Pseudo-reality and pseudo-adjointness of Hamiltonians

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Abstract

We define pseudo-reality and pseudo-adjointness of a Hamiltonian, \( H \), as
\[
\rho H \rho^{-1} = H^* \quad \text{and} \quad \mu H \mu^{-1} = H',
\]
respectively. We prove that the former yields the necessary condition for spectrum to be real whereas the latter helps in fixing a definition for inner-product of the eigenstates. Here we separate out adjointness of an operator from its Hermitian-adjointness. It turns out that a Hamiltonian possessing real spectrum is first pseudo-real, further it could be Hermitian, PT-symmetric or pseudo-Hermitian.

Last few years have witnessed a new scope for even a non-Hermitian Hamiltonians to possess real spectrum. It has been found that when a Hamiltonian, \( H \), is invariant under the joint action of parity \((P : x \rightarrow -x)\) and time-reversal \((T : i \rightarrow -i)\) i.e. \([PT, H] = 0\), there may arise surprisingly two situations. One, when \(PT\) and \(H\) admit common eigenstates and two, when they do not do so. In the former situation one can show that the eigenvalues will be real and in the latter the eigenvalues are conjectured to be complex-conjugate pairs and PT-symmetry is said to be spontaneously broken. One can indeed not tell whether a \(PT\)-symmetric potential has real or complex (conjugate pairs of) energy-eigenvalues, until the wavefunctions are analyzed. This intriguing feature has inspired the pursuit [1-6] of both analytically and numerically solved models of PT-symmetric potentials. Thus, PT-symmetry of a Hamiltonian could at most be a necessary and not the sufficient condition for the reality of eigenvalues.

Further, the phenomenon of real eigenvalues of non-Hermitian Hamiltonians has been found to be connected with the already known concept of pseudo-Hermiticity. A Hamiltonian is pseudo-Hermitian [7-16] if
\[ \eta H \eta^{-1} = H^\dagger. \] (1)

It has also been known that
\[ (E_m^* - E_n) \psi_m^\dagger \eta \psi_n = 0, \quad N_{\eta,n} = \psi_n^\dagger \eta \psi_n. \] (2)

Here we propose to choose matrix notations for a subtle reason that these notations have a separate and explicit sign for the adjoint (transpose) operation. The sign, \(^\dagger\), jointly denotes complex-conjugation, \(^*\), and transpose (adjoint), \(',\) of the operators or vectors. Notice that (2) merely asserts two important features of the eigenstates (i) : If eigenvalues are real and distinct, the eigenstates will be \(\eta\)-orthogonal as \(\psi_m^\dagger \eta \psi_n = \epsilon \delta_{m,n}\). (ii) : Complex eigenvalues will have zero pseudo-norm i.e., \(N_{\eta,n} = 0\). Here, we must bring home the fact that the concept of pseudo-Hermiticity as such does not yield an explicit proof for the reality of eigenvalues (even under any further condition), it can only support real eigenvalues indirectly (see Eq. (2)). This shortcoming of pseudo-Hermiticity which has gone un-noticed both recently and initially [7-16] motivates the present work.

Several PT-symmetric potentials having real spectrum have been found to be parity-pseudo-Hermitian where \(\eta = P\)[8]. Several complex potentials which are both PT-symmetric and non-PT-symmetric have been found to be pseudo-Hermitian when \(\eta = e^{-\theta p_x}\)[9]. This operator affects an imaginary shift in the co-ordinate i.e. : \(\eta x \eta^{-1} = x + i\theta\). Several other Hamiltonians of both the types have been reported [10] to be pseudo-Hermitian under \(\eta = e^{\phi(x)}\) : a gauge-like transformation. It has been proved that if a non-Hermitian operator possesses real eigenvalues then there exists (one can find) a metric of the types \(\eta = OO^\dagger\) [8], or \((OO^\dagger)^{-1}\) [11] under which the Hamiltonian is pseudo-Hermitian. Next, following matrix algebra it has been stated and proved [24] that if a matrix-Hamiltonian has real eigenvalues and a diagonalizing matrix \(D\) then it is pseudo-Hermitian under \(\eta_+ = (DD^\dagger)^{-1}\) and vice versa.

