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Exact *PT*-symmetry is equivalent to Hermiticity

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Abstract

We show that a quantum system possessing an exact antilinear symmetry, in particular *PT*-symmetry, is equivalent to a quantum system having a Hermitian Hamiltonian. We construct the unitary operator relating an arbitrary non-Hermitian Hamiltonian with exact *PT*-symmetry to a Hermitian Hamiltonian. We apply our general results to *PT*-symmetry in finite dimensions and give the explicit form of the above-mentioned unitary operator and Hermitian Hamiltonian in two dimensions. Our findings lead to the conjecture that non-Hermitian *CPT*-symmetric field theories are equivalent to certain nonlocal Hermitian field theories.

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The interest in *PT*-symmetric quantum mechanics [1] has its origin in the idea that since the *CPT* theorem follows from the axioms of local quantum field theory, one might obtain a more general field theory by replacing the axiom of the Hermiticity of the Hamiltonian by the requirement of *CPT*-symmetry. The simplest nonrelativistic example of such theories is the *PT*-symmetric quantum mechanics. During the past five years there have appeared dozens of publications exploring the properties of the *PT*-symmetric Hamiltonians. Among these are a series of articles [2–9] by the present author that attempt to demonstrate that *PT*-symmetry can be understood most conveniently using the theory of pseudo-Hermitian operators (see also [10]). The recent articles of Bender *et al* [11, 12], however, show that the mystery associated with *PT*-symmetry has surprisingly survived the comprehensive treatment offered by pseudo-Hermiticity. The aim of this paper is to provide a conclusive proof that the exact *PT*-symmetry is equivalent to Hermiticity. In particular, we offer a complete treatment of *PT*-symmetry in finite dimensions that clarifies some of the issues raised in [12] and shows that some of the claims made in [12] are not true. We also comment on the nature and possible advantages of non-Hermitian *CPT*-symmetric field theories.

First, we wish to point out that the results of [11] regarding the *PT*-symmetry of Hermitian Hamiltonians follow from the more general result that any diagonalizable pseudo-Hermitian Hamiltonian is *PT*-symmetric where the *P* and *T* are the generalized parity and time-reversal operators [8]. The definitions of *P* and *T* used in [11] were originally given for arbitrary diagonalizable pseudo-Hermitian Hamiltonians in [8]; they are equations (77) and (78) of [8]. The statement that any Hermitian Hamiltonian is *PT*-symmetric is actually not surprising at all. A simple corollary of theorem 2 of [4] is that any Hermitian Hamiltonian has an antilinear symmetry. The proof of this theorem provides an explicit construction of such symmetries. Among them are the (generalized) *PT* and *CPT* symmetries that are considered in great detail in [8].

We start our analysis by considering a linear operator H' that acts in a complex vector space V and commutes with an invertible antilinear operator $\mathcal{X}'$. Then as shown in [3], the eigenvalues of H' are either real or come in complex-conjugate pairs. Furthermore, if we demand that all the eigenvectors of H' are also eigenvectors of $\mathcal{X}'$, i.e., the symmetry generated by $\mathcal{X}'$ is exact, then the eigenvalues of H' are necessarily real. Now, let $\mathcal{H}$ be the (invariant) subspace of V spanned by the eigenvectors of H'. Then by construction the restriction H of H' to $\mathcal{H}$ will be diagonalizable, and the restriction $\mathcal{X}$ of $\mathcal{X}'$ to $\mathcal{H}$ will generate an exact symmetry of H.

Next, suppose that $\langle\, ,\rangle$ is an arbitrary complete positive-definite inner product on $\mathcal{H}$, so that $\mathcal{H}$ is endowed with the structure of a separable Hilbert space. Then H is a diagonalizable operator acting in $\mathcal{H}$ and having a real spectrum. We will identify it as the Hamiltonian of a physical system whose state vectors belong to $\mathcal{H}$. The dynamics of the system is then determined by the Schrödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = H\psi(t). \tag{1}$$

It is tempting to view $\mathcal{H}$ as the Hilbert space for this quantum system. However, in general, H is not a Hermitian operator with respect to the inner product $\langle\, ,\rangle$ of $\mathcal{H}$. Hence, the time evolution generated by H in $\mathcal{H}$ will not be unitary.

