\textbf{\(\mathcal{PT}\)-symmetry and its spontaneous breakdown explained by anti-linearity}

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\textbf{Abstract}

The impact of an anti-unitary symmetry on the spectrum of non-hermitean operators is studied. Wigner’s normal form of an anti-unitary operator is shown to account for the spectral properties of non-hermitean, \(\mathcal{PT}\)-symmetric Hamiltonians. Both the occurrence of single real or complex conjugate pairs of eigenvalues follows from this theory. The corresponding energy eigenstates span either one- or two-dimensional irreducible representations of the symmetry \(\mathcal{PT}\). In this framework, the concept of a spontaneously broken \(\mathcal{PT}\)-symmetry is not needed.

Deep in their hearts, many quantum physicists will renounce hermiticity of operators only reluctantly. However, non-hermitean Hamiltonians are applied successfully in nuclear physics, biology and condensed matter, often modelling the interaction of a quantum system with its environment in a phenomenological way. Since 1998, non-hermitean Hamiltonians continue to attract interest from a conceptual point of view \[1\]: surprisingly, the eigenvalues of a one-dimensional harmonic oscillator Hamiltonian remain real when the complex potential \(\hat{V} = i\hat{x}^3\) is added to it. Numerical, semiclassical, and analytic evidence \[2\] has been accumulated confirming that bound states with real eigenvalues exist for the vast class of complex potentials satisfying \(V^\dagger(\hat{x}) = V(-\hat{x})\). In addition, pairs of complex conjugate eigenvalues occur systematically.

\(\mathcal{PT}\)-symmetry has been put forward to explain the observed energy spectra. The Hamiltonian operators \(\hat{H}\) under scrutiny are invariant under the combined action of parity \(\mathcal{P}\) and time reversal \(\mathcal{T}\),

\[ [\hat{H}, \mathcal{PT}] = 0 \, . \]  

They act on the fundamental observables according to

\[ \mathcal{P} : \begin{cases} \hat{x} \rightarrow -\hat{x} , \\ \hat{p} \rightarrow -\hat{p} , \end{cases} \quad \mathcal{T} : \begin{cases} \hat{x} \rightarrow \hat{x} , \\ \hat{p} \rightarrow -\hat{p} , \end{cases} \]  

(2)
and $T$ anti-commutes with the imaginary unit,
\[ T i = i^* T = -i T. \]

Whenever a $\mathcal{PT}$-symmetric Hamiltonian has a real eigenvalue $E$, the associated eigenstate $|E\rangle$ is found to be an eigenstate of the symmetry $\mathcal{PT}$,
\[ E = E^* : \hat{H}|E\rangle = E|E\rangle, \quad \mathcal{PT}|E\rangle = +|E\rangle. \]  

Occasionally, $\mathcal{PT}|E\rangle = -|E\rangle$ occurs which is equivalent to (4) upon redefining the phase of the state: $\mathcal{PT}(i|E\rangle) = +(i|E\rangle)$. There is no difference between symmetry and anti-symmetry under $\mathcal{PT}$.

However, if the eigenvalue $E$ is complex, the operator $\mathcal{PT}$ does not map the corresponding eigenstate of $\hat{H}$ to itself,
\[ E \neq E^* : \hat{H}|E\rangle = E|E\rangle, \quad \mathcal{PT}|E\rangle \neq \lambda|E\rangle, \text{ any } \lambda. \]  

This situation is described as a ‘spontaneous breakdown’ of $\mathcal{PT}$-symmetry. No mechanism has been identified which would explain this breaking of the symmetry.

