Unbounded $\mathcal{C}$-symmetries and their nonuniqueness

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Abstract

It is shown that if the $\mathcal{C}$ operator for a $\mathcal{PT}$-symmetric Hamiltonian with simple eigenvalues is not unique, then it is unbounded. The fact that the $\mathcal{C}$ operator is unbounded is significant because, while there is a formal equivalence between a $\mathcal{PT}$-symmetric Hamiltonian and a conventionally Hermitian Hamiltonian in the sense that the two Hamiltonians are isospectral, the Hilbert spaces are inequivalent. This is so because the mapping from one Hilbert space to the other is unbounded. This shows that $\mathcal{PT}$-symmetric quantum theories are mathematically distinct from conventional Hermitian quantum theories.

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1. Introduction

The Sturm–Liouville differential-equation eigenvalue problem associated with the non-Hermitian Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 (ix)\varepsilon \quad (0 < \varepsilon < 2)\quad (1)$$

has a positive discrete spectrum [1]. It was conjectured [2]$^4$ that these spectral properties are a consequence of the invariance of $H$ under the combination of the space-reflection operator $\mathcal{P}f(x) = f(-x)$ and the time-reversal operator $\mathcal{T}f(x) = f^*(x)$; that is $[H, \mathcal{PT}] = 0$.

The $\mathcal{PT}$-symmetric Hamiltonian $H$ is not Hermitian$^5$ in the Hilbert space $L_2(\mathbb{R})$ whose inner product is

$$(f, g) \equiv \int_{\mathbb{R}} dx [\mathcal{T}f(x)]g(x) \quad [f, g \in L_2(\mathbb{R})], \quad (2)$$

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$^4$ In these papers there is no upper bound on $\varepsilon$, but here we impose the condition that $\varepsilon < 2$ so that we may treat $\varepsilon$ as a real variable.
$^5$ The terms ‘Hermitian operator’ and ‘self-adjoint operator’ are equivalent.
but $H$ is Hermitian with respect to the $\mathcal{PT}$ inner product

$$
(f, g)_{\mathcal{PT}} \equiv \int_{\mathbb{R}} \text{d}x [\mathcal{PT} f(x)] g(x), \quad [f, g \in L_2(\mathbb{R})],
$$

(3)

where $\mathcal{PT} f(x) = [f(-x)]^*$. The set of functions $L_2(\mathbb{R})$ endowed with the $\mathcal{PT}$ inner product (2) is a Krein space [3] and $H$ is a Hermitian operator in the Krein space $L_2(\mathbb{R})$ with the $\mathcal{PT}$ inner product $(\cdot, \cdot)_{\mathcal{PT}}$. The principal difference between the inner product $(\cdot, \cdot)$ and the $\mathcal{PT}$ inner product $(\cdot, \cdot)_{\mathcal{PT}}$ is that $(\cdot, \cdot)_{\mathcal{PT}}$ is indefinite; that is, there exist nonzero functions $f, g \in L_2(\mathbb{R})$ such that $(f, f)_{\mathcal{PT}} < 0$. Proving that the $\mathcal{PT}$-symmetric Hamiltonian $H$ in (1) has a positive real spectrum is mathematically significant, but $H$ does not have any obvious relevance to physics until it can be shown that $H$ can serve as a basis for a theory of quantum mechanics. To do so one must demonstrate that the Hamiltonian $H$ is Hermitian on a Hilbert space (not a Krein space!) that is endowed with an inner product whose associated norm is positive definite. Only then can one say that the theory is unitary and that it has a probabilistic interpretation.

These problems can be overcome for the $\mathcal{PT}$-symmetric Hamiltonian $H$ by finding a new (hidden) symmetry represented by a linear operator $\mathcal{C}$, which commutes with both the Hamiltonian $H$ and the $\mathcal{PT}$ operator. In terms of $\mathcal{C}$ one must construct a $\mathcal{CPT}$ inner product

$$
(f, g)_{\mathcal{CPT}} \equiv \int_{\mathbb{R}} \text{d}x [\mathcal{CPT} f(x)] g(x),
$$

(4)

whose associated norm is positive definite and show that $H$ is Hermitian with respect to $(\cdot, \cdot)_{\mathcal{CPT}}$. When such a $\mathcal{C}$ operator exists, we say that the $\mathcal{PT}$-symmetry of $H$ is unbroken. Constructing the $\mathcal{C}$ operator is the key step in showing that the time evolution for the Hamiltonian $H$ is unitary.

There have been many attempts to calculate the operator $\mathcal{C}$ [4, 5] or the metric operator $\Theta = \mathcal{CP}$ [6] for the various $\mathcal{PT}$-symmetric models of interest. Because of the difficulty of the problem ($\mathcal{C}$ depends on the choice of $H$), it is not surprising that the majority of the available results are approximate, usually expressed as leading terms of perturbation series. However, these investigations have shown that $\mathcal{C}$ may be unbounded and that its choice is nonunique [7].

In the present paper we study the phenomena of (possible) nonuniqueness and unboundedness of $\mathcal{C}$ for $\mathcal{PT}$-symmetric Hamiltonians in $L_2(\mathbb{R})$. To this end we establish in section 2 a one-to-one correspondence between the collection of operators $\mathcal{C}$ and the collection of all possible $\mathcal{PT}$ orthogonal pairs of maximal positive and maximal negative subspaces of $L_2(\mathbb{R})$, where positivity (and negativity) is understood with respect to the $\mathcal{PT}$ inner product. This is an underlying mathematical structure that allows one to explain the property of boundedness/unboundedness of the operator $\mathcal{C}$.

Our investigations show that this property is crucial. Indeed, if the $\mathcal{C}$ operator for $H$ is bounded, then $H$ is Hermitian on a Hilbert space that coincides with the same set of functions $L_2(\mathbb{R})$ but is endowed with the $\mathcal{CPT}$ inner product that is equivalent to the initial one $(\cdot, \cdot)$. Thus, the $\mathcal{PT}$-symmetric Hamiltonian $H$ can be realized as Hermitian on the same set of states $L_2(\mathbb{R})$ with the help of the right choice of the bounded metric operator $\Theta = \mathcal{CP}$. In this case (and only in this case!) the complete set of eigenfunctions $\{f_n\}$ of $H$ gives rise to a Riesz basis of $L_2(\mathbb{R})$. It should be emphasized that all previous papers [6] devoted to the construction of the metric operator $\Theta$ have dealt with the case of an operator $\mathcal{C}$ that is bounded.

The situation is completely different if $\mathcal{C}$ is unbounded in $L_2(\mathbb{R})$ (see section 3). In this case the metric operator $\Theta$ is not defined on all elements of $L_2(\mathbb{R})$ and the $\mathcal{CPT}$ inner product is not equivalent to the initial one $(\cdot, \cdot)$. This leads to the Hermitian realization of $H$ in a new Hilbert space $\mathcal{H}$ that does not coincide with $L_2(\mathbb{R})$. In fact, the common part of spaces $\mathcal{H}$ and

Reference [8] gives a physical discussion of this phenomenon.
\( L_2(\mathbb{R}) \) contains the linear span \( \mathcal{M} = \text{span}\{f_n\} \) of eigenfunctions of \( H \), and the completion of \( \mathcal{M} \) with respect to the nonequivalent inner products \((\cdot, \cdot)\) and \((\cdot, \cdot)_{CPT} \) leads to different Hilbert spaces \( L_2(\mathbb{R}) \) and \( \mathcal{H} \), respectively. The set of eigenfunctions \( \{f_n\} \) loses the Riesz-basis property in \( L_2(\mathbb{R}) \), but it turns out to be an orthogonal basis in the new space \( \mathcal{H} \). Therefore, in contrast to the case of bounded operators \( C \), a \( CPT \)-symmetric Hamiltonian \( H \) with an unbounded \( C \) operator cannot be similar to a Hermitian Hamiltonian in the Hilbert space \( L_2(\mathbb{R}) \). The nonuniqueness and unboundedness of the \( C \) operator is discussed in detail in sections 4 and 5 and a brief summary is given in section 6.