If we assume that H has a discrete spectrum, then according to theorem 3 of [4] H is Hermitian with respect to a positive-definite inner product $\langle\langle\, ,\rangle\rangle$ on $\mathcal{H}$. Like any other inner product on $\mathcal{H}$, $\langle\langle\, ,\rangle\rangle$ will have the form [13]:

$$\langle\langle\psi,\phi\rangle\rangle = \langle\psi,\eta_+\phi\rangle \qquad \forall\psi,\phi\in\mathcal{H} \tag{2}$$

for some Hermitian, invertible, linear operator $\eta_+ : \mathcal{H}\to\mathcal{H}$. The Hermiticity of H with respect to $\langle\langle\, ,\rangle\rangle$, i.e.,

$$\langle\langle\psi,H\phi\rangle\rangle = \langle\langle H\psi,\phi\rangle\rangle \qquad \forall\psi,\phi\in\mathcal{H} \tag{3}$$

is equivalent to its η_+-pseudo-Hermiticity [2]:

$$H^\dagger = \eta_+ H\eta_+^{-1}. \tag{4}$$

Moreover, the fact that $\langle\langle\, ,\rangle\rangle$ is a positive-definite inner product implies that η_+ is a positive-definite operator. This in turn means that η_+ has a positive square root ρ_+, i.e., there exists a positive Hermitian operator $\rho_+ : \mathcal{H}\to\mathcal{H}$ such that

$$\eta_+ = \rho_+^2. \tag{5}$$

Clearly, ρ_+ is invertible.

Next, let $\tilde{\mathcal{H}}$ denote the span of the eigenvectors of H endowed with the inner product $\langle\langle\, ,\rangle\rangle$. As a vector space $\tilde{\mathcal{H}}$ coincides with $\mathcal{H}$. Therefore we may view ρ_+ as a linear invertible operator mapping $\tilde{\mathcal{H}}$ onto $\mathcal{H}$. We can easily show that for all $\psi,\phi\in\mathcal{H}$,

$$\left\langle\left\langle\rho_+^{-1}\psi,\rho_+^{-1}\phi\right\rangle\right\rangle = \left\langle\rho_+^{-1}\psi,\eta_+\rho_+^{-1}\phi\right\rangle = \left\langle\psi,\rho_+^{-1}\eta_+\rho_+^{-1}\phi\right\rangle = \langle\psi,\phi\rangle.$$

Equivalently, we have for all $\phi\in\mathcal{H}$ and $\tilde\psi\in\tilde{\mathcal{H}}$,

$$\left\langle\left\langle\tilde\psi,\rho_+^{-1}\phi\right\rangle\right\rangle = \langle\rho_+\tilde\psi,\phi\rangle.$$

Comparing this equation with the defining relation for $\rho_+^{-1\dagger}$, namely $\langle\langle\tilde{\psi}, \rho_+^{-1}\phi\rangle\rangle = \langle\rho_+^{-1\dagger}\tilde{\psi}, \phi\rangle$, we see that $\rho_+^{-1\dagger} = \rho_+ = (\rho_+^{-1})^{-1}$. Therefore, $\rho_+^{-1} : \mathcal{H} \to \tilde{\mathcal{H}}$ is a unitary operator; the Hilbert spaces $\mathcal{H}$ and $\tilde{\mathcal{H}}$ are related by a unitary operator. In particular, for every Hamiltonian operator h defining a time evolution in $\mathcal{H}$, we may define a Hamiltonian

$$\tilde{h} := \rho_+^{-1} h \rho_+ \tag{6}$$

acting in $\tilde{\mathcal{H}}$ such that under the action of ρ_+^{-1} the solutions $\psi(t)$ of the Schrödinger equation for the Hamiltonian h are mapped to the solutions $\tilde{\psi}(t)$ of the Schrödinger equation for $\tilde{h}$. The observables $O : \mathcal{H} \to \mathcal{H}$ are also mapped to the observables $\tilde{O} : \tilde{\mathcal{H}} \to \tilde{\mathcal{H}}$ by the unitary similarity transformation

$$\tilde{O} = \rho_+^{-1} O \rho_+. \tag{7}$$

Now, if we set $\tilde{h} = H$, i.e., view H as a Hamiltonian acting in the Hilbert space $\tilde{\mathcal{H}}$, then

$$h := \rho_+ H \rho_+^{-1} \tag{8}$$

will be a Hermitian Hamiltonian acting in the original Hilbert space $\mathcal{H}$. The Hermiticity of h follows from the fact that H is Hermitian with respect to the inner product $\langle\langle\, ,\, \rangle\rangle$ on $\tilde{\mathcal{H}}$, and that ρ_+^{-1} is unitary.

By construction, the Hamiltonians H and h are related by a unitary transformation mapping two different Hilbert spaces with the same vector space structure. Using the terminology of [4], we say that the quantum systems determined by $(\mathcal{H}, h)$ and $(\tilde{\mathcal{H}}, H)$ are related by a pseudo-canonical transformation. Clearly, they are physically equivalent.

In summary, we have shown that if a quantum system has an exact antilinear symmetry (with an invertible symmetry generator) then one can describe the same system using a Hermitian Hamiltonian. This applies to *PT*-symmetric systems whose generator is clearly invertible.

The construction of the unitary operator ρ_+^{-1} requires knowledge of the eigenvectors of the Hamiltonian H. If the Hilbert space is an infinite-dimensional function space and H is a differential operator, then ρ_+^{-1} and consequently the Hamiltonian h are in general nonlocal (non-differential) operators. This suggests that the idea of replacing the Hermiticity condition on the Hamiltonian of a local quantum field theory by its *CPT*-symmetry will probably give rise to a theory which is equivalent to a nonlocal field theory with a Hermitian Hamiltonian. This should not however overshadow the importance of this idea as it suggests the possibility of treating certain nonlocal field theories using equivalent local *CPT*-symmetric field theories with non-Hermitian Hamiltonians.

