Pseudo-Hermitian quantum mechanics

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Abstract. In these lectures, we will describe a systematic procedure for constructing an inner product in a pseudo-Hermitian quantum mechanical system.

In recent years there is a lot of interest in $\mathcal{PT}$ symmetric quantum mechanical theories [1] where $\mathcal{P}$ represents parity or space reflection while $\mathcal{T}$ denotes time reversal. As we know $\mathcal{P}$ represents a linear operator while $\mathcal{T}$ corresponds to an anti-linear operator. As a result, in these theories the Hamiltonian is not Hermitian in the Dirac sense, rather it satisfies

$$H = \mathcal{P}^{-1}H^\dagger \mathcal{P} = \mathcal{P} H^\dagger \mathcal{P}, \quad (1)$$

where we have used the properties of the parity operator in the last step, namely,

$$\mathcal{P}^\dagger = \mathcal{P}, \quad \mathcal{P}^2 = 1. \quad (2)$$

The interest in these theories arises from the fact than even though the Hamiltonians in these theories are not Hermitian, the eigenvalues are real if the ground state of the theory is $\mathcal{PT}$ symmetric. We note that the reality of eigenvalues does not require that the Hamiltonian be Hermitian, namely, Hermiticity is not a necessary condition for eigenvalues to be real. A familiar example of a matrix Hamiltonian which is not Hermitian and yet has real eigenvalues is given by

$$H = \begin{pmatrix} \alpha & \beta \\ 0 & \gamma \end{pmatrix} \neq H^\dagger, \quad \alpha, \beta, \gamma \text{ real},$$

which is not Hermitian, but the eigenvalues of the Hamiltonian are given by $E = \alpha, \gamma$ which are real. In this case, we note that if we define

$$S = \begin{pmatrix} a & \beta \\ \frac{\beta}{a-\gamma} a & d \end{pmatrix}, \quad S^{-1} = \frac{1}{\det S} \begin{pmatrix} d & -\frac{\beta}{a-\gamma} a \\ -\frac{\beta}{a-\gamma} a & a \end{pmatrix},$$

where $a, d$ are arbitrary constants, we can check that

$$H = S^{-1}H^\dagger S, \quad (3)$$

which is quite similar to (1).
Any quantum mechanical system whose Hamiltonian can be related to its adjoint (in the Dirac sense) through a similarity transformation as in (3),

\[ H = S^{-1} H^\dagger S, \quad \Rightarrow \quad SH = H^\dagger S, \]  

(4)
is called a pseudo-Hermitian Hamiltonian \[2\]. It is worth emphasizing that by definition, the similarity transformation is assumed to be bounded so that it does not take us out of the Hilbert space. We note from the definition in (4) that, in particular, when \( S = 1 \), the pseudo-Hermitian Hamiltonian coincides with a Hermitian Hamiltonian. Therefore, Hermitian Hamiltonians define a subset of pseudo-Hermitian Hamiltonians. By taking the (Dirac) adjoint of the defining relation (4), we obtain

\[ H^\dagger = S^\dagger H (S^\dagger)^{-1}, \quad \Rightarrow \quad H = (S^\dagger)^{-1} H^\dagger S^\dagger, \]  

(5)
which shows (compare with (3)) that the similarity transformation \( S \) can be chosen to be Hermitian

\[ S = S^\dagger. \]  

(6)

It is worth emphasizing here that to define the adjoint of an operator, we need a Hilbert space \( \mathcal{H} \) with an inner product such that if \( |\psi\rangle, |\phi\rangle \in \mathcal{H} \)

\[ \langle \phi | H | \psi \rangle = \langle H^\dagger | \phi | \psi \rangle, \]  

(7)
and a Hamiltonian is said to be Hermitian (self-adjoint) if

\[ H = H^\dagger, \]  

(8)
besides technical questions such as domains of the operators etc. Normally, the inner product in quantum mechanics is understood in the Dirac sense, namely, if \( |\psi\rangle, |\phi\rangle \in \mathcal{H} \), then the inner product of the two states is defined to be

\[ \langle \phi | \psi \rangle = \int_{-\infty}^{\infty} dx \langle \phi | x \rangle \langle x | \psi \rangle = \int_{-\infty}^{\infty} dx \phi^*(x) \psi(x). \]  

(9)
This inner product is defined independent of the quantum mechanical system under consideration and has the added advantage that it leads to a positive norm for any quantum mechanical state and we choose physical states to satisfy

\[ \langle \psi | \psi \rangle = \int_{-\infty}^{\infty} dx |\psi(x)|^2 < \infty, \]  

(10)
which allows us to give a probabilistic description for the system.