The $\mathcal{PT}$-symmetric square-well model provides a simple example for this behavior. It describes a particle moving between reflecting boundaries at $x = \pm 1$, in the presence of a piecewise constant complex potential,
\[ V_Z(x) = \begin{cases} iZ, & x < 0, \\ -iZ, & x > 0, \end{cases} \quad Z \in \mathbb{R}. \]  

Acceptable solutions of Schrödinger’s equation must satisfy both the boundary conditions, $\psi(\pm 1) = 0$, and continuity conditions at the origin. As long as the value of the parameter $Z$ is below a critical value, $Z < Z_0$, the eigenvalues $E_n$ of the non-hermitean Hamiltonian $\hat{H} = -\partial_{xx} + V_Z(x)$ are real, and each eigenstate $|\psi_n\rangle$ satisfies the relations (4), with eigenvalues $E_n$ and +1, respectively. Above the threshold, $Z > Z_0$, at least one pair of complex conjugate eigenvalues $E_0$ and $E_0^*$ develops. One of the corresponding eigenstates has the form
\[ \psi_0(x) = \begin{cases} K_p \sinh \kappa(1 - x), & x > 0, \\ K_n \sinh \lambda^*(1 + x), & x < 0, \end{cases} \]  

the complex parameters $\kappa, \lambda, K_n$, and $K_p$ being determined by the boundary and continuity conditions. The state $\psi_0(x)$ is not invariant under $\mathcal{PT}$, i.e. (5) holds.

The purpose of the present contribution is a group-theoretical analysis of $\mathcal{PT}$-symmetry. The properties of $\mathcal{PT}$-symmetric systems are explained in a natural way by taking into account that $\mathcal{PT}$ is not a unitary but an anti-unitary symmetry of a non-hermitean operator. The argument proceeds in three steps. First, Wigner’s normal form of anti-unitary operators is reviewed, i.e. their (irreducible) representations are identified. Second, the properties of non-hermitean operators with anti-unitary symmetry are derived. These results are then shown to account for the characteristic features of $\mathcal{PT}$-symmetric systems.
Wigner develops a normal form of anti-unitary operators $\hat{A}$ in [5]. Anti-unitarity of $\hat{A}$ is defined by the relation

$$\langle \hat{A}\chi |\hat{A}\psi \rangle = \langle \psi |\chi \rangle$$

and it implies anti-linearity,

$$\hat{A}(\alpha |\psi \rangle + \beta |\chi \rangle) = \alpha^* \hat{A}|\psi \rangle + \beta^* \hat{A}|\chi \rangle .$$

which is equivalent to (3). The representation theory of $\hat{A}$ relies on the fact that the square of an anti-unitary operator is unitary:

$$\langle \hat{A}^2\chi |\hat{A}^2\psi \rangle = \langle \hat{A}\psi |\hat{A}\chi \rangle = \langle \chi |\psi \rangle .$$

Therefore, the operator $\hat{A}^2$ has a complete, orthonormal set of eigenvectors $|\Omega \rangle$ with eigenvalues $\Omega$ of modulus one,

$$\hat{A}^2|\Omega \rangle = \Omega|\Omega \rangle , \quad |\Omega | = 1 .$$

It plays the role of a Casimir-type operator labelling different representations of $\hat{A}$. Wigner distinguishes three different types of representations corresponding to the eigenvalues of $\hat{A}^2$: complex $\Omega$ ($\neq \Omega^*$), $\Omega = +1$, or $\Omega = -1$, summarized in Table (1).

1. An eigenstate $|\Omega \rangle$ of $\hat{A}^2$ with eigenvalue $\Omega$ ($\neq \Omega^*$) is not invariant under $\hat{A}$. Instead, the states $|\Omega \rangle$ and $|\Omega^* \rangle \equiv \hat{A}|\Omega \rangle$ constitute a ‘flipping pair’ with complex ‘flipping value’ $\omega$ (and $\omega^*$), where $\omega^2 = \Omega$. They span a two-dimensional space which is closed under the action of $\hat{A}$. Therefore, it carries a two-dimensional representation of $\hat{A}$, denoted by $\Gamma_\omega$, which is irreducible: due to the anti-linearity of $\hat{A}$, no (non-zero) linear combination of the flipping states exist which is invariant under $\hat{A}$.

2. Similarly, if $\hat{A}^2$ has an eigenvalue $\Omega = -1$, then the operator $\hat{A}$ flips the states $|\rangle$ and $|\rangle^* \equiv \hat{A}|\rangle$. The flipping value is $i$, and the associated two-dimensional representation $\Gamma_i$ is not reducible.

