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$\mathcal{PT}$-symmetry and its spontaneous breakdown explained by anti-linearity

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Abstract
The impact of an anti-unitary symmetry on the spectrum of non-Hermitian operators is studied. Wigner's normal form of an anti-unitary operator accounts for the spectral properties of non-Hermitian, $\mathcal{PT}$-symmetric Hamiltonians. The occurrence of either 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.

Keywords: $\mathcal{PT}$-symmetry, anti-linearity, anti-unitarity, invariances, representation theory

Deep in their hearts, many quantum physicists will renounce hermiticity of operators only reluctantly. However, non-Hermitian 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-Hermitian Hamiltonians have continued 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 $\hat{V} = \mathrm{i}\hat{x}^3$ 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 $\mathcal{T}$:

$$[\hat{H}, \mathcal{PT}] = 0. \tag{1}$$

They act on the fundamental observables according to

$$\mathcal{P}: \begin{cases} \hat{x} \to -\hat{x}, \\ \hat{p} \to -\hat{p}, \end{cases} \qquad \mathcal{T}: \begin{cases} \hat{x} \to \hat{x}, \\ \hat{p} \to -\hat{p}, \end{cases} \tag{2}$$

and $\mathcal{T}$ *anti-commutes* with the imaginary unit:

$$\mathcal{T}\mathrm{i} = \mathrm{i}^*\mathcal{T} \equiv -\mathrm{i}\mathcal{T}. \tag{3}$$

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 $\mathcal{PT}$:

$$E = E^*: \qquad \hat{H}|E\rangle = E|E\rangle, \qquad \mathcal{PT}|E\rangle = +|E\rangle. \tag{4}$$

Occasionally, $\mathcal{PT}|E\rangle = -|E\rangle$ occurs [3] which is equivalent to (4) upon redefining the phase of the state: $\mathcal{PT}(\mathrm{i}|E\rangle) = +(\mathrm{i}|E\rangle)$. 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:

$$E \neq E^*: \qquad \hat{H}|E\rangle = E|E\rangle, \qquad \mathcal{PT}|E\rangle \neq \lambda|E\rangle, \tag{5}$$

where λ is any real or complex number. 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 behaviour [4]. It describes a particle moving between reflecting boundaries at $x = \pm 1$, in the presence of a piecewise constant complex potential,

$$V_Z(x) = \begin{cases} \mathrm{i}Z, & x < 0, \\ -\mathrm{i}Z, & x > 0, \end{cases} \qquad Z \in \mathbb{R}. \tag{6}$$

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, $Z < Z_0^c$, the eigenvalues E_n of the non-Hermitian 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, $Z > Z_0^c$, at least one pair of complex conjugate eigenvalues E_0 and E_0^* develops. One of the corresponding eigenstates has the form [4]

$$\psi_0(x) = \begin{cases} K_p \sinh \kappa(1-x), & x > 0, \\ K_n \sinh \lambda^*(1+x), & x < 0, \end{cases} \tag{7}$$

the complex parameters κ, λ, 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-Hermitian* operator. The argument proceeds in three steps. First, Wigner's normal form of anti-unitary operators is reviewed; this amounts to identifying their (irreducible) representations. Second, the properties of non-Hermitian operators with anti-unitary symmetry are derived. These results are then shown to account for the characteristic features of $\mathcal{PT}$-symmetric systems, including the occurrence of both single real and pairs of complex conjugate eigenvalues.