Pseudoanti-Hermiticity [9] and a recipe [12] for construction of pseudo-Hermitian potentials have also been discussed. Clearly, without knowing a metric one can not invoke pseudo-Hermiticity. One can find at least one metric, \(\eta_+\), as stated above. It is also, known that a Hamiltonian could be pseudo-Hermitian under several metrics. These metrics would further help in bringing out the symmetry of the Hamiltonian as \([H, \eta, \eta^{-1}]\) [8,23,24]. These metrics may be real, complex, Hermitian, non-Hermitian, unitary, proper (\(\det(\eta) = 1\)), involutary \((\eta^2 = 1)\) and secular etc.. When a metric does not depend upon the parameters of the Hamiltonian, we call it secular [16].
At this stage of the developments, we find that the adjointness of a Hamiltonian has not been taken into account when we discuss the PT-symmetry or pseudo-Hermiticity of a Hamiltonian. As a result, we find that a potential despite being both PT-symmetric and pseudo-Hermitian and possessing real spectrum does not satisfy (e.g. [10]) the PT-orthogonality (PT-inner-product) [3].

\[(E^*_m - E_n)\Psi_m^{PT}\Psi_n = 0, \quad N_{PT,n} = \Psi^{PT}_n \Psi_n.\]  

(3)

It, however, satisfies \(\eta\)-pseudo-orthogonality condition [2]. This is as though PT-symmetry is not enough to ensure orthogonality of eigenstates. A special analysis has been carried out [15] to uphold PT-symmetry in this regard, eventually it yielded a condition more akin to (2). Moreover, as mentioned above the concept of pseudo-Hermicity at best does not contradict the occurrence of the real eigenvalues nevertheless it does not provide a proof for it. This is achieved here in the present work by introducing the concept of pseudo-reality of Hamiltonians.

In this letter, we introduce the concept of pseudo-reality and pseudo-adjointness of a Hamiltonian by proposing to separate out adjointness of an operator from the Hermitian-adjointness, a subtle point which has been missed out in the developments described above.

Let us first discuss the adjointness of an operator. We propose to use \(\prime\) sign for adjoint and transpose if the Hamiltonian is in differential and matrix form, respectively. The adjoint of a differential operator \(A\) denoted as \(A'\) is defined as [17]

\[u.Av - v.A'u = \frac{dW(u,v)}{dx},\]  

(4)

i.e. the right hand side is an exact differential and \(W\) is called bilinear concomitant [17]. The functions \(u, v\) are two arbitrary vectors form a vector space. Here the dot denotes simple multiplication. Subsequently, we have

\[\left(\frac{d^n}{dx^n}\right)' = (-1)^n \frac{d^n}{dx^n}, \quad n = 1, 2, ...\]  

(5)

Thus for the quantum mechanical operators : position, momentum and kinetic energy, we have

\[(x)' = x, \quad (p_x)' = -p_x, \quad \text{and} \quad (K)' = K.\]  

(6)

Thus, Hamiltonians of the type \(p_x^2/(2m) + V(x)\) are self-adjoint, i.e. \(H = H'\). Usually, we use the concept of Hermitian-adjointness in quantum mechanics, i.e.
\[ (p_x)^\dagger = \left(-i\hbar \frac{d}{dx}\right)' = p_x, \]  
(7)

and call an operator \( A \equiv p_x, K \) and \( x \) to be self-(Hermitian)-adjoint by also noticing that \( \langle A\Psi|\Psi\rangle = \langle \Psi|A^\dagger\Psi \rangle \) [17,18]. The phrase Hermitian is also dropped out from self-(Hermitian)-adjoint and it is taken as granted in Hermitian quantum mechanics. Nevertheless, while investigating the real spectrum of non-Hermitian Hamiltonians, we have to disentangle these two. Apparently, the adjoint transformation brings about a “trivial” change in case of differential operator, however, for a matrix operator it changes rows to columns, which appears to be quite a “non-trivial” action. Notice that, in matrix notation, we have

\[ (Au)'v - u'A'v = 0, \]  
(8)

iff ‘ denotes the transpose of a matrix and dot denotes matrix multiplication. In matrix algebra, incidentally one defines “adjoint” of a matrix as \( \text{Adj}(A) = A^{-1}|A| \), which should be taken as a misnomer for quantum mechanical discussions. Let us keep in mind that \( (p_x)^* = -p_x \) and the following transformations

\[ Tp_xT^{-1} = -p_x = Pp_xP^{-1}, TxT^{-1} = x = P(-x)P^{-1}, TKT^{-1} = K = PKP^{-1}, \]  
(9)

for further discussions.

