Quasi-Hermiticity in infinite-dimensional Hilbert spaces

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Abstract

In infinite-dimensional Hilbert spaces, the application of the concept of quasi-Hermiticity to the description of non-Hermitian Hamiltonians with real spectra may lead to problems related to the definition of the metric operator. We discuss these problems by examining some examples taken from the recent literature and propose a formulation that is free of these difficulties.

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1 Introduction

In the past few years, the study of non-Hermitian Hamiltonians has attracted much interest, because under certain conditions, non-Hermitian Hamiltonians may have a real spectrum and therefore may describe realistic physical systems \cite{1}. Many examples of this kind are known \cite{1,2}. Despite that, the physical interpretation of quantum theories based on non-Hermitian Hamiltonians remains obscure.

Recently, the concepts of quasi- or pseudo-Hermitian operators \cite{3,4} have become very popular in the attempts to overcome the problems to find a physical interpretation for such theories.

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These concepts seem to be adequate to describe systems whose underlying Hilbert space is finite-dimensional. In this paper, we want to point out that they have to be used with some care when applied to the more interesting theories that are defined in infinite-dimensional Hilbert spaces. We show that in many examples that have been discussed in the literature, unbounded metric operators appear, and emphasize that this is incompatible with the concepts of quasi- or pseudo-Hermiticity. Then we demonstrate how these difficulties can be avoided within standard quantum mechanics based on Hermitian operators [5].

2 Quasi- and pseudo-Hermiticity

Given a Hilbert space $\mathcal{H}$ with scalar product $(.,.)$, an operator $A : \mathcal{H} \rightarrow \mathcal{H}$ is called quasi-Hermitian, if there exists an operator $\eta : D_\eta \rightarrow \mathcal{H}$ that has the following properties:

- the domain of definition of $\eta$ is the entire space, $D_\eta = \mathcal{H}$,
- the operator $\eta$ is Hermitian, $\eta^\dagger = \eta$,
- the operator $\eta$ is positive definite, $(\varphi, \eta \varphi) > 0$ for all $\varphi \in \mathcal{H}$, $\varphi \neq 0$,
- $\eta$ is bounded, i.e. for all $\varphi \in \mathcal{H}$ there exists a real, positive $k$ such that $\|\eta \varphi\| \leq k\|\varphi\|$, 
- $\eta A = A^\dagger \eta$.

This definition is taken from the work of Scholtz et al. [3], who give a very thorough discussion of quantum theories based on quasi-Hermitian operators. The importance of this concept lies in the fact that if one introduces a new scalar product with the metric operator $\eta$, such that for arbitrary $\varphi, \psi \in \mathcal{H}$

$$(\varphi, \psi)_\eta := (\varphi, \eta \psi),$$

thereby defining a new Hilbert space $\mathcal{H}_\eta$, then the operator $A$ (which may be non-Hermitian with respect to the original scalar product $(.,.)$) is Hermitian with respect to the new one:

$$(\varphi, A \psi)_\eta = (\varphi, \eta A \psi) = (\varphi, A^\dagger \eta \psi) = (A \varphi, \eta \psi) = (A \varphi, \psi)_\eta.$$  

In this way, the scalar product $(.,.)_\eta$ can serve as the basis of a quantum theory.

The two conditions on the domain of definition and boundedness of $\eta$ are not independent: According to the theorem of Hellinger and Toeplitz [6], any Hermitian operator that is defined on the entire Hilbert space $\mathcal{H}$ is bounded.
A notion closely related to quasi-Hermiticity is pseudo-Hermiticity. Its importance in the current discussion of non-Hermitian Hamiltonians with real spectra has been emphasized in the work of Mostafazadeh [4]. In [4], an operator $A$ is called pseudo-Hermitian, if a Hermitian automorphism $\tilde{\eta}$ exists that fulfills $A^\dagger = \tilde{\eta} A \tilde{\eta}^{-1}$. Being an automorphism, its domain of definition is the entire space, so that (again by virtue of the theorem of Hellinger and Toeplitz) it is bounded. On the other hand, as shown in [3], the $\eta$ appearing in the definition of quasi-Hermiticity is an automorphism, too. Thus quasi-Hermiticity and pseudo-Hermiticity are identical except for the requirement that, contrary to $\tilde{\eta}$, $\eta$ has to be positive-definite [7]. This positive-definiteness of $\eta$ ensures the positive-definiteness of the scalar product (1), and is thus a necessary requirement if one attempts to construct a Hilbert space based on the scalar product (1).

