Explicit Realization of Pseudo-Hermitian and Quasi-Hermitian Quantum Mechanics for Two-Level Systems

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Abstract

We give an explicit characterization of the most general quasi-Hermitian operator $H$, the associated metric operators $\eta_+$, and $\eta_+$-pseudo-Hermitian operators acting in $\mathbb{C}^2$. The latter represent the physical observables of a model whose Hamiltonian and Hilbert space are respectively $H$ and $\mathbb{C}^2$ endowed with the inner product defined by $\eta_+$. Our calculations allows for a direct demonstration of the fact that the choice of an irreducible family of observables fixes the metric operator up to a multiplicative factor.

Key Words: Pseudo-Hermitian, quasi-Hermitian, metric operator, observable, two-level system.

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1. Introduction

Recently there has been a significant interest in devising a unitary quantum theory based on $\mathcal{PT}$-symmetric Hamiltonian operators such as $H = p^2 + ix^3$ that possess a real discrete spectrum [1–4]. A key ingredient that allows for the formulation of such a quantum theory is a spectral theorem proven in [5] (see also [6]) asserting that if a diagonalizable operator $H$ acting in a separable Hilbert space has a discrete spectrum, then its spectrum is real if and only if there is a positive-definite inner product $\langle \cdot, \cdot \rangle_+$ on $\mathcal{H}$ with respect to which $H$ is Hermitian. The inner product $\langle \cdot, \cdot \rangle_+$ may be conveniently expressed in terms of a positive-definite (metric) operator $\eta_+: \mathcal{H} \to \mathcal{H}$ according to

$$\langle \cdot, \cdot \rangle_+ = \langle \cdot | \eta_+ \cdot \rangle,$$

where $\langle \cdot | \cdot \rangle$ is the defining inner product of $\mathcal{H}$. The Hermiticity of $H$ with respect to $\langle \cdot, \cdot \rangle_+$, i.e., the condition $\langle \cdot, H \cdot \rangle_+ = \langle H \cdot, \cdot \rangle_+$, is equivalent to the $\eta_+$-pseudo-Hermiticity [7] of $H$, namely

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

Another equivalent condition to the reality of the spectrum of $H$ is its quasi-Hermiticity [8], i.e., the existence of an invertible operator $\rho: \mathcal{H} \to \mathcal{H}$ such that

$$h := \rho^{-1} H \rho$$
is Hermitian with respect to $\langle \cdot | \cdot \rangle$, i.e., $\langle h | \cdot \rangle = \langle \cdot | \cdot \rangle$. We will call such an operator Hermitian, i.e., use the defining inner product $\langle \cdot | \cdot \rangle$ of $\mathcal{H}$ to determine if an operator is Hermitian or not.

In [8], the authors propose a different approach to quantum mechanics in which the inner product of the physical Hilbert space is not a priori fixed but determined by the choice of sufficiently many appropriate observables. In order to make this statement more precise we first recall a few definitions.

**Definition 1:** Let $\mathcal{H}$ be a separable Hilbert space. Then a set $\mathcal{S} = \{O_\alpha\}$ of bounded linear operators $O_\alpha : \mathcal{H} \rightarrow \mathcal{H}$ is said to be irreducible if there is no proper subspace of $\mathcal{H}$ that is left invariant by all $O_\alpha$’s, i.e., the only subspace $\mathcal{H}'$ of $\mathcal{H}$ satisfying the following condition is $\mathcal{H}$.

\[ O_\alpha \psi' \in \mathcal{H}', \quad \text{for all } \psi' \in \mathcal{H}' \quad \text{and all } O_\alpha \in \mathcal{S}. \]

**Definition 2:** Let $\mathcal{H}$ be a separable Hilbert space. Then a set $\mathcal{S} = \{O_\alpha\}$ of quasi-Hermitian linear operators $O_\alpha : \mathcal{H} \rightarrow \mathcal{H}$ is said to be compatible if there is an invertible bounded operator $\rho : \mathcal{H} \rightarrow \mathcal{H}$ such that $\rho^{-1}O_\alpha \rho$ is Hermitian for all $O_\alpha \in \mathcal{S}$.