We propose to call a Hamiltonian, \( H \), as pseudo-real if

\[ \rho H \rho^{-1} = H^*, \]  
(10)

and pseudo-adjoint if

\[ \mu H \mu^{-1} = H'. \]  
(11)

**Proposition I :**

If a Hamiltonian, \( H \), is pseudo-real (10), then it has real eigenvalues, \( E \), subject to a condition on its eigenstate, \( \Psi \). Recall that \( (AB)^* = A^*B^* \).

**Proof :** Let \( H\Psi = E\Psi \),

\[ \Rightarrow (H\Psi)^* = (E\Psi)^*, \Rightarrow H^*\Psi^* = E^*\Psi^*, \Rightarrow \rho H \rho^{-1}\Psi^* = E^*\Psi^*, \Rightarrow H \rho^{-1}\Psi^* = E^* \rho^{-1}\Psi^*. \quad \Box \]  
(12)

We finally find that
\[ E = E^*, \text{ iff } \rho^{-1} \Psi^* = \epsilon \Psi. \]  

Let us have a quick illustration of what we mean. If \( H_0 = cp_x \), we find that this Hamiltonian is pseudo-real under parity \( P \), it possesses real eigenvalues \( \pm ck \) and the eigenstates are \( \Psi = e^{\pm ikx} \), with \( \epsilon = 1 \).

**Proposition II:**

If a Hamiltonian, \( H \), is pseudo-real (10) and pseudo-adjoint (11), then it is pseudo-Hermitian (1) under

\[ \eta = (\mu \rho^{-1})'. \]

Recall that \( (AB)' = B'A' \).

**Proof:**

\[
\rho H \rho^{-1} = \rho(\mu^{-1}H'\mu)\rho^{-1}, \Rightarrow H^* = \left( \rho\mu^{-1}H'\mu\rho^{-1} \right), \Rightarrow H'^* = (\mu \rho^{-1})' H (\mu \rho^{-1)'). \quad \square
\]

Finally we have

\[
(\mu \rho^{-1})' H \left( (\mu \rho^{-1})' \right)^{-1} = H^\dagger.
\]

Further, the orthogonality of the eigenstates will follow according to (2), which now reads as

\[
(E_m^* - E_n) \Psi_m^\dagger (\mu \rho^{-1})' \Psi_n = 0, \quad N_{\eta,n} = \Psi_n^\dagger (\mu \rho^{-1})' \Psi_n.
\]

Hermiticity of \( H \), follows when we have \( \rho = \mu \). PT-symmetry of the Hamiltonian follows when we have \( \rho = P \) and \( \mu = 1 \). In addition to this, if we treat complex conjugation as \( T \) in (13), we re-discover the fact that eigenvalues of a PT-symmetric potential will be real provided \( PT\Psi = \epsilon \Psi \), i.e \( \Psi \) is also the eigenstate of \( PT \). The Hamiltonians of the type

\[
H_1 = \frac{p_x^2}{2m} + Ve(x) + iVo(x) \quad [1-6],
\]

where \( e \) and \( o \) denote even and odd functions are such examples. For such PT-symmetric potentials, the self-adjointness of \( H \) is implied \( \mu = 1 \), and the following orthogonality condition

\[
(E_m - E_n) \Psi_m^\dagger \Psi_n = 0
\]

will also work, automatically. Notice the absence of \( \dagger \) in (18). One can check that \( H_1 \) possesses real eigenvalues since it is pseudo-real, \( PH_1 P^{-1} = H_1^* \) and the condition (13)
is explicitly satisfied by the energy-eigenstates. Several, exactly solvable models of PT-symmetric potentials [1-6] are available for a verification.

