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Pseudo-Hermiticity of Hamiltonians under gauge-like transformation: real spectrum of non-Hermitian Hamiltonians

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Abstract

We report that it is the pseudo-Hermiticity of Hamiltonians under the gauge-like transformation that underlies the reality of the spectrum and orthogonality of states for the non-Hermitian Hamiltonians type $H_\beta = [p + i\beta v(x)]^2/2m + V(x)$, which could be both $\mathcal{PT}$-symmetric and non-$\mathcal{PT}$-symmetric. Notably, the eigenstates of H_β, when it is $\mathcal{PT}$-symmetric, are *real* and do not satisfy the $\mathcal{PT}$-orthogonality condition. © 2002 Elsevier Science B.V. All rights reserved.

The Hermiticity of a Hamiltonian was supposed to be the necessary condition for the real spectrum until the year 1998 [1]. A conjecture due to Bender and Boettcher [1] has relaxed this condition by introducing the concept of $\mathcal{PT}$-symmetry of the Hamiltonian. Here $\mathcal{P}$ denotes parity operator (space reflection) and $\mathcal{T}$ denotes time-reversal. Let $\chi = \mathcal{PT}$, then $\mathcal{PT}$-symmetry implies $\chi H \chi^{-1} = H$. Such a Hamiltonian has been conjectured to possess a real discrete spectrum if the eigenstates also regard the said symmetry, i.e., $\chi\Psi_n(x) = (-1)^n\Psi_n(x)$. This situation is referred to as $\mathcal{PT}$-symmetry being *unbroken or exact*. Otherwise, spontaneous breaking of $\mathcal{PT}$-symmetry takes place and the eigenvalues are complex conjugate pairs.

The last few years have recorded a lot of numerically [1,2] solved and analytically solvable [3–9] (also see references therein) examples in support of the conjecture. Ref. [9] contains a fully tractable model of a $\mathcal{PT}$-symmetric potential which exhibits both the instances of $\mathcal{PT}$-symmetry *broken* and *unbroken* with respect to a parameter about its critical value. Supersymmetric [5,10] and group theoretic methods [8] have been utilized for $\mathcal{PT}$-symmetric Hamiltonians. The eigenstates for a $\mathcal{PT}$-symmetric Hamiltonian become complex and hence new orthogonality conditions have been suggested [9,11,15]. Real energy band structure arising due to complex, periodic, $\mathcal{PT}$-symmetric potentials has also been reported [12,13]. However, despite the overwhelming evidence, $\mathcal{PT}$-symmetry could not be seen as a necessary condition for the real spectrum of a non-Hermitian Hamiltonian. As a matter of fact, some non-$\mathcal{PT}$-symmetric potentials have been known [3,8] to have a real spectrum. More recent conceptual developments on these topics can be seen in [14–16].

Currently, in a very interesting work [17] Mostafazadeh introduces the concept of pseudo-Hermiticity and points out that all the $\mathcal{PT}$-symmetric Hamil-

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tonians considered so far [1–10] are actually $\mathcal{P}$-pseudo-Hermitian, namely $\mathcal{P}H\mathcal{P}^{-1} = H^\dagger$. Further, it is claimed that generally, it is the η-pseudo-Hermiticity [17]

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

and not the $\mathcal{PT}$-symmetry, of a Hamiltonian which is the necessary condition for its real spectrum. And a new orthogonality (η-orthogonality) condition has been proposed as [17]

$$\left(E_i^* - E_j\right) \int_{-\infty}^{\infty} \Psi_i^*(x) \eta \Psi_j(x)\, dx = 0, \tag{2}$$

which is more general than that given earlier in Refs. [9,15],

$$\left(E_i^* - E_j\right) \int_{-\infty}^{\infty} \Psi_i^{\mathrm{PT}}(x) \Psi_j(x)\, dx = 0, \tag{3}$$