In the following we explore the utility of our findings in the study of *PT*-symmetry in finite dimensions [12], where $\mathcal{H} = \mathbb{C}^D$ for some $D \in \mathbb{Z}^+$.

In [12], the authors explore certain matrix Hamiltonians that they identify with the finite-dimensional analogues of the Hamiltonians studied within the context of *PT*-symmetric quantum mechanics [1]. The analysis of [12] involves considering complex symmetric Hamiltonians H that admit an antilinear symmetry generated by $\mathcal{X} := PT$ where P is a real symmetric matrix satisfying $P^2 = 1$, i.e., it is an involution, and T is complex conjugation $\star$ (for all $\psi \in \mathcal{H}, \star\psi := \psi^*$.) They outline a construction of the most general real symmetric matrix P which is an involution, impose the condition that H commutes with *PT*, restrict to the range of parameters of H where the *PT*-symmetry is exact and define the indefinite *PT* inner product,

$$(\psi|\phi) := [PT\psi]^T \cdot \phi \tag{9}$$

where T stands for the transpose and a dot means matrix multiplication. For the case $D = 2$, they compute the eigenvectors of H, introduce a charge-conjugation operator C, such that H commutes with C and consequently CPT, and show that the CPT inner product,

$$\langle\psi|\phi\rangle := [CPT\psi_a]^T \cdot \phi \tag{10}$$

is positive-definite. Among the statements made in [12] are

Claim 1. A finite-dimensional *PT*-symmetric Hamiltonian (which is a certain complex symmetric matrix) is not unitarily equivalent to any Hermitian matrix Hamiltonian.

Claim 2. The extension to nonsymmetric *PT*-symmetric matrix Hamiltonians cannot be pursued by the methods of the theory of pseudo-Hermitian operators as outlined in [8], because they lead to nonunitary evolutions.

In the remainder of this paper we show how the general results described above explain the findings reported in [12], prove that the claims 1 and 2 are false and discuss an extension of the results of [12] on *PT*-symmetry in finite dimensions to nonsymmetric matrix Hamiltonians.

First, we use the fact that T is complex conjugation and P is a real symmetric involution to show that $(PT)^2 = 1$. This together with the observation that H is a *PT*-symmetric symmetric complex matrix implies

$$H = PT\,H\,PT = P(TH)TP = P\,H^*\,P = PH^\dagger P.$$

Multiplying both sides of this equation from left and right by P and using $P^2 = 1$, we have

$$H^\dagger = P\,H\,P = P\,H\,P^{-1}. \tag{11}$$

Hence H is P-pseudo-Hermitian.

Next, let $\prec\,,\,\succ$ denote the ordinary Euclidean inner product on $\mathcal{H} = \mathbb{C}^D$, i.e.,

$$\prec\psi,\phi\succ := \psi^\dagger \cdot \phi \qquad \forall\psi,\phi \in \mathcal{H} \tag{12}$$

where $\psi^\dagger := \psi^{T*}$. Then in view of equations (9) and (12), and the fact that P is real and symmetric,

$$(\psi|\phi) = [P\psi^*]^T \cdot \phi = \psi^{T*}P \cdot \phi = \prec\psi, P\phi\succ \qquad \forall\psi,\phi \in \mathcal{H}.$$

Therefore the *PT* inner product of [12] is just the pseudo-inner product [2]:

$$\langle\!\langle\psi,\phi\rangle\!\rangle_\eta := \prec\psi, \eta\phi\succ \qquad \forall\psi,\phi \in \mathcal{H}$$

corresponding to the choice $\eta = P$.

Because the eigenvalues of H are real, it is η_+-pseudo-Hermitian for a positive-definite operator η_+, i.e., (4) holds. As discussed in [2, 8], if we introduce $C := \eta_+^{-1}P$, we can use equations (4) and (11) to show

$$[H, C] = H\eta_+^{-1}P - \eta_+^{-1}PH = \eta_+^{-1}H^\dagger P - \eta_+^{-1}H^\dagger P = 0 \tag{13}$$

i.e., C is a linear symmetry generator. Furthermore, if we repeat the arguments leading to equation (75) of [8] we find that the *CPT* inner product is nothing but the η_+ inner product:

$$\langle\psi|\phi\rangle = \prec\psi, \eta_+\psi\succ =: \langle\!\langle\psi,\phi\rangle\!\rangle.$$

As a concrete example, we give an explicit construction of η_+, P and C for the 2×2 Hamiltonians studied in [12], namely

$$H = \begin{pmatrix} r + t\cos\varphi - \mathrm{i}s\sin\varphi & \mathrm{i}s\cos\varphi + t\sin\varphi \\ \mathrm{i}s\cos\varphi + t\sin\varphi & r - t\cos\varphi + \mathrm{i}s\sin\varphi \end{pmatrix} \tag{14}$$

where r, s, t, φ are real parameters and

$$|s| \leqslant |t|. \tag{15}$$

We will also compute the Hermitian matrix h that is unitarily equivalent to H.