The condition that $\rho^{-1}O_\alpha \rho$ is Hermitian is equivalent to the existence of a positive-definite (metric) operator $\eta_+$ such that $O_\alpha$ is $\eta_+$-pseudo-Hermitian [5]. Thus, $\mathcal{S} = \{O_\alpha\}$ is a compatible set if and only if all $O_\alpha$ are $\eta_+$-pseudo-Hermitian for some metric operator $\eta_+$.

We can express the main result of [8] as:

**Theorem:** Up to a multiplicative factor there is a unique positive-definite (metric) operator $\eta_+$ such that all the elements of a compatible irreducible set $\mathcal{S} = \{O_\alpha\}$ of operators is $\eta_+$-pseudo-Hermitian. Equivalently, there is a (positive-definite) inner product $\langle \cdot , \cdot \rangle_+$ on $\mathcal{H}$ such that all $O_\alpha$ are Hermitian with respect to $\langle \cdot , \cdot \rangle_+$, and this inner product is unique up to a trivial multiplicative factor.

The purpose of this article is to conduct a thorough investigation of the implementation of the above-mentioned developments to the simplest nontrivial class of quantum systems, namely the two-level systems for which $\mathcal{H}$ is $\mathbb{C}^2$ endowed with the Euclidean inner product. In particular, we

- compute the most general form of quasi-Hermitian operators,
- find the explicit form of the most general metric operator $\eta_+$ that renders a given quasi-Hermitian operator $\eta_+$-pseudo-Hermitian,
- determine the class of all quasi-Hermitian operators $O$ that together with the given one ($H$) form a compatible irreducible set, and
- show by an explicit calculation how the choice of such an operator fixes $\eta_+$ up to a scale factor.

In the remainder of this paper $\mathcal{H}$ will denote $\mathbb{C}^2$ endowed with the Euclidean inner product, the elements of $\mathcal{H}$ will be represented by column vectors, and the linear operators $L : \mathcal{H} \rightarrow \mathcal{H}$ will be identified with their matrix representations in the standard basis of $\mathbb{C}^2$. In particular, both the identity operator acting in $\mathbb{C}^2$ and the $2 \times 2$ identity matrix will be denoted by $I$.

### 2. Quasi-Hermitian Operators and the Associated Metric Operators

It is clear that every quasi-Hermitian operator $H$ is necessarily diagonalizable and has a real spectrum. These conditions hold if and only if $H$ is $\eta_+$-pseudo-Hermitian for a positive-definite (metric) operator $\eta_+$,
[5, 6]. Furthermore, $H$ is $\eta_+$-pseudo-Hermitian if and only if its traceless part $H_0 := H - \frac{1}{2} \text{tr}(H)I$ is $\eta_+$-pseudo-Hermitian.\footnote{This is because the eigenvalues of $H$ and hence its trace are real.} As a result we can confine our attention to traceless operators:

$$H_0 = \begin{pmatrix} a & b \\ \bar{c} & -a \end{pmatrix} \text{ with } a, b, c \in \mathbb{C}. \quad (4)$$

Next, we use the conditions that $H_0$ is diagonalizable and its eigenvalues are real and have opposite sign to infer that $\det H_0 = -(a^2 + bc)$ is real and non-positive. This in turn implies that the eigenvalues of $H_0$ are given by $\pm E$ where $E := \sqrt{a^2 + bc}$. The case $E = 0$ corresponds to the trivial degenerate case where $H_0$ is the zero operator.

The converse of the above argument also holds, i.e., the condition $a^2 + bc \in \mathbb{R}^+$ ensures that $H$ is a nonzero quasi-Hermitian operator. Relaxing the tracelessness condition, we have the following form for the most general quasi-Hermitian operator acting in $\mathcal{H}$.

$$H = H_0 + qI = \begin{pmatrix} q + a & b \\ c & q - a \end{pmatrix}, \quad (5)$$

where $q \in \mathbb{R}$, $a, b, c \in \mathbb{C}$, and $a^2 + bc \in [0, \infty)$.

