Pseudo-Hermiticity, $\mathcal{PT}$-symmetry, and the Metric Operator*

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Abstract

The main achievements of Pseudo-Hermitian Quantum Mechanics and its distinction with the indefinite-metric quantum theories are reviewed. The issue of the non-uniqueness of the metric operator and its consequences for defining the observables are discussed. A systematic perturbative expression for the most general metric operator is offered and its application for a toy model is outlined.

1 Introduction

Most physicists are surprised by being told that certain non-Hermitian but $\mathcal{PT}$-symmetric Hamiltonians, such as $H = p^2 + ix^3$, have a purely real spectrum. This was also the case for the present author who learned about these Hamiltonian in a seminar given by Miloslav Znojil at Koç University in May 2001. Perhaps the most natural question about these Hamiltonian is whether $\mathcal{PT}$-symmetry, i.e., the condition $[H, \mathcal{PT}] = 0$, ensures the reality of their spectrum. It does not take much effort to see that the answer to this question is a definite No. Indeed $\mathcal{PT}$-symmetry is neither necessary nor sufficient for the reality of the spectrum. Yet it plays a certain interesting role whose true appreciation has required the use of the correct mathematical tools.

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The search for finding a condition which is both necessary and sufficient for the reality of the spectrum has led to a notion of a pseudo-Hermitian operator \[1\] that was slightly different from the one used in the earlier studies particularly in the context of the indefinite-metric quantum theories and the parallel mathematical developments \[2\].

The approach of \[1\] is mainly motivated by the earlier results on the problem of the geometric phase for non-Hermitian Hamiltonians \[3\] and in quantum cosmology \[4\]. According to the definition proposed in \[1\], *H* is called pseudo-Hermitian, if there exists a Hermitian and invertible operator \(\eta\) satisfying

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

(1)

In the same article there also appears the notion of an \(\eta\)-pseudo-Hermitian operator, for the case that one fixes a particular metric operator \(\eta\). It is this notion of \(\eta\)-pseudo-Hermitian operator that coincides with the older definition of a pseudo-Hermitian or \(J\)-Hermitian operator. The distinction may seem to be quite minute, but in the context of \(\mathcal{PT}\)-symmetric QM it has played a most significant role.\(^1\)

As is indicated in the title of \[1\], unlike Hermiticity which is a sufficient condition for the reality of the spectrum, pseudo-Hermiticity (under some rather general technical conditions) is a necessary condition. A condition that was both necessary and sufficient is given in \[5\]. It amounts to supplementing the pseudo-Hermiticity condition with the existence of a metric operator of the form \(\eta_+ = O^\dagger O\), \[5\]. Such a metric operator is clearly positive-definite and defines a positive-definite inner product \(\langle \cdot, \cdot \rangle := \langle \cdot | \eta_+ \cdot \rangle\), where \(\langle \cdot | \cdot \rangle\) is the defining inner product of the Hilbert space in which \(H\) and \(\eta_+\) act. This is made more explicit in \[6\] where a clear picture of the role of the antilinear symmetries such as \(\mathcal{PT}\) is also provided.

\[5\] and \[6\] also offer other equivalent necessary and sufficient conditions for the reality of the spectrum of \(H\). One of these is the condition that \(H\) may be mapped to a Hermitian Hamiltonian by a similarity transformation. It was after publication of \[1, 5, 6\] that the author noticed that the non-Hermitian Hamiltonians having this property are called *quasi-Hermitian*, \[7\]. It is one of the important results of \[1, 5, 6\] that \(\mathcal{PT}\)-symmetric Hamiltonians such as 

\[
H = p^2 + ix^3
\]

are quasi-Hermitian. This result cannot be inferred from those of \[7\].

An important observation made in \[7, 8, 9\] is the non-uniqueness of the metric operator. This problem is especially important when one deals with the observables of the theory. The approach of \[7\] to this problem is different from the one taken in Pseudo-Hermitian QM. In

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\(^1\)Indeed the author’s lack of knowledge about the earlier related publications on the indefinite-metric quantum theories was quite fortunate, for it provided the means to escape being conditioned by the earlier treatments and allowed for proposing a notion of pseudo-Hermiticity that proved more useful in the study of \(\mathcal{PT}\)-symmetric systems.
the metric operator is determined by fixing sufficiently many operators with real spectrum and demanding that they be Hermitian with respect to the inner product defined by the metric operator. In contrast in Pseudo-Hermitian QM, one uses the input data which is the Hamiltonian $H$, to determine the set $\mathcal{U}^+_H$ of all possible positive-definite metric operators $\eta_+$. Any two elements $\eta_{+1}, \eta_{+2}$ of $\mathcal{U}^+_H$ are related via $\eta_{+2} = A^\dagger \eta_{+1} A$, where $A$ is a symmetry generator $[A, H] = 0$. Each element of $\mathcal{U}^+_H$ defines a positive-definite inner product and a complete set of observables that are Hermitian with respect to this inner product. The arbitrariness in the choice of a complete set of observables in [7] is traded for the arbitrariness in the choice of an element of $\mathcal{U}^+_H$. An advantage of the latter approach is that one can explicitly construct the most general positive-definite metric operator and the corresponding observables.

