PT-symmetry entails pseudo-Hermiticity regardless of diagonalizability

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Abstract

We prove that in finite dimensions, a Parity-Time (PT)-symmetric Hamiltonian is necessarily pseudo-Hermitian regardless of whether it is diagonalizable or not. This result is different from Mostafazadeh’s, which requires the Hamiltonian to be diagonalizable. PT-symmetry breaking often occurs at exceptional points where the Hamiltonian is not diagonalizable. Our result implies that PT-symmetry breaking is equivalent to the onset of instabilities of pseudo-Hermitian systems, which was systematically studied by Krein et al. in 1950s. In particular, we show that the mechanism of PT-symmetry breaking is the resonance between eigenmodes with different Krein signatures.

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In quantum physics, observables are assumed to be Hermitian operators. Bender and collaborators [1–3] proposed to relax this fundamental assumption and considered Parity-Time (PT)-symmetric operators. The concept and techniques of PT-symmetry have been applied to many branches of physics [4–19]. Although PT-symmetry was first studied in infinite-dimensional systems, many of the current applications are in finite dimensions.

When discussing PT-symmetry, a related property, pseudo-Hermiticity, is often considered. Pseudo-Hermitian operators were introduced by Dirac and Pauli as a class of non-Hermitian operators [20–22]. Investigating the relation between PT-symmetry and pseudo-Hermiticity may reveal important mathematical and physical structures of non-Hermitian operators. In this regard, Mostafazadeh proved that a diagonalizable PT-symmetric Hamiltonian is pseudo-Hermitian [23–25].

In this paper, we prove that in finite dimensions, a PT-symmetric Hamiltonian is necessarily pseudo-Hermitian regardless of whether it is diagonalizable or not. We first prove that for a Hamiltonian $H$, a sufficient and necessary condition of pseudo-Hermiticity is that $H$ is similar to its Hermitian conjugate $\overline{H}$ (Theorem 2). Then because a PT-symmetric Hamiltonian is similar to its Hermitian conjugate, it is pseudo-Hermitian (Theorem 3). We emphasize that this result is different from Mostafazadeh’s [23–25]. The difference is significant, because our result relaxes the diagonalizability requirement. As we know, most of the interesting PT-symmetry breaking happens at exceptional points where the Hamiltonian is not diagonalizable. Our result is applicable when studying these effects.

As such an application, we show that a theoretical description of PT-symmetry breaking, which is arguably the most important topic in PT-symmetry physics, can be built upon the mathematical work on the instabilities of pseudo-Hermitian systems developed by Krein, Gel’fand and Lidskii [26–28] in 1950s. For a pseudo-Hermitian Hamiltonian, its eigenvalues are symmetric with respect to the real axis. As the system parameters vary, a necessary and sufficient condition for the onset of instability is that two eigenmodes with opposite Krein signatures collide, which is the so-called Krein collision. These results can be directly applied to PT-symmetric Hamiltonians due to Theorem 3, implying that PT-symmetry breaking occurs when and only when eigenmodes with different Krein signatures collide. Note that when PT-symmetry breaking happens, the Hamiltonian can be either diagonalizable or non-diagonalizable. But PT-symmetry is often broken at the exceptional points where the Hamiltonian is not diagonalizable. As an example, we show that the governing equations
of the classical Kelvin-Helmholtz instability, which was proven to be PT-symmetric [19], is pseudo-Hermitian, and the Kelvin-Helmholtz instability is the result of PT-symmetry breaking triggered by the Krein collision.

We start from the definitions of PT-symmetry, pseudo-Hermiticity, and another related concept, i.e., G-Hamiltonian matrix. Consider the linear system specified by a Hamiltonian $H$,

$$\dot{x} = -iHx = Ax,$$  \hspace{1cm} (1)

where $A$ is defined to be a shorthand notation of $-iH$.

The Hamiltonian $H$ in Eq.(1) is called PT-symmetric [1–3] if it commutes with the parity-time operator $PT$, i.e.,

$$PTH - HPT = 0.$$  \hspace{1cm} (2)

Here $P$ is a linear operator satisfying $P^2 = I$ and $T$ is the complex conjugate operator. In the present study, we will focus on finite-dimensional systems, for which $H$, $A$ and $P$ can be represented by matrices, and Eq. (2) is equivalent to

$$P\tilde{H} - \tilde{H}P = 0,$$  \hspace{1cm} (3)

where $\tilde{H}$ denotes the complex conjugates of $H$.

The Hamiltonian $H$ in Eq. (1) is called pseudo-Hermitian [20–22] if there exits a non-singular Hermitian matrix $G$ such that

$$H^\dagger G - GH = 0,$$  \hspace{1cm} (4)

where $H^\dagger$ is the conjugate transpose of the matrix $H$.