We are, of course, quite familiar with quantum mechanical systems where the Hamiltonian is Hermitian. In these lectures we would address the question of whether we can also have a satisfactory quantum mechanical description of a system whose Hamiltonian is pseudo-Hermitian \([3]\)

\[ H = S^{-1} H^\dagger S. \]  

(11)
We note that, in general, the Hamiltonian in this case can have real or complex eigenvalues. The immediate difficulty that arises when \( H \) is not Hermitian is that the time evolution operator \((\hbar = 1)\)

\[ U(t) = e^{-itH}, \]  

(12)
is not unitary with the inner product (9)
\[
\langle \phi(t) | \psi(t) \rangle = \langle \phi(0) | e^{itH^\dagger} e^{-itH} | \psi(0) \rangle \neq \langle \phi(0) | \psi(0) \rangle,
\]
(13)
since \( H \neq H^\dagger \). This would result in nonconservation of probability under time evolution. This is, of course, the standard interpretation for non-Hermitian Hamiltonians and has been used in the past to describe systems with decay of particles. Here we would like to ask if a pseudo-Hermitian system can be defined in such a way that it leads to a probabilistic description together with a unitary evolution.

As we have already mentioned, concepts such as Hermiticity and unitarity are defined with respect to a given inner product. Therefore, the difficulty of nonunitary time evolution can possibly be avoided and we can define a unitary quantum theory if we can have a modified inner product with respect to which the Hamiltonian \( H \) will be Hermitian
\[
H = H^{**},
\]
(14)
where \( H^{**} \) denotes the adjoint with respect to the modified inner product.

Before showing that this is possible let us study the quadratic form
\[
\langle \phi | \psi \rangle_S = \langle \phi | S | \psi \rangle = \langle \phi | S \psi \rangle = \langle S \phi | \psi \rangle,
\]
(15)
where we have used (6) in the last step. We note that this quadratic form reduces to the standard Dirac inner product when \( S = 1 \) as we would like, since in that case the system is described by a Hermitian Hamiltonian. The adjoint with respect to this quadratic form, \( H^* \), would satisfy (see (7) as well as (15))
\[
\langle H^* \phi | \psi \rangle_S = \langle \phi | H \psi \rangle_S = \langle \phi | SH \psi \rangle
\]
\[
= \langle H^\dagger S \phi | \psi \rangle = \langle SS^{-1} H^\dagger S \phi | \psi \rangle
\]
\[
= \langle S^{-1} H^\dagger S \phi | \psi \rangle_S.
\]
(16)
Comparing both sides we conclude that
\[
H^* = S^{-1} H^\dagger S,
\]
(17)
which reduces to \( H^* = H^\dagger \) when \( S = 1 \) as it should (namely, it should correspond to the Dirac adjoint in this case). We note here that the relation (17) is quite general in the sense that if we define a quadratic form with respect to an operator \( q \), then the adjoint \( H^{**} \) with respect to this product would be related to the Dirac adjoint as
\[
H^{**} = q^{-1} H^\dagger q.
\]
(18)
Using (4) (or (11)) we note from (17) that with respect to the quadratic form (15), the Hamiltonian, in fact, becomes Hermitian (self-adjoint)
\[
H^* = H.
\]
(19)

Since \( S \) defines a product with respect to which the Hamiltonian is Hermitian, we expect that time evolution would be unitary with respect to this product
\[
\langle \phi(t) | \psi(t) \rangle_S = \langle \phi(t) | S | \psi(t) \rangle = \langle \phi(0) | e^{itH^\dagger} Se^{-itH} | \psi(0) \rangle
\]
\[
= \langle \phi(0) | S^{-1} e^{itH^\dagger} Se^{-itH} | \psi(0) \rangle
\]
\[
= \langle \phi(0) | e^{itH} e^{-itH} | \psi(0) \rangle
\]
\[
= \langle \phi(0) | S | \psi(0) \rangle = \langle \phi(0) | \psi(0) \rangle_S,
\]
(20)
where we have used (4) in the intermediate step. This shows that time evolution is indeed unitary with respect to this product. However, this modified product does not yet lead to a quantum mechanical description.

To better understand the problem, let us note that if $|\psi_E\rangle$ and $|\psi_{E'}\rangle$ denote two eigenstates of the Hamiltonian ($E, E'$ are in general complex and we denote the complex conjugate with a “bar”) satisfying

$$H|\psi_E\rangle = E|\psi_E\rangle, \quad H|\psi_{E'}\rangle = E'|\psi_{E'}\rangle,$$

then it follows that (we use (4) in the intermediate step)

$$E\langle \psi_{E'}|\psi_E\rangle_S = E\langle \psi_{E'}|S|\psi_E\rangle = \langle \psi_{E'}|SH|\psi_E\rangle = \langle \psi_{E'}|H^\dagger S|\psi_E\rangle = E\langle \psi_{E'}|\psi_E\rangle_S,$$

so that we can write

$$(E - E')\langle \psi_{E'}|\psi_E\rangle_S = 0.$$  \hfill (23)

Therefore, this determines

$$\langle \psi_{E'}|\psi_E\rangle_S = e^{-i\Psi(E)}\delta_{EE'}.$$  \hfill (24)

The exponential factor and, therefore, the product can become negative (for example, if $S$ has negative eigenvalues as in the case of the parity operator $P$ and, therefore, cannot define an inner product. So, although time evolution is unitary with this modified product, the product cannot lead to a probabilistic description. As a result, a quantum mechanical description would not follow.