for a $\mathcal{PT}$-symmetric Hamiltonian. The usual orthogonality condition is

$$(E_i - E_j) \int_{-\infty}^{\infty} \Psi_i^*(x) \Psi_j(x)\, dx = 0. \tag{4}$$

For one-dimensional bound eigenstates an interesting question that can be raised here is whether we can give up the complex-conjugation (the sign of $*$) in the above condition. Usually, it does not matter, as the hitherto discussed eigenstates in the literature have always been real. We mention an unusual instance in the following. More recently, the real spectrum and orthogonality of the complex potentials of both the types $\mathcal{PT}$-symmetric and non-$\mathcal{PT}$-symmetric known so far have been shown to be due to pseudo-Hermiticity under an imaginary shift of the coordinate [18]. The pseudo-Hermiticity has also been seen [18] as an alternative framework when the Hamiltonian is $\mathcal{PT}$-symmetric. In this work we bring out a shortcoming in the framework of $\mathcal{PT}$-symmetric quantum mechanics [1,9,11,15].

In this Letter, we show the inconsistency of the $\mathcal{PT}$-orthogonality condition (3) when a non-Hermitian potential is $\mathcal{PT}$-symmetric and possesses a real spectrum. Considering Hamiltonians of the type

$$H_\beta = \frac{[p + i\beta\nu(x)]^2}{2m} + V(x) \quad (m = 1 = \hbar), \tag{5}$$

we show that pseudo-Hermiticity provides a more general and consistent framework than that of $\mathcal{PT}$-symmetry [1,9,11,15] when a non-Hermitian Hamiltonian possesses a real spectrum. We check that H_β (5) is pseudo-Hermitian by noticing a gauge-like transformation:

$$e^{f(x)}\big[p + i\beta\nu(x)\big]e^{-f(x)} = p - i\beta\nu(x),$$
$$f(x) = -2\beta \int \nu(x)\, dx. \tag{6}$$

Proof.

$$\begin{aligned}
&\big\{p + i\beta\nu(x)\big\}e^{-f(x)} - e^{-f(x)}\big\{p + i\beta\nu(x)\big\} \\
&\quad = \big[p + i\beta\nu(x), e^{-f(x)}\big] \\
&\quad = \big[p, e^{-f(x)}\big] \\
&\quad = i f'(x) e^{-f(x)}.
\end{aligned} \tag{7}$$

Multiplying by $e^{f(x)}$ on both the sides we get

$$e^{f(x)}\big(p + i\beta\nu(x)\big)e^{-f(x)} = p + i\beta\nu(x) + i f'(x). \tag{8}$$

Setting $f(x)$ as stated in Eq. (6), we prove the result. □

Further it also follows that $e^{f(x)}[p + i\beta\nu(x)]^n \times e^{-f(x)} = [p - i\beta\nu(x)]^n$. Now let us take a particular model of a non-Hermitian Hamiltonian:

$$H_\beta = \frac{(p + i\beta x)^2}{2} + \frac{1}{2}\big(\alpha^2 + \beta^2\big)x^2. \tag{9}$$

Let us note that $\mathcal{P}x\mathcal{P}^{-1} = -x$, $\mathcal{P}p\mathcal{P}^{-1} = -p = \mathcal{T}p\mathcal{T}^{-1}$, $\mathcal{T}iI\mathcal{T}^{-1} = -iI$, $x^\dagger = x$, $i^\dagger = -i$ and $p^\dagger = p$ but $p^* = -p$. It may be checked that the Hamiltonian H_β in Eq. (5) possesses the following properties. H_β is non-Hermitian:

$$H_\beta^\dagger \neq H_\beta.$$

However, H_β is *real* as $H_\beta^* = H_\beta$. H_β is $\mathcal{PT}$-symmetric:

$$\chi H_\beta \chi^{-1} = H_\beta.$$

H_β is not $\mathcal{P}$-pseudo-Hermitian:

$$\mathcal{P}H_\beta\mathcal{P}^{-1} \neq H_\beta^\dagger.$$

Also note that $\mathcal{T}H_\beta\mathcal{T}^{-1} \neq H_\beta^\dagger$ and $\chi H_\beta \chi^{-1} \neq H_\beta^\dagger$.