An alternative parametrization of $H_0$ that simplifies its diagonalization is [9]

$$H_0 = E \begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix}, \quad (6)$$

where $E \in [0, \infty)$, $\theta, \varphi \in \mathbb{C}$, $\Re(\theta) \in [0, \pi)$ and $\Re(\varphi) \in [0, 2\pi)$.\footnote{\(\Re\) and \(\Im\) stand for the real and imaginary parts of their argument.} The adjoint $H_0^\dagger$ of $H_0$ and any linearly independent pair of eigenvectors $|\phi_n\rangle$ of $H_0^\dagger$ are given by

$$H_0^\dagger = E \begin{pmatrix} \cos \theta^* & e^{-i\varphi^*} \sin \theta^* \\ e^{i\varphi^*} \sin \theta^* & -\cos \theta^* \end{pmatrix},$$

$$|\phi_1\rangle = n_1 \begin{pmatrix} \cos \frac{\varphi^*}{2} \\ e^{i\varphi^*} \sin \frac{\varphi^*}{2} \end{pmatrix}, \quad |\phi_2\rangle = n_2 \begin{pmatrix} \sin \frac{\varphi^*}{2} \\ -e^{i\varphi^*} \cos \frac{\varphi^*}{2} \end{pmatrix}, \quad (7, 8)$$

where $n_1, n_2 \in \mathbb{C} - \{0\}$ are arbitrary.

The most general positive-definite metric operator $\eta_+$ that renders $H_0$ (and hence $H$) $\eta_+$-pseudo-Hermitian is given by [10, 11]

$$\eta_+ = \sum_{n=1}^2 |\phi_n\rangle\langle\phi_n| = k \begin{pmatrix} au + b & e^{-i\varphi}(u\zeta - \zeta^*) \\ e^{i\varphi}(u^* \zeta^* - \zeta) & e^{i(\varphi - \varphi^{\prime})}(a + bu) \end{pmatrix}, \quad (9)$$

where

$$a := |\cos \frac{\theta}{2}|^2, \quad b := |\sin \frac{\theta}{2}|^2, \quad \zeta := \sin \frac{\theta}{2} \cos \frac{\varphi^*}{2}, \quad k := |n_2|^2, \quad u := |n_1/n_2|^2. \quad (10)$$

Note that the parameters $a, b, \zeta$ are determined by $\theta$ and $\varphi$ that fix $H_0$ while $k$ and $u$ characterize the freedom of the choice of $\eta_+$. In particular, changing $k$ corresponds to a trivial scaling of $\eta_+$ and the associated inner product (1).

For later use we introduce the set $\mathcal{U}_\eta$ consisting of all the metric operators (9) such that $H$ is $\eta_+$-pseudo-Hermitian.
3. Irreducible Sets of Compatible Quasi-Hermitian Operators

Given a linear operator acting in $\mathbb{C}^2$, the eigenspaces associated with each eigenvalue is an invariant subspace of the operator. This implies that a pair of (diagonalizable quasi-Hermitian) operators have a common proper invariant subspace, if they share an eigenvector. In other words, they form an irreducible set, if they have no common eigenvectors. In light of this observation, to construct an irreducible set of compatible quasi-Hermitian operators one needs to supplement a given quasi-Hermitian operator $H$ with a linear operator $H'$ that is $\eta_+$-pseudo-Hermitian for some $\eta_+ \in \mathcal{U}_\eta$ and do not share any eigenvector with $H$.

