Extremely broken generalized $\mathcal{PT}$ symmetry

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Abstract
We discuss some simple Hückel-like matrix representations of non-Hermitian operators with antiunitary symmetries that include generalized $\mathcal{PT}$ (parity transformation followed by time-reversal) symmetry. One of them exhibits extremely broken antiunitary symmetry (complex eigenvalues for all nontrivial values of the model parameter) because of the degeneracy of the operator in the Hermitian limit. These examples illustrate the effect of point-group symmetry on the spectrum of the non-Hermitian operators. We construct the necessary unitary matrices by means of simple graphical representations of the non-Hermitian operators.

Keywords PT symmetry · Antiunitary symmetry · Unitary operators · Group theory

Mathematics Subject Classification 81Q05

1 Introduction
Since the seminal paper by Bender and Boettcher [1] on parity-time symmetry in non-relativistic quantum mechanics, there has been great interest in all kinds of physical problems that lead to $\mathcal{PT}$ -symmetric equations (see [2] and references therein). Strictly speaking, the parity operation is given by $P f(x) = f(-x)$, where $x$ represents the set of coordinates that describe the system. However, in some applications other operators $P$ that satisfy $P^2 = \hat{1}$, where $\hat{1}$ is the identity operator, have served as parity, such as, for example, the $2 \times 2$ matrix representation chosen by Bender [2]. In this way, several fancy names emerged, like partial $\mathcal{PT}$ symmetry [3] or reverse-order partial $\mathcal{PT}$ symmetry [4]. Such kind of pseudo-parity operators are particular cases of the unitary operators that lead to antiunitary symmetries [4–6].

Most studies based on parameter-dependent operators are commonly restricted to the range of model parameter values for which the eigenvalues are real or appear as
complex-conjugate pairs, which gives rise to the so-called unbroken (all the eigenvalues are real) or broken (one or more eigenvalues are complex) $\mathcal{PT}$ symmetry [2] (and references therein). If $\lambda$ is the model parameter then $\mathcal{PT}$ symmetry is unbroken for $0 \leq \lambda < \lambda_c$ and broken for $\lambda > \lambda_c$, where, typically, the Hamiltonian operator is Hermitian for $\lambda = 0$. On the other hand, some authors have searched for $\mathcal{PT}$-symmetric non-Hermitian operators with complex eigenvalues for all non-trivial values of the model parameter [7–9]. It was argued that the occurrence of this kind of extremely broken $\mathcal{PT}$ symmetry, where, for example, $\lambda_c = 0$, is due to the point-group or dynamical symmetry of the physical problem and can be predicted by first-order perturbation theory [7–9].

There has recently been interest in $\mathcal{PT}$-symmetry in molecular systems. Burton et al [10] derived the conditions for $\mathcal{PT}$-symmetry in the context of electronic structure theory within the Hartree-Fock (HF) approximation. These authors showed that the HF orbitals are symmetric with respect to the $\mathcal{PT}$ operator if and only if the effective Fock Hamiltonian is $\mathcal{PT}$-symmetric.

The purpose of this paper is to illustrate the concept of antiunitary symmetry [5] as a generalization of $\mathcal{PT}$ symmetry, as well as the effect of point-group symmetry [11, 12] on the occurrence of extremely broken antiunitary symmetry. As illustrative examples we choose non-Hermitian versions of the Hückel model proposed many years ago for the treatment of conjugated molecules [13, 14] and also $H_n$ structures [14].

In Sect. 2 we summarize the main ideas about antiunitary symmetry; in Sect. 3 we illustrate the effect of point-group symmetry by means of two extremely simple examples based on the Hückel model; finally, in Sect. 4 we summarize the main results and draw conclusions.

## 2 Antiunitary symmetry

The concept of antiunitary symmetry was developed by Wigner [5] some time ago and later invoked in some discussions on generalized $\mathcal{PT}$ symmetry [4, 6, 15]. In this section we introduce it in a way somewhat different from our earlier papers [4, 6].