### 2. Preliminaries and basic properties of \( C \)

We assume that a closed densely defined linear operator \( C \) in \( L_2(\mathbb{R}) \) obeys the relations

\[
C^2 = I, \quad [C, PT] = 0. \tag{5}
\]

Moreover, due to the requirement that the \( CPT \) inner product (4) determines a positive-definite norm, we additionally assume that \( C \) is a positive Hermitian operator in \( L_2(\mathbb{R}) \):

\[
CP > 0, \quad (CP)^\dagger = CP, \tag{6}
\]

where \( \dagger \) means the Dirac adjoint in \( L_2(\mathbb{R}) \) (the adjoint operator with respect to (2)).

The relations in (5) require an additional explanation in the case where \( C \) is unbounded. Precisely, the identity \( C^2 = I \) holds on the domain of definition \( D(C) \) of \( C \); that is, \( C : D(C) \to D(C) \) and \( C^2 f = f \) for all \( f \in D(C) \). Similarly, \( [C, PT] = 0 \) means that \( PT : D(C) \to D(C) \) and \( CPT f = PT C f \) for all \( f \in D(C) \). If \( C \) is bounded, then \( D(C) = L_2(\mathbb{R}) \) and the relations \( C^2 = I \) and \( [C, PT] = 0 \) should hold on the whole \( L_2(\mathbb{R}) \).

The conditions (5) and (6) are equivalent to the following presentation of \( C \):

\[
C = e^{iQ} P, \tag{7}
\]

where \( Q \) is a Hermitian operator in \( L_2(\mathbb{R}) \), which anticommutes with \( P \) and \( T : \{Q, P\} = \{Q, T\} = 0 \).

Our aim now is to establish another description of the operator \( C \) in (7) using the geometric properties of the Krein space \( L_2(\mathbb{R}) \) with the \( CPT \) inner product (3). To this end, we recall [3] that a (closed) subspace \( \mathcal{L} \) of the Hilbert space \( L_2(\mathbb{R}) \) is called positive (uniformly positive) with respect to the \( CPT \) inner product if

\[
(f, f)_{CPT} > 0 \quad \text{and} \quad (f, f)_{CPT} \geq \alpha (f, f) \quad (\alpha > 0)
\]

for all functions \( f \in \mathcal{L} \setminus \{0\} \).

A positive (uniformly positive) subspace \( \mathcal{L} \) is called maximal if \( \mathcal{L} \) is not a proper subspace of a positive (uniformly positive) subspace in \( L_2(\mathbb{R}) \). Negative (uniformly negative) subspaces with respect to the \( CPT \) inner product and the property of their maximality are similarly defined.

Let \( \mathcal{L}_+ \) be a maximal positive subspace of \( L_2(\mathbb{R}) \). Then its \( CPT \) orthogonal complement

\[
\mathcal{L}_- = \mathcal{L}_+^{\perp} = \{f \in L_2(\mathbb{R}) : (f, g)_{CPT} = 0, \forall g \in \mathcal{L}_+\}
\]

is a maximal negative subspace of \( L_2(\mathbb{R}) \), and the direct \( CPT \) orthogonal sum

\[
\mathcal{D} = \mathcal{L}_+^{\perp} \mathcal{L}_- \tag{8}
\]

is a dense linear set in the Hilbert space \( L_2(\mathbb{R}) \). The set \( \mathcal{D} \) coincides with \( L_2(\mathbb{R}) \); that is,

\[
L_2(\mathbb{R}) = \mathcal{L}_+^{\perp} \mathcal{L}_-. \tag{9}
\]

The brackets \([+\cdot\cdot]\) means orthogonality with respect to \( CPT \) inner product.
if and only if $L_+$ is a maximal uniformly positive subspace with respect to the $PT$ inner product. In that case the subspace $L_-$ is a maximal uniformly negative subspace.

In the appendix, we prove the following auxiliary results:

(I) Let $C$ be determined by (7), where $Q$ is a Hermitian operator in $L_2(\mathbb{R})$ such that $\{Q, P\} = \{Q, T\} = 0$. Then the subspaces

$$L_+ = \frac{1}{2}(I + C)D(C), \quad L_- = \frac{1}{2}(I - C)D(C) \quad (10)$$

are $PT$ invariant (that is, $PTL_\pm = L_\pm$) and they form a $PT$ orthogonal sum (8), where $L_+$ and $L_-$ are respectively, maximal positive and maximal negative with respect to the $PT$ inner product. The domain of definition $D(C)$ is described by (8), and the operator $C$ acts as the identity operator on $L_+$ and as the minus identity operator on $L_-$. 

(II) Let the subspaces $L_\pm$ in (8) be $PT$ invariant and let an operator $C$ be defined on (8) as mentioned above; that is, $D(C) = D$ and the restriction of $C$ onto $L_+$ $[L_-]$ coincides with the identity operator (minus identity operator). Then the operator $C$ can also be determined by (7), where $\{Q, P\} = \{Q, T\} = 0$.

It follows from statements (I) and (II) that there exists a one-to-one correspondence between the set of operators $C = e^{Q}P$ with $\{Q, P\} = \{Q, T\} = 0$ and the set of $PT$ orthogonal decompositions (8), where $L_\pm$ are $PT$ invariant and $L_+ [L_-]$ belongs to the collection of all maximal positive (maximal negative) subspaces with respect to the $PT$ inner product. The action of $C = e^{Q}P$ is reduced to the $\pm$ identity operator on $L_\pm$. 

This relationship allows one to describe various classes of $C$. In particular, $C$ is a bounded operator in $L_2(\mathbb{R})$ if and only if the corresponding maximal subspace $L_+ [L_-]$ in (10) is uniformly positive (negative) [9, 15]. In this case $C$ is determined on the whole space $L_2(\mathbb{R})$ due to (9).

3. $PT$-symmetric Hamiltonians with $C$ operators

We begin with some definitions to avoid possible misunderstanding of the results below.

(1) A densely defined operator $H$ in $L_2(\mathbb{R})$ is called a $PT$-symmetric Hamiltonian if $[H, PT] = 0$ and $H$ is Hermitian with respect to the $PT$ inner product (3). The relation $[H, PT] = 0$ means that $PT : D(H) \rightarrow D(H)$ and $HPTf = PTHF$ for all $f \in D(H)$.

(2) We say that a $PT$-symmetric Hamiltonian $H$ has an operator $C = e^{Q}P$ if the commutation relation $[H, C] = 0$ holds. The latter means that

$$D(C) \supset D(H), \quad C : D(H) \rightarrow D(H), \quad H : D(H) \rightarrow D(C) \quad \text{and} \quad HCf = CHf$$

for all $f \in D(H)$. If $C$ is a bounded operator, then the first and third relations are trivial since $D(C) = L_2(\mathbb{R})$.

In general, a $PT$-symmetric Hamiltonian $H$ may have many $C$ operators. However, all of these operators have to be simultaneously unbounded (or bounded) in $L_2(\mathbb{R})$. Let us explain this point. Assume that $H$ has an unbounded operator $C = e^{Q}P$. In this case the operator $C$ is uniquely defined by a certain direct sum (8) in the sense that

$$Cf = C(f_+ + f_-) = f_+ - f_-, \quad \forall f = f_+ + f_- \in D(C) = L_+ [\pm] L_-.$$ \quad (11)

The commutation relation $[H, C] = 0$ means that the domain of definition $D(H)$ is contained in $D(C)$ and that $H$ is decomposed along $L_+ [\pm] L_-$ as follows:

$$H = H_+ + H_-.$$ \quad (12)
where $H_+ = H|_{\mathcal{L}_+} : \mathcal{L}_+ \to \mathcal{L}_+$ and $H_- = H|_{\mathcal{L}_-} : \mathcal{L}_- \to \mathcal{L}_-$ are, respectively, symmetric\(^8\) operators in $\mathcal{L}_+$ and $\mathcal{L}_-$ with respect to the $\mathcal{CPT}$ inner product (4).

