20)

It is easy to verify that the matrix C commutes with \mathcal{PT} and with H and that $C^2 = 1$. The eigenstates of the Hamiltonian are simultaneously eigenstates of C:

$$C|\varepsilon_{+}\rangle = +|\varepsilon_{+}\rangle \qquad C|\varepsilon_{-}\rangle = -|\varepsilon_{-}\rangle.$$
(21)

Using these results, we can define a *new* inner product in which the *bra* states are the CPT conjugates of the *ket* states:

$$\langle \cdot | \equiv [\mathcal{CPT}| \cdot \rangle]^T.$$
⁽²²⁾

The CPT inner product of two states $|a\rangle$ and $|b\rangle$ is now defined as the dot product of the CPT conjugate of $|a\rangle$ and $|b\rangle$:

$$\langle a|b\rangle \equiv [\mathcal{CPT}|a\rangle]^T \cdot |b\rangle. \tag{23}$$

This inner product has the symmetry property $\langle a|b\rangle^* = \langle b|a\rangle$. The advantage of the CPT inner product is that the associated norm is positive definite.

We recover the parity operator

$$\mathcal{P} = \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix} \tag{24}$$

that was used in [4] by choosing $\phi = \pi/2$. All the results that are reported in [4] are also obtained for this choice of ϕ . However, there is an error in [4]. In this reference the parameters *s* and *t* in the Hamiltonian must be identical; they cannot be unequal because then the matrix would not be symmetric and the eigenvectors would not be orthogonal.

What happens if we choose the parity operator \mathcal{P} to have unequal numbers of positive and negative eigenvalues? For example, suppose we take D = 8 and choose $m_+ = 6$ and $m_- = 2$. (Of course, in this case there are only 12 real parameters in \mathcal{P} instead of the 16 parameters that occur in the symmetric case for which $m_+ = m_- = 4$ (see equation (6)). Correspondingly, there are also four fewer parameters in the Hamiltonian.) We have found that the signs of the \mathcal{PT} norms (see (18)) of the eigenstates of the Hamiltonian are exactly the same as the signs of the eigenvalues of \mathcal{P} . However, the *order* of the signs depends on the values of the parameters in H and is unpredictable. The operator \mathcal{C} is exactly what is needed to cancel each of the minus signs in the \mathcal{PT} norms so that the \mathcal{CPT} norms of the eigenstates are all positive.

3. Concluding remarks

The natural question that arises is whether it is possible to have a more general formalism for \mathcal{PT} -symmetric matrix Hamiltonians; that is, to have matrix Hamiltonians with more arbitrary parameters than the number given in (12). There are two possibilities: first, one could consider having an asymmetric matrix Hamiltonian H or an asymmetric parity matrix \mathcal{P} . Second, we could generalize the time reversal operator to include a matrix multiplying the complex conjugation operator.

If the matrix Hamiltonian H is not symmetric, then eigenstates of H corresponding to different eigenvalues will not be orthogonal. This forces us to generalize the \mathcal{PT} inner product $(\cdot|\cdot)$ to include a *weight matrix* W [7]. That is, rather than having an ordinary dot product of vectors, we would have to generalize the definition of the inner product to $(\cdot|W|\cdot)$, where the matrix elements of W are chosen so that

$$(\varepsilon_m | W | \varepsilon_n) = \delta_{mn}. \tag{25}$$

In this case, the matrix W plays the same role as the operator C. The drawback of this generalization is that W will not commute with H. As we now argue, we must reject this generalization of the Hamiltonian because the theory is not unitary: unitarity means that the inner product of two states is independent of time. In the Schrödinger picture the states $|a, 0\rangle$ and $|b, 0\rangle$ at time t = 0 evolve into the states $|a, t\rangle = e^{-iHt}|a, 0\rangle$ and $|b, t\rangle = e^{-iHt}|b, 0\rangle$ at time t. Thus,

$$(a,t] = [\mathcal{PT}|a,t]^T = (a,0)e^{iHt}.$$
(26)

Recalling that *H* commutes with \mathcal{PT} , we see that the inner product between these states will not be independent of time unless $e^{iHt}We^{-iHt} = W$, and this requires that *W* and *H* commute. As *W* and *H* do not commute in a theory described by an asymmetric Hamiltonian, the Hamiltonian must be abandoned as physically unacceptable because time evolution would not be unitary.

Similarly, if we generalize the parity operator to the case of an asymmetric matrix \mathcal{P} , the most general \mathcal{PT} -symmetric H will be asymmetric. Again, we must reject this possibility.

Finally, we ask if it is possible to generalize T so that it is a product of some matrix B and the complex conjugation operator. The condition that $T^2 = 1$ implies that $BB^* = 1$.

The requirement that $[\mathcal{P}, \mathcal{T}] = 0$ imposes the additional constraint $[\mathcal{P}, B] = 0$. These two conditions are so strong that no additional parameters appear in the most general \mathcal{PT} -symmetric matrix Hamiltonian H.

In conclusion, the matrix constructions presented in this paper have changed our views regarding the relationship between hermiticity and \mathcal{PT} symmetry. We do not believe, as has been claimed (see, for example, [8] and references therein), that hermiticity is a special case of \mathcal{PT} symmetry⁴. Rather, based on our study of finite matrices we understand that these are two totally distinct and unitarily inequivalent complex classes of Hamiltonians whose overlap is restricted to the class of real symmetric Hamiltonians. We conjecture that the relationship illustrated in figure 1 continues to be valid even for infinite-dimensional coordinate-space Hamiltonians.

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⁴ The problem with the analysis in [8] is that the norm associated with the inner product is not positive. To observe this nonpositivity, we construct a vector that is a linear combination of eigenvectors of the Hamiltonian: $\mu|\varepsilon_m\rangle + \nu|\varepsilon_n\rangle$, where $m \neq n$ and μ and ν are complex numbers. According to equation (15) in [8], the norm of this vector is $\mu^2 + \nu^2$, which is not positive in general.