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THE METRIC OPERATORS FOR PSEUDO-HERMITIAN HAMILTONIAN

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Abstract

The Hamiltonian of a conventional quantum system is Hermitian, which ensures real spectra of the Hamiltonian and unitary evolution of the system. However, real spectra are just the necessary conditions for a Hamiltonian to be Hermitian. In this paper, we discuss the metric operators for pseudo-Hermitian Hamiltonian which is similar to its adjoint. We first present some properties of the metric operators for pseudo-Hermitian Hamiltonians and obtain a sufficient and necessary condition for an invertible operator to be a metric operator for a given pseudo-Hermitian Hamiltonian. When the pseudo-Hermitian Hamiltonian has real spectra, we provide a new method such that any given metric operator can be transformed into the same positive-definite one and the new inner product with respect to the positive-definite metric operator is well defined. Finally, we illustrate the results obtained with an example.

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1. Introduction

As a fruitful extension of conventional quantum mechanics, pseudo-Hermitian quantum mechanics has developed into a noteworthy area of research, especially PT-symmetric quantum mechanics [3, 4, 8, 23]. This theory has been widely discussed and developed. Consider a quantum system determined by a Hamiltonian H. In order

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to ensure the applicability of the conventional theory of quantum mechanics, it is necessary for H to be diagonalizable with real spectra [16]. However, such a necessary condition can be satisfied even if H is not Hermitian [2, 11]. Mostafazadeh [12] showed that a non-Hermitian Hamiltonian with discrete spectra and a complete biorthonormal system of eigenvectors is pseudo-Hermitian if and only if the spectra are all real, or the complex eigenvalues come in complex conjugate pairs and the geometric multiplicity and the Jordan dimensions of the complex-conjugate eigenvalues coincide. The pseudo-Hermitian Hamiltonian which is defined by a similarity transformation, $H^\dagger = WHW^{-1}$, where W is called a metric operator for H, has developed into a noteworthy area of research, and systems evolving under pseudo-Hermitian dynamics display rich phenomena [7, 9, 10, 22]. In fact, the metric operator for a pseudo-Hermitian Hamiltonian is not unique, and it is worthwhile to discuss the properties of the metric operator and the structure of the set of all metric operators.

Indeed, H is diagonalizable and has real spectra if and only if there exists a positive-definite operator η such that $H^\dagger = \eta H \eta^{-1}$ [13]. The positivity of η implies that H belongs to a special class of pseudo-Hermitian operators called quasi-Hermitian operators [21], while the pseudo-Hermitian operators only require that η is invertible. Then a consistent quantum theory can be built with a new inner product $\langle\cdot|\cdot\rangle_\eta = \langle\cdot|\eta|\cdot\rangle$, and any H satisfying $\langle\cdot|H\cdot\rangle_\eta = \langle H\cdot|\cdot\rangle_\eta$ is Hermitian [12]. Furthermore, putting $\varrho = \sqrt{\eta}$, we have H similar to the Hermitian Hamiltonian, $h := \varrho H \varrho^{-1}$. Hence, the quasi-Hermitian quantum theory that is determined by H admits an equivalent Hermitian description in terms of the (standard) Hilbert space with the Hermitian Hamiltonian h [14, 15]. However, the specific form of h depends on the choice of ϱ, since $\tilde{\varrho} = U\sqrt{\eta}$ also satisfies the condition. This has motivated the search for alternative methods of computing the most general metric operator for a given pseudo-Hermitian Hamiltonian [17, 18, 20]. For a quasi-Hermitian Hamiltonian H, if the given metric operator W is not positive, then the inner product with respect to W is indefinite. While Mostafazadeh [13] ensures that there must exist a positive-definite metric operator, changing the nonpositive metric operator to a positive definite one is an interesting topic to explore.

Since in a finite-dimensional quantum system each Hamiltonian has a matrix presentation with respect to the given orthonormal basis, the Hamiltonian and the corresponding matrix are considered to be identical and there is a growing body of literature that pertains to the finite-dimensional case, such as pseudo-Hermitian random matrix theory, and pseudo-Hermitian spin systems [5, 6, 19]. In this article we discuss the metric operators for pseudo-Hermitian Hamiltonians in finite-dimensional quantum systems. In Section 2 we first establish some properties of the metric operator and obtain a sufficient and necessary condition for an invertible operator to be a metric operator for a given pseudo-Hermitian Hamiltonian according to the vec map. Then in Section 3 we provide a method to change a given metric operator which is not positive-definite to become a positive one when the pseudo-Hermitian Hamiltonian has real spectra. Our findings and conclusions are summarized in Section 4.