We note that if $S$ is positive, then the norm of the state is automatically positive. This is because in this case we can write

$$S = g^\dagger g,$$

so that we can write

$$H = g^{-1}(g^{-1})^\dagger H^\dagger g^\dagger g,$$

or, $$gHg^{-1} = (g^{-1})^\dagger H^\dagger g^\dagger = (gHg^{-1})^\dagger,$$

or, $$h = h^\dagger,$$  \hfill (26)

where we have identified

$$h = gHg^{-1}, \quad h^\dagger = (gHg^{-1})^\dagger.$$  \hfill (27)

Thus, the energy eigenvalue equation can also be written as

$$H|\psi_E\rangle = E|\psi_E\rangle,$$

or, $$gHg^{-1}g|\psi_E\rangle = Eg|\psi_E\rangle,$$

or, $$h(g|\psi_E\rangle) = E(g|\psi_E\rangle).$$  \hfill (28)

As we have seen in (26) $h$ is Hermitian so that we have

$$E = \tilde{E}, \quad \langle \psi_E|S|\psi_E\rangle = \langle \psi_E|g^\dagger g|\psi_E\rangle = |g|\psi_E\rangle|^2 \geq 0.$$  \hfill (29)

However, we are interested in the more general case where $S$ is not necessarily positive. We note here that the exponential factor in (24) cannot vanish since this would imply that the state $|\psi_E\rangle$ would be orthogonal to every state (pseudo eigenstate) and would reduce the dimensionality of
the space. This will contradict the theorem from linear algebra that if $S$ is a bounded operator and \{\ket{\psi_E}\} defines a complete basis, then so does \{\ket{S\psi_E}\}.

We can make the product (15) an inner product if we can remove the exponential factor in (24). This should, of course, be done maintaining the unitary evolution which can be guaranteed by defining a new operator and a new product as follows. Let

$$q = SA, \quad [A, H] = 0,$$

which implies that

$$A = f(H), \quad q^\dagger = A^\dagger S = SS^{-1}f(H^\dagger)S = Sf(H) = SA = q,$$

much like the similarity transformation $S$. (We note here that (31) can also be shown without assuming that $A = f(H)$.) Let us next define a product with respect to the operator $q$ as

$$\langle \phi | \psi \rangle_q = \langle \phi | q \psi \rangle = \langle q\phi | \psi \rangle,$$

which reduces to the Dirac inner product when $q = 1$. From (18) we note that with respect to this product, the adjoint will be given by

$$H^\# = q^{-1}H^\dagger q = A^{-1}S^{-1}H^\dagger SA = A^{-1}HA = H,$$

so that the Hamiltonian will be Hermitian with respect to this product and time evolution will be unitary. As a result, for any operator $A$ commuting with the Hamiltonian, the operator $q$ in (30) would define a product (32) which would maintain the unitary evolution.

Let us next show that we can choose the operator $A$ as well as a suitable Hilbert space carefully so that the product (32) becomes an inner product. Let $P_E$ denote projection operators for states in this space such that

$$P_E\ket{\psi_E'} = \delta_{EE'}\ket{\psi_E'}, \quad \sum_E P_E = 1.$$

Therefore, since $[A, H] = 0$ we can express

$$A = \sum_E c_E P_E, \quad [A, H]\ket{\psi_E} = 0,$$

which implies that we can write

$$A\ket{\psi_E} = c_E\ket{\psi_E}.$$

Namely, the states $\ket{\psi_E}$ are simultaneous eigenstates of $A$ and $H$ and the coefficients of expansion $c_E$ in (36) can be identified with the eigenvalues of $A$.

Using (36) in (30) we can write

$$q = SA = S\sum_E c_E P_E,$$

and it follows from (32) that

$$\langle \psi_E'|\psi_E\rangle_q = \langle \psi_E'|S\sum_{E'} c_{E'} P_{E'}|\psi_E\rangle$$

$$= c_E \langle \psi_E'|S|\psi_E\rangle = c_E e^{-iF(F)} \delta_{EE'}.$$
Here we have used (24) in the last step. It is clear now that if we choose
\[ c_E = e^{iF(E)}, \quad A = \sum_E e^{iF(E)} P_E, \] (40)
then we have
\[ \langle \psi_{E'}|\psi_E \rangle = \delta_{EE'}, \] (41)
so that the product, in fact, becomes an inner product and a quantum mechanical description for the system is possible.

This shows that, while for any arbitrary \( A \) commuting with the Hamiltonian \( H \) the product (32) leads to a unitary evolution, for the particular choice of \( A \) in (40)
\[ q = S \sum_E c_E P_E = S \sum_E e^{iF(E)} P_E = S e^{iF(H)} \sum_E P_E = Se^{iF(H)}, \] (42)
the product with respect to \( q \) (32) is indeed an inner product. Here we have used the completeness relation in (35). This allows us to identify
\[ A = e^{iF(H)} = (\langle \psi_E|\psi_E \rangle)^{-1}, \] (43)
with \( E \to H \) on the right.