The complex quasi-exactly solvable Hamiltonian \[ H_2 = \frac{p_x^2}{2m} - (z \cosh 2x - 3i)^2 \] (19) has first three eigenvalues (real if \( z^2 \leq \frac{1}{4} \)) and eigenfunctions known analytically. \( H_2 \) was termed as PT-symmetric under \( T : i \rightarrow -i \), and \( P : x \rightarrow i\pi/2 - x \). Notice that both the operations do not commute [5]. We find that \( H_2 \) more appropriately is pseudo-real under the transformation \( \rho : x \rightarrow (i\pi/2 - x) \) and self-adjoint (\( \mu = 1 \)). The eigenfunctions [3] can be checked to satisfy the proposed condition (13).

Let us consider the following Hamiltonian
\[ H_3 = \frac{[p_x + i\beta x]^2}{2m} + \frac{1}{2}m\alpha^2 x^2, \] (20) which admits real eigenvalues and real eigenvectors [10]. We find that \( H_3 \) is trivially pseudo-real (10) under \( \rho = 1 \) and we will have real eigenvalues and real eigenfunctions too [10]. Next, \( H_2 \) is pseudo-adjoint (11) as \( e^{-\beta x^2}H_3e^{\beta x^2} = H_3' \). So we have \( \mu = e^{-\beta x^2} = \eta \). Alternatively, we may take \( H_2 \) to be pseudo-real under \( \rho = P \) and then \( \eta = e^{-\beta x^2}P \), also see [15]. Obviously, in both the cases \( H_3 \) would rather be categorized as pseudo-Hermitian despite being PT-symmetric.

Next let us consider the Hermitian Hamiltonian
\[ H_4 = \frac{[p_x - 3\gamma x^2]^2}{(2m)} + \frac{1}{2}m\alpha^2 x^2. \] (21) which has real eigenvalues. One can readily check that \( \rho = \mu = P \), this leads to Hermiticity. We find that \( e^{-2i\gamma x^3}H_4e^{2i\gamma x^3} = H_4^* = H_4' \) that means we again have the situation of Hermiticity where \( \rho = \mu = e^{-2i\gamma x^3} \). Other interesting options are to choose \( \rho = P \) and \( \mu = e^{-2i\gamma x^3} \) or \( \rho = e^{-2i\gamma x^3} \) and \( \mu = P \). In both situations, we have \( \eta = e^{-2i\gamma x^3}P \), see also [14].] The \( \eta \)-norm (2) will be indefinite, \((-1)^n, n = 0, 1, 2,.. \).

Intriguingly, when we choose to see even a Hermitian Hamiltonian (e.g. (21)) as PT-symmetric or pseudo-Hermitian both the norms are indefinite (positive-negative). However, the Hermitian norm , namely, \( \Psi^\dagger \Psi \) remains definite (positive). This point has earlier been revealed and remarked [22,24], however, it is often overlooked (see e.g. [23],[26]).

Complex Morse potential \( V^{C-M}(x) = (A+iB)^2e^{-2x} - (2c+1)(A+iB)e^{-x} \) which is non-PT-symmetric was found [5] to have real eigenvalues. Notice that the real Morse potential is
written as $V^{R-M}(x) = D^2e^{-2x} - (2C + 1)De^{-x}$ and $V^{C-M}(x)$ is nothing but $V^{R-M}(x - ia)$. The Hamiltonian with this potential has been investigated [9] to be pseudo-Hermitian under $\eta = e^{-2ap_x}$. If real potentials $V(x)$ admit real eigenvalues then the potentials $V(x - ia)$ are also found to possess identical eigenvalues. When real and imaginary parts of $V(x - ia)$ are separated out, the re-written potential would actually appear to be “different” and even “unrelated” with $V(x)$. The equivalence of two spectra will be due to the fact that the Hamiltonian $H(x) = p_x^2/(2m) + V(x)$ follows: $e^{-ap_x}H(x - ia)e^{ap_x} = H(x)$. We find that $e^{-2ap_x}H(x - ia)e^{2ap_x} = H(x + ia)$ implying that $\rho = e^{-2ap_x}$ and $\mu = 1$. Thus, both the orthogonality conditions (17) and (18) will be satisfied. We have indefinite norms: $N_{PT,n} = (-1)^n = N_{\eta,n}$.