It follows from (11) and (12) that the range $\mathcal{R}(H - \lambda I)$ ($\lambda \in \mathbb{C}$) is contained in $\mathcal{D}(C)$. Hence,

$$\quad (H - \lambda I)f = g, \quad f \in \mathcal{D}(H) \subset \mathcal{D}(C)$$

may have a solution $f$ only for elements $g \in \mathcal{D}(C) \subset L_2(\mathbb{R})$.

Now, let us suppose that $H$ has a bounded $C$ operator. Then

$$\mathcal{D}(C) = \mathcal{L}_+ \| - \mathcal{L}_- = L_2(\mathbb{R}).$$

The restriction of the $\mathcal{CPT}$ inner product (4) onto $\mathcal{L}_+$ and $\mathcal{L}_-$ coincides with the inner products $(\cdot, \cdot)_{\mathcal{P}\mathcal{T}}$ and $-(\cdot, \cdot)_{\mathcal{P}\mathcal{T}}$ whose associated norms are positive definite, and the operators $H_\pm$ in (12) are Hermitian operators in the Hilbert spaces $\mathcal{L}_+$ and $\mathcal{L}_-$ endowed with the $\mathcal{CPT}$ inner product $(\cdot, \cdot)_{\mathcal{CPT}}$. Thus, $\mathcal{R}(H_+ - \lambda I) = \mathcal{L}_+$ and $\mathcal{R}(H_- - \lambda I) = \mathcal{L}_-$ for all nonreal $\lambda$, and thus (13) has a solution $f$ for any $g \in L_2(\mathbb{R})$. This contradicts the previously established result. Hence, the operator $H$ has no bounded operators $C$.

There is an essential difference between the cases of bounded and unbounded $C$ operators. If a $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian $H$ has a bounded $C$ operator, then its spectrum is real. On the other hand if $C$ is unbounded, then $H$ has real eigenvalues (since $H_\pm$ are symmetric operators in (12) but the restricted solvability of (13) (only for $g \in \mathcal{D}(C) \subset L_2(\mathbb{R})$) leads to the confusing conclusion that all non-real points belong to the continuous spectrum of $H$. The latter does not relate to an inherent structure of $H$, but rather indicates the wrong choice of underlying Hilbert space $L_2(\mathbb{R})$.

4. Reasons for nonuniqueness of $C$ operators

For a given $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian $H$ in $L_2(\mathbb{R})$ there may exist different $C$ operators. Due to statements (I) and (II), the nonuniqueness of $C$ is equivalent to the existence of different decompositions (8) (or (9) for the case of bounded $C$) that reduce the operator $H$.

We analyze the phenomenon of nonuniqueness in detail for the case where $H$ has a complete set of eigenfunctions $\{f_n\}$ in $L_2(\mathbb{R})$. In this context ‘complete set’ means that the linear span of eigenfunctions $\{f_n\}$, that is, the set of all possible finite linear combinations

$$\quad \text{span}\{f_n\} \equiv \left\{ \sum_{n=1}^d c_n f_n : \forall d \in \mathbb{N}, \forall c_n \in \mathbb{C} \right\},$$

is a dense subset in $L_2(\mathbb{R})$.

In general, the completeness of a linearly independent sequence of eigenfunctions $\{f_n\}$ does not mean that $\{f_n\}$ is a Schauder basis\(^9\) of $L_2(\mathbb{R})$. The difference is that the completeness of $\{f_n\}$ allows us to approximate an arbitrary $f \in L_2(\mathbb{R})$ by finite linear combinations $\sum_{n=1}^d c_n f_n \to f$ as $d \to \infty$, where $c_n^d$ depend on the choice of $d$, while the definition of a Schauder basis requires that $c_n^d$ does not depend on $d$.

If a $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian $H$ has a bounded $C$ operator, then the complete linearly independent sequence of eigenfunctions $\{f_n\}$ turns out to be the Riesz basis.\(^10\) Indeed, in the

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\(^8\) In the case of unbounded $C$, we cannot claim that $H_\pm$ are Hermitian (self-adjoint) in $\mathcal{L}_\pm$ because the subspaces $\mathcal{L}_\pm$ are not closed with respect to the $\mathcal{CPT}$ inner product (4).

\(^9\) A sequence $\{f_n\}$ is a Schauder basis for $L_2(\mathbb{R})$ if for each $f \in L_2(\mathbb{R})$, there exist unique scalar coefficients $\{c_n\}$ such that $f = \sum_{n=1}^\infty c_n f_n$ [10].

\(^10\) A Schauder basis $\{f_n\}$ is a Riesz basis if there exist an invertible operator $A$ and an orthonormal basis $\{\psi_n\}$ in $L_2(\mathbb{R})$ such that $f_n = A \psi_n$. 
case of a bounded $C$ operator, the $\mathcal{PT}$-symmetric Hamiltonian $H$ is Hermitian in $L_2(\mathbb{R})$ with respect to the $\mathcal{PT}$ inner product $(\cdot, \cdot)_{\mathcal{PT}}$. Without loss of generality we may assume that the eigenfunctions $\{f_n\}$ of $H$ form an orthonormal system with respect to $(\cdot, \cdot)_{\mathcal{PT}}$. Since the initial inner product $(\cdot, \cdot)$ and the $\mathcal{PT}$ inner product $(\cdot, \cdot)_{\mathcal{PT}}$ are topologically equivalent (when $C$ is bounded!), the completeness of $\{f_n\}$ with respect to $(\cdot, \cdot)$ yields the completeness of $\{f_n\}$ in $L_2(\mathbb{R})$ with respect to $(\cdot, \cdot)_{\mathcal{PT}}$. Hence, $\{f_n\}$ is an orthonormal basis of $L_2(\mathbb{R})$ with respect to $(\cdot, \cdot)_{\mathcal{PT}}$. The equivalence of $(\cdot, \cdot)$ and $(\cdot, \cdot)_{\mathcal{PT}}$ means that the orthonormal basis $\{f_n\}$ is transformed to the Riesz basis of $L_2(\mathbb{R})$ with respect to $(\cdot, \cdot)$. In this case the action of $C$ is completely determined by the sequence of eigenfunctions $\{f_n\}$.

In contrast to the case of bounded $C$, the existence of an unbounded $C$ operator for a $\mathcal{PT}$-symmetric Hamiltonian $H$ means that its complete linearly independent sequence of eigenfunctions $\{f_n\}$ cannot be a Riesz basis of $L_2(\mathbb{R})$.

There are two reasons for the nonuniqueness of the $C$ operator for a $\mathcal{PT}$-symmetric Hamiltonian $H$ with a complete set of eigenfunctions $\{f_n\}$ in $L_2(\mathbb{R})$. One of them can be illustrated even for the matrix case, and it deals with the (possible) appearance of nontrivial neutral elements with respect to the $\mathcal{PT}$ inner product in at least one of eigensubspaces $\ker(H - \lambda I)$.

Let us illustrate this phenomenon by considering a $\mathcal{PT}$-symmetric Hamiltonian $H$ with a Riesz basis $\{f_n\}$ of eigenfunctions and hence with a bounded $C$ operator. We assume that the first $k$ eigenfunctions $f_1, \ldots, f_k$ correspond to the eigenvalue $\lambda_0$. For the sake of simplicity, other eigenvalues $\lambda_1, \lambda_2, \ldots$ of $H$ are assumed to be simple; that is, $\dim \ker(H - \lambda_m) = 1$, $m \in \mathbb{N}$ and hence, $\ker(H - \lambda_m)$ coincides with the span of the function $f_{k+m}$.