As pointed out in [12],

$$\psi_n := \begin{pmatrix} a_n \cos\frac{\varphi}{2} + \mathrm{i} b_n \sin\frac{\varphi}{2} \\ a_n \sin\frac{\varphi}{2} - \mathrm{i} b_n \cos\frac{\varphi}{2} \end{pmatrix} \qquad n = \pm \tag{16}$$

with

$$a_n := \frac{\sin\alpha}{\sqrt{2(1 - n\cos\alpha)\cos\alpha}} \qquad b_n := \frac{(-1 + n\cos\alpha)}{\sqrt{2(1 - n\cos\alpha)\cos\alpha}} \tag{17}$$

and $\alpha := \sin^{-1}(s/t) \in (-\pi/2, \pi/2)$, are linearly independent eigenvectors of H.

We also note that because H is symmetric, $H^\dagger = H^*$. Hence ψ_n^* are eigenvectors of $H^\dagger$. If we let $\phi_n = n\psi_n^*$, we find a pair of linearly independent eigenvectors of $H^\dagger$, namely

$$\phi_n = n \begin{pmatrix} a_n \cos\frac{\varphi}{2} - \mathrm{i} b_n \sin\frac{\varphi}{2} \\ a_n \sin\frac{\varphi}{2} + \mathrm{i} b_n \cos\frac{\varphi}{2} \end{pmatrix} \tag{18}$$

that together with ψ_n form a complete biorthonormal system $\{\psi_n, \phi_n\}$ for the Hilbert space $\mathcal{H} = \mathbb{C}^2$. That is they satisfy

$$\prec\phi_n, \psi_m\succ = \phi_n^\dagger \cdot \psi_m = \delta_{mn} \qquad \psi_+ \cdot \phi_+^\dagger + \psi_- \cdot \phi_-^\dagger = I \tag{19}$$

where I is the identity matrix.

Now, we can compute the positive operator η_+, and the generalized parity $\mathcal{P}$ and charge conjugation $\mathcal{C}$ operators as defined in [8], namely

$$\eta_+ := \phi_+ \cdot \phi_+^\dagger + \phi_- \cdot \phi_-^\dagger \tag{20}$$

$$\mathcal{P} := \phi_+ \cdot \phi_+^\dagger - \phi_- \cdot \phi_-^\dagger \tag{21}$$

$$\mathcal{C} := \psi_+ \cdot \phi_+^\dagger - \psi_- \cdot \phi_-^\dagger. \tag{22}$$

Substituting (16) and (18) in these equations, we find

$$\eta_+ = \begin{pmatrix} \sec\alpha & \mathrm{i}\tan\alpha \\ -\mathrm{i}\tan\alpha & \sec\alpha \end{pmatrix} \tag{23}$$

$$\mathcal{P} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ \sin\varphi & -\cos\varphi \end{pmatrix} \tag{24}$$

$$\mathcal{C} = \begin{pmatrix} \sec\alpha\cos\varphi - \mathrm{i}\tan\alpha\sin\varphi & \sec\alpha\sin\varphi + \mathrm{i}\tan\alpha\cos\varphi \\ \sec\alpha\sin\varphi + \mathrm{i}\tan\alpha\cos\varphi & -\sec\alpha\cos\varphi + \mathrm{i}\tan\alpha\sin\varphi \end{pmatrix}. \tag{25}$$

One can directly check that indeed η_+ and H satisfy (4), i.e., H is η_+-pseudo-Hermitian, and that the eigenvalues of η_+, which are given by $\sec\alpha \pm \tan\alpha = \sqrt{1 + \tan^2\alpha} \pm \tan\alpha$, are positive. Moreover, equations (24) and (25) are identical with the expressions for the parity P and the charge conjugation C given in [12]. We have obtained them by a systematic application of the general results of [8].

Next, we show that contrary to the claims of [12] the quantum system defined by Hamiltonian (14) is equivalent to a quantum system having a Hermitian Hamiltonian h. For this purpose we calculate the positive square root ρ_+ of η_+. The result is

$$\rho_+ = \begin{pmatrix} r_+ & -\mathrm{i}r_- \\ \mathrm{i}r_- & r_+ \end{pmatrix} \tag{26}$$

where

$$r_\pm := \tfrac{1}{2}\left(\sqrt{\sec\alpha - \tan\alpha} \pm \sqrt{\sec\alpha + \tan\alpha}\right).$$

Inserting (14) and (26) in (8), we obtain

$$h = \begin{pmatrix} r + \sqrt{t^2+s^2}\cos\varphi & \sqrt{t^2+s^2}\sin\varphi \\ \sqrt{t^2+s^2}\sin\varphi & r - \sqrt{t^2+s^2}\cos\varphi \end{pmatrix} = rI + \sqrt{t^2+s^2}\,\mathcal{P}. \tag{27}$$

This Hamiltonian is a real symmetric matrix, so it is Hermitian as expected. We also see that it is $\mathcal{P}$-symmetric.