The distinction between quasi- and pseudo-Hermiticity is not always made, see e. g. [4,8,9,10,11]. In our subsequent analysis, we will consider only systems with quasi-Hermitian Hamiltonians.

In finite-dimensional Hilbert spaces $\mathcal{H}$ the condition on the domain of definition of $\eta$ can be easily fulfilled and the boundedness condition always holds. This is the reason why quasi-Hermiticity is so useful in this case. However, in infinite-dimensional Hilbert spaces, the domain of definition of $\eta$ and the boundedness of $\eta$ are important constraints.

If the domain of definition of $\eta$ is smaller than the space $\mathcal{H}$, so that, say, $\varphi$ is not in the domain of definition of $\eta$, whereas $\psi$ is, then $(\varphi, \eta\psi)$ is well-defined, but $(\eta\varphi, \psi)$ is not defined. Therefore, although $\eta$ may be Hermitian, the equation

$$(\varphi, \psi)_\eta = (\psi, \varphi)^*_\eta$$

(3)

does not always make sense. But (3) is one of the fundamental defining relations of a scalar product.

The boundedness of $\eta$ is important, because Hilbert spaces are by definition norm complete. This means that they contain all limits of Cauchy sequences, i. e. sequences $\xi_1, \xi_2, \ldots$ of vectors with the property that for all $\varepsilon > 0$ there exists a positive number $M(\varepsilon)$ such that

$$\|\xi_n - \xi_m\| < \varepsilon \quad \text{for all } n, m > M(\varepsilon) \quad .$$

(4)

Now the norm in (4) explicitly depends on the scalar product chosen in the Hilbert space, $\|\xi_n\| = \sqrt{(\xi_n, \xi_n)}$. A change of the scalar product as in (1) may change the convergence properties of sequences. The requirement of boundedness of $\eta$ just ensures that this does not happen: Given a Cauchy sequence in
the norm implied by $(.,.)$, one finds for the norm $\|\xi_n\|_\eta = \sqrt{(\xi_n, \xi_n)_\eta}$ implied by the scalar product $(.,.)_\eta$:

$$\|\xi_n - \xi_m\|_\eta = \sqrt{(\xi_n - \xi_m, \eta(\xi_n - \xi_m))} \leq \sqrt{\|\xi_n - \xi_m\|_\eta \|\eta(\xi_n - \xi_m)\|}.$$ 

Here we have used the Cauchy-Schwarz inequality. Now $\eta$ is bounded, $\|\eta(\xi_n - \xi_m)\| \leq k\|\xi_n - \xi_m\|$ for some $k$, so that

$$\|\xi_n - \xi_m\|_\eta \leq \sqrt{k} \|\xi_n - \xi_m\|.$$ 

Thus $\xi_1, \xi_2, \ldots$ is a Cauchy sequence with respect to the norm $\|\|_\eta$ if it is a Cauchy sequence with respect to the norm $\|\|$. In [3] it is shown that the converse statement is also true. Therefore, the Hilbert spaces $\mathcal{H}$ and $\mathcal{H}_\eta$ contain the same vectors.