The bounded operator $C$ generates the decomposition (9) of $L_2(\mathbb{R})$, where subspaces $\mathcal{L}_\pm$ are determined by (10).

$$f_n = f_n^+ + f_n^-, \quad f_n^\pm = \frac{1}{2}(I \pm C)L_2(\mathbb{R}),$$

(14)

where $f_n^\pm \in \mathcal{L}_\pm$. The sequences of functions $\{f_n^\pm\}$ are Riesz bases of $\mathcal{L}_\pm$; that is, $\mathcal{L}_+$ and $\mathcal{L}_-$ coincide with the closures of the linear spans of $\{f_n^+\}$ and $\{f_n^-\}$, respectively.

The functions $f_n^\pm$ in (14) are also eigenfunctions of $H$ corresponding to the same eigenvalue. Therefore, due to the simplicity of the eigenvalues $\lambda_m$ ($m \in \mathbb{N}$), the decomposition (14) of the corresponding eigenfunctions $f_{k+m}$ may contain only one nonzero element. This means that

$$f_{k+m} = \begin{cases} f_{k+m}^+ & \text{if } (f_{k+m}, f_{k+m})_{\mathcal{PT}} > 0, \\ f_{k+m}^- & \text{if } (f_{k+m}, f_{k+m})_{\mathcal{PT}} < 0. \end{cases} \quad \forall m \in \mathbb{N}. \quad (15)$$

(The case $(f_{k+m}, f_{k+m})_{\mathcal{PT}} = 0$ is impossible because it gives two linearly independent eigenfunctions $f_{k+m}^\pm$ of $H$, which contradicts the simplicity of $\lambda_m$.) Therefore, the functions $f_{k+m}^\pm$ are uniquely determined by $f_n$ when $n = k + m$.

The span of the first $k$ eigenfunctions $f_1, \ldots, f_k$ coincides with $\ker(H - \lambda_0 I)$. If this finite-dimensional subspace contains nontrivial neutral elements with respect to the $\mathcal{PT}$ inner product, then $\ker(H - \lambda_0 I)$ contains positive elements with respect to the $\mathcal{PT}$ inner product as well as negative ones. This means that $\ker(H - \lambda_0 I)$ admits different $\mathcal{PT}$ orthogonal decompositions onto positive and negative $\mathcal{PT}$ invariant subspaces $\mathcal{M}_\pm$:

$$\ker(H - \lambda_0) = \mathcal{M}_+ \oplus \mathcal{M}_-.$$ One of the possible decompositions is $\mathcal{M}_+ = \text{span}[f_n^+]$ and $\mathcal{M}_- = \text{span}[f_n^-]$, where the elements $f_n^\pm$ are determined by $f_n$ with the use of the decomposition (14). Fixing another

\[\text{One of functions } f_n^\pm \text{ may vanish.} \]
complete set of eigenfunctions \( \mathcal{M}_0^{+} \). With \( \mathcal{PT} \) invariant subspaces \( \mathcal{M}_\pm \), we obtain other decompositions of the functions

\[
f_n = f_n^+ + f_n^- \quad (n = 1, \ldots, k)
\]

onto positive and negative parts with respect to the \( \mathcal{PT} \) inner product.

Let us define \( \mathcal{L}_\pm \) and \( \mathcal{L}'_\pm \), respectively, as the closure (with respect to \( \langle \cdot, \cdot \rangle \)) of the linear spans of the \( \mathcal{PT} \) orthogonal functions

\[
\left[ \{ f_n^+ \}_{n=1}^k \cup \{ f_{k+m}^- \}_{m=1}^\infty \right] \quad \text{and} \quad \left[ \{ f_n^- \}_{n=1}^k \cup \{ f_{k+m}^+ \}_{m=1}^\infty \right].
\]

By this construction, \( \mathcal{L}_\pm \) are maximal positive/negative subspaces with respect to the \( \mathcal{PT} \) inner product, \( \mathcal{L}'_\pm \) are \( \mathcal{PT} \) invariant, and

\[
L_\pm(\mathbb{R}) = \mathcal{L}'_\pm[1+]L_\pm'.
\]

It is clear that \( \mathcal{L}_+ \neq \mathcal{L}'_+ \) and \( \mathcal{L}_- \neq \mathcal{L}'_- \). Therefore, the \( \mathcal{C}' \) operator of \( H \) determined by (17) (that is, \( \mathcal{C}' \mid \mathcal{L}_\pm = I \) and \( \mathcal{C}' \mid \mathcal{L}_\pm' = -I \)) does not coincide with the \( \mathcal{C} \) operator.

Another reason leading to the nonuniqueness of \( \mathcal{C} \) cannot be observed for bounded \( \mathcal{C} \) operators and this phenomenon may appear only for unbounded operators \( \mathcal{C} \).

Indeed, let \( H \) be a \( \mathcal{PT} \)-symmetric Hamiltonian with a complete set of eigenfunctions \( \{ f_n \} \) that correspond to the simple eigenvalues of \( H \). First, suppose that \( H \) has a bounded \( \mathcal{C} \) operator. Then the decomposition (9) holds, where \( \mathcal{L}_\pm \) are determined by (10). Doing the \( \mathcal{PT} \) arrangement of \( \{ f_n \} \) according to (14), we obtain two sequences of functions \( \{ f_n^+ \} \) and \( \{ f_n^- \} \) belonging to \( \mathcal{L}_+ \) and \( \mathcal{L}_- \), respectively. Due to the simplicity of the eigenvalues of \( H \), one of the functions \( f_n^+ \) and \( f_n^- \) in (14) coincides with \( f_n \), while another one is the zero function (see (15)). Thus, the sequences \( \{ f_n^\pm \} \) are the result of the separation of the sequence \( \{ f_n \} \) by the signs of the \( \mathcal{PT} \) inner products \( (f_n, f_n)_{\mathcal{PT}} \).

For the case of bounded \( \mathcal{C} \), it was shown above that \( \{ f_n \} \) can be considered as an orthonormal basis\(^{12} \) of \( L_\pm(\mathbb{R}) \) with respect to the \( \mathcal{CPT} \) inner product \( \langle \cdot, \cdot \rangle_{\mathcal{CPT}} \). Therefore, the sequences \( \{ f_n^+ \} \) and \( \{ f_n^- \} \) are orthonormal bases of the maximal positive subspace \( \mathcal{L}_+ \) and the maximal negative subspace \( \mathcal{L}_- \), respectively. This means that the initial sequence of eigenfunctions \( \{ f_n \} \) determines the unique decomposition (9) that leads to the uniqueness of a bounded operator \( \mathcal{C} \).

To summarize, for a \( \mathcal{PT} \)-symmetric Hamiltonian \( H \) with a complete set of eigenfunctions \( \{ f_n \} \) corresponding to simple eigenvalues, there may exist only one bounded operator \( \mathcal{C} \).

However, the situation is completely different for the case of unbounded operators \( \mathcal{C} \). Precisely, we are going to show below that for a \( \mathcal{PT} \)-symmetric Hamiltonian \( H \) with a complete set of eigenfunctions \( \{ f_n \} \) corresponding to simple eigenvalues, there may exist infinitely many unbounded operators \( \mathcal{C} \). This problem was inspired by the results of [5], where for the \( \mathcal{PT} \)-symmetric Hamiltonian

\[
H = \frac{1}{2}p^2 + \frac{1}{2}\mu^2 q^2 + i\varepsilon q^3
\]

infinitely many operators \( \mathcal{C} \) were constructed by formal perturbative calculation methods.

