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Completeness and orthonormality in $PT$-symmetric quantum systems

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Some $PT$-symmetric non-Hermitian Hamiltonians have only real eigenvalues. There is numerical evidence that the associated $PT$-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 $PT$ symmetry provides a link between the eigenstates of the Hamiltonian and those of its adjoint, forming a dual pair of bases. The charge operator emerges naturally upon expressing the properties of the dual bases in terms of one basis only, and it is shown to be a function of the Hamiltonian.

Hermitian operators have real eigenvalues while non-Hermitian 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-Hermitians Hamiltonians $\hat{H}$ are indeed real [2] if they are invariant under the combined action of self-adjoint parity $P$ and time reversal $T$,

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

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

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

following from Eq. (1) with $\eta=P$. Wigner’s representation theory of antilinear operators [4] provides an alternative explanation if applied to the operator $PT$ [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-Hermitian Hamiltonians (with real eigenvalues only) do not satisfy the standard completeness relations. Numerical evidence [6] suggests that one has instead

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

the functions $\phi_n(x) = \langle x|E_n \rangle$ being energy eigenstates of a particle on the real line subjected to a $PT$-symmetric potential such as $V(x)=x^2(ix)^\nu, \nu>0$ [7]. Whether the completeness relation (3) 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].

$$(f,g)=\int_C dx [PTf(x)]g(x),$$

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

$$\langle \phi_n, \phi_m \rangle=(−1)^n \delta_{mn},$$

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 $C$. Its position representation is given by

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

Then, the redefined inner product

$$\langle f|g \rangle=\int_C dx [CPTf(x)]g(x),$$

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

$$\sum_n [CPT \phi_n(x)] \phi_n(y)=\delta(x-y).$$

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

The purpose of this contribution is, first, to prove that relations such as Eq. (3) exist for all $PT$-symmetric system with real eigenvalues. Second, the origin of the operator $C$ 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 Eqs. (3) and (4)] are nothing but
biorthonormality and completeness for a pair of dual bases associated with $\hat{H}$. It is due to the system’s $PT$ 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-Hermitian Hamiltonian $\hat{H}$ with a discrete spectrum [12]. The operators $\hat{H}$ and its adjoint $\hat{H}^\dagger$ have complete sets of eigenstates:

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

(9)

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

$$\sum_n |E^n\rangle\langle E_n| = \sum_n |E_n\rangle\langle E^n| = \mathbb{I},$$

(10)

and as dual bases, they satisfy orthonormality relations,

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

(11)

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

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

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

(12)

Multiplication by $\langle E_m|$ from the left and using the adjoint of the second equation in Eq. (9) with $E^n = E_n$ leads to

$$(E_m - E_n)|E^n\rangle\langle E^n|(PT|E_n\rangle) = 0.$$  

(13)

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

$$PT|E_n\rangle = |E_n\rangle \quad \text{or} \quad \phi_n^\dagger(-x) = \phi_n(x).$$

(14)

$PT$ symmetry of a non-Hermitian 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,

$$\hat{H}^\dagger = P\hat{H}P.$$

(15)

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

$$|E^n\rangle = s_n P|E_n\rangle, \quad s_n = \pm 1.$$  

(16)

This relation is crucial to derive the numerically observed completeness and orthogonality relations. To see that Eq. (16) holds, an argument similar to the derivation of Eq. (14) will be given. Write $\hat{H}^\dagger = P\hat{H}P$ in the second equation of (9), multiply it with $P$, use $P^2 = I$ and recall that $E^n = E_n^* = E_n$:

$$\hat{H}(P|E^n\rangle) = E_n(P|E^n\rangle).$$

(17)

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

$$|E^n\rangle = c_n P|E_n\rangle, \quad c_n \in \mathbb{C}.$$  

(18)

This also follows from multiplying Eq. (17) by $\langle E^m|$ from the left and using the adjoint of the second equation in Eq. (9) with $E^m = E_n$:

$$(E_m - E_n)\langle E^m|(P|E^n\rangle) = 0.$$  

(19)

The numbers $c_n$ must, in fact, be real since the states $|E_n\rangle$ and $|E^n\rangle$ are a normalized pair: using $P^2 = I$ and Eq. (18) implies

$$1 = \langle E^n|E_n\rangle = \langle E^n|P^2|E_n\rangle = c_n^* c_n^{-1} \langle E_n|E_n\rangle = c_n c_n^{-1},$$

(20)

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 Eq. (18) with its own adjoint, giving $\langle E^m^n|E^m\rangle = c_n^{-1} \langle E_m|E_n\rangle$, or

$$c_n = s_n \left(\frac{\langle E^m|E^n\rangle}{\langle E_m|E_n\rangle}\right)^{1/2}, \quad s_n = \pm 1,$$

(21)

consistent with Eq. (20) because the scalar products are positive. The square root can always be given the value 1 by rescaling the eigenstates of $\hat{H}$ and $\hat{H}^\dagger$. For each dual pair, let

$$|E_n\rangle \rightarrow \lambda_n |E_n\rangle \quad \text{and} \quad |E^n\rangle \rightarrow \lambda_n^{-1}|E^n\rangle, \quad 0 < \lambda_n < \infty,$$

