Pseudo-Hermiticity versus $PT$-Symmetry II: A complete characterization of non-Hermitian Hamiltonians with a real spectrum

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Abstract

We give a necessary and sufficient condition for the reality of the spectrum of a non-Hermitian Hamiltonian admitting a complete set of biorthonormal eigenvectors.

Recently, we have explored in [1] the basic mathematical structure underlying the spectral properties of $PT$-symmetric Hamiltonians [2]. In particular, we have shown that these properties are associated with a class of more general (not necessarily Hermitian) Hamiltonians $H$ satisfying

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

(1)

where $^\dagger$ denotes the adjoint of the corresponding operator and $\eta$ is a Hermitian invertible linear operator. We have termed such a Hamiltonian `\(\eta\)-pseudo-Hermitian.' Hermitian and the $PT$-symmetric Hamiltonians that admit a complete set of biorthonormal eigenvectors constitute subsets of the set of pseudo-Hermitian Hamiltonians. For a $PT$-symmetric Hamiltonian, the exactness of $PT$-symmetry ensures the reality of the energy spectrum. The purpose of this article is to provide a complete characterization of the Hamiltonians that

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have a real spectrum assuming that they are endowed with a complete set of biorthonormal eigenvectors.

By definition, a $PT$-symmetric Hamiltonian has a symmetry given by an anti-linear operator, namely $PT$. It is well-known that if a Hamiltonian satisfies

$$[H, A] = 0,$$  \hspace{1cm} (2)

for an anti-linear operator $A$, then

\[ \star \text{ either the eigenvalues of } H \text{ are real or they come in complex conjugate pairs.} \]

Furthermore, an eigenvalue of $H$ is real provided that a corresponding eigenvector is invariant under the action of $A$, i.e., Eq. (3) together with

$$H|E\rangle = E|E\rangle,$$  \hspace{1cm} (3)

and

$$A|E\rangle = |E\rangle$$  \hspace{1cm} (4)

imply $E \in \mathbb{R}$. Therefore, a Hamiltonian with an anti-linear symmetry has a real spectrum if the symmetry is exact.

In Ref. [1], we have shown that every pseudo-Hermitian Hamiltonian has the property $\star$. Furthermore, for Hamiltonians with a complete set of biorthonormal eigenvectors this property is the necessary and sufficient condition for pseudo-Hermiticity. This, in particular, means that pseudo-Hermiticity is a necessary condition for having a real spectrum, but it is not sufficient. In the following we give the necessary and sufficient condition for the reality of the spectrum of any Hamiltonian that admits a complete set of biorthonormal eigenvectors. We shall only consider the case of discrete spectra. The generalization to continuous spectra does not seem to involve major difficulties.

We first recall the defining properties of a Hamiltonian admitting a complete set of biorthonormal eigenvectors [3]. If a Hamiltonian $H$ has a complete set of biorthonormal
eigenvectors \(\{|\psi_n\rangle, |\phi_n\rangle\}\), then

\[
H|\psi_n\rangle = E_n|\psi_n\rangle, \quad H^\dagger|\phi_n\rangle = E_n^*|\phi_n\rangle,
\]

(5)

\[
\langle \phi_m|\psi_n \rangle = \delta_{mn},
\]

(6)

\[
\sum_n |\psi_n\rangle \langle \phi_n| = 1,
\]

(7)

where \(n\) is the spectral label, \(\delta_{mn}\) denotes the Kronecker delta function, and 1 is the identity operator.

**Theorem:** Let \(H : \mathcal{H} \to \mathcal{H}\) be a Hamiltonian that acts in a Hilbert space \(\mathcal{H}\), has a discrete spectrum, and admits a complete set of biorthonormal eigenvectors \(\{|\psi_n\rangle, |\phi_n\rangle\}\). Then the spectrum of \(H\) is real if and only if there is an invertible linear operator \(O : \mathcal{H} \to \mathcal{H}\) such that \(H\) is \(OO^\dagger\)-pseudo-Hermitian.

**Proof:** Let \(\{|n\rangle\}\) be a complete orthonormal basis of \(\mathcal{H}\), i.e.,

\[
\langle m|n \rangle = \delta_{mn}, \quad \sum_n |n\rangle \langle n| = 1,
\]

(8)

and \(O : \mathcal{H} \to \mathcal{H}\) and \(H_0 : \mathcal{H} \to \mathcal{H}\) be defined by

\[
O := \sum_n |\psi_n\rangle \langle n|, \quad H_0 := \sum_n E_n |n\rangle \langle n|.
\]

(9)

Then, in view of (3) – (4), \(O\) is invertible with the inverse given by

\[
O^{-1} = \sum_n |n\rangle \langle \phi_n|,
\]

(10)

and

\[
O^{-1}HO = H_0.
\]

(11)

Now suppose that the spectrum of \(H\) is real. Then, \(H_0\) is Hermitian, and taking the adjoint of both sides (III), we have

\[
O^{-1}HO = O^\dagger H^\dagger O^{-1\dagger}
\]

(12)
or alternatively

\[ H = (OO^\dagger)H^\dagger(OO^\dagger)^{-1}. \]  \hspace{1cm} (13)

This equation shows that \( H \) is \( OO^\dagger \)-pseudo-Hermitian. This completes the proof of necessity. Next we suppose that \( H \) is \( OO^\dagger \)-pseudo-Hermitian. Then (13) and consequently (12) hold. On the other hand, in view of (1) and (4), we have

\[ H_0 = O^{-1}HO, \quad H_0^\dagger = O^\dagger H^\dagger O^{-1}\dagger. \]

Therefore, (12) implies that \( H_0 \) is Hermitian, and the eigenvalues \( E_n \) are all real. \( \square \)

It should be emphasized that the characterization of the non-Hermitian Hamiltonians with a real spectrum given by the preceding theorem applies to the Hamiltonians that admit a complete biorthonormal system of eigenvectors. A generalization of this result to the case of arbitrary Hamiltonians is not known.

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