We begin the present discussion with the complex conjugation operator $K$ defined by

$$K |f\rangle = |f\rangle^*,$$  \hfill (1)

where $|f\rangle$ belongs to the physical vector space and * stands for complex conjugation. Obviously, $K^2 = \hat{1}$. From the well known properties of complex conjugation we have

$$K (|f\rangle + |g\rangle) = K |f\rangle + K |g\rangle,$$
$$Kc |f\rangle = c^* K |f\rangle,$$  \hfill (2)

where $|g\rangle$ also belongs to the physical vector space and $c$ is a complex number.
If $H$ is a non-Hermitian operator, then it follows from $KHK | f \rangle = KH | f \rangle^* = H^* | f \rangle$ that

\[ KHK = H^*. \]  

(3)

Suppose that there is a unitary operator $U$ ($U^\dagger = U^{-1}$, $U^\dagger$ being the adjoint of $U$) that satisfies

\[ U^\dagger H U = H^* = KHK. \]  

(4)

Therefore,

\[ A^{-1} H A = H, \]  

(5)

where $A = UK$ is said to be an antiunitary symmetry of the physical system represented by $H$. Equation (5) is equivalent to

\[ [H, A] = H A - A H = 0. \]  

(6)

It is worth noticing that $A$ satisfies Eq. (2).

In some cases, there is a set of unitary operators $S_U = \{U_j, j = 1, 2, \ldots, N\}$ that satisfy Eq. (4) and we can, therefore, construct a set of antiunitary operators $S_A = \{A_j = U_j K, j = 1, 2, \ldots, N\}$ that leave $H$ invariant as in Eq. (5). One can easily verify that $U_i U_j \notin S_U$ because $(U_i U_j)^\dagger H U_i U_j = H$. On the other hand, $A_i A_j \in S_A$.

If $|\psi\rangle$ is an eigenvector of $H$ with eigenvalue $E$

\[ H |\psi\rangle = E |\psi\rangle, \]  

(7)

then

\[ [H, A] |\psi\rangle = H A |\psi\rangle - A H |\psi\rangle = H A |\psi\rangle - AE |\psi\rangle = H A |\psi\rangle - E^* A |\psi\rangle = 0. \]  

(8)

In other words: if $E$ is an eigenvalue of $H$ with eigenvector $|\psi\rangle$ then $E^*$ is an eigenvalue of $H$ with eigenvector $A |\psi\rangle$.

If

\[ A |\psi\rangle = a |\psi\rangle, \]  

(9)

where $a$ is a complex number, for all the eigenvectors of $H$, we say that the antiunitary symmetry is unbroken because it follows from Eq. (8) that $H |\psi\rangle = E^* |\psi\rangle$ and $E = E^*$. If, on the other hand, $|\psi\rangle$ and $A |\psi\rangle$ are linearly independent (for at least one eigenvector of $H$), then $E^*$ is an eigenvalue $H$ with eigenvector $A |\psi\rangle$ and we say that the $\mathcal{PT}$ symmetry is broken.
In order to identify the antiunitary symmetries of a given operator $H$ we just look for unitary operators $U$ that satisfy Eq. (4). In the following section we illustrate this point by means of some simple examples.

## 3 Simple examples

In this section, we consider simple matrix representations of non-Hermitian operators. Our first illustrative example is given by the matrix

$$H_p(\gamma) = \begin{pmatrix} i\gamma & 1 & 0 & 1 \\ 1 & -i\gamma & 1 & 0 \\ 0 & 1 & i\gamma & 1 \\ 1 & 0 & 1 & -i\gamma \end{pmatrix},$$  

(10)

where $\gamma$ is real, that may be related to a Hückel model for a cyclic molecule [13, 14] with complex diagonal elements. To facilitate the construction of unitary matrices that satisfy (see the general Eq. (4))

$$U^\dagger H U = H^*,$$  

(11)

we resort to the graphical representation of $H_p$ shown in Fig. 1. It is worth mentioning that we will refer to unitary matrices for the sake of generality, but in fact all the matrices discussed in what follows are real and, consequently, orthogonal.