Let us briefly illustrate the principal idea. Assume that a \( \mathcal{PT} \)-symmetric Hamiltonian \( H \) with a complete set of eigenfunctions \( \{ f_n \} \) corresponding to simple eigenvalues has an unbounded \( \mathcal{C} \) operator. Then, the direct sum (8) of the subspaces \( \mathcal{L}_\pm \) from (10) determines the domain of \( \mathcal{C} \). Repeating the previous arguments, we separate the sequence \( \{ f_n \} \) by the sign of the \( \mathcal{PT} \) inner products \( (f_n, f_n)_{\mathcal{PT}} \). The obtained sequences \( \{ f_n^\pm \} \) belong to \( \mathcal{L}_\pm \).

Let \( \mathcal{L}'_+ \) and \( \mathcal{L}'_- \) be the closure of span\( \{ f_n^+ \} \) and span\( \{ f_n^- \} \) with respect to the initial inner product \( \langle \cdot, \cdot \rangle \). By this construction, \( \mathcal{L}'_+ \subset \mathcal{L}_+ \) and the direct \( \mathcal{PT} \) orthogonal sum

\[
\mathcal{D}' = \mathcal{L}'_+[+]\mathcal{L}'_-
\]

12 After the normalization procedure.
is a dense set in $L^2_{\text{c}}(\mathbb{R})$ (due to the completeness of $\{f_n\}$). However, it may happen that $\mathcal{L}'_\pm$ are proper subspaces of $\mathcal{L}_\pm$ (that is, $\mathcal{L}'_\pm \subset \mathcal{L}_\pm$ and $\mathcal{L}'_\pm \neq \mathcal{L}_\pm$). This phenomenon was first observed by Langer [12]. His paper provides a mathematically rigorous explanation based on the fact that the $\mathcal{CPT}$ inner product $(\cdot, \cdot)_{\mathcal{CPT}}$ is singular with respect to the initial inner product $(\cdot, \cdot)$.

If $\mathcal{L}'_\pm \subset \mathcal{L}_\pm$, then the positive $\mathcal{L}'_+$ and negative $\mathcal{L}'_-$ subspaces with respect to the $\mathcal{PT}$ inner product do not have the property of maximality, and hence the direct sum (18) does not define an operator $\mathcal{C}$ with properties (5) and (6). The positive $\mathcal{L}'_+$ and negative $\mathcal{L}'_-$ subspaces in (18) can be extended to maximal positive and maximal negative subspaces in different ways that lead to the nonuniqueness of $\mathcal{C}$. (One of the possible extensions are the subspaces $\mathcal{L}'_\pm$ mentioned above.) These phenomena are discussed in detail in the next section.

5. An example of $\mathcal{PT}$-symmetric Hamiltonians $H$ with different unbounded operators $\mathcal{C}$

Let $\{\gamma_n^+\}$ and $\{\gamma_n^-\}$ be orthonormal bases of real functions in the sets of even $L^2_{\text{even}}$ and odd $L^2_{\text{odd}}$ functions of $L^2_{\text{c}}(\mathbb{R})$, respectively. In particular, we can choose the even and odd Hermite functions. Any function $\phi \in L^2_{\text{c}}(\mathbb{R})$ has the representation $\phi = \sum_{n=0}^{\infty} (c_n^+ \gamma_n^+ + c_n^- \gamma_n^-)$, where the sequences $\{c_n^\pm\}$ are elements of the Hilbert space $l_2$; that is, $\sum_{n=1}^{\infty} |c_n^\pm|^2 < \infty$. The operator

$$T\phi = \sum_{n=1}^{\infty} \text{i} \alpha_n (c_n^+ \gamma_n^- - c_n^- \gamma_n^+), \quad \alpha_n = (-1)^n \left(1 - \frac{1}{n}\right)$$

plays a key role in our construction and has many useful properties that can be directly deduced from (19). In particular, $T$ is a Hermitian contraction in $L^2_{\text{c}}(\mathbb{R})$ that anticommutes with $\mathcal{P}$ and $\mathcal{T}$ (that is, $H' = H$, $\|T\phi\| < \|\phi\|$ if $\phi \neq 0$, and $(T, \mathcal{P}) = (T, \mathcal{T}) = 0$). The anticommutation with $\mathcal{P}$ means that $T$ interchanges the sets of even and odd functions: $T : L^2_{\text{even}} \rightarrow L^2_{\text{odd}}$ and vice versa. Denote

$$\mathcal{L}_+ = \{f^+ = \gamma^+ + T \gamma^+ : \gamma^+ \in L^2_{\text{even}}\}, \quad \mathcal{L}_- = \{f^- = \gamma^- + T \gamma^- : \gamma^- \in L^2_{\text{odd}}\}.$$

Since $(T, \mathcal{P}) = (T, \mathcal{T}) = 0$, the subspaces $\mathcal{L}_\pm$ are $\mathcal{PT}$ invariant and $\mathcal{PT} f^+ = T(\gamma^+ - T \gamma^+) \quad \gamma^+ \in L^2_{\text{even}}, \quad \mathcal{PT} f^- = T(-\gamma^- + T \gamma^-) \quad \gamma^- \in L^2_{\text{odd}}$

Hence,

$$(f^+, f^-)_{\mathcal{PT}} = (\gamma^+ - T \gamma^+, \gamma^- + T \gamma^-) = (\gamma^+, T \gamma^-) - (T \gamma^+, \gamma^-) = (T \gamma^+, \gamma^-) - (T \gamma^+, \gamma^-) = 0.$$

Thus the subspaces $\mathcal{L}_\pm$ are $\mathcal{PT}$ orthogonal.

The subspace $\mathcal{L}_+$ is positive with respect to the $\mathcal{PT}$ inner product $(\cdot, \cdot)_{\mathcal{PT}}$ because

$$(f^+, f^+)_{\mathcal{PT}} = (\gamma^+ - T \gamma^+, \gamma^+ + T \gamma^+) = (\gamma^+, \gamma^+) - (T \gamma^+, \gamma^+) = \sum_{n=1}^{\infty} (1 - \alpha_n^2)|c_n^+|^2 > 0,$$

where $\gamma^+ = \sum_{n=1}^{\infty} c_n^+ \gamma_n^+$. However, $(f^+, f^+)_{\mathcal{PT}}$ is not topologically equivalent to the initial inner product

$$(f^+, f^+) = (\gamma^+ + T \gamma^+, \gamma^+ + T \gamma^+) = (\gamma^+, \gamma^+) + (T \gamma^+, T \gamma^+) = \sum_{n=1}^{\infty} (1 + \alpha_n^2)|c_n^+|^2$$

on $\mathcal{L}_+$ because $\lim_{n \rightarrow \infty} (1 - \alpha_n^2) = \lim_{n \rightarrow \infty} \frac{1}{2} \left(2 - \frac{1}{n}\right) = 0$. Thus, the subspace $\mathcal{L}_+$ cannot be uniformly positive.
The property of maximality of \( \mathcal{L}_+ \) with respect to \( (\cdot, \cdot)_{PT} \) follows from the theory of Krein spaces \([13]\) and the formula \((20)\). Similar arguments show that \( \mathcal{L}_- \) is a maximally negative subspace with respect to \( (\cdot, \cdot)_{PT} \). The obtained direct sum \((8)\) of \( \mathcal{L}_\pm \) is densely defined in \( L_2(\mathbb{R}) \) and the corresponding operator \( \mathcal{C} \) is determined by \((A.4)\). Elementary calculations using \((19)\) and \((A.4)\) lead to the conclusion that

\[
\mathcal{C}\phi = \sum_{n=1}^{\infty} \frac{1}{1 - \alpha_n^2} \left( \left( 1 + \alpha_n^2 \right)c_n^+ + 2i\alpha_n c_n^- \right) y_n^+ + \left[ - \left( 1 + \alpha_n^2 \right)c_n^- + 2i\alpha_n c_n^+ \right] y_n^- .
\]  

