P, T, PT, and CPT invariance of Hermitian Hamiltonians

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Abstract

Currently, it has been claimed that certain Hermitian Hamiltonians have parity (P) and they are PT-invariant. We propose generalized definitions of time-reversal operator (T) and orthonormality such that all Hermitian Hamiltonians are P, T, PT, and CPT invariant. The PT-norm and CPT-norm are indefinite and definite respectively. The energy-eigenstates are either E-type (e.g., even) or O-type (e.g., odd). C mimics the charge-conjugation symmetry which is recently found to exist for a non-Hermitian Hamiltonian. For a Hermitian Hamiltonian it coincides with P.

The Hamiltonians which are invariant under the joint transformation of Parity ($x \rightarrow -x$) and Time-reversal ($i \rightarrow -i$) are called PT-invariant. It has been conjectured [1] that such Hamiltonians possess real discrete energy-eigenvalues provided the PT symmetry is unbroken. PT-symmetry is called unbroken or exact if the energy-eigenstates are also simultaneous eigenstates of PT. On the other hand when PT-symmetry is spontaneously broken the energy-eigenvalues are complex conjugate pairs. Multipronged investigations supporting this conjecture have been extensively carried out [1-3]. Consequently, the condition of Hermiticity for a Hamiltonian to possess real eigenvalues gets relaxed. It is remarkable that it is discrete symmetries of an Hamiltonian which seem to decide if the eigenvalues will be real.

The real eigenvalues of the PT-symmetric potential can now be found to be connected to the concept of $\eta$—distorted inner-product $\langle \psi | \eta \psi \rangle$ [4] which culminated in 50s-60s into the concept of pseudo-Hermiticity [5] of a Hamiltonian
\[ \eta H \eta^{-1} = H^\dagger, \]  

(1)

wherein it is known [5] that the distinct real eigenvalues have \( \eta \)-orthogonal eigenvectors. The complex eigenvalues are known to have zero \( \eta \)-norm. Recently, several PT-symmetric potentials have been pointed out to be P-pseudo-Hermitian [6]. Several other classes of non-Hermitian Hamiltonians which are both PT-symmetric and non-PT-symmetric Hamiltonians have been argued to be pseudo-Hermitian under \( \eta = e^{-\theta p} \) and \( \eta = e^{-\phi(x)} \) [7]. Pseudo-Hermiticity has been found to be more general when non-Hermitian Hamiltonians have real eigenvalues. However, the notion of PT-symmetry is physically more appealing which could provide contact with physical systems and situations. Recently, by constructing \( 2 \times 2 \) pseudo-Hermitian matrices a new pseudo-unitary group and new ensembles of Gaussian-random matrices have been proposed [8]. New energy-level-spacing-distribution functions hence obtained [8] are expected to represent the spectral fluctuations of PT-symmetric systems.

A real central potential in three dimensions and real a symmetric (under space reflection) potentials in one dimension are automatically PT symmetric. It is the real, non-symmetric potential in one dimension which by admitting real eigenvalues would disallow a conjecture that Hermitian potentials are PT-symmetric. However, currently for Hamiltonians of the type \( \mathcal{H} = \frac{p^2}{(2m)} + V(x) \) two fundamental claims have been made: \( C_1 \) : “Hermitian Hamiltonians, \( \mathcal{H} \), have Parity” and \( C_2 \) : “Hermitian Hamiltonians, \( \mathcal{H} \), are PT-invariant (converse not true).” [9] These claims are fundamentally important as they connect the discrete symmetry (PT-symmetry) of the Hamiltonian to the reality of eigenvalues in the conventional quantum mechanics. In this Letter, we shall examine, extend and consolidate these claims further. Let us remark that this PT-symmetry of a Hermitian Hamiltonian [9] in contrast to the conjecture of Bender and Boettcher [1] essentially includes the individual P and T invariance of a Hamiltonian.