A quantum system described by the Hamiltonian H that is viewed as acting in the Hilbert space $\mathcal{H}$ obtained by endowing $\mathbb{C}^2$ with the inner product (2), which is the same as the *CPT* inner product, may be equally well described by the Hermitian Hamiltonian h viewed as acting in $\mathbb{C}^2$ endowed with the Euclidean inner product (12). There is simply no advantage in considering the Hamiltonians of the form (14) and imposing the condition that they should generate a unitary time evolution. This condition leads one to the study of the well-understood two-level Hermitian Hamiltonians [14].

Next, we wish to point out that the most general *PT*-symmetric matrix Hamiltonians (with *PT* to be understood as the generalized parity–time-reversal operator [8]) are the pseudo-Hermitian matrices. Among these are the quasi-Hermitian Hamiltonians [8, 15] that have an unbroken *PT*-symmetry. But these are related to Hermitian Hamiltonians via similarity transformations by invertible matrices. Each matrix Hamiltonian (acting in $\mathbb{C}^D$ and) having an exact *PT*-symmetry lives in an orbit of the adjoint action of the group $GL(D, \mathbb{C})$ on the $u(D)$ subalgebra of the Lie algebra $\mathcal{G}\ell(D, \mathbb{C})$. In particular it is diagonalizable. More general *PT*-symmetric Hamiltonians may or may not be diagonalizable. Because the exponential of i times a pseudo-Hermitian matrix is necessarily pseudo-unitary and all the pseudo-unitary matrices are obtained in this way [9], one can use the general characterization of pseudo-unitary matrices given in [9] to determine the number of independent real parameters in the most general pseudo-Hermitian matrix. Note however that if a pseudo-Hermitian matrix has a broken *PT*-symmetry so that it has complex eigenvalues or it is not diagonalizable, then it cannot be used as a Hamiltonian capable of supporting a unitary evolution. In this case one can easily show that there is no positive-definite inner product in which this Hamiltonian is Hermitian. This in turn means [2] that for any choice of positive-definite inner product on $\mathbb{C}^D$, there are solutions of the Schrödinger equation whose norm will depend on time.

For $D \times D$ matrix Hamiltonians with exact *PT*-symmetry one can easily count the maximum number of free real parameters. But what is important is the number of independent parameters corresponding to physically distinct Hamiltonians. The similarity transformations by invertible matrices are essentially gauge transformations relating physically equivalent Hamiltonians. Therefore, there are as many physically distinct $D \times D$ matrix Hamiltonians with exact *PT*-symmetry as physically distinct Hermitian $D \times D$ matrix Hamiltonians. The latter have at most D^2 real parameters[1]. The fact that the authors of [12] obtain a smaller number is because they confine their study to symmetric complex matrices. As we argued above one can consistently apply the results of [8] to consider nonsymmetric *PT*-symmetric Hamiltonians that support unitary evolutions provided that the *PT*-symmetry is not broken.

In [7], we provide a complete analysis of general 2×2 pseudo-Hermitian Hamiltonians. In particular, we show that the number of free parameters in a traceless diagonalizable 2×2

[1] One can diagonalize a Hermitian Hamiltonian by a unitary transformation and transform it into a traceless matrix by a time-dependent phase transformation of the state vectors [14]. This implies that distinct unitary physical systems having a $D \times D$ matrix Hamiltonian are uniquely determined by $D - 1$ free parameters. These may be identified with the transition energies.

pseudo-Hermitian Hamiltonian having real eigenvalues is 5. Allowing for a nonzero trace is equivalent to adding a pseudo-Hermitian matrix that is proportional to the identity matrix, i.e., $a_0 I$ for some $a_0 \in \mathbb{R}$. Hence the number of free real parameters in the most general diagonalizable 2×2 pseudo-Hermitian Hamiltonian H with real eigenvalues is 6. As we show in [8], we can construct the generalized parity $\mathcal{P}$, time reversal $\mathcal{T}$ and charge conjugation $\mathcal{C}$ operators and show that H has $\mathcal{PT}$-, $\mathcal{C}$- and $\mathcal{CPT}$-symmetries. These symmetry generators are involutions, i.e., $(\mathcal{PT})^2 = \mathcal{C}^2 = (\mathcal{CPT})^2 = I$. However, the operators $\mathcal{P}$ and $\mathcal{T}$ are involutions ($\mathcal{P}^2 = \mathcal{T}^2 = I$) provided that the eigenvectors of H and $H^\dagger$ fulfil certain conditions (see statement 6 of lemma 1 in [8]). In the following, instead of trying to satisfy these conditions, we will first identify T with complex conjugation $\star$ and use a direct method of constructing the most general 2×2 matrix Hamiltonian admitting an exact *PT*-symmetry for an indefinite Hermitian involution P (this means that $P^\dagger = P = P^{-1}$ and P has real eigenvalues of opposite sign), so that PT is also an involution. We will then extend our analysis to the most general case where T is an arbitrary Hermitian, antilinear, involution.

