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.

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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,

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

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

$$\eta\hat{H}\eta^{-1}=\hat{H}^{\dagger}, \tag{2}$$

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

$$\sum_n (-1)^n \phi_n(x)\phi_n(y)=\delta(x-y), \tag{3}$$

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 $V(x)=x^2(ix)^{\nu},\nu\geqslant 0$ [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],

$$(f,g)=\int_{\mathcal{C}} dx[PTf(x)]g(x), \tag{4}$$

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

$$(\phi_m,\phi_n)=(-1)^n\delta_{mn}, \tag{5}$$

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 C. Its position representation is given by

$$C(x,y)=\sum_n \phi_n(x)\phi_n(y). \tag{6}$$

Then, the redefined inner product

$$\langle f|g\rangle=\int_{\mathcal{C}} dx[CPTf(x)]g(x), \tag{7}$$

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

$$\sum_n [CPT\phi_n(x)]\phi_n(y)=\delta(x-y). \tag{8}$$

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

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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:

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

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

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

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

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

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

$$(E_m - E_n)\langle E^m|(PT|E_n\rangle) = 0. \tag{13}$$

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 $|E_n\rangle \to e^{-i\varphi_n/2}|E_n\rangle$ implies—as is well known—that one can always write

$$PT|E_n\rangle = |E_n\rangle \quad \text{or} \quad \phi_n^*(-x) = \phi_n(x). \tag{14}$$

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,

$$\hat{H}^\dagger = P\hat{H}P. \tag{15}$$

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

$$|E^n\rangle = s_n P|E_n\rangle, \quad s_n = \pm 1. \tag{16}$$

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 $P^2 = \hat{I}$ and recall that $E^n = E_n^* = E_n$:

$$\hat{H}(P|E^n\rangle) = E_n(P|E^n\rangle). \tag{17}$$

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,

$$|E^n\rangle = c_n P|E_n\rangle, \quad c_n \in \mathbb{C}. \tag{18}$$

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 $E^m \equiv E_m$:

$$(E_m - E_n)\langle E^m|(P|E^n\rangle) = 0. \tag{19}$$

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

$$1 = \langle E^n|E_n\rangle = \langle E^n|P^2|E_n\rangle = c_n^* c_n^{-1}\langle E_n|E^n\rangle = c_n^* c_n^{-1}, \tag{20}$$

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 ± 1. To see this, multiply each side of Eq. (18) with its own adjoint, giving $\langle E^n|E^n\rangle = c_n^2\langle E_n|E_n\rangle$, or

$$c_n = s_n\left(\frac{\langle E^n|E^n\rangle}{\langle E_n|E_n\rangle}\right)^{1/2}, \quad s_n = \pm 1, \tag{21}$$

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

$$|E_n\rangle \to \lambda_n|E_n\rangle \quad \text{and} \quad |E^n\rangle \to \lambda_n^{-1}|E^n\rangle, \quad 0 < \lambda_n < \infty, \tag{22}$$

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

$$c_n = s_n\left(\frac{1}{\lambda_n^4}\frac{\langle E^n|E^n\rangle}{\langle E_n|E_n\rangle}\right)^{1/2} \equiv s_n \quad \text{if} \quad \lambda_n = \left(\frac{\langle E^n|E^n\rangle}{\langle E_n|E_n\rangle}\right)^{1/4}. \tag{23}$$

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 $\langle E_n|$ and solve for $s_n \equiv s_n^{-1}$, giving

$$s_n = \langle E_n|P|E_n\rangle. \tag{24}$$

Using Eq. (16), it is straightforward to derive completeness relations which involve the states of *one* basis only. Rewrite Eq. (10) by means of Eq. (16) as

$$\sum_n |E_n\rangle\langle E^n| = \sum_n s_n |E_n\rangle\langle E_n|P = \hat{I}, \tag{25}$$

and take its matrix elements in the position representation

$$\sum_n s_n \phi_n(x)\phi_n^*(-y) = \sum_n s_n \phi_n(x)\phi_n(y) = \delta(x-y), \tag{26}$$

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 $\hat{H}^\dagger$,

$$\sum_n s_n \phi^n(x)\phi^n(y) = \delta(x-y). \tag{27}$$

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,

$$\begin{aligned}\langle E^n|E_m\rangle &= s_n\langle E_n|P|E_m\rangle\\ &= s_n\int dx\,\phi_n^*(-x)\phi_m(x)\\ &= s_n\int dx\,\phi_n(x)\phi_m(x)\\ &= \delta_{nm},\end{aligned} \tag{28}$$

or, using the notation from Eq. (4),

$$(\phi_n,\phi_m) = s_n\delta_{nm}, \tag{29}$$

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

Suppose we wanted to write an operator version of Eq. (16). Define an operator C_s by

$$C_s = \sum_k s_k|E_k\rangle\langle E^k|. \tag{30}$$

Its eigenstates are $|E_n\rangle$ since

$$C_s|E_n\rangle = \sum_k s_k|E_k\rangle\langle E^k|E_n\rangle = s_n|E_n\rangle, \tag{31}$$

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

$$|E^n\rangle = s_nP|E_n\rangle = PC_s|E_n\rangle, \tag{32}$$

one can transform the scalar product of dual states, using Eq. (14) twice,

$$\begin{aligned}\langle E_m|E^n\rangle &= \langle E_m|PC_s|E_n\rangle\\ &= \langle E_m|P\int dx|x\rangle\langle x|C_s|E_n\rangle\\ &= \int dx\,\phi_m^*(-x)C_s\phi_n(x)\\ &= \int dx\,\phi_m(x)[C_sPT\phi_n(x)]\\ &= \delta_{mn}.\end{aligned} \tag{33}$$

Defining $C_s=C$ 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

$$\begin{aligned}\delta(x-y) &= \sum_n \langle x|P|E^n\rangle\langle E_n|P|y\rangle\\ &= \sum_n C_s\phi_n(x)\phi_n^*(-y) = \sum_n [C_sPT\phi_n(x)]\phi_n(y),\end{aligned} \tag{34}$$

which reproduces Eq. (8), identical to Eq. (13) of Ref. [6]. By taking matrix elements of Eq. (30), the position representation of the operator $C_s(x,y)$ is found to agree with Eq. (6).

There is, in fact, a simple way to express the operator C_s, which follows from comparing Eq. (30) with the "diagonal" representation of the Hamiltonian,

$$\hat{H} = \sum_n E_k|E_k\rangle\langle E^k|. \tag{35}$$

Introducing a function $f(x)$ such that

$$f(E_k) = s_k, \quad n=1,2,\dots, \tag{36}$$

one finds that the operator C_s is nothing but a function of the Hamiltonian,

$$\begin{aligned}C_s &= \sum_n s_k|E_k\rangle\langle E^k|\\ &= \sum_n f(E_k)|E_k\rangle\langle E^k|\\ &= f\left(\sum_n E_k|E_k\rangle\langle E^k|\right)\\ &= f(\hat{H}).\end{aligned} \tag{37}$$

Therefore, C_s 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.

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