The unitary matrix

$$U_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$  

(12)

that produces the transformation

$$U_1 \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} c_2 \\ c_1 \\ c_4 \\ c_3 \end{pmatrix},$$  

(13)

already satisfies Eq. (11). Since this matrix satisfies $U_1^2 = I$, where $I$ is the $4 \times 4$ identity matrix, it is a good candidate for generalized parity $P = P = U_1$. In order to realize how to construct the unitary matrices in a straightforward way, note that this one is just a representation of a rotation of $\pi$ radians about an axis through the middle of the sides $1-2$ and $3-4$ of the square in Fig. 1.
Another candidate for generalized parity is

\[ U_2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \]  

that leads to

\[ U_2 \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} c_4 \\ c_3 \\ c_2 \\ c_1 \end{pmatrix}. \]  

Note that \( U_2^2 = I \) because it is a rotation of \( \pi \) about an axis through the middle of the square sides 1 – 4 and 2 – 3. The unitary matrices just derived are not the only ones that satisfy Eq. (11).

The unitary matrix

\[ U_3 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \]  

gives rise to the cyclic permutation

\[ U_3 \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} c_2 \\ c_3 \\ c_4 \\ c_1 \end{pmatrix}. \]
It is a representation of a rotation of $\pi/2$ about an axis through the center of the square in Fig. 1. For this reason, $U_3^4 = I$ which gives rise to two more matrices that satisfy Eq. (11): $U_4 = U_3^2$ and $U_5 = U_3^3$. It is clear that $U_3^4 U_1 U_3 = U_2$ because the axes associated to $U_1$ and $U_2$ are perpendicular. Although $U_3^4 = I$, it is not a suitable candidate for generalized $PT$ symmetry because $U_3^{-1}HU_3 = H$.

The existence of more than one candidate for generalized parity is a good reason for speaking of antiunitary symmetry instead of $PT$ symmetry or generalized $PT$ symmetry [15], thus avoiding fancy names like partial $PT$ symmetry [3] or reverse-order partial $PT$ symmetry [4], even when the former was observed experimentally [16].

There are two matrices that satisfy $U_j^{-1}HU_j = H$, $j = 6, 7$, which represent unitary symmetries, and are unsuitable for the construction of antiunitary operators. They are the matrix representations of the rotations of $\pi$ about axes through opposite vertices of the square in Fig. 1.

The eigenvalues of the matrix (10) are

$$E_1(\gamma) = -E_4(\gamma) = -\sqrt{4 - \gamma^2}, \quad E_2(\gamma) = -E_3(\gamma) = -i\gamma,$$

that show that the antiunitary symmetries constructed above are broken for all $\gamma \neq 0$ (which we have chosen to call extremely broken $PT$ symmetry). The reason is the degeneracy of $H_P(0)$ as discussed elsewhere for other non-Hermitian models [7–9]. Note that perturbation theory yields a $\gamma^2$-power series for $E_1$ and $E_4$ and a $\gamma$-power series (only one term) for $E_2$ and $E_3$. Once again, we appreciate that degeneracy is the cause of the extremely broken antiunitary symmetry. The degeneracy when $\gamma = 0$ is due to the point-group symmetry of $H_P(0)$ as this matrix is invariant under all the transformations $U_j^\dagger H_P(0)U_j = H_P(0)$ given by $G_8 = \{I, U_j, j = 1, 2, \ldots, 7\}$. This set of 8 matrices is a group isomorphic to $C_{4v}$ that includes a two-dimensional irreducible representation $E$ [11, 12]. Figure 2 shows the eigenvalues of $H_P(\gamma)$ for some values of the model parameter. It is clear that the two complex eigenvalues stem from the degenerate ones $E_2(0) = E_3(0)$ as argued in previous papers about other non-Hermitian models [7–9].