According to the claim \( C_1 \) Hermitian Hamiltonians, \( \mathcal{H} \), have parity [9]. If \( \mathcal{H} \) is a Hermitian Hamiltonian with an eigenvalue equation

\[ \mathcal{H}\Psi_n = E_n\Psi_n. \]  

(2)

The completeness and orthonormality of the eigenstates read as

\[ \sum_{n=0}^{\infty} |\Psi_n\rangle \langle \Psi_n| = 1, \langle \Psi_m|\Psi_n\rangle = \delta_{m,n}. \]  

(3)
The parity operator $P$ has been proposed \[9\] as

$$P = \sum_{n=0}^{\infty} (-1)^n |\Psi_n \rangle \langle \Psi_n|.$$  

It can be shown that $P$ is involutary and it commutes with $\mathcal{H}$ and its eigenvalues are $\pm 1$ i.e.,

$$P^2 = 1, [P, \mathcal{H}] = 0, P|\Psi_n \rangle = (-)^n |\Psi_n \rangle.$$  

For the Hamiltonians of the type $H_S = \frac{p^2}{2m} + V_S(x)$ where $V_S(x)$ is symmetric under space-reflection this proposal works well as the eigenstates will be symmetric (anti-symmetric) as $n$ is even (odd). Imagine, if $V_S(x)$ is slightly distorted to make it non-symmetric ($V_{N-S}(x)$), this potential will have the same number of bound-states but now they can no more be classified as even/odd functions of space variable despite their quantum numbers being even/odd. The claim $C_1$ that all Hermitian Hamiltonian have parity would break down.

When there exists a symmetry in the system one can classify the state and a certain kind of order can be observed. When this symmetry is broken, we loose the order and would find it difficult to classify the states again. Thus, we propose a new classification scheme of the states for the potential $V_{N-S}(x)$ to revive the claim $C_1$. We term the states as Extraordinary-type (E-type) when the wavefunctions satisfy a condition that $\Psi_n(x = -L)\Psi_n(x = R) > 0$ and Ordinary-type (O-type) when we have $\Psi_n(x = -L)\Psi_n(x = R) < 0$. Here, $L, R$ are the large asymptotic distances on either side of the potential. Therefore, one can now state that all Hermitian Hamiltonians have a generalized parity (4) wherein the states are either E-type or O-type. The E-type (O-type) of states have even (odd) number of nodes. It may be well to recall that in Bohr-Sommerfeld or WKB quantization of the Hamiltonian, the quantum number $n$ is set even and odd alternatively to get the complete spectrum irrespective of the symmetry of the potential. These methods do seem to have a generalized sense built in them. Let us remark that the Hamiltonians of the type $[p - \phi]^2/(2m) + V(x)$ could be treated as $H_{N-S}$.

The most interesting aspect of the $\eta-$norm ($\langle \Psi | \eta \Psi \rangle$) [4,5] or PT-norm is its indefiniteness (positive-negative) [3] ($\langle \Psi | P \Psi \rangle$) as against the positive definiteness of the usual (unitary, Hermitian) norm ($\langle \Psi | \Psi \rangle$). Since the norm represents the quantum mechanical probability, an indefinite PT or $\eta-$ norm is taken to be very seriously. In this regard, a current proposal [10] that the negativity of the PT-norm indicates a hidden symmetry which would mimic [11]
charge-conjugation symmetry (C) such that CPT-norm is positive definite is very appealing. Consequent to this a pseudo-Hermitian $(1) \ 2 \times 2$ matrix Hamiltonian has been demonstrated to be C,PT,CPT invariant by constructing $P = \eta, T = K_0$ and C in an interesting way [10].

It becomes natural to put the claims ($C_{1,2}$) in this more general perspective for the sake of consistency. Since the potentials considered in [9] are real and therefore the PT-invariance of Hermitian Hamiltonians is automatic. We find that the definition of $T$ as $K_0$ [10], if extended to the Hermitian matrix Hamiltonians, would actually disprove the claim $C_2$. To be both consistent and rigorous, one actually requires a generalized definition a la (4) of an anti-linear, involutary operator associated with time-reversal symmetry $T$.

