Completeness and Orthonormality in $\mathcal{PT}$-symmetric Quantum Systems

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June 2003

Abstract

Some $\mathcal{PT}$-symmetric non-hermitean Hamiltonians have only real eigenvalues. There is numerical evidence that the associated $\mathcal{PT}$-invariant energy eigenstates satisfy an unconventional completeness relation. An ad hoc scalar product among the states is positive definite only if a recently introduced ‘charge operator’ is included in its definition. A simple derivation of the conjectured completeness and orthonormality relations is given. It exploits the fact that $\mathcal{PT}$-symmetry provides an additional link between the eigenstates of the Hamiltonian and those of its adjoint, which form a dual pair of bases. The ‘charge operator’ emerges naturally upon expressing the properties of the dual bases in terms of one basis only.

Hermitean operators have real eigenvalues while non-hermitean ones may have complex eigenvalues. Numerical and analytical results indicated the possibility to compensate the non-hermiticity of a Hamiltonian by the presence of an additional symmetry [1]. The spectra of many non-hermiteans Hamiltonians $\hat{H}$ are indeed real [2] if they are invariant under the combined action of self-adjoint parity $\mathcal{P}$ and time reversal $\mathcal{T}$,

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

and if the energy eigenstates are invariant under the operator $\mathcal{PT}$. Pairs of complex conjugate eigenvalues are compatible with $\mathcal{PT}$-symmetry as well but the eigenstates of $\hat{H}$ are no longer invariant under $\mathcal{PT}$. It is possible to explain these observations by the concept of pseudo-hermitean operators [3] which satisfy

$$\eta \hat{H} \eta^{-1} = \hat{H}^\dagger,$$

following from Eq. (1) with $\eta = \mathcal{P}$. Wigner’s representation theory of anti-linear operators [4] provides an alternative explanation if applied to the operator $\mathcal{PT}$ [5].
What is more, the group theoretical approach explains the fate of energy eigenstates if they are not invariant under the action of PT, and a complete classification of PT-invariant subspaces emerges.

PT-symmetric systems possess at least two other intriguing features. First, the eigenstates of PT-symmetric non-hermitean Hamiltonians (with real eigenvalues only) do not satisfy the standard completeness relations. Numerical evidence [6] suggests that one has instead

$$\sum_n (-1)^n \phi_n(x)\phi_n(y) = \delta(x - y),$$

(3)

the functions $\phi_n(x) \equiv \langle x | E_n \rangle$ being energy eigenstates of a particle on the real line subjected to a PT-symmetric potential such as $V(x) = x^2(ix)^\nu, \nu \geq 0$ [7]. Whether the completeness (3) relation is valid has been called a ‘major open mathematical question for PT-symmetric Hamiltonians’ [8]. Second, a ‘natural inner product’ of functions $f(x)$ and $g(x)$ associated with PT-symmetric systems has been proposed [9],

$$(f, g) = \int dx [\mathcal{P}\mathcal{T} f(x)] g(x),$$

(4)

where the integration is along an appropriate path, possibly in the complex-$x$ plane [6]. This scalar product implies that energy eigenstates can have a negative norm,

$$(\phi_m, \phi_n) = (-1)^n \delta_{mn}.$$

(5)

which makes it difficult to maintain the familiar probabilistic interpretation of quantum theory [9] and gave rise to discussions about the state space of PT-symmetric systems [10].

In an attempt to base an extension of quantum mechanics [6] on systems with PT-symmetry a remedy against the indefinite metric in Hilbert space has been proposed in the form of a linear ‘charge operator’ $\mathcal{C}$. Its position representation is given by

$$\mathcal{C}(x, y) = \sum_n \phi_n(x)\phi_n(y).$$

(6)

Then, the redefined inner product

$$\langle f | g \rangle = \int_C dx [\mathcal{C}\mathcal{T}\mathcal{P} f(x)] g(x),$$

(7)

is positive definite, and the completeness relation (3) turns into

$$\sum_n [\mathcal{C}\mathcal{T}\mathcal{P} \phi_n(x)]\phi_n(y) = \delta(x - y).$$

(8)

These relations are also consistent with results obtained for pseudo-hermitean operators [3, 11].