2. The two golden rules

A physical system which is determined by a Hamiltonian is a Hilbert space (a complex vector space with inner product), and the Hamiltonian corresponds to a linear operator. Suppose that $H \in B(\mathbb{C}^d)$ is a Hamiltonian, $H^\dagger$ is the adjoint of H, H^T is the transpose of H, $|\psi\rangle$ is a unit column vector, $\langle\psi| = (|\psi\rangle)^\dagger$ is a unit row vector.

DEFINITION 2.1 [12]. Let $H \in B(\mathbb{C}^d)$. If there exists an invertible operator W such that $H^\dagger = WHW^{-1}$, then H is called a *pseudo-Hermitian Hamiltonian* and W is called a *metric operator* for H.

We note from the Definition 2.1 that, in particular, when $W = I$, the pseudo-Hermitian Hamiltonian coincides with a Hermitian Hamiltonian. Therefore, all Hermitian Hamiltonians form a subset of the set of pseudo-Hermitian Hamiltonians.

We now present some results about the pseudo-Hermitian Hamiltonian and its metric operators.

THEOREM 2.2. *Let H be a pseudo-Hermitian Hamiltonian on $B(\mathbb{C}^d)$ with a metric operator W.*

(i) *The spectra of H are all real or complex conjugate pairs.*
(ii) *$W^\dagger$ is also a metric operator for H, and a Hermitian metric operator for H can always be determined.*
(iii) *For any $\lambda \in \mathbb{R}\backslash\{0\}$, λW is a metric operator for H.*
(iv) *If M is another metric operator for H and $W + M$ is invertible, then $W + M$ is a metric operator for H.*
(v) *If an invertible operator A commutes with H, then $WA^k (k \in \mathbb{N})$ are metric operators for H.*
(vi) *If an invertible operator B commutes with $H^\dagger$, then $B^k W (k \in \mathbb{N})$ are metric operators for H.*

PROOF. Let H be a pseudo-Hermitian Hamiltonian with a metric operator W, that is, $H^\dagger = WHW^{-1}$.

(i) Because the spectra of H and $H^\dagger$ are complex conjugate to each other and a similarity transformation does not change the spectra, the spectra of H are all real or complex conjugate pairs.
(ii) From $H^\dagger = WHW^{-1}$ it follows that $H = (W^\dagger)^{-1}H^\dagger W^\dagger$ and $H^\dagger = W^\dagger H(W^\dagger)^{-1}$. Thus, $W^\dagger$ is also a metric operator for H. If the given W is Hermitian, then that is true. Otherwise, there exists a $\theta \in \mathbb{R}$ such that $-\mathrm{e}^{2\mathrm{i}\theta} I \neq W^{-1}W^\dagger$; put

$$\tilde{W} = \mathrm{e}^{\mathrm{i}\theta}W + \mathrm{e}^{-\mathrm{i}\theta}W^\dagger.$$

Then $\tilde{W}$ is Hermitian and satisfies $H^\dagger\tilde{W} = \tilde{W}H$. Since the spectra of $W^{-1}W^\dagger$ does not contain $-\mathrm{e}^{2\mathrm{i}\theta}$, the inverse of $\tilde{W}$ is $\mathrm{e}^{-\mathrm{i}\theta}[I + \mathrm{e}^{-2\mathrm{i}\theta}W^{-1}W^\dagger]^{-1}W^{-1}$. Hence, $\tilde{W}$ is a metric operator for H.

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(iii) This follows from the definition of the pseudo-Hermitian Hamiltonian.
(iv) This follows from the definition of the pseudo-Hermitian Hamiltonian.
(v) By the definition of the pseudo-Hermitian Hamiltonian and since $AH = HA$, we have $(WA)H = WHA = H^\dagger(WA)$. Thus, for all $k \in \mathbb{N}$, $W_k = WA^k$ are metric operators for H.
(vi) This is similar to (v).

The proof is now complete. □

In order to understand the metric operators for a given pseudo-Hermitian Hamiltonian operator, we introduce the operator–vector correspondence as follows. We know that

$$\mathrm{vec} : L(\mathbb{X}, \mathbb{Y}) \to \mathbb{Y} \otimes \mathbb{X}$$

is the linear bijection and isometry, mapping an operator to a vector [1]. For $u \in \mathbb{X}$ and $v \in \mathbb{Y}$, we have

$$\mathrm{vec}(uv^\dagger) = u \otimes \bar{v},$$

where the bar denotes the complex conjugate.