The eigenvalue problem, $H_\beta \Psi_n(x) = E_n \Psi_n(x)$, gets transformed in accordance with

$$e^{f(x)/2} H_\beta e^{-f(x)/2} = H_{\mathrm{SHO}} = \frac{p^2}{2} + \frac{(\alpha^2+\beta^2)x^2}{2}. \tag{10}$$

Here $f(x) = -\beta x^2$, the wavefunction $\Psi_n(x)$ gets transformed as

$$\Psi_n(x) = \exp\bigl(\beta x^2/2\bigr)\Phi_n(x), \tag{11}$$

where $\Phi_n(x)$ are the well known eigenfunctions of simple harmonic oscillator. One, therefore, obtains

$$E_n = \left(n + \frac{1}{2}\right)\sqrt{\alpha^2+\beta^2}, \quad n = 0, 1, 2, \ldots, \tag{12}$$

and the energy-eigenfunctions

$$\Psi_n(x) = N_n \exp\Bigl[-\Bigl(\sqrt{\alpha^2+\beta^2} - \beta\Bigr)x^2/2\Bigr] \times H_n\bigl[x\bigl(\alpha^2+\beta^2\bigr)^{1/4}\bigr], \tag{13}$$

which are such that $\Psi_n(\pm\infty) = 0$, as long as $\alpha \neq 0$. Here $H_n(z)$ are the Hermite polynomials. Notice that the eigenfunctions are *real* and normalizable. Consequently, the orthonormality condition becomes

$$\int_{-\infty}^{\infty} \exp\bigl(-\beta x^2\bigr)\Psi_m(x)\Psi_n(x)\,dx = \delta_{m,n}, \tag{14}$$

and the normalization coefficient in Eq. (13) can be chosen as $N_n = (\alpha^2+\beta^2)^{1/8}/\sqrt{2^n n!\sqrt{\pi}}$. Remarkably, the $\mathcal{PT}$-symmetric model Hamiltonian (5) does not satisfy the $\mathcal{PT}$-orthogonality (3), instead, we have Eq. (14) being satisfied. The failure of eigenstates (13) of the $\mathcal{PT}$-symmetric Hamiltonian (5) to satisfy the $\mathcal{PT}$-orthogonality (3) indicates a theoretical shortcoming in the framework of $\mathcal{PT}$-symmetry. It is here that we invoke the η-pseudo-Hermiticity (1) [17] by carefully noticing that $\exp(-\beta x^2) H_\beta \exp(+\beta x^2) = H_\beta^\dagger$ resembling an imaginary shift of momentum and a "gauge"-like transformation of the Hamiltonian. Next, we check that eigenfunctions (13) satisfy

$$\langle \Psi_m | \eta \Psi_n \rangle = \langle \eta \Psi_m | \psi_n \rangle. \tag{15}$$

Therefore, η in Eq. (15) is a Hermitian linear automorphism according to Definition 1 in Ref. [17]. It may be stated that the states in Eq. (15) may be two arbitrary elements of some other inner product vector-space. Eventually, the Hamiltonian H_β (5) is η-pseudo-Hermitian according to Eq. (1). Now, let us emphasize that Eq. (14), which has been independently obtained, is nothing but the η-orthonormality condition of Eq. (2) as suggested in Ref. [17]:

$$\int_{-\infty}^{\infty} \Psi_m^*(x)\eta\Psi_n(x)\,dx = \delta_{m,n}. \tag{16}$$

By replacing β by $i\gamma$ in Eq. (5), we get a Hermitian Hamiltonian:

$$H_\gamma = \frac{(p-\gamma x)^2}{2} + \frac{1}{2}\bigl(\alpha^2 - \gamma^2\bigr)x^2. \tag{17}$$