Let $T = \star$, then the equation $(PT)^2 = I$ may be written as $P = \star P \star = P^*$. Therefore, P is a real Hermitian (equivalently a real symmetric) matrix. Moreover, the condition that P is an indefinite involution implies that its eigenvalues are ± 1. This is sufficient to establish that

$$P = O\sigma_3 O^{-1} \tag{28}$$

where σ_3 is the diagonal Pauli matrix (see (29) below) and O is some special orthogonal matrix, i.e., $O \in SO(2)$. O is in particular unitary and as any other unitary matrix may be written as the exponential of i times a linear combination of the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{29}$$

The fact that O is a real matrix then implies that it has the form

$$O = \mathrm{e}^{-\mathrm{i}\varphi\sigma_2/2} \tag{30}$$

for some $\varphi \in [0, 2\pi)$. Inserting (30) in (28), we have

$$P = \mathrm{e}^{-\mathrm{i}\varphi\sigma_2/2}\sigma_3\, \mathrm{e}^{\mathrm{i}\varphi\sigma_2/2} = \cos\varphi\sigma_3 + \sin\varphi\sigma_1. \tag{31}$$

To establish the second equality in (31) we used the identity [14]:

$$\mathrm{e}^{-\mathrm{i}\vartheta\sigma_i/2}\sigma_j\, \mathrm{e}^{\mathrm{i}\vartheta\sigma_2/2} = \cos\vartheta\sigma_j + \sin\vartheta \sum_{k=1}^{3} \epsilon_{ijk}\sigma_k \qquad \forall i \neq j \tag{32}$$

where $\vartheta \in \mathbb{C}$ and ϵ_{ijk} is the totally antisymmetric Levi-Civita symbol with $\epsilon_{123} = 1$. Equation (31) is identical to (24), as expected [12].

Next, we note that the *PT*-symmetry of H (i.e., $[H, PT] = 0$) together with $(PT)^2 = 1$ and $P^2 = 1$ implies

$$H^* = P\,H\,P. \tag{33}$$

Defining

$$H_0 := O^{-1} H O \tag{34}$$

and using (28), (30) and (33), we find

$$H_0^* = \sigma_3 H_0 \sigma_3. \tag{35}$$

As any 2×2 complex matrix, H_0 may be written as a linear combination of the identity matrix and the Pauli matrices, $H_0 = a_0 I + \sum_{i=1}^{3} a_i\sigma_i$, with $a_0, a_1, a_2, a_3 \in \mathbb{C}$. Substituting this equation in (35) and using (29) we see that a_0, a_2, a_3 must be real and a_1 must be imaginary.

Letting $\alpha_1 := \mathrm{i}a_1 \in \mathbb{R}$, we then have

$$H_0 = a_0 I - \mathrm{i}\alpha_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3 = \begin{pmatrix} a_0 + a_3 & -\mathrm{i}(\alpha_1 + a_2) \\ \mathrm{i}(-\alpha_1 + a_2) & a_0 - a_3 \end{pmatrix}. \tag{36}$$

Next, we use (30), (32), (34) and (36) to compute

$$H = OH_0O^{-1} = a_0 I - (a_3 \sin\varphi + \mathrm{i}\alpha_1\cos\varphi)\sigma_1 + a_2\sigma_2 + (a_3\cos\varphi - \mathrm{i}\alpha_1\sin\varphi)\sigma_3. \tag{37}$$

If we relabel the parameters according to

$$r := a_0 \qquad s := -\alpha_1 \qquad t := a_3 \qquad u := a_2$$

and insert (29) in (36), we obtain

$$H = \begin{pmatrix} r + t\cos\varphi - \mathrm{i}s\sin\varphi & t\sin\varphi + \mathrm{i}(s\cos\varphi - u) \\ t\sin\varphi + \mathrm{i}(s\cos\varphi + u) & r - t\cos\varphi + s\mathrm{i}\sin\varphi \end{pmatrix}. \tag{38}$$

As seen from this equation, H has five free real parameters. The condition of the exactness of the PT-symmetry implies that the eigenvalues of H are real. These are also the eigenvalues of H_0. The fact that the eigenvalues of H_0 are real implies that the determinant of the traceless part of H_0 must be either zero or negative. In view of (36) this yields $s^2 - t^2 - u^2 = \alpha_1^2 - a_2^2 - a_3^2 \leqslant 0$. If $s^2 - t^2 - u^2 = 0$, either $H = H_0 = 0$ or H_0 and consequently H are not diagonalizable [7]. Requiring that H is a nonzero diagonalizable Hamiltonian so that it supports a nontrivial (nonstationary) unitary time evolution (with respect to some positive-definite inner product on $\mathbb{C}^2$) is equivalent to the condition $s^2 - t^2 - u^2 < 0$, alternatively

$$|s| < \sqrt{t^2 + u^2}. \tag{39}$$

Now, suppose that condition (39) is satisfied so that H is diagonalizable and has real eigenvalues $E_\pm$. Let $\psi_\pm$ be a pair of linearly independent eigenvectors of H, so that $H\psi_\pm = E_\pm\psi_\pm$. Acting with both sides of $[PT, H] = 0$ on $\psi_\pm$, we can easily show that $PT\psi_\pm$ are also eigenvectors of H with eigenvalue $E_\pm$. There are two possibilities.