THEOREM 2.3. *Let $H \in B(\mathbb{C}^d)$ be a pseudo-Hermitian Hamiltonian and $W \in B(\mathbb{C}^d)$ be invertible. Then W is a metric operator for H if and only if*

$$(I \otimes H^T - H^\dagger \otimes I)\mathrm{vec}(W) = 0.$$

PROOF. *Necessity*. Let W be a metric operator for H. Then $H^\dagger = WHW^{-1}$ and

$$\mathrm{vec}(H^\dagger W) = \mathrm{vec}(WH).$$

Using the property of the vec mapping,

$$\mathrm{vec}(AXB^T) = (A \otimes B)\mathrm{vec}(X),$$

we have

$$(H^\dagger \otimes I)\mathrm{vec}(W) = (I \otimes H^T)\mathrm{vec}(W).$$

Thus,

$$(I \otimes H^T - H^\dagger \otimes I)\mathrm{vec}(W) = 0.$$

Sufficiency. Let W satisfy $(I \otimes H^T - H^\dagger \otimes I)\mathrm{vec}(W) = 0$. Then

$$(I \otimes H^T)\mathrm{vec}(W) = (H^\dagger \otimes I)\mathrm{vec}(W)$$

and

$$\mathrm{vec}(WH) = \mathrm{vec}(H^\dagger W).$$

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Since the vec mapping is a linear bijection, we have $WH = H^{\dagger}W$. Since W is invertible, it is a metric operator for H. This completes the proof. □

REMARK 2.4. When $S \in B(\mathbb{C}^{d^2})$ commutes with $I \otimes H^T - H^{\dagger} \otimes I$, we have that $S(\text{vec}(W))$ is also an eigenvector of $I \otimes H^T - H^{\dagger} \otimes I$ corresponding to eigenvalue 0. If S is invertible, then $\text{vec}^{-1}(S(\text{vec}(W)))$ is a metric operator for H. When H is invertible, we have the following results.

(i) Take $S = I \otimes H^T$ and $I \otimes H^T(\text{vec}(W)) = \text{vec}(WH)$. Then $\check{W} = WH$ is a metric operator for H. Moreover, we see that it is consistent with Theorem 2.2(v); here, we take $A = H$.
(ii) Take $S = H^{\dagger} \otimes I$ and $H^{\dagger} \otimes I(\text{vec}(W)) = \text{vec}(H^{\dagger}W)$. Then $\hat{W} = H^{\dagger}W$ is a metric operator for H, and it is consistent with Theorem 2.2(vi); here, we take $B = H^{\dagger}$.
(iii) Take $S = H^{\dagger} \otimes H^T$ and $H^{\dagger} \otimes H^T(\text{vec}(W)) = \text{vec}(H^{\dagger}WH)$. Then $\check{W} = H^{\dagger}WH$ is a metric operator for H.

Furthermore, for all $k \in \mathbb{N}$, WH^k, $(H^{\dagger})^k W$ and $(H^{\dagger})^k WH^k$ are Hermitian if the metric operator W for H is Hermitian.

For example, when $H = \left(\begin{smallmatrix} \mathrm{i} & 1 \\ 2 & -\mathrm{i} \end{smallmatrix}\right)$, we have

$$I \otimes H^T - H^{\dagger} \otimes I = \begin{pmatrix} 2\mathrm{i} & 2 & -2 & 0 \\ 1 & 0 & 0 & -2 \\ -1 & 0 & 0 & 2 \\ 0 & -1 & 1 & -2\mathrm{i} \end{pmatrix}.$$

By calculation, the eigenvalue zero of the operator $(I \otimes H^T - H^{\dagger} \otimes I)$ has multiplicity 2, and $\alpha_1 = (0, 1, 1, 0)^T$ and $\alpha_2 = (2, -2\mathrm{i}, 0, 1)^T$ are two linear independent eigenvectors of $I \otimes H^T - H^{\dagger} \otimes I$. Then we obtain two metric operators for H:

$$W_1 = \text{vec}^{-1}(\alpha_1) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad W_2 = \text{vec}^{-1}(\alpha_2) = \begin{pmatrix} 2 & -2\mathrm{i} \\ 0 & 1 \end{pmatrix}.$$

For any nonzero linear combination β of α_1 and α_2, if $\text{vec}^{-1}(\beta)$ is invertible, then $\text{vec}^{-1}(\beta)$ is also a metric operator for H. We see that the metric operator W_2 as above is not Hermitian. From the proof of Theorem 2.2(ii) a new Hermitian metric operator,

$$\tilde{W_2} = e^{\mathrm{i}\pi/3}W_2 + e^{-\mathrm{i}\pi/3}W_2^{\dagger} = \begin{pmatrix} 2 & \sqrt{3} - \mathrm{i} \\ \sqrt{3} + \mathrm{i} & 1 \end{pmatrix}$$

as $\theta = \pi/3$, is obtained for H.