The results in Eqs. (12), (13), and (14) consequently change to

$$E_n = \left(n + \frac{1}{2}\right)\sqrt{\alpha^2-\gamma^2}, \quad \alpha > \gamma, \quad n = 0, 1, 2, \ldots, \tag{18}$$

$$\Psi_n(x) = M_n \exp\Bigl[-\Bigl(\sqrt{\alpha^2-\gamma^2} - i\gamma\Bigr)x^2/2\Bigr] \times H_n\bigl[x\bigl(\alpha^2-\gamma^2\bigr)^{1/4}\bigr], \tag{19}$$

and

$$\int_{-\infty}^{\infty} \exp\bigl(-i\gamma x^2\bigr)\Psi_m(x)\Psi_n(x)\,dx = \delta_{m,n}, \tag{20}$$

with the normalization coefficient given as $M_n = (\alpha^2-\gamma^2)^{1/8}/\sqrt{2^n n!\sqrt{\pi}}$. Notice the real eigenvalues (18) but complex eigenfunctions (19) of the Hermitian Hamiltonian (17). Remarkably, the usual connection between the nodal structure with the quantum number n does not hold any more. Even the ground state may have nodes for some values of γ. Eigenvalues (18) possess an interesting feature of becoming complex (conjugate) at the cost of eigenfunction (19) being delocalized as it would not vanish at $x = \pm\infty$. This interesting phase-transition of eigenvalues from real to complex takes place when $\gamma > \gamma_{\text{critical}}$ $(= \alpha)$.

Though we do have $\exp(-i\gamma x^2) H_\gamma \exp(+i\gamma x^2) = H_\gamma = H_\gamma^\dagger$, we cannot assume $\exp(-i\gamma x^2)$ as a Hermitian linear automorphism, η, as eigenstates (19) or some other states from an inner product vector space do not satisfy condition (15). Also, states (19) with this choice of η would also not satisfy the η-orthonormality condition (2). It is here that we resolve to call H_γ Hermitian and not η-pseudo-Hermitian. Incidentally, the orthonormality condition as displayed in Eq. (20) is the same as the usual orthonormality condition as per Eq. (4), i.e.,

$$\int_{-\infty}^{\infty} \Psi_m^*(x)\Psi_n(x)\,dx = \delta_{m,n}. \tag{21}$$

For discrete states the pressing need for the complex-conjugation in Eq. (21), when the Hamiltonian is Hermitian, can be realized here. Usually, in one-dimensional problems where the discrete states are real it does not matter at all.

A distinctive feature of eigenstates (13) of the $\mathcal{PT}$-symmetric Hamiltonian (5) so far [1–10] is that they are *real*. Usually, the operations † (Hermitian self-adjoint) and $*$ (complex-conjugation) are treated to be the same—a simplification which shows up later when one deals with presently discussed Hamiltonians like $H = p^2 + V(x,p)$. With this in mind, we propose to resolve the real (complex) eigenstates of a non-Hermitian (Hermitian) Hamiltonian.

Proposition. *Let H be a Hamiltonian (operator) admitting an eigenvalue problem. We claim that the eigenfunctions can be real only when H is real and the eigenvalues are real. Also, if H is not real and further, if its eigenvalues are real, its eigenfunctions cannot be real.*

Proof. Let $\mathcal{H}$ be a real Hamiltonian such that $\mathcal{H}^* = \mathcal{H}$ with real eigenvalues, E_n. We have $\mathcal{H}\Psi_n = E_n\Psi_n$. Noticing that the *complex-conjugation* does not *transpose*, i.e., $(\mathcal{H}\mathcal{G})^* = \mathcal{H}^*\mathcal{G}^*$, we have $\mathcal{H}\Psi_n^* = E_n\Psi_n^*$, thus proving that $\Psi_n^* = \Psi_n$ $\forall n$, in the absence of degeneracy. We may also deduce that $C_1\Psi_n + C_2\Psi_n^*$ will be an eigenfunction. Next, by choosing $C_1 = C_2 = C$ and $C_1 = -C_2 = C/i$, we can manage to have real eigenfunctions. It is now trivial to see that $\psi_n^* \neq \psi_n$, if $\mathcal{H}^* \neq \mathcal{H}$. □