We shall first consider the problem of the characterization of a general quasi-Hermitian operator that is compatible with $H$. In other words, we shall construct the most general quasi-Hermitian operator, $H' = H'_0 + q' I$ with

$$H'_0 = \begin{pmatrix} a' & b' \\ c' & -a' \end{pmatrix},$$

$a', b', c' \in \mathbb{C}, a'^2 + b'c' \in [0, \infty)$ and $q' \in \mathbb{R}$, such that $H'^\dagger = \eta_+ H' \eta_+^{-1}$ for a metric operator $\eta_+$ of the form (9). This in turn implies $H'^\dagger_0 = \eta_+ H'_0 \eta_+^{-1}$ or alternatively

$$H'^\dagger_0 \eta_+ = \eta_+ H'_0.$$  \hspace{1cm} (12)

This relation leads to four complex equations for the three unknowns $a'$, $b'$ and $c'$. These equations that involve the fixed complex constants $\theta, \varphi$ (alternatively $a, b, \zeta$) and the free real positive parameter $u$ are not independent. They can be reduced to the following three simpler equations.

$$\Im(\lambda b') = r \Im(a'),$$ \hspace{1cm} (13)

$$\Im(\lambda c'^*) = s \Im(a'),$$ \hspace{1cm} (14)

$$sb' - r c'^* = 2\lambda^* \Re(a'),$$ \hspace{1cm} (15)

where

$$\lambda := e^{i\varphi} (u\zeta^* - \zeta), \quad r := e^{2\Im(\varphi)}(a + bu), \quad s := au + b.$$ \hspace{1cm} (16)

The parameters $a', b'$, and $c'$ entering the expression for $H'_0$ are furthermore subject to the constraint $a'^2 + b'c' \in [0, \infty)$, i.e.,

$$\Re(a'^2 + b'c') \geq 0,$$ \hspace{1cm} (17)

$$\Im(a'^2 + b'c') = 0.$$ \hspace{1cm} (18)

Note, however, that in view of the $\eta_+$-pseudo-Hermiticity of $H'_0$ and the positive-definiteness of $\eta_+$, $H'_0$ is Hermitian with respect to the positive-definite inner product (1). This in turn implies that it is diagonalizable and has a real spectrum. As a result, we expect conditions (17) and (18) not to lead to any further restrictions on the possible values of $a'$, $b'$, and $c'$. In the following we shall first solve (13)–(15) and check by explicit calculation that indeed (17) and (18) are automatically satisfied.

Before exploring (13)–(15), we note the following useful identity:

$$\zeta = \frac{1}{2} \left( \sin[\Re(\theta)] + i \sinh[\Im(\theta)] \right).$$ \hspace{1cm} (19)

which follows from (10) upon the application of Euler’s formula. We can use (19) to infer the equivalence of the conditions: $\theta = 0$ and $\zeta = 0$. Another consequence of (19) is that for all nonzero values of $\zeta$, $\lambda = 0$ if and only if $\zeta^*/\zeta$ is real and equal to $u$. In this case, $\zeta$ and hence $\theta$ must be real and $u = 1$.

\^{3}Recall that $\Re(\theta) \in [0, \pi)$. 

440
Now, we are in a position to analyze (13)–(15), (17) and (18). We do this by considering the following two cases separately.

**Case 1** \( \lambda = 0 \): This is equivalent to setting (1) \( \zeta = \theta = 0 \), or (2) \( \zeta, \theta \in \mathbb{R} \) and \( u = 1 \). In this case (13)–(15) yield

\[
\Im(a') = 0, \quad c' = r^{-1}s \, b'^* = \left( \frac{au + b}{a + bu} \right) e^{-2\alpha(\varphi)} b'^*,
\]

where \( \Re(a') = a' \) and \( b' \) are respectively real and complex free parameters. In view of (20), it is not difficult to check that indeed (17) and (18) are automatically satisfied.