In the following section, for a pseudo-Hermitian Hamiltonian H, the corresponding metric operator W may always be chosen to be Hermitian, that is, $W = W^{\dagger}$.

3. The results of metric operators for pseudo-Hermitian Hamiltonian

In this section we assume that the Hamiltonian $H \in B(\mathbb{C}^d)$ has different eigenvalues. Let H admit a complete biorthonormal set of eigenvectors $\{|E_n\rangle, |\hat{E}_n\rangle\}$. Then it satisfies the following defining relations:

$$H|E_n\rangle = \gamma_n|E_n\rangle, \quad H^\dagger|\hat{E}_n\rangle = \overline{\gamma_n}|\hat{E}_n\rangle, \tag{3.1}$$

$$\langle\hat{E}_n|E_m\rangle = \delta_{nm}, \tag{3.2}$$

$$\sum_n |\hat{E}_n\rangle\langle E_n| = \sum_n |E_n\rangle\langle\hat{E}_n| = I. \tag{3.3}$$

Here, δ_{nm} stands for the Kronecker delta function, and I is the identity operator. In view of equations (3.1)–(3.3), we have

$$H = \sum_n \gamma_n|E_n\rangle\langle\hat{E}_n|, \quad H^\dagger = \sum_n \overline{\gamma_n}|\hat{E}_n\rangle\langle E_n|. \tag{3.4}$$

In addition, if H is a pseudo-Hermitian Hamiltonian with metric operator W, that is, $H^\dagger = WHW^{-1}$, put

$$\langle x|y\rangle_W = \langle x|W|y\rangle, \quad \text{for all } |x\rangle, |y\rangle \in \mathbb{K}.$$

Then, for any m,n,

$$\gamma_n\langle E_m|E_n\rangle_W = \langle E_m|WH|E_n\rangle = \langle E_m|H^\dagger W|E_n\rangle = \overline{\gamma_m}\langle E_m|E_n\rangle_W,$$

and we can write

$$(\gamma_n - \overline{\gamma_m})\langle E_m|E_n\rangle_W = 0. \tag{3.5}$$

Therefore, this determines

$$\langle E_m|E_n\rangle_W = \rho_{m,n}e^{\mathrm{i}\theta(m,n)}\delta_{\gamma_n,\overline{\gamma_m}}, \tag{3.6}$$

where $\rho_{m,n} = |\langle E_m|E_n\rangle_W| \geq 0$ and $\theta(m,n) = \mathrm{Arg}(\langle E_m|E_n\rangle_W)$ is the argument of $\langle E_m|E_n\rangle_W$.

If there exists an eigenvalue $\gamma_j \notin \mathbb{R}$, then $\langle E_j|E_j\rangle_W = 0$. In this case, it is impossible to define an inner product with respect to W. If all eigenvalues are real, the product in equation (3.6) which can be become negative due to this exponential factor (for example, W has negative eigenvalues), cannot define an inner product. In fact, the quadratic form in equation (3.6) satisfies the inner product conditions except positive-definiteness, because the metric operator W is not necessarily positive, and H is Hermitian with respect to this quadratic form since

$$\langle x|H|y\rangle_W = \langle x|WH|y\rangle = \langle x|H^\dagger W|y\rangle = \langle Hx|W|y\rangle = \langle Hx|y\rangle_W.$$

Thus, when the spectra of pseudo-Hermitian Hamiltonian are all real, it is significant to find a positive metric operator such that equation (3.6) is a well-defined inner product, and the non-Hermitian Hamiltonian can be exchanged for the Hermitian case. Besides, the existence of this positive metric operator was shown by Mostafazadeh [13], who proved that the spectra of H are real if and only if there is a positive invertible linear operator η such that $H^{\dagger} = \eta H \eta^{-1}$.

Hence, for a pseudo-Hermitian Hamiltonian H with real spectra, we provide in the following a method to change the given nonpositive metric operator ($W \ngtr 0$) into a positive one ($\eta > 0$).