While (43), in principle, identifies the operator \( A \) and determines \( q \) in (42), in practice the construction of \( q \) using conventional ideas from quantum mechanics is nontrivial. So, let us describe a systematic method for constructing \( q \) in complicated theories. Let us consider the operator equation
\[ H\sigma_E = E\sigma_E + \sigma_E k_E, \] (44)
and its adjoint (by multiplying with appropriate inverse operators)
\[ H^\dagger (\sigma_E^{-1})^\dagger = \bar{E}(\sigma_E^{-1})^\dagger + (\sigma_E^{-1})^\dagger k_E^\dagger. \] (45)
\( \sigma_E \) and \((\sigma_E^{-1})^\dagger\) are called generators for the eigenstates of \( H \) and \( H^\dagger \) respectively if
(i) there exists at least one state \( |\psi \rangle \) such that
\[ k_E|\psi \rangle = 0, \quad \sigma_E|\psi \rangle \neq 0, \quad \forall E \in \text{Spect}(H). \] (46)
(ii) there exists at least one state \( |\phi \rangle \) satisfying
\[ k_E^\dagger|\phi \rangle = 0, \quad \text{with} \ (\sigma_E^{-1})^\dagger|\phi \rangle \neq 0, \quad \text{and} \ (\psi|\phi \rangle \neq 0, \quad \forall E \in \text{Spect}(H). \] (47)
(iii) \( \sigma_E \) has an inverse \( \sigma_E^{-1} \), at least on the reference state \( |\psi \rangle \), such that
\[ \sigma_E^{-1}\sigma_E|\psi \rangle = |\psi \rangle, \] (48)
and an adjoint inverse \((\sigma_E^{-1})^\dagger\) is well defined at least on the reference state \( |\phi \rangle \) This requirement is so that \( |\psi_E \rangle = \sigma_E|\psi \rangle \) is invertible in the sense that \( |\psi \rangle = \sigma_E^{-1}|\psi_E \rangle \).

It follows now from (44) as well as (46) that
\[ H\sigma_E|\psi \rangle = E\sigma_E|\psi \rangle + \sigma_E k_E|\psi \rangle = E\sigma_E|\psi \rangle, \] (49)
which allows us to identify the eigenstates of \( H \) as
\[ |\psi_E \rangle = \sigma_E|\psi \rangle, \quad H|\psi_E \rangle = E|\psi_E \rangle. \] (50)
This is reminiscent of the harmonic oscillator where we can identify the reference state with the ground state with the generators corresponding to \((a^\dagger)^n\) up to normalization factors. Similarly, from (45) as well as (47) we can identify the eigenstates of \(H^\dagger\) to correspond to
\[
|\phi_E\rangle = (\sigma_E^{-1})^\dagger|\phi\rangle, \quad H^\dagger|\phi_E\rangle = E|\phi_E\rangle, \quad H^\dagger|\phi_E\rangle = E|\phi_E\rangle. \tag{51}
\]
Some comments are in order here. Since \(H\) is not Hermitian, we have two sets of eigenstates
\[
H|\psi_E\rangle = E|\psi_E\rangle, \quad H^\dagger|\phi_E\rangle = E|\phi_E\rangle, \tag{52}
\]
and we have to construct generators for both these sets of states. If \(H = H^\dagger\), then the two sets of states would coincide, but when \(H\) is pseudo-Hermitian, the two sets would be related by some operator which we will see shortly to correspond to \(q\).

From the definition of a pseudo-Hermitian system (4) we note that
\[
E = H|\psi_E\rangle, \quad \text{or} \quad SH|\psi_E\rangle = H^\dagger(S|\psi_E\rangle) = E(S|\psi_E\rangle), \tag{53}
\]
so that comparing with (51) and (52) we can write
\[
|\phi_E\rangle = (\sigma_E^{-1})^\dagger|\phi\rangle = \alpha_E S|\psi_E\rangle, \tag{54}
\]
where \(\alpha_E\) is a constant. Taking the inner product with \(|\psi_E\rangle\) we obtain
\[
\langle\psi_E|\phi_E\rangle = \langle\psi|\sigma_E^\dagger(\sigma_E^{-1})^\dagger|\phi\rangle = \alpha_E \langle\psi|\psi_E\rangle_S
\]
\text{or, } \alpha_E e^{-iF(E)} = \langle\psi|\phi\rangle. \tag{55}
\]
If we choose the normalization
\[
\langle\psi|\phi\rangle = 1, \tag{56}
\]
then (54) and (55) determine
\[
\alpha_E = e^{iF(E)}, \quad |\phi_E\rangle = S e^{iF(E)}|\psi_E\rangle = S A|\psi_E\rangle = q|\psi_E\rangle. \tag{57}
\]
Furthermore, following (57), let us define
\[
|\phi\rangle = q_0|\psi\rangle, \quad \text{such that } \langle\psi|\phi\rangle = \langle\psi|q_0|\psi\rangle = 1. \tag{58}
\]