**Case 2** \( \lambda \neq 0 \): where either (3) \( u \neq 1 \) and \( \zeta, \theta \neq 0 \), or (4) \( \zeta \) and \( \theta \) are not real. In this case we can simplify (15) by multiplying its both sides by \( \lambda \). Then the imaginary part of the resulting equation is automatically satisfied by virtue of (13) and (14), and its real part yields

\[
s \Re(\lambda b') - r \Re(\lambda c'^*) = 2|\lambda|^2 \Re(a').
\]

We can solve (13), (14), and (21) to obtain:

\[
b' = \lambda^{-1} \left[ w + ir \Im(a') \right] = e^{-i\varphi} w + ie^{-i\varphi} (a + bu) \Im(a'),
\]

\[
c' = (r \lambda^*)^{-1} \left[ sw - 2|\lambda|^2 \Re(a') - ir s \Im(a') \right] = e^{i\varphi} [(au + b)e^{-2\alpha(\varphi)} w - 2i u \zeta - \zeta^* |\lambda|^2 \Re(a') - i (a + bu) (au + b) \Im(a')] (u \zeta - \zeta^*) (a + bu),
\]

where \( w \in \mathbb{R} \) and \( a' \in \mathbb{C} \) are arbitrary. Next, we impose the constraints (17) and (18). In view of the fact that \( \lambda \neq 0 \), (18) is equivalent to

\[
\Im[|\lambda|^2 a^2 + (\lambda b')(\lambda c'^{*})] = 0.
\]

Expressing the left-hand side of this relation in terms of the real and imaginary parts of \( \lambda b' \) and \( \lambda c'^* \) and making use of (13), (14) and (21), we have checked that (24) is automatically satisfied. Finally imposing (17) yields

\[
|\lambda|^2 \left[ \Re(a')^2 - \Im(a')^2 - 2r^{-1} w \Re(a') \right] + r s \Im(a')^2 + r^{-1} s w^2 \geq 0.
\]

We shall next prove that this inequality is also satisfied for all \( w \in \mathbb{R} \) and \( a' \in \mathbb{C} \) irrespective of values of \( \theta, \varphi \) and \( u \). To do this we first view (25) as a quadratic polynomial in \( \Im(a') \). This polynomial will be non-negative if we can prove that it does not have two distinct real roots. This is equivalent to the condition:

\[
D \geq 0,
\]

where

\[
D := \frac{|\lambda|^2 [\Re(a')^2 - 2r^{-1} w \Re(a')] + r^{-1} s w^2}{rs - |\lambda|^2} = \frac{|\lambda|^2 \left[ \Re(a')^2 - r^{-1} w^2 + r^{-2} w^2 (rs - |\lambda|^2) \right]}{rs - |\lambda|^2}.
\]

As seen from this relation, in order to show that \( D \geq 0 \) we just need to check that \( rs - |\lambda|^2 \) is non-negative. Employing (10), (16), and the elementary trigonometric identities

\[
\cos^2 \frac{\theta}{2} = \frac{1 + \cos \theta}{2}, \quad \sin^2 \frac{\theta}{2} = \frac{1 - \cos \theta}{2},
\]

441
we have

\[ rs - |\lambda|^2 = e^{2\Im(\varphi)}[(a + bu)(au + b) - |u\zeta - \zeta^*|^2] \]
\[ = e^{2\Im(\varphi)} u \left( |\cos \frac{\theta}{2}|^2 + |\sin \frac{\theta}{2}|^2 + 2\Re \left[ \cos^2 \frac{\theta}{2} \sin^2 \frac{\theta}{2} \right] \right) \]
\[ = e^{2\Im(\varphi)} u. \quad (28) \]

Hence \( rs - |\lambda|^2 > 0 \), and (26) and (25) are always satisfied.

In summary, the traceless quasi-Hermitian operators \( H'_0 \) that together with \( H_0 \) (respectively \( H \)) form a compatible set involve, in addition to the complex parameters \( \theta, \varphi \) of \( H_0 \) and the real positive parameter \( u \) of \( \eta_+ \), three free real parameters. For Case 1, these can be taken as \( \Re(a') \), \( \Re(b') \) and \( \Im(a') \). For Case 2, one can choose \( \Re(a') \), \( \Im(a') \) and \( w \) (or alternatively \( \Re(b') \)).