To this end, we would like to switch over to matrix notation of eigenstates $\Psi_n$. Let us recall that we can have three operations over $\Psi_n$ i.e., complex-conjugation ($\Psi_n^*$), transpose operation ($\Psi_n'$) and both together as $\Psi_n^\dagger$ which denotes the Dirac’s bra-vector : $(\Psi_n | = | \Psi_n\rangle^\dagger$. Without loss of generality, we assume the Hamiltonian to be a $2 \times 2$ matrix with eigenvalue equation as $H\Psi_n = E_n\Psi_n$ $(n = 0, 1)$, so we have

$$\Psi_0^\dagger\Psi_0^\dagger + \Psi_1^\dagger\Psi_1^\dagger = 1, \Psi_n^\dagger\Psi_m = \delta_{m,n}. \quad (6)$$

The parity operator (4) becomes

$$P = \Psi_0^\dagger\Psi_0^\dagger - \Psi_1^\dagger\Psi_1^\dagger \quad (7)$$

yielding

$$P^2 = (\Psi_0^\dagger\Psi_0^\dagger - \Psi_1^\dagger\Psi_1^\dagger - \Psi_0^\dagger\Psi_1^\dagger + \Psi_0^\dagger\Psi_1^\dagger) = (\Psi_0^\dagger\Psi_0^\dagger + \Psi_1^\dagger\Psi_1^\dagger) = 1, \quad (8)$$

and $[P, H] = PH - HP = 0, P\Psi_n = (-)^n\Psi_n. \quad (9)$

We propose the anti-linear time-reversal operator $T$ as

$$T = UK_0 = (\Psi_0^\dagger\Psi_0^\dagger + \Psi_1^\dagger\Psi_1^\dagger) K_0. \quad (10)$$

Here, $K_0$ is the complex-conjugation operator i.e., $K_0(AB + CD) = A^*B^* + C^*D^*$. the operator $T$ is involutary

$$T^2 = UK_0UK_0 = (\Psi_0^\dagger\Psi_0^\dagger + \Psi_1^\dagger\Psi_1^\dagger) = 1. \quad (11)$$
T commutes with H

\[ [T, H] = TH - HT = 0, T\Psi_n = \Psi_n. \]  

(12)

Using (7) and (10), we construct PT or TP operators as

\[ PT = (\Psi_0 \Psi_0' - \Psi_1 \Psi_1') K_0 = TP, \]  

(13)

which has the following properties :

\[ (PT)^2 = 1, [PT, H] = 0, PT\Psi_n = (-1)^n \Psi_n. \]  

(14)

We now define a general \( \chi \)-orthonormality and \( \chi \)-norm as

\[ (\chi \Psi_m)^\dagger \Psi_n = C_{m,n} \delta_{m,n}, N_\chi = (\chi \Psi)^\dagger \Psi, \]  

(15)

\( C_{m,n} \) is indefinite (positive-negative). \( \chi \) in the above equation denotes discrete symmetry operators (P, T, and PT) of the Hermitian Hamiltonian, i.e \([\chi, H] = 0\). Thus for a Hermitian Hamiltonian \( H \) we get

\[ N_{PT,n} = (-1)^n, n = 0, 1, \]  

(16)

which is indefinite. The indefiniteness of PT-norm when the Hamiltonian is non-Hermitian, PT-symmetric (pseudo-Hermitian) has motivated a novel identification of charge-Conjugation symmetry, \( C \), in order to make the CPT-norm definite [10].

In our case when the Hamiltonian is Hermitian, choosing one from \( \Psi^\dagger, \Psi' \) and other from \( \Psi^*, \Psi \), one can construct only two distinct and nontrivial involutary operators \( P \) and \( T \). One can therefore not associate with a Hermitian Hamiltonian third distinct linear involutary operator which could possibly be charge-conjugation-operator \( C \) such that \( C^2 = 1 \). Notice that by setting \( C = P \), we find that \( N_{CPT} (\chi = CPT = P^2T = T) \) in (15) is positive definite and Hamiltonian is CPT-invariant i.e., \([H,\text{CPT}]=[H,P^2T]=[H,T]=0\).