THEOREM 3.1. *Let H be a pseudo-Hermitian Hamiltonian with real spectra. For any metric operator W for H, it can be transformed into $\eta = \sum_n |\hat{E}_n\rangle\langle\hat{E}_n|$.*

PROOF. Let the eigenvalues of H be all real, that is, $\gamma_n \in \mathbb{R}$ for all n. By equation (3.4),

$$H = \sum_n \gamma_n |E_n\rangle\langle\hat{E}_n|, \quad H^{\dagger} = \sum_n \gamma_n |\hat{E}_n\rangle\langle E_n|. \tag{3.7}$$

Put

$$P_n = |E_n\rangle\langle\hat{E}_n| \tag{3.8}$$

and

$$A = \sum_n a_n P_n, \quad a_n \in \mathbb{R}\backslash\{0\}. \tag{3.9}$$

We have

$$A^{-1} = \sum_n \frac{1}{a_n} P_n,$$

$$AH = \sum_n a_n |E_n\rangle\langle\hat{E}_n| H = H \sum_n a_n |E_n\rangle\langle\hat{E}_n| = HA$$

and

$$A|E_n\rangle = a_n|E_n\rangle.$$

So $|E_n\rangle$ are simultaneous eigenstates of A and H, and the coefficients of expansion a_n in equation (3.9) are indeed the eigenvalues of A. Take

$$\eta = WA.$$

Then

$$\eta^{\dagger} = A^{\dagger} W = WW^{-1} \sum_n \bar{a}_n P_n^{\dagger} W = WA = \eta.$$

Since A commutes with H, we get that η is also a metric operator for H by Theorem 2.2(v). Next define

$$\langle\phi|\psi\rangle_\eta = \langle\phi|\eta|\psi\rangle.$$

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We have

$$\langle E_m|E_n\rangle_\eta = a_n\langle E_m|E_n\rangle_W.$$

Since W is invertible and Hermitian, by equation (3.6), we have

$$\langle E_m|E_n\rangle_W = \begin{cases} 0, & m \neq n, \\ \langle E_m|W|E_m\rangle \in \mathbb{R}\backslash 0, & m = n. \end{cases}$$

Then

$$\langle E_m|E_n\rangle_W = \tilde{\rho}_n\delta_{m,n},$$

where $\tilde{\rho}_n$ are positive or negative real numbers. Thus,

$$\langle E_m|E_n\rangle_\eta = a_n\tilde{\rho}_n\delta_{m,n}.$$

If we choose the coefficients of A as

$$a_n = \frac{1}{\tilde{\rho}_n},$$

then

$$\langle E_m|E_n\rangle_\eta = \delta_{m,n}. \tag{3.10}$$

By this method of constructing η, we have

$$\eta = WA = W\sum_j a_jP_j = \sum_j \frac{W}{\langle E_j|E_j\rangle_W}|E_j\rangle\langle\hat{E}_j|.$$

According to equation (3.3),

$$W\sum_n |E_n\rangle\langle\hat{E}_n| = \sum_n |\hat{E}_n\rangle\langle E_n|W,$$

and multiplying $|E_j\rangle$ yields

$$W|E_j\rangle = |\hat{E}_j\rangle\langle E_j|W|E_j\rangle.$$

Thus,

$$\eta = \sum_j |\hat{E}_j\rangle\langle\hat{E}_j|. \tag{3.11}$$

This completes the proof. □

We see that η is positive-definite, $\langle\cdot|\cdot\rangle_\eta = \langle\cdot|\eta|\cdot\rangle$ is a well-defined inner product, and the eigenstates of H form an orthonormal basis by equation (3.10). Indeed, the positive-definite metric operator η we obtained in equation (3.11) which was shown by Mostafazadeh [13], satisfies our Theorem 2.3. By equation (3.7) and vec mapping,

$$I \otimes H^T - H^\dagger \otimes I = I \otimes \sum_n \gamma_n\overline{|\hat{E}_n\rangle\langle E_n|} - \sum_n \gamma_n|\hat{E}_n\rangle\langle E_n| \otimes I,$$