From this analysis we see that for every \(E\) we can write
\[
|\phi_E\rangle = q|\psi_E\rangle = (\sigma_E^{-1})^\dagger|\phi\rangle \tag{59}
\]
or,
\[
q \sigma_E|\psi\rangle = (\sigma_E^{-1})^\dagger q_0|\psi\rangle. \tag{59}
\]
Therefore, we determine
\[
q = \sum_E (\sigma_E^{-1})^\dagger q_0 \sigma_E^{-1} P_E, \tag{60}
\]
so that
\[
q|\psi_E\rangle = \sum_{E'} (\sigma_{E'}^{-1})^\dagger q_0 \sigma_{E'}^{-1} P_{E'}|\psi_E\rangle
= \sum_{E'} (\sigma_{E'}^{-1})^\dagger q_0 \sigma_{E'}^{-1} \delta_{E'E} |\psi_E\rangle
= (\sigma_E^{-1})^\dagger q_0 \sigma_E^{-1} \sigma_E |\psi\rangle = (\sigma_E^{-1})^\dagger q_0 |\psi\rangle
= (\sigma_E^{-1})^\dagger |\phi\rangle = |\phi_E\rangle, \tag{61}
\]

and that
\[ \langle \psi_{E'} | \psi_E \rangle_q = \langle \psi_{E'} | S A | \psi_E \rangle = e^{iF(E)} \langle \psi_{E'} | \psi_E \rangle_S = e^{iF(E)} e^{-iF(E')} \delta_{E E'} = \delta_{E E'}, \quad (62) \]
as we would expect.

This construction of the operator \( q \) and the inner product works for any pseudo-Hermitian Hamiltonian with real or complex eigenvalues. Furthermore, since Hermitian Hamiltonians define a subset of pseudo-Hermitian Hamiltonians, it should work for such systems as well leading to \( q = 1 \) and reducing the inner product (32) to the standard Dirac inner product.

Let us check this in the case of the harmonic oscillator where the Hamiltonian has the form
\[ H = \frac{1}{2} (p^2 + x^2 - 1) = a^\dagger a = H^\dagger. \quad (63) \]

This is a Hermitian Hamiltonian with real energy eigenvalues
\[ H | \psi_{En} \rangle = H | \psi_n \rangle = E_n | \psi_n \rangle = n | \psi_n \rangle, \quad E_n = n = 0, 1, 2, \ldots, \]
\[ | \psi_n \rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} | \psi_0 \rangle, \quad a | \psi_0 \rangle = 0, \]
\[ \langle \psi_m | \psi_n \rangle = \delta_{mn}. \quad (64) \]

In this case, we can identify the reference state with the ground state which leads to
\[ | \psi \rangle = | \psi_0 \rangle, \quad \sigma_{En} = \sigma_n = \frac{(a^\dagger)^n}{\sqrt{n!}}. \quad (65) \]

Using the standard commutation relations between the annihilation and creation operators we obtain
\[ [H, \sigma_n] = [a^\dagger a, \frac{(a^\dagger)^n}{\sqrt{n!}}] = n \frac{(a^\dagger)^n}{\sqrt{n!}}, \]
or,
\[ H \sigma_n = n \sigma_n + \sigma_n H. \quad (66) \]

Comparing with (44) we now determine
\[ k_n = H, \quad k_n | \psi \rangle = H | \psi \rangle = 0. \quad (67) \]

Since the ground state is already normalized (see (64)), it follows from (58) that in this Hermitian case,
\[ q_0 = 1, \quad \text{leading to} \quad | \phi \rangle = | \psi \rangle = | \psi_0 \rangle. \quad (68) \]

Furthermore, the inverses of the generators are easily seen to correspond to
\[ \sigma_n^{-1} = \frac{\sigma_n}{\sqrt{n!}}, \quad \text{so that} \quad \sigma_n^{-1} \sigma_n | \psi \rangle = | \psi \rangle. \quad (69) \]

Furthermore, the projection operators on to the energy states are given by
\[ P_n = | \psi_n \rangle \langle \psi_n |, \quad \sum_n P_n = 1, \quad (70) \]
which follows from the completeness of the harmonic oscillator states. Furthermore, $P_n$ can be checked to satisfy

$$(\sigma_n^{-1})^\dagger(\sigma_n)^{-1}P_n = \frac{(a_1)^n (a)^n}{\sqrt{n!} \sqrt{n!}} P_n = P_n. \tag{71}$$

It follows now from (60) that

$$q = \sum_n (\sigma_n^{-1})^\dagger q_0 \sigma_n^{-1} P_n = \sum_n \frac{(a_1)^n (a)^n}{\sqrt{n!} \sqrt{n!}} P_n = \sum_n P_n = 1,$$

and

$$\langle \psi_m | \psi_n \rangle_q = \langle \psi_m | q | \psi_n \rangle = \langle \psi_m | \psi_n \rangle = \delta_{mn}. \tag{72}$$

Our construction indeed reduces to the standard inner product for a Hermitian Hamiltonian.