Let us re-emphasize that the definition of \( T \) assumed as \( K_0 \) in Ref. [10] fails to prove the \( T \) and PT-invariance of a Hermitian matrix Hamiltonian. Here, we are able to define \( T \) and norm as in Eq.(10) and Eq. (15) respectively which salvages this problem and one can prove the claimed [9] PT-symmetry of Hermitian Hamiltonian in general. In the illustration below this point is being brought out.
Illustration:

Let the Hermitian Hamiltonian be modelled as

\[ H = \begin{bmatrix} a & b + ic \\ b - ic & a \end{bmatrix}, \]  

(17)

The eigenvalues are \( E_{0,1} = a \pm \sqrt{b^2 + c^2} \) and the normalized eigenvectors are

\[ \Psi_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{i\theta} \\ 1 \end{bmatrix}, \quad \Psi_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{i\theta} \\ -1 \end{bmatrix} \]  

(18)

where \( \theta = \tan^{-1}(c/b) \). Using (7) and (10) \( P \) and \( T \) can be constructed as

\[ P = \begin{bmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{bmatrix}, \quad T = \begin{bmatrix} e^{2i\theta} & 0 \\ 0 & 1 \end{bmatrix} K_0, \quad PT = \begin{bmatrix} 0 & e^{i\theta} \\ e^{i\theta} & 0 \end{bmatrix} K_0 \]  

(19)

One can readily verify the involutions : \( P^2 = 1 = T^2 = (PT)^2 \) and commutations revealing the discrete symmetries of \( H : [P,H]=[T,H]=[PT,H]=0 \). One can confirm that \( \Psi_{0,1} \) are also the eigenstates of \( P,T, \) and \( PT \). One can see that \( N_{PT,n} = (-1)^n \). However, following the Ref. [10], if we assume \( T=K_0 \), it can be quickly be seen that \( [T,H] \neq 0 \neq [PT,H] \). The PT-orthonormality as defined in [10] which in matrix notation reads as \( (PK_0\Psi_0)\Psi_1 \) does not vanish and becomes complex ! This justifies our definitions of \( T \) and \( \chi \)-orthonormality given in (10) and (15) respectively. Let us point out that generalization to \( N \times N \) matrix Hamiltonians is straightforward i.e.,

\[ P = \sum_{n=0}^{N} (-1)^n \Psi_n \Psi_n^\dagger, \quad T = \left( \sum_{n=0}^{N} \Psi_n \Psi_n^\dagger \right) K_0 \]  

(20)

Thus, by employing our proposed definitions of \( T \) and \( \chi \)-orthonormality in (10) and (15) we could establish and demonstrate that Hermitian Hamiltonians are \( P \)-symmetric, \( T \)-symmetric, \( PT \)-symmetric, \( CPT \)-symmetric and the eigenstates are either \( E \)-type or \( O \)-type. \( PT \)-norm (\( CPT \)-norm) is indefinite (definite). In the light of this work one now requires the definitions of linear (\( C,P \)) and anti-linear operator \( T \) when the Hamiltonian is pseudo-Hermitian matrix [8] possessing real eigenvalues. As the basis for a pseudo-Hermitian Hamiltonian is known to be bi-orthonormal (\( \Psi,\Phi \)) [5], this gives a possible handle for constructing one more involutary operator \( C \) other than \( P \) and \( T \). Thus found definitions of \( P, T, \) and \( C \) and orthonormality are expected to be consistent with the definitions discussed.
here (7,10,15). In fact, the new definitions ought to contain the present ones as a special case. These constructions, however, turn out to be quite elusive presently. It is instructive to note that matrix notations are not only handy but also are more transparent and general than Dirac’s notations of bras and kets. This feature brings the present work closer to the discrete symmetries \( \mathcal{P}, \mathcal{T} \) and \( \mathcal{C} \) which are discussed in relativistic field theory [11].