The matrix $A = -iH$ in Eq. (1) is called G-Hamiltonian [26–28] if there exist a non-singular Hermitian matrix $G$ and a Hermitian matrix $S$ such that

$$A = iG^{-1}S.$$  \hspace{1cm} (5)

The concept of pseudo-Hermiticity was first introduced by Dirac and Pauli in 1940s [20–22]. G-Hamiltonian matrix was defined by Krein et al. in 1950s [26–28] in the study of linear dynamical systems satisfying the G-Hamiltonian condition (5). For finite-dimensional systems, these two concepts are equivalent.
**Theorem 1.** For a finite-dimensional system \( \dot{x} = -iHx = Ax \), \( H \) is pseudo-Hermitian if and only if \( A \) is a G-Hamiltonian matrix.

The proof of Theorem 1 is straightforward according to the definitions of pseudo-Hermitian and G-Hamiltonian matrices. But we give this fact the status of a theorem to highlight the exact equivalence between these two concepts independently defined by physicists and mathematicians. We will mostly use the terminology of pseudo-Hermiticity exclusively hereafter.

Now we establish a necessary and sufficient condition for pseudo-Hermiticity.

**Theorem 2.** For a matrix \( H \in \mathbb{C}^{n \times n} \), it is pseudo-Hermitian if and if only it is similar to its complex conjugate \( \bar{H} \).

**Proof.** Necessity is easy to prove. If a Hamiltonian is pseudo-Hermitian, i.e., satisfying Eq. (4), then \( H = G^{-1}H^\dagger G \). Thus matrix \( H \) is similar to \( H^\dagger \), and also to \( \bar{H} \).

We prove the sufficiency by constructing the Hermitian matrix \( G \). Matrix \( H \) can be written as

\[
H = Q^{-1}JQ, \tag{6}
\]

where \( J \) is its Jordan canonical form and \( Q \) is a reversible matrix. The Jordan canonical form consists of several Jordan blocks of the form

\[
J(\lambda) = \begin{pmatrix}
\lambda & 1 \\
& \ddots & \ddots \\
& & \ddots & \ddots \\
& & & \lambda & 1 \\
& & & & \lambda
\end{pmatrix}_{m \times m}. \tag{7}
\]

When \( m = 1 \), the Jordan block \( J(\lambda) \) is reduced to \( \lambda \). If \( H \) is similar to \( \bar{H} \), then its eigenvalues are symmetric with respect to the real axis, and they are either real numbers or complex number pairs of the form \( \lambda = a + bi \) and \( \bar{\lambda} = a - bi \), where \( a \) and \( b \) are real numbers. Accordingly, there are two kinds of matrix blocks

\[
F_1 = J(a) = \begin{pmatrix}
a & 1 \\
& \ddots & \ddots \\
& & \ddots & \ddots \\
& & & a & 1 \\
& & & & a
\end{pmatrix}_{m \times m} \quad \text{and} \quad F_2 = \begin{pmatrix}
J(a + bi) & 0 \\
0 & J(a - bi)
\end{pmatrix}_{2l \times 2l}. \tag{8}
\]
The Jordan matrix can now be expressed as $J = \text{Diag}(M_1, M_2, \cdots, M_k)$, where $M_j$ is in the form of $F_1$ or $F_2$. In the following, we prove that both types of matrix blocks are pseudo-Hermitian. For both types of matrix blocks, we find that Hermitian matrix

$$G'_j = \begin{pmatrix} 0 & \cdots & 0 & 1 \\ \vdots & \ddots & \ddots & \ddots \\ 0 & \ddots & \ddots & \ddots \\ 1 & 0 & \cdots & 0 \end{pmatrix}$$

satisfies the condition $M_j^\dagger G'_j - G'_j M_j = 0$, i.e., $M_j$ is pseudo-Hermitian. Next we construct a larger Hermitian matrix $G'$ using $G'_j$ as follows,

$$G' = \text{Diag}(G'_1, G'_2, \cdots, G'_k),$$

and the Jordan canonical form of $H$ satisfies $J^\dagger G' - G' J = 0$. Let

$$G = Q^\dagger G' Q,$$

and we obtain

$$H^\dagger G - G H = (Q^{-1} J Q)^\dagger G - G Q^{-1} J Q$$

$$= Q^\dagger J^\dagger Q^{-1} Q' G' Q - Q^\dagger G' Q Q^{-1} J Q$$

$$= Q^\dagger (J^\dagger G' - G' J) Q$$

$$= 0,$$

where $G$ is a non-singular Hermitian matrix. This completes the proof that $H$ is pseudo-Hermitian.