1. $E_+ = E_1$. Then H is a real multiple of the identity matrix, i.e., $H = E_+ I$, and we can select $\psi_+ = \pi_+$ and $\psi_- = \mathrm{i}\pi_-$, where $\pi_\pm$ are a pair of eigenvectors of P with eigenvalue ± 1. It is obvious that $H\psi_\pm = E\psi_\pm$ and $PT\psi_\pm = P[\pm\psi_\pm] = \psi_\pm$.
2. $E_+ \neq E_-$. Then $PT\psi_\pm = N_\pm\psi_\pm$ for some $N_\pm \in \mathbb{C} - \{0\}$, and we can always rescale the eigenvectors $\psi_\pm$ and choose the phases of $N_\pm$ so that $PT\psi_\pm = \psi_\pm$.

This shows that (39) is the necessary and sufficient condition for the exactness of PT-symmetry.

The symmetric Hamiltonian (14) and condition (15) ensuring its exact PT-symmetry are special cases of the Hamiltonian (38) and condition (39). Because the Hamiltonians (14) and (38) differ by $u\sigma_2$, one may wonder if they are related by a unitary similarity transformation. In order to see that this is indeed the case, we let $t' \in \mathbb{R}^+$ and $\beta \in [0, 2\pi)$ be given by

$$t' := \sqrt{t^2 + u^2} \qquad \sin\beta := \frac{u}{\sqrt{t^2 + u^2}} \qquad \cos\beta := \frac{t}{\sqrt{t^2 + u^2}}$$

and introduce

$$H' := \begin{pmatrix} r + t'\cos\varphi - \mathrm{i}s\sin\varphi & \mathrm{i}s\cos\varphi + t'\sin\varphi \\ \mathrm{i}s\cos\varphi + t'\sin\varphi & r - t'\cos\varphi + \mathrm{i}s\sin\varphi \end{pmatrix} \tag{40}$$

$$U_1 := \mathrm{e}^{\mathrm{i}\varphi\sigma_2/2}\,\mathrm{e}^{\mathrm{i}\beta\sigma_2/2}\,\mathrm{e}^{-\mathrm{i}\varphi\sigma_2/2}. \tag{41}$$

Then using (32) we can show that

$$H' = \mathrm{e}^{\mathrm{i}\varphi\sigma_2/2}(rI + \mathrm{i}s\,\sigma_1 + t'\sigma_3)\,\mathrm{e}^{-\mathrm{i}\varphi\sigma_2/2} \tag{42}$$

$$H = U_1 H' U_1^{-1} \tag{43}$$

where H is the Hamiltonian (38). Equation (43) indicates that the Hamiltonian (38) may be mapped to a symmetric Hamiltonian of the form (14) by a unitary transformation. A direct consequence of this observation is that the Hamiltonians (38) are also equivalent to the Hermitian Hamiltonians (27); in view of (8) and (43) we have

$$H = U_2 h' U_2^{-1} \tag{44}$$

where $U_2 := U_1 \rho_+'^{-1}$, ρ_+' is the matrix (26) with $\alpha \in (-\pi/2, \pi/2)$ given by $\alpha = \sin^{-1}(s/t')$, and h' is the Hamiltonian (27) with t replaced by t'. Because U_1 is a unitary matrix, U_2 viewed as an operator mapping $\mathbb{C}^2$ endowed with the inner product (2) to $\mathbb{C}^2$ endowed with the Euclidean inner product (12) is unitary. Therefore, equation (44) establishes the unitary equivalence of the Hamiltonians (38) to the Hermitian Hamiltonians of the form (27).

Next, we wish to construct the most general 2×2 Hamiltonians admitting an exact *PT*-symmetry such that P and T are general Hermitian (respectively linear and antilinear) commuting involutions. To do this, we first recall that the Hermiticity condition for an antilinear operator T has the form [16]

$$\prec\psi, T\phi\succ = \prec\phi, T\psi\succ \qquad \forall\psi, \phi \in \mathcal{H} = \mathbb{C}^2 \tag{45}$$

and that any antilinear operator acting in $\mathbb{C}^2$ may be expressed as

$$T = \tau\star \tag{46}$$

for some linear operator $\tau : \mathbb{C}^2 \to \mathbb{C}^2$. Then imposing the condition that T is an involution, i.e., $T^2 = 1$ and using (45), we can show that

$$\tau^\dagger = \tau^{-1} = \tau^*. \tag{47}$$

In other words, τ is a complex, symmetric, unitary matrix. Writing τ as the exponential of i times a linear combination of I and the Pauli matrices and requiring that it is symmetric yields the general form of τ, namely

$$\tau = \mathrm{e}^{\mathrm{i}\gamma}[\cos\xi I + \mathrm{i}\sin\xi(\cos\zeta\sigma_1 + \sin\zeta\sigma_3)] \tag{48}$$

where $\gamma, \xi, \zeta \in [0, 2\pi)$.