(22)

a transformation which does not change orthonormality of the bases since $\langle E_n|E^n\rangle$ remains invariant. Eq. (21), however, turns into

$$c_n = s_n \left(\frac{1}{\lambda_n^2} \frac{\langle E^m|E^n\rangle}{\langle E_m|E_n\rangle}\right)^{1/2} \quad \text{if} \quad \lambda_n = \left(\frac{\langle E^m|E^n\rangle}{\langle E_m|E_n\rangle}\right)^{1/4}.$$  

(23)

The signature $s = (s_1, s_2, \ldots)$ depends on the actual Hamiltonian as a discussion of finite-dimensional $PT$-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 $PT$ symmetry have been determined. Multiply Eq. (16) with $|E_n\rangle$ and solve for $s_n = s_n^{-1}$, giving

$$s_n = \langle E_n|P|E_n\rangle.$$  

(24)

Using Eq. (16), it is straightforward to derive completeness relations which involve the states of one basis only.
\[ \sum_n |E_n\rangle\langle E^n| = \sum_n s_n |E_n\rangle\langle E_n| P = I, \quad (25) \]

and take its matrix elements in the position representation
\[ \sum_n s_n \phi_n(x) \phi^*_n(-y) = \sum_n s_n \phi_n(x) \phi_n(y) = \delta(x-y), \quad (26) \]

where PT invariance (14) 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 \( \hat{H} \),
\[ \sum_n s_n \phi_n^*(x) \phi_n^*(y) = \delta(x-y). \quad (27) \]

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 Eq. (16) and PT-invariance,
\[ \langle E^n|E_m\rangle = s_n \langle E_n|P|E_m\rangle \\
= s_n \int dx \phi_n^*(-x) \phi_m(x) \\
= s_n \int dx \phi_n(x) \phi_m(x) \\
= \delta_{nm}, \quad (28) \]

or, using the notation from Eq. (4),
\[ (\phi_n, \phi_m) = s_n \delta_{nm}, \quad (29) \]

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

Suppose we wanted to write an operator version of Eq. (16). Define an operator \( C_x \) by
\[ C_x = \sum_k s_k |E_k\rangle\langle E^k| \quad (30) \]

Its eigenstates are \( |E_n\rangle \) since
\[ C_x |E_n\rangle = \sum_k s_k |E_k\rangle \langle E^k|E_n\rangle = s_n |E_n\rangle \quad (31) \]

and its eigenvalues \( s_n \) coincide indeed with the signs of the “PT norm,” a property of the charge operator \( C \) pointed out in Ref. [6]. Writing
\[ |E^n\rangle = s_n P |E_n\rangle = PC_s |E_n\rangle, \quad (32) \]

one can transform the scalar product of dual states, using Eq. (14) twice,
\[ \langle E_m|E^n\rangle = \langle E_m|PC_s|E_n\rangle \\
= \langle E_m|P \int dx |x\rangle\langle x|C_s|E_n\rangle \\
= \int dx \phi^*_m(-x) C_s \phi_n(x) \\
= \int dx \phi_m(x) [C_s PT \phi_n(x)] \\
= \delta_{mn}. \quad (33) \]

Defining \( C_x = C \) if \( s_n = (-1)^n \), this equation justifies Eq. (7) for energy eigenstates. Furthermore, the first completeness relation in Eq. (10) implies through Eq. (32) that
\[ \delta(x-y) = \sum_n \langle x|P|E^n\rangle\langle E_n|P|y\rangle \\
= \sum_n C_s \phi_n(x) \phi^*_n(-y) = \sum_n [C_s PT \phi_n(x)] \phi_n(y), \quad (34) \]

which reproduces Eq. (8), identical to Eq. (13) of Ref. [6].

By taking matrix elements of Eq. (30), the position representation of the operator \( C_x(x, y) \) is found to agree with Eq. (6).

There is, in fact, a simple way to express the operator \( C_x \), which follows from comparing Eq. (30) with the “diagonal” representation of the Hamiltonian,
\[ \hat{H} = \sum_n E_k |E_k\rangle\langle E^k|, \quad (35) \]

Introducing a function \( f(x) \) such that
\[ f(E_k) = s_k, \quad n = 1, 2, \ldots, \quad (36) \]

one finds that the operator \( C_x \) is nothing but a function of the Hamiltonian,
\[ C_x = \sum_n s_k E_k \langle E^k| \\
= \sum_n f(E_k) \langle E^k| \\
= f \left( \sum_n E_k |E_k\rangle\langle E^k| \right) \\
= f(\hat{H}). \quad (37) \]

Therefore, \( C_x \) commutes with the Hamiltonian, and it will not be Hermitian, consistent with Eq. (30).

In summary, it has been shown that the dual bases of PT-symmetric quantum systems with non-Hermitian Hamiltonians enjoy a particularly simple relation (16). 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-Hermitian 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 constructive conclusion, one would need to find a natural interpretation of the linear, idempotent charge operator $C$. This appears difficult in the framework of nonrelativistic quantum mechanics: in spite of having eigenvalues $s_n = \pm 1$ only, the operator $C$ is neither self-adjoint nor unitary while the familiar operator of charge conjugation used in field theory is unitary.

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