The theorem is proved by constructing a non-singular Hermitian matrix $G$ for the similarity transformation between $H$ and $\tilde{H}$. But $G$ is not unique. For a given $H$, we can find more than one non-singular Hermitian matrices $G$. In practice, one does not need to follow the construction procedure given in Theorem 2 to find $G$. It is often found by direct calculation.

**Theorem 3.** For finite-dimensional systems, a PT-symmetric Hamiltonian $H$ is necessarily pseudo-Hermitian.

**Proof.** By the definition of PT-symmetry, i.e., Eq. (3), $H$ is similar to $\tilde{H}$. Thus, according to Theorem 2, it is pseudo-Hermitian.

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Theorem 3 is the main theorem in this paper, and we would like to emphasize again that it holds regardless of whether $H$ is diagonalizable or not. We note that Mostafazadeh’s result \cite{23-25}, which states that diagonalizable PT-symmetric Hamiltonians are pseudo-Hermitian, is different from Theorem 3.

As an application of Theorem 3, we investigate the mechanism of PT-symmetry breaking in the framework of pseudo-Hermiticity. Theorem 3 implies that PT-breaking is equivalent to the onset of instabilities of pseudo-Hermitian matrices, which was systematically studied by Krein, Gel’fand and Lidskii \cite{26-28} in 1950s. Specifically, the instability analysis of pseudo-Hermitian matrices gives a comprehensive description on how real eigenvalues of $H$ evolve into conjugate pairs of complex eigenvalues as the system parameters vary. Here we briefly summarize the main results. (i) The eigenvalues of a pseudo-Hermitian Hamiltonian $H$ are symmetric with respect to real axis. They are either real numbers or complex conjugate pairs. (ii) Let $\psi$ be an eigenmode (or eigenvector) of $H$, Krein product of $\psi$ can be defined as \cite{26-28}

$$\langle \psi, \psi \rangle = \psi^\dagger G \psi.$$ 

The sign of the Krein product is called Krein signature. It was found that the physical meaning of the Krein product is action \cite{29}, which is partially indicated by the fact that its dimension is \text{[energy]} \times \text{[time]}. We will also refer to the Krein product as action, especially in the context of physics. (ii) The eigenvalues of $H$ can be classified according to the Krein products of the corresponding eigenvectors. An $r$-fold real eigenvalue $\lambda$ of $H$ with its eigen-subspace $V_\lambda$ is called the first kind if all eigenmodes of $\lambda$ have positive actions, i.e., $\langle y, y \rangle > 0$ for any $y \neq 0$ in $V_\lambda$. It is called the second kind if all eigenmodes of $\lambda$ have negative actions. If there exists a zero-action eigenmode, then $\lambda$ is called an eigenvalue of mixed kind \cite{28}. If an eigenvalue is the first kind or the second kind, it’s called definite. (iii) The number of each kind of eigenvalues is determined by the Hermitian matrix $G$. Let $p$ be the number of positive eigenvalues and $q$ be the number of negative eigenvalues of the matrix $G$, then any pseudo-Hermitian Hamiltonian has $p$ eigenvalues of first kind and $q$ eigenvalues of second kind (counting multiplicity). (iv) The finite-dimensional pseudo-Hermitian Hamiltonian is strongly stable if and only if all of its eigenvalues lie on the real axis and are definite. Here, a pseudo-Hermitian Hamiltonian is strongly stable means that eigenvalues of all pseudo-Hermitian Hamiltonians in an open neighborhood of the parameter space lie on the real axis. As a result, a pseudo-Hermitian Hamiltonian becomes unstable when and only when
a positive-action mode resonates with a negative-action mode. This is a process known as the Krein collision.

Applying these results to PT-symmetric Hamiltonians, we see that PT-symmetry breaking can happen only when a repeated eigenvalue appears as a result of two eigenmodes resonate. However, if two eigenmodes with the same sign of action resonate, then there is no PT-symmetry breaking. PT-symmetry breaking is triggered only when a positive-action mode resonates with a negative-action mode.

Let’s look at an example. The governing equations for the classical Kelvin-Helmholtz instability in fluid dynamics was shown to be a complex system with the following PT-symmetric Hamiltonian [19]

\[
H = \begin{pmatrix}
-k(-u_{10}\rho_{10} - 2u_{20}\rho_{20} + u_{10}\rho_{20}) & -i|k|(u_{10} - u_{20})^2\rho_{20} + ig(\rho_{20} - \rho_{10}) \\
\rho_{10} + \rho_{20} & \rho_{10} + \rho_{20} \\
-i|k| & ku_{10}
\end{pmatrix}.
\]  

(13)