Let us next apply our construction to a simple $2 \times 2$ matrix Hamiltonian which is pseudo-Hermitian. Let us consider the Hamiltonian

$$H = \begin{pmatrix} re^{i\theta} & se^{i\phi} \\ te^{-i\phi} & re^{-i\theta} \end{pmatrix} \neq H^\dagger, \quad r, s, t, \theta, \phi \text{ real}. $$

This Hamiltonian is not Hermitian. However, if we define a matrix

$$S = \begin{pmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{pmatrix} = S^{-1} = S^\dagger,$$

we can check that

$$H = S^{-1} H^\dagger S, \tag{73}$$

so that the Hamiltonian is pseudo-Hermitian. Note that this Hamiltonian is not $\mathcal{PT}$ symmetric (unless $s = t, \phi = 0$) where the parity operator is defined by

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and time reversal $\mathcal{T}$ corresponds to complex conjugation. However, we note that we can define a modified parity operation

$$\overline{\mathcal{P}} = \begin{pmatrix} 0 & \sqrt{\frac{t}{s}} \\ \sqrt{\frac{s}{t}} & 0 \end{pmatrix} = \overline{\mathcal{P}}^{-1},$$

and the model is $\overline{\mathcal{P}} \mathcal{T}$ symmetric ($\mathcal{T}$ is complex conjugation). For $s = t$, $\overline{\mathcal{P}} \rightarrow \mathcal{P}$, but note that although $\overline{\mathcal{P}}^2 = 1$, unless $s = t$

$$\overline{\mathcal{P}}^\dagger \neq \mathcal{P}, \quad \mathcal{P} H \mathcal{P} = H^* \neq H^\dagger, \tag{74}$$

as in (1).

The eigenvalues of $H$ are determined to be

$$\det\begin{pmatrix} re^{i\theta} - E & se^{i\phi} \\ te^{-i\phi} & re^{-i\theta} - E \end{pmatrix} = 0,$$

whose roots are given by

$$E^2 - 2Er \cos \theta + r^2 - st = 0,$$

or, $E_\pm = r \cos \theta \pm \sqrt{st - r^2 \sin^2 \theta}. \tag{75}$
Therefore, for \( st > r^2 \sin^2 \theta \), the energy eigenvalues are real while for \( st < r^2 \sin^2 \theta \), the two energy eigenvalues are complex conjugates of each other (for \( st = r^2 \sin^2 \theta \) the Hamiltonian cannot be diagonalized). Let us discuss only the case with real eigenvalues for simplicity, the complex case is also straightforward.

Let us define

\[
Q = \sqrt{st - r^2 \sin^2 \theta}, \quad st = Q^2 + r^2 \sin^2 \theta = (Q + ir \sin \theta)(Q - ir \sin \theta),
\]

so that we can write

\[
E_{\pm} = r \cos \theta \pm Q = \bar{E}_{\pm}, \text{ real.}
\]

We can work out the the eigenstates corresponding to the two eigenvalues easily and they have the forms

\[
|\psi_{E_+}\rangle = \frac{1}{\sqrt{s + t}} \begin{pmatrix} (\frac{1}{2})^{\frac{1}{2}} \sqrt{Q + ir \sin \theta} e^{i\phi} \\ (\frac{1}{2})^{\frac{1}{2}} \sqrt{Q - ir \sin \theta} e^{-i\phi} \end{pmatrix},
\]

\[
|\psi_{E_-}\rangle = \frac{i}{\sqrt{s + t}} \begin{pmatrix} (\frac{1}{2})^{\frac{1}{2}} \sqrt{Q - ir \sin \theta} e^{i\phi} \\ -(\frac{1}{2})^{\frac{1}{2}} \sqrt{Q + ir \sin \theta} e^{-i\phi} \end{pmatrix}.
\]

The projection operators in this case can be determined to correspond to

\[
P_{E_+} = \frac{1}{2Q}(H - E_-) = \frac{1}{2Q} \begin{pmatrix} Q + ir \sin \theta & se^{i\phi} \\ te^{-i\phi} & Q - ir \sin \theta \end{pmatrix},
\]

\[
P_{E_-} = -\frac{1}{2Q}(H - E_+) = \frac{1}{2Q} \begin{pmatrix} Q - ir \sin \theta & -se^{i\phi} \\ -te^{-i\phi} & Q + ir \sin \theta \end{pmatrix},
\]

which satisfy

\[
P_{E_+} + P_{E_-} = \frac{1}{2Q}(E_+ - E_-) 1 = \frac{1}{2Q} \times 2Q 1 = 1.
\]

Therefore, the projection operators project on to complementary spaces. Furthermore, they satisfy the relations

\[
P_{E_+} = S^{-1} P_{E_+}^\dagger S, \quad P_{E_-} = S^{-1} P_{E_-}^\dagger S.
\]

Let us choose the reference state to be

\[
|\psi\rangle = |\psi_{E_-}\rangle, \quad \Rightarrow \quad \sigma_{E_-} = 1 = \sigma_{E_-}^{-1}.
\]

Furthermore, from the form of the eigenstates in (78) and the definition

\[
|\psi_{E_+}\rangle = \sigma_{E_+} |\psi_{E_-}\rangle = \sigma_{E_+} |\psi_{E_-}\rangle,
\]

we determine that

\[
\sigma_{E_+} = \begin{pmatrix} 0 & i \sqrt{\frac{1}{2}} e^{i\phi} \\ -i \sqrt{\frac{1}{2}} e^{-i\phi} & 0 \end{pmatrix} = \sigma_{E_+}^{-1}, \quad S \sigma_{E_+} = -\sigma_{E_+}^\dagger S.
\]