Hence, the real Hamiltonian (5) (which is non-Hermitian) possesses real eigenvalues (12) and real eigenfunctions (13). The non-real Hamiltonian (17) (which is Hermitian) possesses real eigenvalues and complex eigenfunctions. The example of the elementary linear momentum operator, p, could be more pedagogic: it is not real, hence with real eigenvalues, k, it admits only complex eigenfunctions, e^{ikx}.

If the real functions $f(x)$ and $g(x)$ are odd and even, respectively, the $\mathcal{PT}$-symmetric Hamiltonian

$$\mathcal{H}_\beta = \frac{1}{2}\big[p + i\beta f(x)\big]^2 + \frac{\alpha^2}{2}g(x) + \frac{\beta^2}{2}f^2(x) \tag{22}$$

will be η-pseudo-Hermitian and η will be given as $\exp[-2\beta\int f(x)\,dx]$. For such Hamiltonians (22) the pseudo-Hermiticity means that the "gauge"-transformed Hamiltonian is identical to its adjoint. The eigenstates of $\mathcal{H}_\beta$ will be only η-orthonormal if the spectrum is real. When $f(x) = \tanh(x)$ and $g(x) = \tanh^2(x)$, one will have an exactly solvable model. Notice that $f(x)$ and $g(x)$ need not be of the specified parities if $\mathcal{H}_\beta$ is desired to be only η-pseudo-Hermitian. For example, one may choose $f(x) = [1-\exp(x)]$ and $g(x) = [1-\exp(x)]^2$ for an analytically solvable model which is not $\mathcal{PT}$-symmetric. These two pseudo-Hermitian models can be analytically checked to have real eigenvalues. Their eigenstates will be real since their Hamiltonian (22) is *real*. Also, by letting $\beta = i\gamma$ in (22), we get $\mathcal{H}_\gamma$ and by choosing $f(x)$ and $g(x)$ as above we can have real eigenvalues because $\mathcal{H}_\gamma$ is Hermitian. But since $\mathcal{H}_\gamma$ is *not real*, it will have complex eigenstates.

In the context of (de)localization phase transitions in non-Hermitian quantum mechanics, Hatano and Nelson [19] have proposed a non-Hermitian Hamiltonian

$$\mathcal{H}_{\mathrm{H-N}} = \frac{(p+ig)^2}{2m} + V(x), \tag{23}$$

where g is real and $V(x)$ is real and random. It is known [19] that Hamiltonian (23) admits real eigenvalues if $g < g_c$ and complex eigenvalues if $g > g_c$, g_c being some model-dependent critical value. This is analogous to the behaviour of a $\mathcal{PT}$-symmetric Hamiltonian [1]. A fully analytically solvable complex potential which is both $\mathcal{PT}$-symmetric and P-pseudo-Hermitian exhibiting a transition from real to complex conjugate spectrum is available in Ref. [9]. One may readily check that Hamiltonian (23) is not invariant under the $\mathcal{PT}$-transformation. We would like to remark that Hamiltonian (23) is actually pseudo-Hermitian under the gauge-like transformation $e^{-2gx}\mathcal{H}_{\mathrm{H-N}} \times e^{2gx} = \mathcal{H}^\dagger_{\mathrm{H-N}}$, with Hermitian linear automorphism, η $(= e^{-2gx})$. Consequently, Hamiltonian (23) can admit real or complex or both kinds of eigenvalues. It may be stressed here that pseudo-Hermiticity [17] is only *necessary* and not the *sufficient* condition for a Hamiltonian to possess real eigenvalues. Other interesting properties of Hamiltonian (23), its eigenvalues and eigenfunctions have been discussed in Ref. [16].