Norm of the eigenstates is required to be positive definite for a probabilistic interpretation of quantum mechanics. In this regard the existence of $\eta_+$ in the form $(DD^\dagger)^{-1/2}[24]$ for a pseudo-Hermitian Hamiltonian possessing real eigenvalues is very important. Currently, the indefiniteness of pseudo-norms is proposed to indicate the presence of a Hidden symmetry, $C$ [19], which mimics charge-conjugation symmetry $C$ [20]. It has also been proposed that it is the $CPT - norm$ that will be positive definite. Consequently, the Hermitian Hamiltonians are $P-, T-, PT-$, and $CPT-$ invariant [22] and pseudo-Hermitian Hamiltonians are $C-, PT-$, and $CPT-$ invariant [24]. $PT-$ and $CPT-$ norms are indefinite and definite respectively. In these works [19,21,22,24] one is actually talking about generalized discrete symmetry operators: $C, P$, and $T$ [23].

Recently, $2 \times 2$ pseudo-Hermitian matrix Hamiltonians [16] have been found to give rise to a certain novelties in the random matrix theory. In this theory, to study fluctuation properties of energy-spectrum hitherto one has modeled Hamiltonians as real-symmetric or Hermitian matrices. More recently such simple $2 \times 2$ matrix Hamiltonians are being found handy in bringing out interesting features of PT-symmetry [25,26].

In the following, we take up examples of simple pseudo-Hermitian matrices, for further demonstration of the pseudo-reality and pseudo-adjointness of Hamiltonians.

$$H_5 = \begin{bmatrix} a + ib & c & \\ c & a - ib & \end{bmatrix}, \quad H_6 = \begin{bmatrix} a + c & ib & \\ ib & a - c & \end{bmatrix}, \quad H_7 = \begin{bmatrix} a & i(b - c) & \\ i(b + c) & a & \end{bmatrix}; \quad c^2 > b^2 \quad (22)$$

The eigenvalues of these matrices are $a \pm \sqrt{c^2 - b^2}$. In the following, we make an interesting use of Pauli matrices. For $H_5$, we find that $\rho = \sigma_x, \mu = 1$, so $H_5$ is pseudo-Hermitian under $\eta = \sigma_x$. One can check that $H_6$ is pseudo-real under $\rho = \sigma_z$ and $H_6 = H_6'$, so it is pseudo-
Hermitian under $\eta = \sigma_z$ as we have $\mu = 1$ again. The Hamiltonian $H_7$ is pseudo-adjoint under $\sigma_x$ and it is pseudo-real under $\sigma_z$ to display pseudo-Hermiticity under $\eta = \sigma_y$.

Let us define a real diagonal matrix $E = \text{diag}[E_1, E_2, E_3, ..., E_n]$, i.e., $E^* = E$ and $E' = E$

**Proposition III:**
If a complex Hamiltonian, $H$, possessing real spectrum is diagonalizable by an operator $D$, it is pseudo-real (10) under $\rho = D^*D^{-1}$ (converse is also true).

**Proof:**

\[
D^{-1}HD = E, \Rightarrow D^{-1}H^*D^* = E^*, \Rightarrow D^{-1}\rho H\rho^{-1}D^* = E \Rightarrow \rho = D^*D^{-1}. \quad \square \tag{23}
\]

Note an interesting property of $\rho$ namely $\rho \rho^* = 1$.

**Proposition IV:**
If a Hamiltonian is diagonalizable by an operator $D$, it is pseudo-adjoint (11) under $\mu = (DD')^{-1}$.