3. Two different situations arise if there is an eigenstate $|1 \rangle$ of $\hat{A}^2$ with eigenvalue $+1$. The state $\hat{A}|1 \rangle$ is either a multiple of itself or not. In the first case, the space spanned by $|1 \rangle$ is invariant under $\hat{A}$ and hence carries a one-dimensional representation $\gamma_\omega$ of $\hat{A}$. When redefining the phase of the state appropriately, one obtains an eigenstate $|1 \rangle$ of $\hat{A}$ with eigenvalue $+1$. In the second case, the two states $|+ \rangle \equiv |1 \rangle$ and $|+^* \rangle \equiv \hat{A}|1 \rangle$ provide a flipping pair with flipping value $\omega = +1$, and hence a representation $\Gamma_+$. This representation, however, is reducible due to the reality of the flipping value: the linear combinations $|1_r \rangle = |+ \rangle + |+^* \rangle$ and $|1_i \rangle = i(|+ \rangle - |+^* \rangle)$ are both eigenstates of $\hat{A}$ with eigenvalue $+1$. 
Table 1: Representations \( \Gamma \) of the operator \( \hat{A} \)

| \( \Omega \equiv \omega^2 \) | \( \Gamma \) | action of \( \hat{A} \) | \( \dim \Gamma \) |
|---|---|---|---|
| \( \Omega \neq \Omega^* \) | \( \Gamma_+ \) | \( \hat{A}|\Omega\rangle = \omega^*|\Omega^*\rangle \) | 2 |
| \( \hat{A}|\Omega^*\rangle = \omega|\Omega\rangle \) |
| -1 | \( \Gamma_- \) | \( \hat{A}|\rangle = -i|\rangle \) | 2 |
| \( \hat{A}|\rangle = +i|\rangle \) |
| +1 | \( \Gamma_+ \) | \( \hat{A}|\rangle = +|\rangle \) | 2 |
| \( \hat{A}|\rangle = +|\rangle \) |
| +1 | \( \gamma_+ \) | \( \hat{A}|1\rangle = +|1\rangle \) | 1 |
| \( \hat{A}|\rangle = +|\rangle \) |

Consequently, a Hilbert space \( \mathcal{H} \) naturally decomposes into a direct product of invariant subspaces, each invariant under the action of the anti-unitary operator \( \hat{A} \),

\[
\mathcal{H} = \Gamma_+ \otimes N_+ \otimes \Gamma_- \otimes N_- \otimes \Gamma_+ \otimes N_+ \otimes \gamma_+ \otimes n_+ ;
\]

the nonnegative integers \( N_+ \), \( N_- \) and \( n_+ \) are related to the degeneracies of the eigenvalues \( \Omega (\neq \Omega^*) \) and \( \Omega = \pm 1 \) of the operator \( \hat{A}^2 \). The corresponding decomposition of a vector \( |\psi\rangle \in \mathcal{H} \) is the closest analog of an expansion into the eigenstates of a hermitean (or unitary) operator. Surprisingly, two-dimensional irreducible representations of \( \hat{A} \) exist although there is only one generator, \( \hat{A} \). No ‘good quantum number’ exists which would label the states spanning these representations.

A (diagonalizable) non-hermitean Hamiltonian \( \hat{H} \) with a discrete spectrum \( \mathcal{H} \) and its adjoint \( \hat{H}^\dagger \) each have a complete set of eigenstates:

\[
\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle , \quad \hat{H}^\dagger|\psi_n\rangle = E^*_n|\psi_n\rangle ,
\]

with complex conjugate eigenvalues related by \( E^n = E^*_n \). They form a bi-orthonormal basis in \( \mathcal{H} \), as they provide two resolutions of unity,

\[
\sum_n |\psi^n\rangle \langle \psi_n| = \sum_n |\psi_n\rangle \langle \psi^n| = \hat{I} ,
\]

and satisfy orthogonality relations,

\[
\langle \psi_m|\psi^n\rangle = \delta^n_m .
\]