There are two different (currently known) methods of constructing the most general positive-definite metric operator. the first method employs the approach pursued in the proof of the spectral theorems of [1, 5, 6] and involves constructing a complete biorthonormal system $\{ | \psi_n \rangle, | \phi_n \rangle \}$ where $| \psi_n \rangle$ and $| \phi_n \rangle$ are eigenvectors of $H$ and $H^\dagger$, respectively. For an explicit application of this method see [10, 11]. The second method uses the fact that any positive-definite operator $\eta_+$ has a Hermitian logarithm, i.e., there is a Hermitian operator $Q$ such that

$$\eta_+ = e^{-Q}. \tag{2}$$

Inserting this relation in (1), using the Baker-Campbell-Hausdorff formula,

$$e^{-Q} H e^Q = H + \sum_{k=1}^{\infty} \frac{1}{k!} [H, Q]_k, \tag{3}$$

where $[H, Q]_1 := [H, Q]$ and $[H, Q]_{k+1} := [[H, Q]_k, Q]$ for all $k \geq 1$, and assuming

$$H = H_0 + \epsilon H_1, \quad Q = \sum_{j=1}^{\infty} Q_j \epsilon^j, \tag{4}$$

where $\epsilon \in \mathbb{R}$, $H_0$ and $Q_j$ are $\epsilon$-independent Hermitian operators and $H_1$ is an $\epsilon$-independent anti-Hermitian operator, one obtains and iteratively solves a system of operator equations for $Q_j$ using perturbation theory. An explicit application of this method is given in [12].

The $\mathcal{CPT}$-inner product introduced in [13] is just an example of the inner products $\langle \cdot, \cdot \rangle_+ = \langle \cdot | \eta_+ \rangle$ where $\eta_+$ has been chosen in a particular form, namely that $\mathcal{C} := \eta_+^{-1} \mathcal{P}$ is an involution (squares to one), [9, 14]. The subsequent construction of the $\mathcal{C}$-operator in [13] uses the same

\[2\text{Note that, as shown in [1], } P\mathcal{T}\text{-symmetric systems such as those considered in [13] are } P\text{-pseudo-Hermitian. Because their spectrum is real they are also } \eta_+\text{-pseudo-Hermitian for some positive-definite metric operator } \eta_+, \]
approach as in the first method mentioned above. A variation of the second perturbative method is introduced in [16]. But because the authors confine their attention to the $\mathcal{CPT}$-inner product they miss a large class of alternative and equivalently admissible positive-definite metric operators (inner products).

As shown in [17], using (1) – (4) one can derive

$$\epsilon H_1 = \sum_{\ell=1} \sum_{k=1} \sum_{j=1} \frac{(-1)^{j-k}}{k!2^m} \binom{m}{j} [H_0, Q^k]_j + \mathcal{O}(\epsilon^{\ell+1}),$$

where $\ell \in \mathbb{Z}^+$, $\binom{m}{j} = \frac{m!}{j!(m-j)!}$, and $\mathcal{O}(\epsilon^\ell)$ stands for terms of order $\ell$ or higher in powers of $\epsilon$. This equation together with perturbative expansion of $Q$ given in [1] allows for a systematic derivation of the operator equations for $Q_j$. For example, setting $\ell = 1, 2, 3$ in [1] and using [1], we find

$$[H_0, Q_1] = -2H_1, \quad [H_0, Q_2] = 0, \quad [H_0, Q_3] = \frac{1}{12} [H_0, Q_1]_3.$$  \hspace{1cm} (6)

Comparing these relations with those obtained in [16, 12], we see that the choice of the $\mathcal{CPT}$-inner product corresponds to setting $Q_2 = 0$ (and putting certain restrictions on $Q_1$, $Q_3$, etc.) Now, suppose that $H_0 = p^2$ and $H_1 = iv(x)$ for a real-valued $v$. Then in the position representation, Eqs. (3) and their analogs for $Q_4, Q_5, \cdots$ take the form of a iteratively decoupled system of non-homogeneous $(1 + 1)$-dimensional wave equations:

$$(-\partial_x^2 + \partial_y^2)Q_j(x, y) = R_j(x, y),$$

where $Q_j(x, y) = \langle x|Q_j|y \rangle$ and $R_j$ only involve $Q_1, Q_2, \cdots, Q_{j-1}, [17]$. In view of the fact that the $(1 + 1)$-dimensional wave equation has an explicit solution, this system can be iteratively solved. Note that $R_2 = 0$, hence $Q_2(x, y) = f_2(x - y) + g_2(x + y)$ where $f_2$ and $g_2$ are any complex-valued functions that due to Hermiticity of $Q_2$ satisfy: $\Re[f_2](-x) = \Re[f_2](x)$, $\Im[g_2](x) = c_2 \in \mathbb{R}$, and $\Im[f_2](-x) = -\Im[f_2](x) - 2c_2$.

As an example consider the potential: $v(x) = 0$ for $x \notin [-1, 1]$ and $v(x) = -\text{sign}(x)$ for $x \in [-1, 1]$. Then the general solution of (7) for $j = 1$ is

$$Q_1(x, y) = \frac{i}{8}(|x + y + 2| + |x + y - 2| - 2|x + y| - 4)\text{sign}(x - y) + f_1(x - y) + g_1(x + y),$$

where $f_1$ and $g_1$ have the same properties as $f_2$ and $g_2$. The appearance of the functions $f_1, f_2, g_2$ in the expression for $Q_1$ and $Q_2$ is a manifestation of the non-uniqueness of the metric operator. Similar constructions exists for the cases where $H_0 = p^2 + v_0$ for a real-valued $v_0$. Further details are given in [17].
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