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By equation (3.7) and vec mapping,

$$I \otimes H^T - H^\dagger \otimes I = I \otimes \sum_n \gamma_n \overline{|\hat{E}_n\rangle\langle E_n|} - \sum_n \gamma_n |\hat{E}_n\rangle\langle E_n| \otimes I,$$

$$\mathrm{vec}(\eta) = \sum_j |\hat{E}_j\rangle \otimes \overline{|\hat{E}_j\rangle},$$

followed by biorthogonality relation equation (3.2), we have

$$(I \otimes H^T - H^\dagger \otimes I)(\mathrm{vec}(\eta)) = \sum_n \gamma_n |\hat{E}_n\rangle \otimes \overline{|\hat{E}_n\rangle} - \sum_n \gamma_n |\hat{E}_n\rangle \otimes \overline{|\hat{E}_n\rangle} = 0.$$

Moreover, since η is positive-definite, there exists an operator ρ such that $\eta = \rho^\dagger\rho$. Put

$$\rho = \sum_j |e_j\rangle\langle \hat{E}_j|,$$

where $\{|e_j\rangle\}$ is the standard basis of $\mathbb{C}^d$. Then

$$\rho^{-1} = \sum_j |E_j\rangle\langle e_j|$$

and

$$(\rho H \rho^{-1})^\dagger = \sum_j r_j |e_j\rangle\langle e_j| = \rho H \rho^{-1}.$$

Hence, H is similar to a Hermitian operator.

As we know, the eigenvalues of pseudo-Hermitian Hamiltonians are all real or complex conjugate pairs. When there exists a pair of nonreal eigenvalues $\gamma_j = \overline{\gamma_k}$ such that

$$W|E_j\rangle = \langle E_k|W|E_j\rangle|\hat{E}_k\rangle,$$

we get

$$\eta = \sum_{t \neq j,k} |\hat{E}_t\rangle\langle \hat{E}_t| + \delta_{\gamma_j,\overline{\gamma_k}} (|\hat{E}_k\rangle\langle \hat{E}_j| + |\hat{E}_j\rangle\langle \hat{E}_k|), \tag{3.12}$$

which is not positive-definite. In this case, $\langle E_j|E_j\rangle_\eta = \langle E_k|E_k\rangle_\eta = 0$. Thus, it is impossible to define an orthonormal basis with respect to the metric operator η.

Let us next apply our construction to a simple 2×2 matrix Hamiltonian which is pseudo-Hermitian. Consider the Hamiltonian

$$H = \begin{pmatrix} re^{\mathrm{i}\theta} & se^{\mathrm{i}\phi} \\ te^{-\mathrm{i}\phi} & re^{-\mathrm{i}\theta} \end{pmatrix} \neq H^\dagger, \quad r, s, t, \theta, \phi \in \mathbb{R},$$

and the given metric operator

$$W = \begin{pmatrix} 0 & e^{\mathrm{i}\phi} \\ e^{-\mathrm{i}\phi} & 0 \end{pmatrix} = W^\dagger.$$

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Clearly, $WH = H^\dagger W$. The eigenvalues of W are $\lambda_{W\pm} = \pm 1$ which means $W \not> 0$, so the inner product $\langle\cdot|\cdot\rangle_W = \langle\cdot|W|\cdot\rangle$ is not well defined. The eigenvalues of H are

$$\gamma_\pm = r\cos\theta \pm \sqrt{st - r^2\sin^2\theta}.$$

Therefore, for $st > r^2\sin^2\theta$, the eigenvalues are real, while for $st < r^2\sin^2\theta$, the eigenvalues are complex conjugates of each other (for $st = r^2\sin^2\theta$, the Hamiltonian cannot be diagonalized).

Case 1. For $st > r^2\sin^2\theta$, the eigenvalues of Hamiltonian H are

$$\gamma_\pm = r\cos\theta \pm \sqrt{st - r^2\sin^2\theta} \in \mathbb{R}.$$

Then H is quasi-Hermitian, and there must exist a positive-definite metric operator. The eigenstates of H corresponding to the two eigenvalues are

$$|E_\pm\rangle = \frac{1}{\sqrt{2(st - r^2\sin^2\theta)}}\begin{pmatrix} se^{\mathrm{i}\phi/2} \\ \big(-\mathrm{i}r\sin\theta \pm \sqrt{st - r^2\sin^2\theta}\big)e^{-\mathrm{i}\phi/2}\end{pmatrix},$$

the eigenstates of $H^\dagger$ corresponding to the two eigenvalues are

$$|\hat{E}_\pm\rangle = \frac{1}{\sqrt{2}\big(\sqrt{st - r^2\sin^2\theta} \pm \mathrm{i}r\sin\theta\big)}\begin{pmatrix} te^{\mathrm{i}\phi/2} \\ \big(\mathrm{i}r\sin\theta \pm \sqrt{st - r^2\sin^2\theta}\big)e^{-\mathrm{i}\phi/2}\end{pmatrix},$$