Let the non-hermitean operator \( \hat{H} \) have an anti-unitary symmetry \( \hat{A} \),

\[
[\hat{H}, \hat{A}] = 0 .
\]
Then the unitary operator $\hat{A}^2$ commutes with $\hat{H}$, and it has eigenvalues $\Omega$ of modulus one. Consequently, there are simultaneous eigenstates $|n, \Omega\rangle$ of $\hat{H}$ and $\hat{A}^2$:

$$\hat{H}|n, \Omega\rangle = E_n|n, \Omega\rangle, \quad \hat{A}^2|n, \Omega\rangle = \Omega|n, \Omega\rangle, \quad E_n \in \mathbb{C}. \quad (17)$$

For simplicity, the eigenvalues $\Omega$ are assumed discrete and not degenerate. Wigner’s normal form of anti-unitary operators suggests to consider three cases separately:

- $\Omega \neq \Omega^*$ The state $|n, \Omega^\ast\rangle \equiv \omega \hat{A}|n, \Omega\rangle$, $\omega^2 = \Omega$, (18) is a second eigenstate of $\hat{A}^2$, with eigenvalue $\Omega^\ast$. The states \{\( |n, \Omega\rangle, |n, \Omega^\ast\rangle \}\) provide a flipping pair under the action of the operator $\hat{A}$,

$$\hat{A}|n, \Omega\rangle = \omega^\ast |n, \Omega^\ast\rangle \text{, } \hat{A}|n, \Omega^\ast\rangle = \omega |n, \Omega\rangle, \quad (19)$$
carrying the representation $\Gamma_*$. No degeneracy of the eigenvalue $E_n$ is implied by the anti-unitary $\hat{A}$-symmetry of $\hat{H}$. However, the non-hermitean Hamiltonian has a second eigenstate $|n, \Omega^\ast\rangle$ with eigenvalue $E_n^\ast$,

$$\hat{H}|n, \Omega^\ast\rangle = E_n^\ast |n, \Omega^\ast\rangle, \quad (20)$$
as follows from multiplying the first equation of (17) with $\hat{A}$ and $\omega$.

- $\Omega = -1$ Formally, the results for the representation $\Gamma_-$ are obtained from the previous case by setting $\omega = i$. Again, a pair of complex conjugate eigenvalues is found, and the associated flipping pair spans a two-dimensional representation space.

- $\Omega = +1$ This case is conceptually different from the previous ones as two possibilities arise. Consider the state $|n, +\rangle$, an eigenvector of both $\hat{H}$ and $\hat{A}^2$ with eigenvalues $E_n$ and $+1$, respectively. It satisfies Eqs. (17) with $\Omega \to +$. If, on the one hand, applying $\hat{A}$ to $|n, +\rangle$ results in $e^{i\phi}|n, +\rangle$, then the state $|n, 1\rangle \equiv e^{-i\phi/2}|n, +\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue $+1$,

$$\hat{A}|n, 1\rangle = |n, 1\rangle. \quad (21)$$

This occurrence of the one-dimensional representation $\gamma_+$ forces the associated eigenvalue $E_n$ of $\hat{H}$ to be real since

$$E_n|n, 1\rangle = \hat{H}\hat{A}|n, 1\rangle = \hat{A}\hat{H}|n, 1\rangle = E_n^\ast |n, 1\rangle. \quad (22)$$

If, on the other hand, $|n, +^\ast\rangle \equiv \hat{A}|n, +\rangle$ is not a multiple of $|n, +\rangle$, then these states combine to form the representation $\Gamma_+$, the flipping value being $+1$. Further, the state $|n, +^\ast\rangle$ is an eigenstate of the Hamiltonian with eigenvalue $E_n^\ast$. As the flipping number is real, linear combinations of $|n, +\rangle$ and $|n, +^\ast\rangle$ do exist which are eigenstates of $\hat{A}$—however, they are not eigenstates of $\hat{H}$. Consequently, the anti-unitary symmetry of the Hamiltonian makes itself felt (on a subspace with $(\mathcal{PT})^2 = + \hat{I}$) by either a single real eigenvalue or a pair of two complex conjugate eigenvalues.