The defining relation (44) leads to

\[
H \sigma_{E_-} = E_- \sigma_{E_-} + \sigma_{E_+} k_{E_-}, \quad \Rightarrow \quad k_{E_-} = \sigma_{E_-}^{-1} (H - E_-) \sigma_{E_-} = 2QP_{E_+},
\]

\[
H \sigma_{E_+} = E_+ \sigma_{E_+} + \sigma_{E_-} k_{E_+}, \quad \Rightarrow \quad k_{E_+} = \sigma_{E_+}^{-1} (H - E_+) \sigma_{E_+} = -2QP_{E_+}.
\]
Similarly, analyzing the eigenstates of $H^*$, we determine that
\[ |\phi\rangle = \frac{-s+t}{2Q} S|\psi\rangle = q_0|\psi\rangle, \quad \Rightarrow \quad q_0 = -\frac{s+t}{2Q}, \tag{86} \]
where the normalization is chosen so that $\langle \psi | \phi \rangle = 1$ (see (56). With all this information, we can now determine $q$ from (60)
\[
q = (\sigma_{E_+}^{-1})^* q_0 \sigma_{E_+}^{-1} P_{E_+} + (\sigma_{E_-}^{-1})^* q_0 \sigma_{E_-}^{-1} P_{E_-}
\]
\[
= -\frac{s+t}{2Q} [\sigma_{E_+}^* S \sigma_{E_+} P_{E_+} + S P_{E_-}] = \frac{s+t}{2Q} S(P_{E_+} - P_{E_-})
\]
\[
= \frac{s+t}{2Q} \begin{pmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{pmatrix} \begin{pmatrix} t & e^{i\phi} \\ -i r \sin \theta & -i r \sin \theta \end{pmatrix}
\]
\[
= \frac{s+t}{2Q} \begin{pmatrix} t & e^{i\phi} \\ -i r \sin \theta e^{-i\phi} & s \end{pmatrix}. \tag{87}
\]
It can be checked now that
\[
\langle \psi_{E_i} | \psi_{E_j} \rangle_q = \delta_{E_i E_j}, \quad i, j = \pm. \tag{88}
\]
This analysis can be extended to the case of complex eigenvalues in a straightforward manner. (This can also be extended to $n \times n$ matrix systems.)

The construction that we have described seems to require a knowledge of the energy eigenstates of the theory (so that we can construct the generators of energy eigenstates). However, we cannot solve most quantum mechanical systems. In this case, we determine the energy eigenstates perturbatively. Therefore, following our ideas we can construct the $q$-operator or the inner product perturbatively. The pseudo-Hermitian systems differ from Hermitian systems in this respect. Namely, the inner product in a Hermitian system is given independent of the dynamics whereas in a pseudo-Hermitian system it depends on the dynamics of the system.

Let us consider a pseudo-Hermitian quantum system (with real eigenvalues) whose Hamiltonian can be written as
\[ H = H_0 + \epsilon V(x), \tag{89} \]
where $H_0$ can be solved exactly and $\epsilon$ is a small perturbation parameter. Of course, $H_0$ can be Hermitian or non-Hermitian. However, in most examples, it can be chosen to be Hermitian which we consider for simplicity. Let us denote the generators of eigenstates of $H_0$ by $\sigma_E^{(0)}$ so that we can write
\[ |\psi_E^{(0)}\rangle = \sigma_E^{(0)}|\psi\rangle, \quad P_E^{(0)} = |\psi_E^{(0)}\rangle\langle \psi_E^{(0)}|, \tag{90} \]
where $|\psi\rangle$ denotes the reference state. Since $H_0$ is assumed to be Hermitian, as we have shown in the case of the harmonic oscillator (see (68) and (72))
\[ q_0 = \mathbb{1}, \quad |\phi\rangle = |\psi\rangle, \quad q^{(0)} = \sum_E (\sigma_E^{(0)-1})^* q_0 \sigma_E^{(0)-1} P_E^{(0)} = \mathbb{1}. \tag{91} \]

The perturbative expansion of the eigenstates of the total Hamiltonian is given by
\[ |\psi_E\rangle = \sum_i \epsilon^i |\psi_E^{(i)}\rangle, \tag{92} \]
where $|\psi_E^{(i)}\rangle$ denotes the $i$th order correction to the state $|\psi_E^{(0)}\rangle$. As we know in standard quantum mechanics, the corrections at any order can be chosen to be orthogonal to the state
\[ \langle \psi_E^{(0)} | \psi_E^{(i)} \rangle = 0, \quad i > 0. \tag{93} \]
With this, the correction to the energy eigenstate at any order can be determined recursively as \((i > 0)\)

\[
|\psi_E^{(i)}\rangle = \sum_{E' \neq E} \frac{1}{E^{(0)} - E^{(0)}} \left[ \langle \psi_E^{(0)} | V_{E'}^{(i-1)} - \sum_{j=1}^{i-1} E^{(j)} \langle \psi_E^{(0)} | \psi_E^{(i-j)} \rangle \right] \\
= R^{(i)}|\psi_E^{(0)}\rangle = R^{(i)}\sigma_E^{(0)}|\psi\rangle = \sigma_E^{(i)}|\psi\rangle, \\
E^{(i)} = \langle \psi_E^{(0)} | V | \psi_E^{(i-1)} \rangle,
\]