and

$$\langle\hat{E}_i|E_j\rangle = \delta_{ij}, \quad i, j \in \{+,-\}.$$

The operator P in this case can be determined according to

$$\begin{aligned} P_+ = |E_+\rangle\langle\hat{E}_+| = {}& \frac{1}{2\sqrt{st - r^2\sin^2\theta}} \\ & \times \begin{pmatrix} \sqrt{st - r^2\sin^2\theta} + \mathrm{i}r\sin\theta & se^{\mathrm{i}\phi} \\ te^{-\mathrm{i}\phi} & \sqrt{st - r^2\sin^2\theta} - \mathrm{i}r\sin\theta \end{pmatrix}, \\ P_- = |E_-\rangle\langle\hat{E}_-| = {}& \frac{1}{2\sqrt{st - r^2\sin^2\theta}} \\ & \times \begin{pmatrix} \sqrt{st - r^2\sin^2\theta} - \mathrm{i}r\sin\theta & -se^{\mathrm{i}\phi} \\ -te^{-\mathrm{i}\phi} & \sqrt{st - r^2\sin^2\theta} + \mathrm{i}r\sin\theta \end{pmatrix}. \end{aligned}$$

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The coefficients $a_\pm$ of A are

$$a_+ = \frac{1}{\langle E_+|E_+\rangle_W} = \frac{\sqrt{st - r^2\sin^2\theta}}{s},$$
$$a_- = \frac{1}{\langle E_-|E_-\rangle_W} = \frac{-\sqrt{st - r^2\sin^2\theta}}{s}$$

and

$$A = \frac{\sqrt{st - r^2\sin^2\theta}}{s}(P_+ - P_-) = \frac{1}{s}\begin{pmatrix} \mathrm{i}r\sin\theta & se^{\mathrm{i}\phi} \\ te^{-\mathrm{i}\phi} & -\mathrm{i}r\sin\theta \end{pmatrix}.$$

Thus,

$$\eta = WA = \frac{1}{s}\begin{pmatrix} t & -\mathrm{i}r\sin\theta e^{\mathrm{i}\phi} \\ \mathrm{i}r\sin\theta e^{-\mathrm{i}\phi} & s \end{pmatrix}.$$

It can now be checked that

$$\langle E_m|E_n\rangle_\eta = \delta_{n,m}, \quad m, n = \pm.$$

Therefore, $\{|E_\pm\rangle\}$ is an orthonormal basis with respect to new inner product $\langle\cdot|\cdot\rangle_\eta$ in $\mathbb{C}^2$. We see that

$$\eta = |\hat{E}_+\rangle\langle\hat{E}_+| + |\hat{E}_-\rangle\langle\hat{E}_-|.$$

Case 2. For $st < r^2\sin^2\theta$, the eigenvalues of H are

$$\gamma_\pm = r\cos\theta \pm \mathrm{i}\sqrt{r^2\sin^2\theta - st} \notin \mathbb{R},$$

the eigenstates corresponding to two eigenvalues are

$$|E_\pm\rangle = \frac{1}{\sqrt{2(r^2\sin^2\theta - st)}}\begin{pmatrix} se^{\mathrm{i}\phi/2} \\ -\mathrm{i}\big(r\sin\theta \mp \sqrt{r^2\sin^2\theta - st}\big)e^{-\mathrm{i}\phi/2} \end{pmatrix},$$

the eigenstates of $H^\dagger$ corresponding to the two eigenvalues are

$$|\hat{E}_\pm\rangle = \frac{-1}{\sqrt{2}\big(\sqrt{r^2\sin^2\theta - st} \pm r\sin\theta\big)}\begin{pmatrix} te^{\mathrm{i}\phi/2} \\ \mathrm{i}\big(r\sin\theta \mp \sqrt{r^2\sin^2\theta - st}\big)e^{-\mathrm{i}\phi/2} \end{pmatrix},$$

and

$$\langle\hat{E}_\pm|E_\pm\rangle = \delta_{ij}, \quad i, j \in \{+, -\}.$$

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The operator P in this case can be determined according to