A real Hamiltonian may further be Hermitian, non-Hermitian or pseudo-Hermitian. We have brought home the facts that real Hamiltonians with real eigenvalues can have real eigenfunctions. Similarly, non-real Hamiltonians with real eigenvalues will not have real eigenfunctions. The present non-Hermitian models highlight the fact that pseudo-Hermiticity is a more general and consistent framework than that of the $\mathcal{PT}$-symmetry. However, for a given non-Hermitian Hamiltonian, with real spectrum, the main problem consists in identifying the *Hermitian linear automorphism*, η, but for which the pseudo-Hermiticity [17] cannot proceed. In this Letter, we have proposed "gauge"-pseudo-Hermiticity as $\eta(x)H(\eta(x))^{-1} = H^\dagger$. Earlier, we have claimed the operator, $e^{-\theta p}$, causing an imaginary shift of the coordinate [18], as a Hermitian linear automorphism to explain the real spectrum and orthogonality of all the potentials of both types, $\mathcal{PT}$-symmetric and non-$\mathcal{PT}$-symmetric, known so far [1–10]. The Hamiltonians, H_β, turn out to be a special class of non-Hermitian Hamiltonians which have both the eigenvalues and eigenstates as real. Interestingly, it turns out that the non-random, Hermitian Hamiltonians, e.g., H_γ (17) and $\mathcal{H}_\gamma$ (Eq. (22) with $\beta = i\gamma$) display a (de)localization phase transition as the eigenvalues change from real to complex and the bound eigenstates become delocalized. For instance, see the eigenvalues in Eq. (18), where $\gamma_{\text{critical}} = \alpha$.

References

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

[2] C.M. Bender, S. Boettcher, P.N. Meisinger, J. Math. Phys. 40 (1999) 2201;
C.M. Bender, S. Boettcher, H.F. Jones, V.M. Savage, J. Phys. A: Math. Gen. 32 (1999) 6771.

[3] F. Cannata, G. Junker, J. Trost, Phys. Lett. A 246 (1998) 219.

[4] M. Znojil, Phys. Lett. A 259 (1999) 220;
M. Znojil, J. Phys. A: Math. Gen. 33 (2000) L61.

[5] B. Bagchi, R. Roychoudhury, J. Phys. A: Math. Gen. 33 (2000) L1.

[6] A. Khare, B.P. Mandal, Phys. Lett. A 272 (2000) 53.

[7] G. Levai, M. Znojil, J. Phys. A: Math. Gen. 33 (2000) 7165.

[8] B. Bagchi, C. Quesne, Phys. Lett. A 273 (2000) 285.

[9] Z. Ahmed, Phys. Lett. 282 (2001) 343;
Z. Ahmed, 287 (2001) 295.

[10] B. Bagchi, S. Mallik, C. Quesne, R. Roychoudhury, quant-ph/010795.

[11] C.M. Bender, F. Cooper, P.N. Meisinger, V.M. Savage, Phys. Lett. A 259 (1999) 224.

[12] C.M. Bender, G.V. Dunne, P.N. Meisinger, Phys. Lett. A 252 (1999) 272.

[13] Z. Ahmed, Phys. Lett. A 286 (2001) 231.

[14] M. Znojil, math-ph/0104012.

[15] G.S. Japaridze, quant-ph/0104077.

[16] R. Kretschmer, L. Szymanowski, quant-ph/0105054.

[17] A. Mostafazadeh, math-ph/0107001, J. Math. Phys., to appear;
A. Mostafazadeh, math-ph/0110016.

[18] Z. Ahmed, Phys. Lett. A 290 (2001) 19, quant-ph/0108016.

[19] N. Hatano, D.R. Nelson, Phys. Rev. Lett. 77 (1996) 570;
N. Hatano, D.R. Nelson, Phys. Rev. B 56 (1997) 8651;
N. Hatano, D.R. Nelson, Phys. Rev. B 58 (1998) 8384;
J. Feinberg, A. Zee, Phys. Rev. E 59 (1999) 6433.