Next, we return to the discussion of the irreducibility of a set of compatible quasi-Hermitian operators. As we mentioned above two operators \( H \) and \( H' \) form an irreducible set, if they lack a common eigenvector. This is equivalent to the condition

\[ \det([H, H']) \neq 0, \quad (29) \]

where \([,] \) denotes the commutator. It is easy to see that (29) is equivalent to

\[ \det([H_0, H'_0]) \neq 0, \quad (30) \]

where \( H_0 \) and \( H'_0 \) are the traceless parts of \( H \) and \( H' \), respectively. Substituting (4) and (11) in (30), we find

\[ (bc' - cb')^2 - 4(ab' - ba')(ac' - ca') \neq 0. \quad (31) \]

Let \( C_n \) denote the moduli space of the quasi-Hermitian operator \( H' \) that are compatible with \( H \). Every point in \( C_n \) is parameterized by the free parameters \( q' \in \mathbb{R} \) that equals \( \text{tr}(H')/2 \), \( u \in \mathbb{R}^+ \) that enters in the expression for the allowed metric operators \( \eta_+ \), and the three free real variables: \( \Re(a') \), \( \Re(b') \) and \( \Im(a') \) for Case 1 and \( \Re(a') \), \( \Im(a') \) and \( w \) (or alternatively \( \Re(b') \)) for Case 2. The moduli space \( M_n \) of the quasi-Hermitian operators \( H' \) that are compatible with \( H \) and together with \( H \) constitute an irreducible set is the subset of \( C_n \) that exclude the values of the latter three variables for which the left-hand side of (31) vanishes. \( C_n - M_n \) is a three dimensional subspace of \( C_n \). Hence a generic choice for \( H' \in C_n \) will belong to \( M_n \); \( H \) and \( H' \) will form an irreducible set.

Finally, we consider fixing an element \( H' \) of \( M_n - \{ H \} \), i.e., selecting particular values for \( q', a', b', c' \) that fulfill (13)–(15) and (31). We wish to explain why in this case the value of \( u \) is uniquely determined and hence \( \eta_+ \) is fixed up to the scaling factor \( k \). Consider Case 1 above. If \( \theta \neq 0 \), then \( u = 1 \) necessarily. If \( \theta = 0 \), then we can solve for \( u \) in the second equation in (20). The latter is linear in \( u \), hence its solution is unique. Next, consider Case 2. Then we can similarly solve (22) for \( u \). Again this equation is linear in \( u \) and its solution is unique.

4. Concluding Remarks

In this paper we have provided an explicit characterization of the most general quasi-Hermitian operator \( H \), the associated metric operators \( \eta_+ \), and \( \eta_+ \)-pseudo-Hermitian operators acting in \( \mathbb{C}^2 \). We have derived a quantitative condition that singles out the operators \( H' \) that together with \( H \) form an irreducible set of compatible quasi-Hermitian operators, and demonstrated how a choice of \( H \) and \( H' \) fixes the metric operator up to a scale factor.

In pseudo-Hermitian quantum mechanics [12], a quantum system is constructed by choosing a Hamiltonian operator \( H \) (from among the set of quasi-Hermitian operators) and a metric operator \( \eta_+ \) that renders
the Hamiltonian $\eta_+$-pseudo-Hermitian. The latter specifies the physical Hilbert space of the system. The physical observables are represented by $\eta_+$-pseudo-Hermitian operators $H'$. In quasi-Hermitian quantum mechanics [8], instead of choosing $H$ and $\eta_+$ one chooses $H$ and another element of the space $\mathcal{M}_H$ of all quasi-Hermitian operators that together with $H$ form an irreducible set of compatible operators.

As we demonstrated, by explicit calculations for a general two-level quantum system, employing quasi-Hermitian quantum mechanics requires carrying out all the constructions of the pseudo-Hermitian quantum mechanics. In this sense, the former is not more practical than the latter.

It is occasionally argued that quasi-Hermitian quantum mechanics is more physically relevant because it involves fixing the Hilbert space after choosing a set of physical observables. We wish to emphasize that the physical interpretation of an operator cannot be achieved before fixing the structure of the Hilbert space it acts in. Therefore, as far as the physical aspects of both pseudo- and quasi-Hermitian formulations of quantum mechanics are concerned, they are on equal grounds.

References