$$P_+ = |E_+\rangle\langle\hat{E}_+| = \frac{1}{2\sqrt{r^2\sin^2\theta - st}} \times \begin{pmatrix} \sqrt{r^2\sin^2\theta - st} + r\sin\theta & -\mathrm{i}se^{\mathrm{i}\phi} \\ -\mathrm{i}te^{-\mathrm{i}\phi} & \sqrt{r^2\sin^2\theta - st} - r\sin\theta \end{pmatrix},$$

$$P_- = |E_-\rangle\langle\hat{E}_-| = \frac{1}{2\sqrt{r^2\sin^2\theta - st}} \times \begin{pmatrix} \sqrt{r^2\sin^2\theta - st} - r\sin\theta & \mathrm{i}se^{\mathrm{i}\phi} \\ \mathrm{i}te^{-\mathrm{i}\phi} & \sqrt{r^2\sin^2\theta - st} + r\sin\theta \end{pmatrix}.$$

According to equation (3.5), we have

$$(\gamma_- - \overline{\gamma_+})\langle E_+|E_-\rangle_W = 0, \quad (\gamma_+ - \overline{\gamma_-})\langle E_-|E_+\rangle_W = 0.$$

Since $\gamma_- = \overline{\gamma}_+$, we have

$$\langle E_+|E_+\rangle_W = 0, \quad \langle E_-|E_-\rangle_W = 0.$$

The coefficients $a_\pm$ of A are

$$a_+ = \frac{1}{\langle E_-|E_+\rangle_W} = \frac{-\mathrm{i}\sqrt{r^2\sin^2\theta - st}}{s},$$
$$a_- = \frac{1}{\langle E_+|E_-\rangle_W} = \frac{\mathrm{i}\sqrt{r^2\sin^2\theta - st}}{s}$$

and

$$A = \frac{-\mathrm{i}\sqrt{st - r^2\sin^2\theta}}{s}(P_+ - P_-) = \frac{-1}{s}\begin{pmatrix} \mathrm{i}r\sin\theta & se^{\mathrm{i}\phi} \\ te^{-\mathrm{i}\phi} & -\mathrm{i}r\sin\theta \end{pmatrix}.$$

Thus,

$$\eta = WA = \frac{-1}{s}\begin{pmatrix} t & -\mathrm{i}r\sin\theta e^{\mathrm{i}\phi} \\ \mathrm{i}r\sin\theta e^{-\mathrm{i}\phi} & s \end{pmatrix},$$

which is also not positive-definite. Furthermore,

$$\langle E_+|E_+\rangle_\eta = 0, \quad \langle E_-|E_-\rangle_\eta = 0, \quad \langle E_+|E_-\rangle_\eta = 1,$$

and

$$\eta = |\hat{E}_+\rangle\langle\hat{E}_-| + |\hat{E}_-\rangle\langle\hat{E}_+|.$$

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4. Conclusion

In this work, the metric operators for pseudo-Hermitian Hamiltonians on $B(\mathbb{C}^d)$ are discussed and some properties of the metric operators are obtained. Under the condition that $H \in B(\mathbb{C}^d)$ is a pseudo-Hermitian Hamiltonian and $W \in B(\mathbb{C}^d)$ is invertible, W is a metric operator for H if and only if

$$(I \otimes H^T - H^\dagger \otimes I)\mathrm{vec}(W) = 0.$$

This provides a method for calculating a metric operator for a pseudo-Hermitian Hamiltonian. Furthermore, when a pseudo-Hermitian Hamiltonian has real spectra, Theorem 3.1 states that any given metric operator can be transformed into a positive-definite one as

$$\eta = \sum_{j=1}^{d} |\hat{E}_j\rangle\langle\hat{E}_j|.$$

Moreover, the positive-definite metric operator by this method is not unique, provided that we change the construction of P_j in equation (3.8). If we put

$$P_j = p_j|E_j\rangle\langle\hat{E}_j|, \quad p_j > 0,$$

then the positive-definite metric operator is

$$\eta_1 = \sum_{j=1}^{d} p_j|\hat{E}_j\rangle\langle\hat{E}_j|.$$

When there exists a pair of nonreal eigenvalues of a pseudo-Hermitian Hamiltonian, equation (3.12) provides an expression for the metric operator η. In fact, consider

$$\eta_2 = \sum_t |\hat{E}_t\rangle\langle\hat{E}_t| + \delta_{\gamma_j,\bar{\gamma}_k}\mathrm{i}(|\hat{E}_k\rangle\langle\hat{E}_j| - |\hat{E}_j\rangle\langle\hat{E}_k|),$$

where i makes η_2 Hermitian. It can be checked that η_2 is also a metric operator for H.

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