The purpose of this contribution is, first, to prove that relations such as (3) exist for all PT-symmetric system with real eigenvalues. Second, the origin of the operator $\mathcal{C}$ will be identified, which directly explains both why Eq. (7) defines indeed a positive inner product and why Eq. (8) is a valid completeness relation. To cut a long story
short, the last two equations (as well as (3) and (4)) are nothing but bi-orthonormality and completeness for a pair of dual bases associated with $\hat{H}$. It is due to the system’s $\mathcal{PT}$-symmetry and the occurrence of real eigenvalues only that these two relations acquire a special form which involves the elements \{\phi_n(x)\} of one basis only.

Consider a (diagonalizable) non-hermitean Hamiltonian $\hat{H}$ with a discrete spectrum \[12\]. The operators $\hat{H}$ and its adjoint $\hat{H}^\dagger$ have complete sets of eigenstates:

$$\hat{H}|E_n\rangle = E_n|E_n\rangle, \quad \hat{H}^\dagger|E^n\rangle = E^n|E^n\rangle, \quad n = 1, 2, \ldots, \tag{9}$$

with, in general, complex conjugate eigenvalues, $E^n = E^n^*$. The eigenstates constitute bi-orthonormal bases in $\mathcal{H}$ with two resolutions of unity,

$$\sum_n |E^n\rangle\langle E_n| = \sum_n |E_n\rangle\langle E^n| = \hat{I}, \tag{10}$$

and as dual bases, they satisfy orthonormality relations,

$$\langle E^n|E_m\rangle = \langle E_m|E^n\rangle = \delta_{nm}, \quad m, n = 1, 2, \ldots \tag{11}$$

A priori, nothing is known about scalar products such as $\langle E_n|E_m\rangle$.

Consider now a $\mathcal{PT}$-invariant Hamiltonian, i.e., Eq. (1) holds, and assume all eigenvalues to be real and non-degenerate. Multiply the first equation of (9) with the operator $\mathcal{PT}$ so that

$$\hat{H}(\mathcal{PT}|E_n\rangle) = E_n(\mathcal{PT}|E_n\rangle). \tag{12}$$

Consequently, the state $\mathcal{PT}|E_n\rangle$ must equal $|E_n\rangle$ apart from a factor $d_n$. Since $(\mathcal{PT})^2|E_n\rangle = |E_n\rangle = |d_n|^2|E_n\rangle$, the numbers $d_n$ equal phase factors $e^{i\phi_n}$, say. Redefining $|E_n\rangle \rightarrow e^{i\phi_n/2}|E_n\rangle$ implies—as is well-known—that one can always write

$$\mathcal{PT}|E_n\rangle = |E_n\rangle \quad \text{or} \quad \phi_n^*(-x) = \phi_n(x). \tag{13}$$

$\mathcal{PT}$-symmetry of a non-hermitean Hamiltonian $\hat{H}$ leads to particular relation between the operator and its adjoint $\hat{H}^\dagger$. As mentioned earlier, the adjoint of $\hat{H}$ can be obtained from applying parity to it,

$$\hat{H}^\dagger = \mathcal{P}\hat{H}\mathcal{P}. \tag{14}$$

It will be shown now that a simple relation between the states $|E_n\rangle$ and $|E^n\rangle$ results, viz.,

$$|E^n\rangle = s_n\mathcal{P}|E_n\rangle, \quad s_n = \pm 1. \tag{15}$$

This relation is crucial to derive the numerically observed completeness and orthogonality relations. To see that (15) holds, an argument similar to the derivation of Eq. (13) will be given. Write $\hat{H}^\dagger = \mathcal{P}\hat{H}\mathcal{P}$ in the second equation of (9), multiply it with $\mathcal{P}$, use $\mathcal{P}^2 = \hat{I}$ and recall that $E^n = E^n^* = E_n$:

$$\hat{H}(\mathcal{P}|E^n\rangle) = E_n(\mathcal{P}|E^n\rangle). \tag{16}$$
Comparison with the first equation of (9) shows that the states \( \mathcal{P}|E_n^\prime \rangle \) and \(|E_n\rangle \) are both eigenstates of \( \hat{H} \), with \textit{the same} non-degenerate eigenvalue \( E_n \). Consequently, they must be proportional to each other,

\[
|E_n^\prime \rangle = c_n \mathcal{P}|E_n\rangle , \quad c_n \in \mathbb{C} .
\]  