As we will discuss in the next section, many examples of metric operators $\eta$ found in the literature are not bounded. This complicates the situation considerably. Let us first illustrate this with a very simple example: Consider an infinite set $\psi_1, \psi_2, \ldots$ of orthonormal vectors in some Hilbert space $\mathcal{H}$,

$$(\psi_n, \psi_m) = \delta_{nm} \quad \text{for all } n, m .$$

Within $\mathcal{H}$, define the infinite sequence $\xi_1, \xi_2, \ldots$ with

$$\xi_n = \frac{\psi_n}{\sqrt{n}} \quad \text{for all } n . \quad (5)$$

Since $\|\xi_n - \xi_m\| = \sqrt{1/n + 1/m}$, this sequence is a Cauchy sequence, thus its limit in $\mathcal{H}$ exists,

$$\lim_{n \to \infty} \xi_n \in \mathcal{H}$$

(actually $\lim_{n \to \infty} \xi_n = 0$ in $\mathcal{H}$). Now consider the unbounded linear operator $\eta$ defined by

$$\eta \psi_n := n \psi_n \quad \text{for all } n \quad (6)$$

and the Hilbert space $\mathcal{H}_\eta$ with the new scalar product $(\varphi, \psi)_\eta = (\varphi, \eta \psi)$. For the sequence (5) one now finds $\|\xi_n - \xi_m\|_\eta = \sqrt{2}$ for all $n \neq m$, so that the limit $\lim_{n \to \infty} \xi_n$ does not exist in $\mathcal{H}_\eta$. In other words, the Hilbert spaces $\mathcal{H}$ and $\mathcal{H}_\eta$ consist of different vectors.
3 Examples

In this section we want to discuss various examples of $\eta$ operators taken from the recent literature.

In [8] (see also [9]) the positive-definite operator

$$\eta = e^{-\theta p}$$

(7)

where $p$ is the momentum operator and $\theta$ is a real number, is used to show that the complex Morse potential

$$V(x) = (A + iB)^2 e^{-2x} - (2C + 1)(A + iB) e^{-x}$$

(8)

($A$, $B$ and $C$ being real) is quasi-Hermitian. Indeed, for $\theta = 2 \arctan(B/A)$, one obtains

$$e^{-\theta p} V(x) e^{\theta p} = V(x + i\theta) = (V(x))^\dagger$$

But (7) is not an automorphism in the space $L_2(-\infty, \infty)$ of square-integrable functions. If one defines

$$(\varphi, \psi)_\eta := (\varphi, \eta \psi)_{L_2} \equiv \int_{-\infty}^{\infty} dx \, \varphi^*(x) (\eta \psi)(x)$$

(9)

as a new scalar product for all $\varphi, \psi \in L_2$, one immediately faces inconsistencies: Take

$$\varphi(x) = \exp(x - e^x) \in L_2 \quad , \quad \psi(x) = e^{-x^2} \in L_2 \quad \text{and} \quad \eta = e^{-\pi p}$$

The matrix element

$$(\varphi, \eta \psi)_{L_2} = \int_{-\infty}^{\infty} dx \, e^{x-e^x} e^{-x^2-2i\pi x + \pi^2}$$

is well-defined since the integrand vanishes for $x \to \pm \infty$ at least exponentially. But

$$(\eta \varphi, \psi)_{L_2} = - \int_{-\infty}^{\infty} dx \, e^{x+e^x} e^{-x^2}$$
is not defined, since the integrand vanishes for $x \to -\infty$, but diverges for $x \to \infty$. The reason is (as in (3)) that although $\varphi \in L_2$, the function $(\eta \varphi)(x) = \varphi(x + i\pi) = -\exp(x + e^x)$ is not in $L_2$. Thus, despite the “Hermitean appearance” of $\eta$, the statement $(\varphi,\psi)^*_\eta = (\psi,\varphi)_\eta$ does not hold for all square-integrable functions.