Wigner develops a normal form of anti-unitary operators $\hat{A}$ in [5]. Anti-unitarity of $\hat{A}$ is defined by the relation

$$\langle \hat{A}\chi|\hat{A}\psi\rangle = \langle\psi|\chi\rangle. \tag{8}$$

Anti-unitarity implies anti-linearity:

$$\hat{A}(\alpha|\psi\rangle + \beta|\chi\rangle) = \alpha^*\hat{A}|\psi\rangle + \beta^*\hat{A}|\chi\rangle, \tag{9}$$

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*:

$$\langle \hat{A}^2\chi|\hat{A}^2\psi\rangle = \langle\hat{A}\psi|\hat{A}\chi\rangle = \langle\chi|\psi\rangle. \tag{10}$$

Let the operator $\hat{A}^2$ have a *discrete* spectrum (according to Wigner, operators with a *continuous* spectrum can be treated similarly [5]). Then it has a complete, orthonormal set of eigenvectors $|\Omega\rangle$ with eigenvalues Ω of modulus one:

$$\hat{A}^2|\Omega\rangle = \Omega|\Omega\rangle, \qquad |\Omega| = 1. \tag{11}$$

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

(1) An eigenstate $|\Omega\rangle$ of $\hat{A}^2$ with eigenvalue Ω ($\neq \Omega^*$) 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' ω (and ω^*), 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 Γ_*, which is *irreducible*: due to the anti-linearity of $\hat{A}$, no (non-zero) linear combination of the flipping states exist which would be invariant under $\hat{A}$.

Table 1. Representations Γ of the operator $\hat{A}$.

$\Omega \equiv \omega^2$	Γ	Action of $\hat{A}$	Dim Γ
$\Omega \neq \Omega^*$	Γ_*	$\hat{A}\|\Omega\rangle = \omega^*\|\Omega^*\rangle$ $\hat{A}\|\Omega^*\rangle = \omega\|\Omega\rangle$	2
-1	Γ_-	$\hat{A}\|-\rangle = -\mathrm{i}\|-^*\rangle$ $\hat{A}\|-^*\rangle = +\mathrm{i}\|-\rangle$	2
+1	Γ_+	$\hat{A}\|+\rangle = +\|+^*\rangle$ $\hat{A}\|+^*\rangle = +\|+\rangle$	2
+1	γ_+	$\hat{A}\|1\rangle = +\|1\rangle$	1

(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 $\omega = \sqrt{-1} = \mathrm{i}$, and the associated two-dimensional representation Γ_- 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 γ_+ 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 Γ_+. This representation, however, is *reducible* due to the reality of the flipping value: the linear combinations $|1_r\rangle = |+\rangle + |+^*\rangle$ and $|1_i\rangle = \mathrm{i}(|+\rangle - |+^*\rangle)$ are both eigenstates of $\hat{A}$ with eigenvalue +1.

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 $\hat{A}$:

$$\mathcal{H} = \Gamma_*^{\otimes N_*} \otimes \Gamma_-^{\otimes N_-} \otimes \Gamma_+^{\otimes N_+} \otimes \gamma_+^{\otimes n_+}; \tag{12}$$

the non-negative integers N_*, $N_\pm$, and n_+ account for the degeneracies of the eigenvalues Ω ($\neq \Omega^*$) and $\Omega = \pm 1$ of the operator $\hat{A}^2$. The corresponding decomposition of a vector $|\psi\rangle \in \mathcal{H}$ is the closest analogue of an expansion into the eigenstates of a Hermitian (or unitary) operator. In contrast to the representation theory of linear operators, *two*-dimensional irreducible representations of $\hat{A}$ exist, although there is only one generator, $\hat{A}$. However, there is no 'good quantum number' which would label the states spanning these representations.

A (diagonalizable) *non-Hermitian* Hamiltonian $\hat{H}$ with a discrete spectrum [6] and its adjoint $\hat{H}^\dagger$ each have a complete set of eigenstates:

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \qquad \hat{H}^\dagger|\psi^n\rangle = E^n|\psi^n\rangle, \tag{13}$$