According to Theorem 3, it is also a pseudo-Hermitian Hamiltonian satisfying Eq. (4). With straightforward calculation, we find the following Hermitian matrix

\[
G = \begin{pmatrix}
-|k| & 0 & 0 \\
0 & -|k|(u_{10} - u_{20})^2\rho_{20} - g(\rho_{20} - \rho_{10}) & \rho_{10} + \rho_{20} \\
0 & \rho_{10} + \rho_{20} & ku_{10}
\end{pmatrix}.
\]  

(14)

such that \(H^\dagger G - GH = 0\). The eigenvalues of \(H\) are

\[
a_1 = \frac{k(\rho_{10}u_{10} + \rho_{20}u_{20}) - \sqrt{\Delta}}{\rho_{10} + \rho_{20}},
\]

\[
a_2 = \frac{k(\rho_{10}u_{10} + \rho_{20}u_{20}) + \sqrt{\Delta}}{\rho_{10} + \rho_{20}},
\]

(15)

and the corresponding eigenvectors are

\[
\phi_1 = \left(-\frac{ik\rho_{20}(u_{10} - u_{20}) + \sqrt{\Delta}}{|k|(\rho_{10} + \rho_{20})}, 1\right),
\]

\[
\phi_2 = \left(-\frac{ik\rho_{20}(u_{10} - u_{20}) - \sqrt{\Delta}}{|k|(\rho_{10} + \rho_{20})}, 1\right),
\]

(16)

where \(\Delta = -|k|g(\rho_{10}^2 - \rho_{20}^2) - k^2\rho_{10}\rho_{20}(u_{10} - u_{20})^2\). The Krein signatures, or the signs of actions, of the eigenvalues of \(H\) can be determined by the Hermitian matrix \(G\). When

\[
\tau \equiv \frac{|k|(u_{10} - u_{20})^2\rho_{20} - g(\rho_{20} - \rho_{10})}{\rho_{10} + \rho_{20}} < 0,
\]
FIG. 1. PT-symmetry breaking occurs when a positive-action eigenmode (red) resonates with a negative-action eigenmode (green).

Both eigenvalues of $G$ are negative and the PT-symmetric Hamiltonian $H = iA$ is stable. When $\tau > 0$, one of the eigenvalues of $G$ is positive and the other one is negative. Thus one eigenvalue of $H$ have a positive action and the other one has a negative action, and the resonance between them will result in PT-symmetry breaking. Let’s use a numerically calculated examples to observe the breaking of PT-symmetry. We plot the process in Fig.1 by fixing $u_{10} = 1$, $\rho_{10} = 2$, $\rho_{20} = 3$, $k = 1$ and $g = 3$, and varying $u_{20}$ from 2.3 to 2.7. When $u_{20} = 2.3$, the eigenvalues of $H$ are all real numbers, one of which has a positive action (marked by $M_+$) and the other one has a negative action (marked by $M_-$) in Fig.1(a). Fig.1(b) shows that as $u_{20}$ increases, $M_+$ and $M_-$ move towards each other. Increasing $u_{20}$ to $\sqrt{5}/2 + 1 = 2.58114$, eigenmodes $M_+$ and $M_-$ collide on the real axis, as shown in Fig.1(c). Because the resonance is between modes with different sign of actions, the eigenvalues of $H$ split into a pair symmetric with respect to the real axis and the PT-symmetry is broken. Fig.1(d) shows that the two eigenvalues of $H$ move out of real axis when $u_{20} = 2.7$.

In summary, we have proved that for finite-dimensional systems, a PT-symmetric Hamiltonian is necessarily pseudo-Hermitian regardless of whether it is diagonalizable or not. This result is stronger than Mostafazadeh’s [23,25], which requires that the Hamiltonian is diag-
onalizable. As we know, PT-symmetry breaking often happens at exceptional points where the Hamiltonian is not diagonalizable. The fact that a PT-symmetric Hamiltonian is always pseudo-Hermitian implies that PT-symmetry breaking is equivalent to the onset of instabilities of pseudo-Hermitian matrices. Therefore, the systematic results by Krein et al. on how a pseudo-Hermitian system becomes unstable [26, 28] can be directly applied to the process of PT-symmetry breaking. In particular, we showed that PT-symmetry breaking is triggered when and only when two eigenmodes with different signs of actions resonate. This process is illustrated using the example of the classical Kelvin-Helmholtz instability.

We finish our discussion with an observation. Theorem 3 asserts that a PT-symmetric matrix is necessarily pseudo-Hermitian. One wonders whether the reverse is true. If the $P$ operator in the definition of PT-symmetry (2) is not required to be a parity transformation, i.e., $P^2 = I$, then a pseudo-Hermitian matrix is also PT-symmetric according to Theorem 2. In this case, PT-symmetry and pseudo-Hermitian are equivalent, at least in finite dimensions. We note that essentially all the spectrum properties associated with PT-symmetry are still valid when the requirement of $P^2 = I$ is removed.

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