(17)

The numbers \( c_n \) must, in fact, be \textit{real} since the states \(|E_n\rangle \) and \(|E_n^\prime \rangle \) are a normalized pair: using \( \mathcal{P}^2 = \mathcal{I} \) and (15) implies

\[
1 = \langle E_n^\prime |E_n \rangle = \langle E_n^\prime |\mathcal{P}^2|E_n \rangle = c_n^* c_n^{-1} \langle E_n |E_n^\prime \rangle = c_n^* c_n^{-1} ,
\]

(18)

that is, \( c_n = c_n^* \). Furthermore, the dual bases can always be chosen in such a way that the numbers \( c_n \) will take the values \( \pm 1 \). To see this, multiply each side of (17) with its own adjoint, giving \( \langle E_n^\prime |E_n^\prime \rangle = c_n^2 \langle E_n |E_n \rangle \), or

\[
c_n = s_n \left( \frac{\langle E_n |E_n \rangle}{\langle E_n^\prime |E_n \rangle} \right)^{1/2} , \quad s_n = \pm 1 ,
\]

(19)

consistent with (18) because the square root can always be given the value one by rescaling the eigenstates of \( \hat{H} \) and \( \hat{H}^\dagger \). For each dual pair, let

\[
|E_n \rangle \rightarrow \lambda_n |E_n \rangle \quad \text{and} \quad |E_n^\prime \rangle \rightarrow \lambda_n^{-1} |E_n^\prime \rangle , \quad 0 < \lambda_n < \infty , \quad (20)
\]

a transformation which does not change orthonormality of the bases since \( \langle E_n |E_n^\prime \rangle \) remains invariant. Eq. (19), however, turns into

\[
c_n = s_n \left( \frac{1}{\lambda_n^4} \langle E_n |E_n \rangle \right)^{1/2} \equiv s_n \quad \text{if} \quad \lambda_n = \left( \frac{\langle E_n |E_n^\prime \rangle}{\langle E_n^\prime |E_n \rangle} \right)^{1/4} .
\]

(21)

The \textit{signature} \( s = (s_1, s_2, \ldots) \) depends on the actual Hamiltonian as a discussion of finite-dimensional \( \mathcal{PT} \)-symmetric systems [13] shows. Here is a simple way to calculate the numbers \( s_n \) once the eigenfunctions \( \phi_n(x) = \langle x | E_n \rangle \) of a Hamiltonian with \( \mathcal{PT} \)-symmetry have been determined. Multiply Eq. (15) with \( |E_n \rangle \) and solve for \( s_n \equiv s_n^{-1} \):

\[
s_n = \langle E_n | \mathcal{P} | E_n \rangle .
\]

(22)

Using (15), it is straightforward to derive completeness relations which involve the states of \textit{one} basis only. Rewrite (10) by means of (15) as

\[
\sum_n |E_n \rangle \langle E_n^\prime | = \sum_n s_n |E_n \rangle \langle E_n | \mathcal{P} = \mathcal{I} ,
\]

(23)

and take its matrix elements in the position representation

\[
\sum_n s_n \phi_n(x) \phi_n^*(y) = \sum_n s_n \phi_n(x) \phi_n(y) = \delta(x - y) ,
\]

(24)

where \( \mathcal{PT} \)-invariance (13) has been used. The result agrees with the expression (3) if \( s_n = (-1)^n \). In a similar way, one can derive a completeness relation for the eigenstates of \( \hat{H}^\dagger \),

\[
\sum_n s_n \phi_n^*(x) \phi_n(y) = \delta(x - y) .
\]