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:

$$\sum_n |\psi^n\rangle\langle\psi_n| = \sum_n |\psi_n\rangle\langle\psi^n| = \hat{I}, \tag{14}$$

and satisfy orthogonality relations:

$$\langle\psi_m|\psi^n\rangle = \delta_m^n. \tag{15}$$

Let the non-Hermitian operator $\hat{H}$ have an anti-unitary symmetry $\hat{A}$:

$$[\hat{H}, \hat{A}] = 0. \tag{16}$$

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

$$\hat{H}|n, \Omega\rangle = E_n|n, \Omega\rangle, \qquad \hat{A}^2|n, \Omega\rangle = \Omega|n, \Omega\rangle, \tag{17}$$

with complex energies $E_n \in \mathbb{C}$. For simplicity, the eigenvalues Ω are assumed discrete and not degenerate. Wigner's normal form of anti-unitary operators suggests considering three cases separately: complex Ω ($\neq \Omega^*$) and $\Omega = \pm 1$.

(1) $\Omega \neq \Omega^*$. The state

$$|n, \Omega^*\rangle \equiv \omega\hat{A}|n, \Omega\rangle, \qquad \omega^2 = \Omega, \tag{18}$$

is a second eigenstate of $\hat{A}^2$, with eigenvalue Ω^*. The states $\{|n, \Omega\rangle, |n, \Omega^*\rangle\}$ provide a *flipping pair* under the action of the operator $\hat{A}$:

$$\hat{A}|n, \Omega\rangle = \omega^*|n, \Omega^*\rangle, \qquad \hat{A}|n, \Omega^*\rangle = \omega|n, \Omega\rangle, \tag{19}$$

carrying the representation Γ_*. No degeneracy of the eigenvalue E_n is implied by the anti-unitary $\hat{A}$-symmetry of $\hat{H}$. However, the non-Hermitian Hamiltonian has a second eigenstate $|n, \Omega^*\rangle$ with eigenvalue E_n^*:

$$\hat{H}|n, \Omega^*\rangle = E_n^*|n, \Omega^*\rangle, \tag{20}$$

as follows from multiplying the first equation of (17) with $\hat{A}$ and ω.

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

(3) $\Omega = +1$. 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 equations (17) with $\Omega \to +$. On the one hand, if applying $\hat{A}$ to $|n, +\rangle$ results in $\mathrm{e}^{\mathrm{i}\phi}|n, +\rangle$, then the state $|n, 1\rangle \equiv \mathrm{e}^{-\mathrm{i}\phi/2}|n, +\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue +1:

$$\hat{A}|n, 1\rangle = |n, 1\rangle. \tag{21}$$

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

$$E_n|n, 1\rangle = \hat{H}\hat{A}|n, 1\rangle = \hat{A}\hat{H}|n, 1\rangle = E_n^*|n, 1\rangle. \tag{22}$$

If, on the other hand, the state $|n, +^*\rangle \equiv \hat{A}|n, +\rangle$ is *not* a multiple of $|n, +\rangle$, then these two states combine to form the representation Γ_+, the flipping value being +1. Further, the state $|n, +^*\rangle$ is an eigenstate of the Hamiltonian with eigenvalue E_n^*. As the flipping number is real, linear combinations of $|n, +\rangle$ and $|n, +^*\rangle$ 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 $\hat{A}^2 = +\hat{I}$ via either a single real eigenvalue or a pair of two complex conjugate eigenvalues.

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

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

$$\hat{A} = \mathcal{PT}, \tag{23}$$

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, Γ_*, $\Gamma_\pm$, or γ_+, is realized. Various explicit examples will be given now.

For parameters $Z < Z_0^c$, 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 γ_+, compatible with $(\mathcal{PT})^2 = +\hat{I}$.

For $Z > Z_0^C$, the energy eigenstate $\psi_0(x) \equiv \langle x|E_0, +\rangle$ in (7) 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 Γ_+, and the presence of two complex energy eigenvalues, E_0 and E_0^*, is justified. Equations (5) can be completed to read

$$E \neq E^*: \qquad \begin{aligned} \hat{H}|E_0, +\rangle &= E_0|E_0, +\rangle, \\ \hat{H}|E_0, +^*\rangle &= E_0^*|E_0, +^*\rangle, \end{aligned} \tag{24}$$

and, simultaneously,

$$\begin{aligned} \mathcal{PT}|E_0, +\rangle &= +|E_0, +^*\rangle, \\ \mathcal{PT}|E_0, +^*\rangle &= +|E_0, +\rangle. \end{aligned} \tag{25}$$

Consequently, $\mathcal{PT}$-symmetry is not broken, but at $Z = Z_0^c$ the system switches between the representations Γ_+ and γ_+, with a corresponding change of the energy spectrum.