Another example is provided by Hamiltonians of the form

$$H = \frac{(p - \phi(x))^2}{2m} + V(x)$$

(10)

where $\phi(x)$ is a complex function and $V(x)$ is real. Similar models are investigated in [10,12,13]. A special case of (10) is the model of Hatano and Nelson [14], which is obtained for $\phi(x) = -ig = \text{const}$. For (10) the positive-definite metric operator

$$\eta = \exp \left( 2 \int_{x_0}^{x} \text{d}y \, \text{Im} \phi(y) \right)$$

with arbitrary $x_0$ can be chosen (see [10,12,13]). Depending on the choice of $\phi(x)$, this operator may be unbounded [10].

As a last example, we refer to [13], where among other models the case $H = p^2 + V(x)$,

$$V(x) = -g^2(x) + k - i \frac{dg}{dx}, \quad \eta = g(x) - i \frac{d}{dx}$$

(11)

with real $g(x)$ and $k$ is investigated. The potential in (11) is related to supersymmetric quantum mechanics. The operator $\eta$ in (11) is an example of a metric operator that is not positive-definite. It is also not bounded; even for well-behaved $g(x)$, the derivative will spoil the boundedness.

4 Construction without metric operator

In the previous sections we have shown that an unbounded metric operator $\eta$ cannot be used to define a consistent Hilbert space structure. Now we give an alternative construction which is not based on the introduction of an $\eta$ operator as in (1) from the very beginning.

Consider the following situation: We are given a (non-Hermitian) Hamiltonian $H$, an infinite, discrete set of eigenvectors $\psi_n$ of $H$ that are elements
of a Hilbert space $\tilde{\mathcal{H}}$ (endowed with the scalar product $(\cdot,\cdot)_{\tilde{\mathcal{H}}}$) and have real eigenvalues $E_n$.

The space $\tilde{\mathcal{H}}$ may be the space $L_2(-\infty,\infty)$, but in general this will not be the case. We emphasize that we do not assume any form of completeness of the $\psi_n$ such as, e.g., the existence of a complete biorthonormal set of eigenvectors [4]. Assumptions like this are often made, but to our knowledge, in the examples of non-Hermitian Hamiltonians with real spectra treated in the literature, their validity is not examined.

We start the construction by considering the vector space $\mathcal{V}$ that is defined as the span (the set of finite superpositions) of the vectors $\psi_1, \psi_2, \ldots$. We can define a scalar product $(\cdot,\cdot)_{\mathcal{V}}$ in $\mathcal{V}$ that fulfills

$$(\psi_n, \psi_m)_{\mathcal{V}} = \delta_{nm} \quad \text{for all } n,m$$

(possibly of the form $(\psi_n, \psi_m)_{\mathcal{V}} = (\psi_n, \eta \psi_m)_{\tilde{\mathcal{H}}}$). The completion of $\mathcal{V}$ with respect to its norm (i.e. the combination of $\mathcal{V}$ with all limits of Cauchy sequences of vectors in $\mathcal{V}$) yields a separable Hilbert space $\mathcal{H}$ [6,5,15]. In this space

- the set $\{\psi_1, \psi_2, \ldots\}$ is a complete orthonormal system of vectors and
- the Hamiltonian $H$ (more precisely the closed extension of the restriction of $H$ to $\mathcal{V}$) is Hermitian.

The last property can be easily seen by noting that all vectors in $\mathcal{H}$ are (possibly infinite) superpositions of the eigenvectors $\psi_n$, e.g. $\varphi = \sum_n c_n \psi_n$, $\psi = \sum_n \tilde{c}_n \psi_n$, thus

$$(\varphi, H \psi)_{\mathcal{H}} = \sum_{n,m} c_n^* \tilde{c}_m (\psi_n, H \psi_m)_{\mathcal{H}} = \sum_n c_n^* \tilde{c}_n E_n$$

and $(H \varphi, \psi)_{\mathcal{H}}$ gives the same result, provided both $\varphi$ and $\psi$ are in the domain of definition of $H$. Owing to these properties of $\mathcal{H}$, this space can be used for a consistent quantum-mechanical formulation.