REFERENCES

1. C.M. Bender and S. Boettcher, Phys. Rev. Lett. 80 (1998) 5243;

2. M. Znojil, Phys. Lett. A 259 (1999) 220; 264 (1999) 108.
   C. M. Bender, G. V. Dunne, P. N. Meisinger, Phys. Lett. A 252 (1999) 253.
   H.F. Jones, Phys. Lett. A 262 (1999) 242.
   B. Bagchi and R. Roychoudhury, J. Phys. A : Math. Gen. A 33 (2000) L1.
   G. Levai and M. Znojil, J. Phys. A : Math. Gen. 33 (2000) 7165.
   A. Khare and B.P. Mandal, Phys. Lett. A 272 (2000) 53.
   B. Bagchi and C. Quesne, Phys. Lett. A 273 (2000) 285.
   R. Kretschmer and L. Symanowaski, ‘The interpretation of quantum mechanical models with non-Hermitian Hamiltonians and real spectra’, arXive quant-ph/0105054
   Z. Ahmed, Phys. Lett. A: 282 (2001) 343; 287 (2001) 295; 286 (2001) 231.
   R.S. Kaushal, J. Phys. A: Math. Gen, 34 (2001) L709.
   R.S. Kaushal and Parthasarathi, J. Phys. A : Math. Gen. 35 (2002) 8743.
   Z. Ahmed,’Discrete symmetries, Pseudo-Hermiticity and pseudo-unitarity’, in DAE (India) symposium on Nucl. Phys. Invited Talks eds., A.K.Jain and A. Navin, vol 45 A (2002) 172.

3. Z. Ahmed, ‘A generalization for the eigenstates of complex PT-invariant potentials with real discrete eigenvalues’ (unpublished) (2001).
   M. Znojil, ‘Conservation of pseudo-norm in PT-symmetric quantum mechanics’, arXive quant-ph/0104012.
   B. Bagchi, C. Quesne and M. Znojil, Mod. Phys. Lett. A16 (2001) 2047.
   G.S. Japaridze, J. Phys. A : Math. Gen. 35 (2002) 1709.
4. P.A.M. Dirac, Proc. Roy. Soc. London A 180 (1942) 1.
   W. Pauli, Rev. Mod. Phys. 15 (1943) 175.
   T.D. Lee, Phys. Rev. 95 (1954) 1329.
   S.N. Gupta, Phys. Rev. 77 (1950) 294.
   K. Bleuler, Helv. Phys. Act. 23 (1950) 567.

5. R. Nevanlinna, Ann. Ac. Sci. Fenn. 1 (1952) 108; 163 (1954) 222.
   L.K. Pandit, Nouvo Cimento (supplimento) 11 (1959) 157.
   E.C.G. Sudarshan, Phys. Rev. 123 (1961) 2183.
   M.C. Pease III, Methods of matrix algebra (Academic Press, New York, 1965).
   T.D. Lee and G.C. Wick, Nucl. Phys. B 9 (1969) 209.
   F.G. Scholtz, H. B. Geyer and F.J.H. Hahne, Ann. Phys. 213 (1992) 74.

6. A. Mostafazadeh, J. Math. Phys. 43 (2002) 205; 43 (2002) 2814; 43 (2002) 3944.

7. Z. Ahmed, Phys. Lett. A 290 (2001) 19; 294 (2002) 287.

8. Z. Ahmed and S.R. Jain, “Pseudo-unitary symmetry and the Gaussian pseudo-unitary
   ensemble of random matrices”, arXiv quant-ph/0209165 (also submitted to Phys. Rev.
   E).
   Z. Ahmed and S.R. Jain, “Gaussian ensembles of 2 × 2 pseudo-Hermitian random
   matrices” to appear in J. Phys. A: Math. Gen. (2003, The special issue on Random
   Matrices).
   Z. Ahmed, “An ensemble of non-Hermitian Gaussian-random 2 × 2 matrices admitting
   the Wigner surmise” to appear in Phys. Lett. A (PLA 12155) 2003.

9. C.M. Bender, P.N. Meisinger and Q. Wang, “All Hermitian Hamiltonians have parity”,
   arXive quant-ph/0211123, J. Phys. A : Math. Gen. 36 (2003) 1029.

10. C.M. Bender, D.C. Brody and H.F. Jones, “Complex extension of quantum mechanics”,
    arXiv quant-ph/2010076, Phys. Rev. Lett. 89 (2002) 270401.

11. J.D. Bjorken and S. D. Drell, Relativistic quantum fields (McGraw-Hill, New
    York, 1965) ch. 15, pp. 107-123.