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

$$\hat{H}_M = \hat{p}^2 - (\zeta \cosh 2x - \mathrm{i}M)^2, \qquad \zeta \in \mathbb{R}, \tag{26}$$

M taking positive integer values. Each operator $\hat{H}_M$ is invariant under the combined action of $\mathcal{PT}$ where $\mathcal{P}$ is the parity about the point $a = \mathrm{i}\pi/2$: $x \to \mathrm{i}\pi/2 - x$. 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 relevant.

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

$$\psi_+(x) = \Psi(x)\cosh x \equiv \langle x|E_+, -\rangle, \tag{27}$$

$$\psi_-(x) = \Psi(x)\sinh x \equiv \langle x|E_+, -^*\rangle, \tag{28}$$

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

$$\mathcal{PT}\psi_+(x) = -\mathrm{i}\psi_-(x), \qquad \mathcal{PT}\psi_-(x) = \mathrm{i}\psi_+(x), \tag{29}$$

and the twofold application of $\mathcal{PT}$ gives (-1). Hence, the representation Γ_- is realized. Similarly, for $M = 4$, four eigenstates form two flipping pairs, i.e. two representations Γ_-, 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

$$\psi(x) = \Psi(x)\sinh 2x,$$
$$\psi_{\pm}(x) = \Psi(x)(A\cosh 2x \pm \mathrm{i}B), \tag{30}$$

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 $\mathrm{i}\psi_{\pm}(x) \equiv \langle x|E_{\pm}\rangle$ 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 γ_+. If $\zeta = 1/2$, the eigenvalues $E_{\pm}$ turn degenerate, and the eigenstates given in (30) merge: $\mathrm{i}\psi_+(x) = \mathrm{i}\psi_-(x) \equiv \varphi(x)$. However, a second, independent $\mathcal{PT}$-invariant solution of Schrödinger's equation can be found:

$$\phi(x) = \Psi(x)\int_{x_0}^{x} \mathrm{d}y\, \frac{\mathrm{e}^{-\mathrm{i}\varphi(y)/2}}{\varphi^2(y)}. \tag{31}$$

The solutions $\{\varphi, \phi\}$ transform according to $\gamma_+ \otimes \gamma_+ \equiv \Gamma_+^d$. So far, the representation Γ_* has apparently not been realized in $\mathcal{PT}$-symmetric quantum systems—a possible explanation is the constraint $\mathcal{T}^2 = \pm 1$ for time reversal [9].

In summary, the representation theory of anti-unitary symmetries of non-Hermitian '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, Γ_* or $\Gamma_{\pm}$. However, no simultaneous eigenstates of the Hamiltonian and the symmetry operator in the two-dimensional $\hat{A}$-invariant subspaces can be identified—only 'flipping pairs' of states. Furthermore, single real eigenvalues may occur, related to the multiple occurrence of the one-dimensional representation γ_+. This is the situation considered in [10] where the reality of a $\mathcal{PT}$-invariant Hamiltonian has been shown under the assumption that $\hat{A}$-invariant states exist. 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 the case for a unitary or Hermitian symmetry, the presence of an anti-unitary symmetry, $[\hat{H}, \hat{A}] = 0$, 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. It will be worthwhile to reflect upon the proposed 'complex extension' of quantum mechanics [11] and its relation to pseudo-hermiticity [12] in the light of representation theory of anti-unitary operators. Finally, the present approach provides a new perspective on the suggested modification of the scalar product in Hilbert space [13] which will be presented elsewhere [14] in detail.

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