(25)
The orthonormality condition for dual states turns into a relation which has been interpreted as the existence of a non-positive scalar product among the eigenstates of $\hat{H}$. Simply write the scalar product (11) in the position representation, using (15) and $\mathcal{PT}$-invariance,

$$\langle E^n | E_m \rangle = s_n \langle E_n | \mathcal{P} | E_m \rangle = s_n \int dx \: \phi_n^*(-x) \phi_m(x)$$

$$= s_n \int dx \: \phi_n(x) \phi_m(x) = \delta_{nm},$$

(26)

or, using the notation from (4),

$$\langle \phi_n, \phi_m \rangle = s_n \delta_{nm},$$

(27)

which is again consistent with $s_n = (-1)^n$.

Suppose we wanted to write an operator version of (15). Define an operator $\mathcal{C}_s$ by

$$\mathcal{C}_s = \sum_k s_k |E_k\rangle \langle E^k|.$$  

(28)

Its eigenstates are $|E_n\rangle$ since

$$\mathcal{C}_s |E_n\rangle = \sum_k s_k |E_k\rangle \langle E^k|E_n\rangle = s_n |E_n\rangle,$$

(29)

and its eigenvalues $s_n$ coincide indeed with the signs of the ‘$\mathcal{PT}$-norm,’ a property of the ‘charge operator’ $\mathcal{C}$ pointed out in [6]. Writing

$$|E^n\rangle = s_n \mathcal{P} |E_n\rangle = \mathcal{P} \mathcal{C}_s |E_n\rangle,$$

(30)

one can transform the scalar product of dual states, using (13) twice,

$$\langle E_m | E^n \rangle = \langle E_m | \mathcal{P} \mathcal{C}_s | E_m \rangle = \langle E_m | \mathcal{P} \int dx \: |x\rangle \langle x| \mathcal{C}_s | E_m \rangle$$

$$= \int dx \: \phi_m^*(-x) \mathcal{C}_s \phi_n(x) = \int dx \: \phi_m(x) [\mathcal{C}_s \mathcal{P} \mathcal{T} \phi_n(x)] = \delta_{nm}.$$

(31)

Defining $\mathcal{C}_s = \mathcal{C}$ if $s_n = (-1)^n$, this equation justifies (7) for energy eigenstates. Furthermore, the first completeness relation in (10) implies through (30) that

$$\delta(x-y) = \sum_n \langle x| \mathcal{P} |E^n\rangle \langle E_n| \mathcal{P} |y \rangle$$

$$= \sum_n \mathcal{C}_s \phi_n(x) \phi_n^*(-y) = \sum_n [\mathcal{C}_s \mathcal{P} \mathcal{T} \phi_n(x)] \phi_n(y),$$

(32)

which reproduces (8), identical to Eq. (13) of [6]. By taking matrix elements of Eq. (28), the position representation of the operator $\mathcal{C}_s(x, y)$ is found to agree with (6).

In summary, it has been shown that the dual bases of $\mathcal{PT}$-symmetric quantum systems with non-hermitean Hamiltonians enjoy a particularly simple relation (15). As a consequence, it is possible to formulate completeness and orthonormality relations which invoke the elements of one basis only. These relations are inherited
from the dual pair of bases providing them thus with a sound mathematical footing. Structurally similar relations can be derived for any pseudo-hermitean Hamiltonian.

It is a different question whether this mathematical structure—call it ‘complex extension’ of quantum mechanics [6], for example—is realized in nature. To draw a positive conclusion, one would need to find a natural interpretation of the linear, idempotent ‘charge operator’ $C$. This appears difficult in the framework of non-relativistic quantum mechanics: in spite of having real eigenvalues $s_n$ only, the operator $C$ is neither self-adjoint nor unitary while the familiar operator of charge conjugation $\hat{C}$ used in field theory is unitary.

References


[8] See the first paper in [7].