Let us fix the function \( \chi \in L_2(\mathbb{R}) \),

\[
\chi = \sum_{n=1}^{\infty} \frac{1}{n^\delta} \left( y_n^+ + y_n^- \right), \quad \frac{1}{2} < \delta \leq \frac{3}{2}
\]

and set

\[
M_{\text{even}} = \{ y^+ \in L_2^{\text{even}} : (y^+, \chi) = 0 \}, \quad M_{\text{odd}} = \{ y^- \in L_2^{\text{odd}} : (y^-, \chi) = 0 \}.
\]  

The functions \( y^+ = \sum_{n=1}^{\infty} c_n^+ y_n^+ \in M_{\text{even}} \) and \( y^- = \sum_{n=1}^{\infty} c_n^- y_n^- \in M_{\text{odd}} \) can be also characterized by the condition

\[
\sum_{n=1}^{\infty} c_n^+ n^\delta = \sum_{n=1}^{\infty} c_n^- n^\delta = 0.
\]  

The subspaces

\[
\mathcal{L}_+ = \{ f^+ = y^+ + Ty^+ : y^+ \in M_{\text{even}} \}, \quad \mathcal{L}_- = \{ f^- = y^- + Ty^- : y^- \in M_{\text{odd}} \}
\]  

are proper subspaces of \( \mathcal{L}_+ \) and \( \mathcal{L}_- \), respectively (since \( M_{\text{even}} \subset L_2^{\text{even}} \) and \( M_{\text{odd}} \subset L_2^{\text{odd}} \)). Therefore, the subspaces \( \mathcal{L}_{\pm} \) lose the property of maximality. We will show that the direct sum \((8)\) of \( \mathcal{L}_{\pm} \) is densely defined in \( L_2(\mathbb{R}) \). To this end, we suppose that a function \( y = \sum_{n=1}^{\infty} (y_n^+ y_n^+ + y_n^- y_n^-) \) is orthogonal to \( (18) \). It follows from \((19)\) and \((25)\) that the condition \( y \perp \mathcal{L}_{\pm} \) is equivalent to the relations

\[
\sum_{n=1}^{\infty} (y_n^+ - i\alpha_n y_n^-) c_n^+ = \sum_{n=1}^{\infty} (y_n^- + i\alpha_n y_n^+) c_n^- = 0,
\]

where \( \{c_n^\pm\} \) are arbitrary elements of the Hilbert space \( L_2 \) that also satisfy \((24)\); that is, \( \{c_n^\pm\} \) are orthogonal to the element \((1/n^\delta)\) in \( L_2 \). This means that

\[
y_n^+ - i\alpha_n y_n^- = \frac{k_1}{n^\delta}, \quad y_n^- + i\alpha_n y_n^+ = \frac{k_2}{n^\delta},
\]

where the constants \( k_1 \) do not depend on \( n \). It follows from \((26)\) that

\[
\frac{1}{n} \left( 2 - \frac{1}{n} \right) y_n^+ = (1 - \alpha_n^2) y_n^+ = (k_1 + i\alpha_n k_2) \frac{1}{n^\delta}.
\]  

Since the sequence \( \{y_n^\pm\} \) belongs to the Hilbert space \( L_2 \) and \( \delta \leq \frac{3}{2} \), the relation \((27)\) is possible for \( k_1 = k_2 = 0 \) only. Then \( y = 0 \) and the direct sum \((18)\) is densely defined in \( L_2(\mathbb{R}) \).

The next step involves the interpretation of \( \mathcal{L}_\pm \) as the closure of linear spans of \( PT \) orthogonal functions \( \{f^\pm_n\} \). These functions can be determined in different ways. A 'constructive' approach uses \((19)\) to establish that

\[
(I - T^2)\phi = \sum_{n=1}^{\infty} (1 - \alpha_n^2) \left( c_n^+ y_n^+ + c_n^- y_n^- \right) \quad [\phi \in L_2(\mathbb{R})].
\]
Thus, \( f_{n}^{+} = \gamma_{n}^{+} + T \gamma_{n}^{+} \), \( f_{n}^{-} = \gamma_{n}^{-} + T \gamma_{n}^{-} \).

The functions \( \{ f_{n}^{+} \} \) are \( \mathcal{PT} \) orthogonal. Indeed, \((f_{n}^{+}, f_{m}^{+})_{\mathcal{PT}} = 0 \) because \( f_{n}^{+} \in \mathcal{L}_{+}^{a} \) by the construction and thus the subspaces \( \mathcal{L}_{+}^{a} \) are \( \mathcal{PT} \) orthogonal. Furthermore,

\[
(f_{n}^{+}, f_{m}^{+})_{\mathcal{PT}} = (\gamma_{n}^{+} - T \gamma_{m}^{+}, \gamma_{m}^{+} + T \gamma_{m}^{+}) = ((I - T^{2})\gamma_{n}^{+}, \gamma_{m}^{+}) = \mu_{n}(\gamma_{n}^{+}, \gamma_{m}^{+}) = \mu_{n}\delta_{nm},
\]

where \( \mu_{n} \) is the eigenvalue of \( P_{even}(I - T^{2})P_{even} \), which corresponds to the eigenfunction \( \gamma_{n}^{+} \in \mathcal{M}_{even} \). Similarly,

\[
(f_{n}^{-}, f_{m}^{-})_{\mathcal{PT}} = (-\gamma_{n}^{-} + T \gamma_{m}^{-}, \gamma_{m}^{-} + T \gamma_{m}^{-}) = -((I - T^{2})\gamma_{n}^{-}, \gamma_{m}^{-}) = -\mu_{n}(\gamma_{n}^{-}, \gamma_{m}^{-}) = -\tilde{\mu}_{n}\delta_{nm},
\]

where \( \tilde{\mu}_{n} \) is the eigenvalue of \( P_{odd}(I - T^{2})P_{odd} \), which corresponds to the eigenfunction \( \gamma_{n}^{-} \in \mathcal{M}_{odd} \). Hence, the functions \( \{ f_{n}^{\pm} \} \) are \( \mathcal{PT} \) orthogonal.

Assume that a function \( f^{+} \in \mathcal{L}_{+,a} \) is orthogonal to \( \text{span}\{ f_{n}^{+} \} \). Then \( f^{+} = \gamma^{+} + T \gamma^{+} \) (due to \((25)) and

\[
0 = (f^{+}, f^{+}) = (\gamma^{+} + T \gamma^{+}, \gamma_{n}^{+} + T \gamma_{n}^{+}) = (\gamma^{+}, \gamma_{n}^{+}) + (T \gamma^{+}, T \gamma_{n}^{+}) = (\gamma^{+}, (I + T^{2}) \gamma_{n}^{+}) = (2 - \mu_{n})(\gamma^{+}, \gamma_{n}^{+}),
\]

where \( 2 - \mu_{n} \neq 0 \). This means that the function \( \gamma^{+} \in \mathcal{M}_{even} \) is orthogonal to the basis \( \{ \gamma_{n}^{+} \} \) of \( \mathcal{M}_{even} \). Hence, \( \gamma^{+} = 0 \) and the closure of span\(\{ f_{n}^{+} \}\) coincides with \( \mathcal{L}_{+,a} \). Similar arguments show that the closure of span\(\{ f_{n}^{-} \}\) coincides with \( \mathcal{L}_{-,a} \). We interpret \( \{ f_{n}^{\pm} \} \) as eigenfunctions of a Hamiltonian \( H \). Since the direct sum \((18) \) is a dense subset in \( L_{2}(\mathbb{R}) \), the same property holds true for span\(\{ f_{n}^{\pm} \}\). Hence \( \{ f_{n}^{\pm} \} \) is a complete system of eigenfunctions of \( H \) in \( L_{2}(\mathbb{R}) \).