**Proof:**

\[
D^{-1}HD = E, \Rightarrow D'HD^{-1}' = E', \Rightarrow D'\mu H\mu^{-1}D^{-1}' = E \Rightarrow \mu = (DD')^{-1}. \quad \square \tag{24}
\]

**Proposition V:**
If a Hamiltonian $H$ possessing real spectrum is pseudo-real under $\rho = D^*D^{-1}$ and pseudo-adjoint under $\mu = (DD')^{-1}$, it is pseudo Hermitian under $\eta = (DD')^{-1}$ (Converse is also true).

The proof follows straight from Proposition II. When $H$ is Hermitian $D$ will be unitary ($U^\dagger = U^{-1}$). We find that $\rho = U^\dagger U = \mu$ and $\eta = 1$. Note that $\mu$ is self-adjoint i.e., $\mu = \mu^\dagger$.

**Illustration:**

The following Hamiltonian $H_8$

\[
H_8 = \begin{bmatrix} a + ib & c + id \\ c - id & a - ib \end{bmatrix}, \quad \Psi_1 = \begin{bmatrix} -e^{-i\theta} \\ e^{-i\phi} \end{bmatrix}, \quad \Psi_2 = \begin{bmatrix} e^{i\theta} \\ e^{-i\phi} \end{bmatrix}, \quad \Phi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \Phi_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{25}
\]

is pseudo-real under $\sigma_x$ and possesses real eigenvalues $a \mp e$, where $e = \sqrt{c^2 + d^2 - b^2}$ if $c^2 + d^2 > b^2$. Here $\Psi_n$ are eigenvectors of $H$ and $\Phi_n$ provides a fundamental orthonormal basis. $D$ can be constructed as $D = \sum_n \Psi_n^\dagger \Phi_n$. We find the expressions for $\rho, \mu$ and $\eta_+$ are

\[
\rho = \begin{bmatrix} 1 & -2ie^{i\phi}\sin\theta \\ 0 & e^{2i\phi} \end{bmatrix}, \quad \mu = \frac{\sec^2\theta}{2} \begin{bmatrix} 1 & -ie^{i\phi}\sin\theta \\ -i\sin\theta e^{i\phi} \cos2\theta e^{2i\phi} \end{bmatrix}, \quad \eta_+ = \frac{\sec^2\theta}{2} \begin{bmatrix} 1 & -i\sin\theta e^{i\phi} \\ i\sin\theta e^{-i\phi} & 1 \end{bmatrix}. \tag{26}
\]
We have introduced $\theta = \tan^{-1}(b/e)$ and $\phi = \tan^{-1}(d/c)$. This illustration also displays the non-uniqueness of $\rho$. Using $\rho = \sigma_x$ and $\mu$ as in (26), we can construct $\eta = (\mu \sigma_x)'$. This metric $\eta$ will satisfy the orthogonality condition (2), however, it does not yield the $\eta$-norm (2) of the vectors $\Psi_n$ as real, whereas $\eta^+$-norm will be real and positive definite.

The PT-symmetric potentials in finite basis space yield finite dimensional matrix Hamiltonians. In this regard, it is interesting to note that two-dimensional and three-dimensional matrix Hamiltonians obtained [27] for the potentials of the type $V(x) = ix^{2n+1}$ are pseudo-real where $\rho = \sigma_z$ and

$$\rho = \begin{bmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 1
\end{bmatrix}, \quad (27)$$

respectively. Some more interesting aspects of finite, D-dimensional, PT-symmetric Hamiltonians have recently been discussed [25,26].

In the end, we conclude that Hamiltonians having real discrete spectrum are first pseudo-real (10), further they could be Hermitian, PT-symmetric or pseudo-Hermitian. The separation of adjointness of an operator from the Hermitian-adjointness is something which is natural when one investigates real spectrum of non-Hermitian Hamiltonians. Consequent to this, we find that the Hamiltonians will have real spectrum if they are pseudo-real provided the eigenstates meet the condition (13). Further, the proposed pseudo-adjointness (11) helps in fixing the inner-product of the states. And this brings pseudo-reality to its logical end, that is, $\eta$-pseudo-Hermiticity, however, not without enriching and supplementing it with a relaxed necessary condition (10) and a crucial axillary condition (13) on the eigenstates for real eigenvalues. We wish that the simple examples presented here would help in further extensions by providing a deeper insight in to this subject.

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