If any of the two-dimensional representations $\Gamma_*$ or $\Gamma_{\pm}$ occurs and the associated eigenvalue happens to be real, the anti-unitary symmetry implies a twofold degeneracy.
of the energy eigenvalue. Again, the symmetry provides no additional label, and simultaneous eigenstates of \( \hat{H} \) and \( \hat{A} \) can be constructed for \( \Gamma_+ \) only. These cases will be denoted by \( \Gamma^+_\varphi \) or \( \Gamma^+_{\varphi} \).

It will be shown now that the properties of \( \mathcal{PT} \)-symmetric quantum systems are consistent with the representation theory of non-hermitean Hamiltonians possessing an anti-unitary symmetry. Upon identifying

\[
A = \mathcal{PT},
\]  

one needs to check the value of \((\mathcal{PT})^2\) when applied to eigenstates of the Hamiltonian in order to decide which of the representations \( \Gamma_\varphi \), \( \Gamma_{\varphi}^\pm \), or \( \gamma_+ \), is realized. Various explicit examples will be given now.

For parameters \( Z < Z_0^\mathcal{C} \), the eigenvalues of the \( \mathcal{PT} \)-symmetric square-well are real throughout, and the operators \( \hat{H} \) and \( \mathcal{PT} \) have common eigenstates. Thus, the relations (4) correspond to a multiple occurrence of the representation \( \gamma_+ \), compatible with \( (\mathcal{PT})^2 = +i\hat{I} \).

For \( Z > Z_0^\mathcal{C} \), the energy eigenstate \( \psi_0(x) \equiv \langle x|E_0, + \rangle \) in (6) satisfies \((\mathcal{PT})^2|E_0, + \rangle = +|E_0, + \rangle \). Therefore, the states \( |E_0, + \rangle \) and \( |E_0, +^* \rangle \equiv \mathcal{PT}|E_0, + \rangle \) carry a representation \( \Gamma_+ \), and the presence of two complex energy eigenvalues, \( E_0 \) and \( E_0^* \), is justified. Eqs. (3) can be completed to read:

\[
E \neq E^* : \quad \begin{aligned}
\hat{H}|E_0, + \rangle &= E_0|E_0, + \rangle, \\
\mathcal{PT}|E_0, + \rangle &= +|E_0, +^* \rangle, \\
\hat{H}|E_0, +^* \rangle &= E_0^*|E_0, +^* \rangle, \\
\mathcal{PT}|E_0, +^* \rangle &= +|E_0, + \rangle.
\end{aligned}
\]  

(24)

Consequently, \( \mathcal{PT} \)-symmetry is not broken but at \( Z = Z_0^\mathcal{C} \) the system switches between the representations \( \Gamma_+ \) and \( \gamma_+ \), with a corresponding change of the energy spectrum.

The following examples are taken from a discrete family of non-hermitean operators [7],

\[
\hat{H}_M = \hat{p}^2 - (\zeta \cosh 2x - iM)^2, \quad \zeta \in \mathbb{R},
\]  

(25)

\( M \) taking positive integer values. Each operator \( \hat{H}_M \) is invariant under the combined action of \( \mathcal{PT} \) where \( \mathcal{P} \) is parity about the point \( a = i\pi/2 \): \( x \to i\pi/2 - x \). Due to the reflection about a point off the real axis, the operators \( \mathcal{P} \) and \( \mathcal{T} \) do not commute as has been pointed out in [8]. However, this fact is not essential here since only the anti-unitary character of the symmetry \( \mathcal{PT} \) is essential.