Earlier discussions of the effect of point-group symmetry on antiunitary symmetry [7–9] suggest that a model with less symmetry than (10) may exhibit real eigenvalues. One such model is given by the Hückel-like open chain in Fig. 3 that represents the matrix

$$H_O(\gamma) = \begin{pmatrix} i\gamma & 1 & 0 & 0 \\ 1 & -i\gamma & 1 & 0 \\ 0 & 1 & i\gamma & 1 \\ 0 & 0 & 1 & -i\gamma \end{pmatrix}.$$

In this case, the unitary matrix (14) is the sole candidate for an antiunitary symmetry because it is the only one that satisfies Eq. (11), i.e. $U_2^\dagger H_O U_2 = H_O^\ast$. As indicated above, $U_2$ is also a candidate for generalized parity.
The eigenvalues of $H_O$ are

$$E_1 = -E_4 = -\frac{1}{\sqrt{2}} \sqrt{-2\gamma^2 + \sqrt{5} + 3}, \quad E_2 = -E_3 = -\frac{1}{\sqrt{2}} \sqrt{-2\gamma^2 - \sqrt{5} + 3}. \quad (20)$$

There are four exceptional points $\gamma_{EP} = \pm \left(\sqrt{5} - 1\right) / 2, \pm \left(\sqrt{5} + 1\right) / 2$ and, consequently, all the eigenvalues are real when $|\gamma| < \left(\sqrt{5} - 1\right) / 2 \approx 0.618$. They are shown in Fig. 4 that confirms the argument put forward above. Note that $H_O(0)$ does not exhibit degenerate states because of its lower symmetry $C_2$ (the point-group being $G_2 = \{I, U_2\}$) with two one-dimensional irreducible representations [11, 12].
The operator

\[
H_{O2}(\gamma) = \begin{pmatrix}
i\gamma & 0 & 1 & 0 \\
0 & i\gamma & 1 & 1 \\
1 & 1 & -i\gamma & 0 \\
0 & 1 & 0 & -i\gamma \\
\end{pmatrix},
\]

(21)

exhibits the same antiunitary symmetry based on \(U_2\). The two matrices \(H_O\) and \(H_{O2}\) are similar because they are related as \(VH_OV = H_{O2}\) by means of the unitary matrix

\[
V = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
\end{pmatrix}, \quad V^2 = I.
\]

(22)

For this reason they are isospectral. The matrices (19) and (21) are associated to the same graphical representation given in Fig. 3 with a different labelling of the sites.

Some non-Hermitian operators with tridiagonal matrix representations exhibit real eigenvalues because they can be transformed into Hermitian operators by means of suitable transformations [17]. However, the arguments put forward in that paper cannot be applied to present matrices that exhibit complex diagonal elements.

4 Conclusions

Throughout this paper it has been our purpose to make two points. First, if the chosen candidate for the parity operator \(P\) is not a true parity it is convenient to refer to it simply as a unitary operator and use the term antiunitary symmetry instead of \(PT\) symmetry. The reason is that in many cases there are more than one unitary operator \(U\) satisfying \(U^2 = \hat{1}\) that may be candidates for generalized \(P\) as shown in Sect. 3 and also in a
previous article [4]. In this way we avoid fancy names like partial $\mathcal{PT}$ symmetry or reverse-order partial $\mathcal{PT}^\dagger$ symmetry [4]. Second, we show another example of a non-Hermitian operator, Eq. (10), that exhibits extremely broken antiunitary symmetry. As in the case of other models discussed in previous papers [7–9], the reason is the symmetry of the operator in the Hermitian limit ($\gamma = 0$ in the present case) that exhibits degenerate eigenvectors. As argued there, first-order perturbation theory is a suitable tool for verifying whether the eigenvalues are complex for small values of the model parameter.

It is worth mentioning recent studies of maximal symmetry breaking in even $\mathcal{PT}$-symmetric lattices [18] (and references therein) although such effect does not appear to be related to the point-group symmetry of the lattice.

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Author Contributions FMF wrote the main manuscript text, carried out all the calculations and prepared the figures

Declarations

Conflict of interest The authors declare no competing interests.

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