(94)

where we have identified

\[
\sigma_E^{(i)} = R^{(i)}\sigma_E^{(0)}. 
\]

(95)

To any order we can write

\[
R = \sum_{i=0} e^{i} R^{(i)}, \quad R^{(0)} = 1, \\
\sigma_E = \sum_{i=0} e^{i} \sigma_E^{(i)} = \sum_{i=0} e^{i} R^{(i)} \sigma_E^{(0)} = R \sigma_E^{(0)}. 
\]

(96)

By taking the adjoint we can determine the corrections to the eigenstates of \(H^\dagger\) to any order to be

\[
|\phi_E\rangle = (R^{-1})^{\dagger}|\phi_E^{(0)}\rangle = (R^{-1})^{\dagger}(\sigma_E^{(0)-1})^{\dagger}|\phi\rangle = (R^{-1})^{\dagger}(\sigma_E^{(0)-1})^{\dagger}|\psi\rangle \\
= ((R \sigma_E^{(0)})^{-1})^{\dagger}|\psi\rangle = (\sigma_E^{-1})^{\dagger}|\psi\rangle. 
\]

(97)

As a result, we determine

\[
q = \sum_E (\sigma_E^{-1})^{\dagger}q_0 \sigma_E^{-1} P_E \\
= \sum_E (R^{-1})^{\dagger}(\sigma_E^{(0)-1})^{\dagger} \sigma_E^{(0)-1} R^{-1} P_E \\
= (R^{-1})^{\dagger} \sum_E (\sigma_E^{(0)-1})^{\dagger} \sigma_E^{(0)-1} P_E R^{-1} \\
= (R^{-1})^{\dagger} q^{(0)} R^{-1} = (R^{-1})^{\dagger} R^{-1}. 
\]

(98)

Thus \(q\) depends only on the perturbation operator \(R\) for systems with real eigenvalues. If \(H_0\) were not Hermitian, then \(q^{(0)}\) would be nontrivial which would have to be determined.

As an application of this formalism, let us consider the \(\mathcal{PT}\) symmetric theory

\[
H = \frac{1}{2}(p^2 + x^2 - 1) + i\epsilon x^3 = H_0 + \epsilon V(x). 
\]

(99)

In this case, \(H_0\) is the harmonic oscillator Hamiltonian which we have already studied.

\[
|\psi_n^{(0)}\rangle = \sigma_n^{(0)}|\psi_0\rangle = \sigma_n^{(0)}|\psi\rangle, \quad E_n^{(0)} = n. 
\]

(100)

To first order in perturbation, we have

\[
|\psi_n^{(1)}\rangle = \sum_{m \neq n} \frac{1}{E_n^{(0)} - E_m^{(0)}} \langle \psi_m^{(0)} | V | \psi_n^{(0)} \rangle |\psi_m^{(0)}\rangle \\
= \sum_{m \neq n} \frac{1}{n - m} \langle \psi_m^{(0)} | i\epsilon x^3 | \psi_n^{(0)} \rangle |\psi_m^{(0)}\rangle. 
\]

(101)
Using the definitions of the annihilation and creation operators,
\[ x = \frac{1}{\sqrt{2}}(a + a^\dagger), \quad p = -\frac{i}{\sqrt{2}}(a - a^\dagger), \]
we can evaluate the first order correction to the energy eigenstate to be
\[ |\psi_n^{(1)}\rangle = \frac{i}{2^{4/2}} \left[ -\frac{2}{3}(a - a^\dagger)^3 + \{(a + a^\dagger)^2(a - a^\dagger)^2\} \right] |\psi_n^{(0)}\rangle, \tag{103} \]
where we have defined
\[ \{A^2B\} = \frac{1}{3}(A^2 + ABA + BA^2). \tag{104} \]

Using (102) we can rewrite (103) also as
\[ |\psi_n^{(1)}\rangle = -\left( \frac{2}{3}p^3 + x^2p - ix \right) |\psi_n^{(0)}\rangle, \tag{105} \]
so that we can identify
\[ R^{(1)} = -\left( \frac{2}{3}p^3 + x^2p - ix \right). \tag{106} \]

To this order, therefore, we can determine
\[
\begin{align*}
    R &= \left( 1 - \epsilon \left( \frac{2}{3}p^3 + x^2p - ix \right) \right), \\
    q &= (R^{-1})^\dagger R^{-1} = \left( 1 - \epsilon \left( \frac{2}{3}p^3 + x^2p - ix \right) \right)^\dagger \left( 1 + \epsilon \left( \frac{2}{3}p^3 + x^2p - ix \right) \right) \\
    &= 1 + \epsilon \left( \frac{2}{3}p^3 + x^2p + ix \right) + \epsilon \left( \frac{2}{3}p^3 + x^2p - ix \right) + O(\epsilon^2) \\
    &= 1 + \epsilon \left( \frac{4}{3}p^3 + px^2 + x^2p \right) + O(\epsilon^2). \tag{107}
\end{align*}
\]
This perturbative construction of \( q \) (and, therefore, the inner product) can be carried out systematically to any order in perturbation.

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[1] It is impossible to refer to the large number of papers on this subject. Therefore, we only refer to three main reviews where references to other papers can be found.
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