Next, we introduce the unitary symmetric matrix

$$U := \mathrm{e}^{\mathrm{i}\gamma/2}\,\mathrm{e}^{\mathrm{i}\xi(\cos\zeta\sigma_1 + \sin\zeta\sigma_3)/2}. \tag{49}$$

Then in view of the identity

$$\mathrm{e}^{\mathrm{i}\varrho\sum_{i=1}^3 n_i\sigma_i} = \cos\varrho I + \mathrm{i}\sin\varrho\sum_{i=1}^3 n_i\sigma_i$$

where $\varrho \in \mathbb{R}$ and n_i are the components of a unit vector $\hat{n} \in \mathbb{R}^3$, we can check that

$$\tau = U^2. \tag{50}$$

Substituting this equation in (46) and making use of the fact that U is both unitary and symmetric, so that $U^* = U^\dagger = U^{-1}$, we have

$$T = U^2\star = U\star(\star U\star) = U\star U^* = U\star U^{-1}. \tag{51}$$

Equations (51) reduce the analysis of the general *PT*-symmetric 2×2 Hamiltonians H with T given by (46) to that of the Hamiltonians (38). In order to see this, we introduce

$$\check{T} := U^{-1}TU = \star \qquad \check{P} := U^{-1}PU \qquad \check{H} := U^{-1}HU. \tag{52}$$

In view of the fact that U is a unitary matrix, it is easy to see that $\check{P}$ is an indefinite Hermitian involution, $\check{P}\check{T}$ is an antilinear involution (so that $[\check{P}, \check{T}] = 0$) and that $\check{H}$ has an exact

$\check{P}\check{T}$-symmetry. Because $\check{T} = \star$, the matrices $\check{P}$ and $\check{H}$ have the general form (31) and (38) respectively. Therefore, according to (52) the most general 2×2 Hamiltonian admitting an exact *PT*-symmetry such that *P* and *T* are general Hermitian (respectively linear and antilinear) commuting involutions is given by

$$H = U\check{H}U^{-1} \tag{53}$$

where *U* is the unitary matrix (49) and $\check{H}$ is given by the right-hand side of (38).

Because $\check{H}$ is a Hamiltonian of the form (38), according to (44) it may be mapped to a Hermitian Hamiltonian of the form (27) by a unitary transformation. This observation together with equation (53) and the fact that *U* is a unitary matrix, indicates that the most general 2×2 Hamiltonian having exact *PT*-symmetry is related to a Hermitian 2×2 Hamiltonian by a unitary transformation.

In this paper we showed that if the Hamiltonian of a quantum system has an exact *PT*-symmetry and supports a unitary time evolution, then the same system may be described using a Hermitian Hamiltonian. This provides the following answer to the question, 'Must a Hamiltonian be Hermitian?' posed in the title of [17]: 'The Hamiltonian need not be Hermitian in a given inner product, but if one demands unitarity then one can describe the same quantum system using a Hermitian Hamiltonian'.

If the Hilbert space is finite dimensional, in general, there is no practical difference between non-Hermitian Hamiltonians supporting unitary evolutions and Hermitian Hamiltonians. For the case that the Hilbert space is an infinite-dimensional function space, again such a non-Hermitian Hamiltonian can be mapped to a physically equivalent Hermitian Hamiltonian. But the latter is generally a nonlocal (non-differential) operator. In other words, a local Hamiltonian which is non-Hermitian with respect to a given (positive-definite) inner product $\prec , \succ$ will support a unitary evolution with respect to another (positive-definite) $\langle , \rangle$ inner product if and only if it is physically equivalent to a Hamiltonian which is Hermitian with respect to the original inner product $\prec, \succ$. The only advantage of exploring exact *PT*-symmetric (quasi-Hermitian) Hamiltonians is that the corresponding equivalent Hermitian Hamiltonians may be nonlocal operators whose study is generally more difficult. This observation also suggests a similar scenario for the non-Hermitian *CPT*-symmetric local field theories, namely that such a theory is equivalent to a Hermitian nonlocal field theory. A direct implication of this statement is that non-Hermitian *CPT*-symmetric local field theories are expected to share the appealing properties of nonlocal field theories, but since they are local field theories they may prove to be much simpler to study.

Finally, we wish to point out that one can also consider time-dependent exact *PT*-symmetric (quasi-Hermitian) Hamiltonians. The issue of the unitarity of the time evolution for this kind of Hamiltonian is more subtle. It plays an interesting role in the solution of the Hilbert space problem for certain quantum cosmological models [18].

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