Since $\mathcal{H}$ is an infinite-dimensional, separable Hilbert space, it is unitarily equivalent to any other infinite-dimensional, separable Hilbert space [6], in particular to the space $L_2(-\infty,\infty)$. This means that an isomorphism $T : \mathcal{H} \rightarrow L_2(-\infty,\infty)$ must exist with

$$(\varphi, \psi)_{\mathcal{H}} = (T\varphi, T\psi)_{L_2} \quad \text{for all } \varphi, \psi \in \mathcal{H} \quad .$$

With the help of the transformation $T$, one can define the Hamiltonian $\hat{H} = THT^{-1}$ that maps from $L_2$ to $L_2$, and its eigenvectors $\hat{\psi}_n = T\psi_n \in L_2$. The
operator $\hat{H}$ is Hermitian in $L^2$: For $\hat{\varphi}, \hat{\psi}$ in the domain of definition of $\hat{H}$ one has

$$(\hat{\varphi}, \hat{H}\hat{\psi})_{L^2} = (T^{-1}\hat{\varphi}, HT^{-1}\hat{\psi})_{\mathcal{H}} = (HT^{-1}\hat{\varphi}, T^{-1}\hat{\psi})_{\mathcal{H}}$$

$$= (T^{-1}\hat{H}\hat{\varphi}, T^{-1}\hat{\psi})_{\mathcal{H}} = (\hat{H}\hat{\varphi}, \hat{\psi})_{L^2}. $$

This is just a consequence of the unitary equivalence of the spaces $\mathcal{H}$ and $L^2(-\infty, \infty)$; it is merely a matter of taste whether the theory is formulated in $\mathcal{H}$ or $L^2(-\infty, \infty)$.

This construction is very general, so that not every possible transformation $T$ can be expected to be physically meaningful. See [5] for a discussion of this aspect. Note that

- any reference to a metric operator $\eta$ has disappeared from the construction; we are only using the reality of the spectrum of $H$.
- still, in cases in which it is possible to talk about the Hermitian adjoint of $T$, one has $(\varphi, \psi)_{\mathcal{H}} = (\varphi, T^\dagger T\psi)_{L^2}$, which looks like $\eta = T^\dagger T$. In fact, decompositions of $\eta$ like this are often used, because they guarantee the positive semi-definiteness of $\eta$ [4,9,11].

Let us apply this construction to the examples mentioned in Section 3: For the complex Morse potential (8), the transformation

$$T = e^{-\theta p/2}$$

renders the potential Hermitian in the space $L^2(-\infty, \infty)$:

$$\hat{V} = TVT^{-1} = (A^2 + B^2) e^{-2x} - (2C + 1)\sqrt{A^2 + B^2} e^{-x} = \hat{V}^\dagger. $$

The Schrödinger equation for this real Morse potential has the usual, well-known eigenfunctions $\hat{\psi}_n \in L^2(-\infty, \infty)$. Therefore, the functions

$$\psi_n(x) = (T^{-1}\hat{\psi}_n)(x) = \hat{\psi}_n(x - i\theta/2) \in \mathcal{H},$$

which are not necessarily square-integrable, are the eigenfunctions of the Schrödinger equation for the complex Morse potential (8).

It is crucial to realize that $T$ is not something like the square-root of $\eta$ in (7) [15]. It is a map from $\mathcal{H}$ to $L^2$, whereas $\eta$ would have to be an automorphism $\mathcal{H} \to \mathcal{H}$. As such, $T$ is always bounded, $\|T\| = 1.$
The example (10) can also be handled easily: The transformation

\[ T = \exp \left( -i \int_{x_0}^{x} dy \phi(y) \right) \]

gives

\[ \hat{H} = THT^{-1} = \frac{p^2}{2m} + V(x) = \hat{H}' \quad . \] (15)

This transformation can be factorized into \( T = T_gT_u \), with \( T_g = \exp(-i \int_{x_0}^{x} dy \ \text{Re} \phi(y)) \) and \( T_u = \exp(\int_{x_0}^{x} dy \ \text{Im} \phi(y)) \). Here the first term \( T_g \) is just a usual, unitary gauge transformation (thus an automorphism), its contribution cancels in (13). The second term \( T_u \) is the non-trivial part that will in general map between different Hilbert spaces.