For \( M = 2 \), two complex conjugate eigenvalues \( E_+ \) and \( E_- = E_+^* \) of \( \hat{H}_2 \) exist, with associated eigenstates

\[
\psi_+(x) = \Psi(x) \cosh x \equiv \langle x|E_+, - \rangle, \quad \psi_-(x) = \Psi(x) \sinh x \equiv \langle x|E_+, -^* \rangle,
\]  

(26)

and a \( \mathcal{PT} \)-invariant function \( \Psi(x) = \exp([i/2]\zeta \cosh 2x] \). These states are a flipping pair with flipping value \( i \),

\[
\mathcal{PT}\psi_+(x) = -i\psi_-(x), \quad \mathcal{PT}\psi_-(x) = i\psi_+(x),
\]  

(27)

and the twofold application of \( \mathcal{PT} \) gives \((-1)\). Hence, the representation \( \Gamma_- \) is realized. Similarly, for \( M = 4 \), four eigenstates form two flipping pairs, i.e. two representations \( \Gamma_- \), each being associated with a pair of complex conjugate eigenvalues.
For $M = 3$, three different real eigenvalues of the Hamiltonian $\hat{H}_3$ have been obtained analytically if $\zeta^2 < 1/4$. The corresponding eigenfunctions are given by
\begin{equation}
\psi(x) = \Psi(x) \sinh 2x, \quad \psi_\pm(x) = \Psi(x) (A \cosh 2x \pm iB),
\end{equation}
with real coefficients $A$ and $B$. Under the action of $\mathcal{PT}$, the state $\psi(x)$ is mapped to itself, while $\psi_\pm(x)$ each acquire an additional minus sign. Therefore, the states $\psi(x) \equiv \langle x | E, + \rangle$ and $i\psi_\pm(x) \equiv \langle x | E_\pm \rangle$ are simultaneous eigenstates of $\hat{H}$ and $\mathcal{PT}$ with eigenvalues $+1$. The part of Hilbert space spanned by these three states transforms according to three copies of the representation $\gamma_+$. If $\zeta = 1/2$, the eigenvalues $E_\pm$ turn degenerate, and the eigenstates given in (28) merge, $i\psi_+(x) = i\psi_-(x) \equiv \varphi(x)$. However, a second, independent $\mathcal{PT}$-invariant solution of Schrödinger’s equation can be found,
\begin{equation}
\phi(x) = \Psi(x) \int_{x_0}^{x} dy \frac{e^{-i\varphi(y)/2}}{\varphi^2(y)}.
\end{equation}
The solutions $\{\varphi, \phi\}$ transform according to $\gamma_+ \otimes \gamma_+ \equiv \Gamma_+^d$. So far, the representation $\Gamma_+$ has apparently not been realized in $\mathcal{PT}$-symmetric quantum systems—a possible explanation is the constraint $T^2 = \pm 1$ for time reversal [3].

In summary, the representation theory of anti-unitary symmetries of non-hermitean ‘Hamiltonians’ has been developed on the basis of Wigner’s normal form of anti-unitary operators. Typically, energy eigenvalues come in complex conjugate pairs, and the associated eigenstates of the Hamiltonian span a two-dimensional space carrying one of the two-dimensional representations $\Gamma_+$, or $\Gamma_\pm$. Furthermore, a single real eigenvalue may occur, related to a one-dimensional representation $\gamma_+$. In this case a single $\hat{A}$-invariant energy eigenstate state exists while there are no simultaneous eigenstates of the Hamiltonian and the symmetry operator in the two-dimensional $\hat{A}$-invariant subspaces. Instead, flipping pairs of states can be identified. Generally, the symmetry does not imply the existence of degenerate eigenvalues—only if the Hamiltonian happens to have a real eigenvalue, a two-dimensional degenerate subspace may exist occasionally. These results naturally explain the properties of eigenstates and eigenvalues of $\mathcal{PT}$-symmetric quantum systems. In particular, it is not necessary to invoke the concept of a spontaneously broken $\mathcal{PT}$-symmetry. Contrary to a unitary or hermitean symmetry, the presence of an anti-unitary symmetry does not imply the existence of a set of simultaneous eigenstates of $\hat{H}$ and $\mathcal{PT}$—simply because an anti-linear operator is not guaranteed to have a complete set of eigenstates. Finally, the present approach provides a new perspective on the suggested modification of the scalar product in Hilbert space [10] which will be presented elsewhere [11] in detail.

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