The Hamiltonian \( H \) is \( \mathcal{PT} \)-symmetric because its eigenfunctions \( f_{n}^{a} \) are also eigenfunctions of \( \mathcal{PT} \). This property of \( f_{n}^{a} \) follows from the construction above. Indeed, the operator \( T \) commutes with \( \mathcal{PT} \) (since \( \{ T, P \} = \{ T, T \} = 0 \)), and the subspaces \( \mathcal{L}_{\pm}^{a} \) in \( (20) \) are \( \mathcal{PT} \) invariant. The same holds true for the subspaces \( \mathcal{M}_{even} \) and \( \mathcal{M}_{odd} \). (This follows from \((23) \) and the definition of \( \chi \).) The orthogonal projections \( P_{even} \) and \( P_{odd} \) commute with \( \mathcal{PT} \). Hence, the operators \( P_{even}(I - T^{2})P_{even} \) and \( P_{odd}(I - T^{2})P_{odd} \) commute with \( \mathcal{PT} \) and their eigenfunctions \( \{ \gamma_{n}^{\pm} \} \) are eigenfunctions of \( \mathcal{PT} \) (because they have simple eigenvalues!).

Thus, \( f_{n}^{+} = \gamma_{n}^{+} + T \gamma_{n}^{+} \) and \( f_{n}^{-} = \gamma_{n}^{-} + T \gamma_{n}^{-} \) are eigenfunctions of \( \mathcal{PT} \).

The complete set of eigenfunctions \( \{ f_{n}^{\pm} \} \) of \( H \) determines the direct sum \((18) \) (because \( \mathcal{L}_{+,a} \) and \( \mathcal{L}_{-,a} \) are the closures of span\(\{ f_{n}^{+} \}\) and span\(\{ f_{n}^{-} \}\), respectively). However, as shown above, the subspaces \( \mathcal{L}_{\pm}^{a} \) are not maximal with respect to the \( \mathcal{PT} \) inner product. Thus, \((18) \) cannot define an operator \( \mathcal{C} \) with properties \((5), (6) \) in \( L_{2}(\mathbb{R}) \). Let us explain this point. To this end we denote by \( \mathcal{C} \) an operator with the domain of definition \( \mathcal{D}(\mathcal{C}) = \mathcal{L}_{\pm}^{a}[\pm] \) that acts as the identity (minus identity) operator on \( \mathcal{L}_{+}^{a} \) (\( \mathcal{L}_{-}^{a} \)). The subspaces \( \mathcal{L}_{\pm}^{a} \) are \( \mathcal{PT} \) invariant because \( f_{n}^{+} \) are eigenfunctions of \( \mathcal{PT} \).

Thus, the operator \( \mathcal{C} \) satisfies the conditions \((5) \):

\[
\mathcal{C}^{2} f = f, \quad \mathcal{C}^{+} \mathcal{PT} f = \mathcal{PT} \mathcal{C} f \quad [f \in \mathcal{D}(\mathcal{C})] \quad \text{and} \quad \mathcal{C}^{+} H g = H \mathcal{C} g \quad [g \in \mathcal{D}(H)].
\]

\(^{(13)}P_{even} \) and \( P_{odd} \) are orthogonal projections onto \( \mathcal{M}_{even} \) and \( \mathcal{M}_{odd} \) in \( L_{2}(\mathbb{R}) \).
where $\mathcal{D}(H)$ is contained in $\mathcal{D}(\mathcal{C}')$ by the definition of $H$. However, $\mathcal{C}'$ cannot satisfy (6) and, as a result, $\mathcal{C}'$ cannot be presented as (7). Indeed, the assumption that $\mathcal{C}' = e^{Q}\mathcal{P}$, where $e^{Q}$ is a Hermitian operator, leads to the conclusion$^{14}$ that the subspaces $\mathcal{L}'_{\pm}$ have the form

$$\mathcal{L}'_{+} = \{ f^+ = \gamma^+ + T\gamma^+: \gamma^+ \in L^2_{\text{even}} \}, \quad \mathcal{L}'_{-} = \{ f^- = \gamma^- + T\gamma^-: \gamma^- \in L^2_{\text{odd}} \},$$

where $T = \tanh \frac{Q}{2}$ is a Hermitian strong contraction defined on $L_2(\mathbb{R})$. This contradicts the original presentation (25) of $\mathcal{L}_{\pm}$, where $T$ is defined on $M_{\text{even}} \oplus M_{\text{odd}} \subset L_2(\mathbb{R})$. In particular, the operator $T$ in (25) is not defined on $\gamma \in L_2(\mathbb{R})$.

Therefore, the metric operator $e^{Q} = \mathcal{C}'\mathcal{P}$ determined by the eigenfunctions $\{ f^\pm_n \}$ of $H$ cannot be Hermitian. This obstacle can be removed if we extend $\mathcal{L}'_{\pm}$ to maximal positive/negative subspaces $\mathcal{L}_{\pm}$ with respect to the $\mathcal{P}\mathcal{T}$ inner product. In this case the operator $\mathcal{C}'$ is extended to an operator $\mathcal{C}$ with properties (5), (6) (that is, we guarantee the Hermiticity of the metric operator $\mathcal{C}\mathcal{P}$ by extending the domain $\mathcal{D}(\mathcal{C}')$).

Additional calculations with the use of theorem 4 in [17] show that if the parameter $\delta$ in (22) satisfies the condition $1 < \delta \leq \frac{1}{2}$, then the pair $\mathcal{L}'_{+}[\mp] \mathcal{L}'_{-}$ can be extended to different pairs of maximal positive/negative subspaces $\mathcal{L}_{\pm}[\mp] \mathcal{L}_{\mp}$. In this case we have different extensions $\mathcal{C} \supset \mathcal{C}'$ that satisfy (5) and (6). These extensions are different unbounded $\mathcal{C}$ operators for the $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian $H$ defined above. One of the possible extensions is the operator $\mathcal{C}$ defined by (21). The corresponding pair of maximal subspaces $\mathcal{L}_{\pm}$ is determined by (20).

On the other hand, if $\frac{1}{2} < \delta \leq 1$, then the extension of $\mathcal{L}'_{+}[\mp] \mathcal{L}'_{-}$ to a maximal pair $\mathcal{L}_{+}[\mp] \mathcal{L}_{\mp}$ is unique. The subspaces $\mathcal{L}_{\pm}$ are determined by (20) and the formula (21) provides the unique extension $\mathcal{C} \supset \mathcal{C}'$ with properties (5) and (6). In this case the $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian $H$ has the unique unbounded operator $\mathcal{C}$.

6. Conclusions

This paper shows that if the $\mathcal{C}$ operator for a $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian with simple eigenvalues is nonunique, then it is unbounded. (A bounded $\mathcal{C}$ operator can be constructed for finite-matrix Hamiltonians and for Hamiltonians generated by differential expressions with $\mathcal{P}\mathcal{T}$-symmetric point interactions.) As a consequence, the mapping between a conventionally Hermitian Hamiltonian and a $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian having real eigenvalues is unbounded. Thus, while there is a formal mapping between the Hilbert spaces of the two theories, the mapping does not map all of the vectors in the domain of one Hamiltonian into the domain of the other Hamiltonian. Consequently, even if the conventionally Hermitian Hamiltonian and the $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian are isospectral, they are mathematically inequivalent theories. Thus, at a fundamental mathematical level a $\mathcal{P}\mathcal{T}$-symmetric Hamiltonian describes a theory that is new. It is an open question whether it is possible to design physical experiments that can detect the differences between these two theories.

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Note added in proof. Our results here extend to more general classes of $\mathcal{P}\mathcal{T}$-symmetric Hamiltonians if we modify slightly the definition of $\mathcal{C}$ in section 3. Let $\mathcal{S}$ be a linear subset of $\mathcal{D}(H)$ such that the closure of the restriction of $H$
onto $S$ coincides with $H$. We say that a $PT$-symmetric Hamiltonian $H$ has an operator $C = e^{i\varphi}P$ if the commutation relation $H C f = C H f$ holds for all $f \in S \subset D(H)$. This means that $D(C) \supset S, \quad C : S \rightarrow S, \quad H : S \rightarrow D(C)$.