For the case of the supersymmetric model (11), we restrict the discussion to \( k = 0 \). Then the Hamiltonian can be written in the factorized form

\[ H = (p - g(x))(p + g(x)) \quad . \]

Defining \( G(x) = \int_{x_0}^{x} dy g(y) \), one can apply a gauge transformation (note that \( g(x) \) is a real function):

\[ e^{iG(x)} H e^{-iG(x)} = (p - 2g(x))p \quad . \]

Multiplying this with \( \sqrt{p} \) and \( \sqrt{p}^{-1} \) from the left and right, respectively, one obtains the operator

\[ \hat{H} = \sqrt{p} \ e^{iG(x)} H e^{-iG(x)} \sqrt{p}^{-1} = p^2 - 2\sqrt{p} g(x) \sqrt{p} \]

\[ = p^2 - 2pg(x + i/(2p)) = p^2 - 2g(x - i/(2p))p \] (16)

\[ = p^2 - 2pg(x + i/(2p)) \quad . \] (17)

The expressions (17) are valid for analytic \( g(x) \). They can be derived by noting that \( \sqrt{p} x \sqrt{p} = p(x + i/(2p)) \), which generalizes by induction to \( \sqrt{p} x^n \sqrt{p} = p(x + i/(2p))^n \). The relations (17) show that \( \hat{H} \) is Hermitian in \( L_2 \). Therefore, the transformation \( T : \mathcal{H} \to L_2 \) can be chosen to be

\[ T = \sqrt{p} \ e^{iG(x)} \quad . \]

Due to the appearance of \( \sqrt{p} \) and \( 1/p \) in (16) and (17), the Hamiltonian \( \hat{H} \) may not be well-defined. One may, however, attempt to solve the Schrödinger
equation in the representation in which \( p \) is diagonal. It should then be possible to give a well-defined meaning to (16) or (17). But the details of such a construction depend on the choice of \( g(x) \) in (11) and go beyond the scope of the present paper.

Equation (16) provides an example in which the Hermitian Hamiltonian \( \hat{H} \) assumes a rather unusual form that cannot be interpreted as a sum of kinetic and potential energy if the operators \( x \) and \( p \) have their usual meaning.

Let us emphasize that the construction outlined above can be applied in situations in which previous analyses have led to unbounded metric operators. Besides this, it is not necessary to assume any form of completeness for the eigenfunctions of the Hamiltonian. Therefore, this approach offers an alternative to the recent application of the theory of quasi-Hermitian operators to the study of non-Hermitian Hamiltonians with real spectra [4].

5 Conclusions and outlook

In this paper we have demonstrated that the notion of quasi-Hermiticity cannot be used to define a consistent quantum theory if the requirement of the boundedness of the metric operator \( \eta \) is not fulfilled. Some examples in which unbounded metric operators are used to describe theories with non-Hermitian Hamiltonians and real spectra have been discussed in detail. In order to map such theories in a consistent way to Hermitian theories, we have presented an alternative formulation that is based only on the unitary equivalence of infinite-dimensional, separable Hilbert spaces. This unitary equivalence ensures the existence of a transformation \( T \) that maps a given non-Hermitian Hamiltonian with real spectrum to a Hermitian one via a similarity transformation.

An interesting question that we have not addressed here concerns the uniqueness of the transformation \( T \). It has been shown in [3] that a (bounded) metric operator \( \eta \) is only uniquely defined if an appropriately chosen \textit{set of observables} is considered. The same is true for the transformation \( T \). In [5] some attempts to find such a set of observables have been discussed. In our opinion this aspect has not received enough attention yet, but will be crucial for the understanding of theories with non-Hermitian Hamiltonians.
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