For a $PT$-symmetric Hamiltonian $H$ having a complete set of eigenfunctions $\{f_n\}$ corresponding to real simple eigenvalues, this definition works as follows: Let $S$ be the linear span of eigenfunctions $\{f_n\}$. The set $S$ is dense in $L^2(\mathbb{R})$ and the closure of $\{H f_n\}$ coincides with $H$. Since $H$ is Hermitian with respect to the $PT$ inner product $(\cdot, \cdot)_{PT}$, the eigenfunctions $f_n$ are $PT$-orthogonal: $(f_n, f_m)_{PT} = 0 (m \neq n)$. The completeness of $\{f_n\}$ implies that every eigenfunction $f_n$ is either positive $(f_n, f_m)_{PT} > 0$ or negative $(f_n, f_m)_{PT} < 0$ with respect to $(\cdot, \cdot)_{PT}$.

We separate the sequence $\{f_n\}$ according to the sign of the $PT$ inner products: $f_n = f_n^+ \pm i f_n^- = f_n^+(1 + \mathbb{P}) f_n \pm i f_n^- (1 - \mathbb{P}) f_n$ and denote by $L^+_n, L^-_n$ the closure of span $\{f_n^\pm\}$ (span $\{f_n^\pm\}$). The $PT$-invariant subspaces $L^+_n$ are positive or negative with respect to the $PT$ inner product and they form the direct $PT$ orthogonal sum (18).

If the eigenfunctions $\{f_n\}$ of $H$ form a Riesz basis, then $L^+_n$ are maximal uniformly positive (negative) subspaces, and the decomposition (18) becomes the decomposition (9) and defines a unique bounded operator $\mathcal{C}$ for $H$. If the eigenfunctions $\{f_n\}$ are not a Riesz basis but are a Schauder basis, then the subspaces $L^+_n$ lose the property of uniform positivity (negativity) but these subspaces are still maximal positive (negative) [13]. In this case, the decomposition (18) takes the form (8). This means that (18) correctly defines a unique unbounded operator $\mathcal{C}$ for $H$. For Riesz and Schauder bases the action of $\mathcal{C}$ is completely determined by the eigenfunctions $\{f_n\}$ of $H$.

In general, when $\{f_n\}$ is a complete set of eigenfunctions, it may happen that the subspaces $L^+_n$ are only positive (negative). If so, the decomposition (18) cannot properly define an operator $\mathcal{C} = e^{i\varphi}P$ and we must extend $L^+_n$ to maximal positive (negative) subspaces. The (possible) nonuniqueness of such extensions leads to the nonuniqueness of unbounded operators $\mathcal{C}$ for $H$.

**Appendix**

To show the equivalence of statements (I) and (II), we consider the $PT$ orthogonal decomposition of $L_2(\mathbb{R})$ onto its even $L^2_{even}$ and odd $L^2_{odd}$ subspaces

$$L_2(\mathbb{R}) = L^2_{even} + L^2_{odd},$$  \hspace{1cm} (A.1)

which are, respectively, maximal positive and maximal negative with respect to $(\cdot, \cdot)_{PT}$. The subspaces $L^+_n$ and $L^-_n$ in (8) are also maximal positive and maximal negative and their ‘deviation’ from $L^2_{even}$ and $L^2_{odd}$ is described by a Hermitian strong contraction $T$, which anticommutes with $\mathbb{P}$ [15]. To be precise,

$$L^+_n = \{f^+ = \gamma^+ + T\gamma^+ : \gamma^+ \in L^2_{even}\}, \quad L^-_n = \{f^- = \gamma^- + T\gamma^- : \gamma^- \in L^2_{odd}\}. \hspace{1cm} (A.2)$$

Denote by $P_\pm$ the projection operators onto $L^\pm_n$ in $L_2(\mathbb{R})$. The operators $P_\pm$ are defined on the linear set $\mathcal{D} = \bigcup L^\pm_n$ and

$$P_+(f^+ + f^-) = f^+, \quad P_-(f^+ + f^-) = f^-, \quad [f^\pm \in \mathcal{L}^\pm].$$

These operators $P_\pm : \mathcal{D} \rightarrow \mathcal{L}^\pm$ can also be determined by the formulas

$$P_+ = (I - T)^{-1}(P_{even} - TP_{odd}), \quad P_- = (I - T)^{-1}(P_{odd} - TP_{even}), \hspace{1cm} (A.3)$$

where $P_{even} = \frac{1}{2}(I + \mathbb{P})$ and $P_{odd} = \frac{1}{2}(I - \mathbb{P})$ are projections on $L^2_{even}$ and $L^2_{odd}$.

Let us prove (A.3). First, we note that $P_{even} T = TP_{odd}$ since $[T, \mathbb{P}] = 0$. Then, for any function $\phi = \gamma^+ + \gamma^- [\gamma^+ \in L^2_{even}, \gamma^- \in L^2_{odd}]$ from $L_2(\mathbb{R})$, we have

$$P_+ (I + T) \phi = (I + T)\gamma^+ + (I + T)P_{odd} \phi = (I - T)^{-1} P_{even} (I - T)^{-1} P_{odd} \phi = (I - T)^{-1} P_{even} (I - T)^{-2} P_{odd} \phi = (I - T)^{-1}(P_{even} - TP_{odd})(I + T)\phi,$$

which establishes the first formula in (A.3) because $(I + T)L_2(\mathbb{R}) = \mathcal{D}$ due to (A.1) and (A.2). The second formula is proved by similar arguments.

**Proof of statement (II).** Let the subspaces $L^\pm_n$ in (8) be $PT$ invariant and let $\mathcal{C}$ act as the identity operator on $L^\pm_n$. Then, using (A.3), we obtain

$$\mathcal{C} = P_+ - P_- = (I - T)^{-1}(P_{even} - TP_{odd} - P_{odd} + TP_{even}) = (I - T)^{-1}(I + T)\mathbb{P}. \hspace{1cm} (A.4)$$
The spectrum of $T$ is contained in the segment $[-1,1]$ and $\pm 1$ cannot be eigenvalues of $T$ because $T$ is a Hermitian strong contraction. In such a case

$$(I - T)^{-1}(I + T) = e^{Q}, \text{ where } Q = s(T) \text{ and } s(\lambda) = \ln \frac{1 + \lambda}{1 - \lambda},$$

is a Hermitian operator in $L_2(\mathbb{R})$.

It follows from (A.2) that the $PT$ invariance of $\mathcal{L}_\pm$ is equivalent to the commutation relation $[T, PT] = 0$. Then $[e^{Q}, PT] = 0$ and hence, $[Q, PT] = 0$.

On the other hand, the condition $[T, P] = 0$ implies that the spectral function $E_\lambda$ of $T$ satisfies the relation $PE_\lambda = E_\lambda P$ for any interval $\Delta$ of $\mathbb{R}$ [16]. Using this relation and the fact that $s(\lambda) = \ln \frac{1 + \lambda}{1 - \lambda}$ is an odd function on $[-1,1]$, we obtain

$$PQ = P \int_{[-1,1]} s(\lambda) dE_\lambda = \int_{[-1,1]} s(\lambda) dE_{-\lambda} P = -\int_{[-1,1]} s(-\lambda) dE_{-\lambda} P = -QP.$$ 

Hence, $[Q, P] = 0$. Combining this with $[Q, PT] = 0$ we conclude that $[Q, T] = 0$. Thus $C$ is determined by (7), where $[Q, P] = (Q, T) = 0$.

**Proof of statement (I).** Let $C$ be determined by (7). In this representation, $e^{Q}$ is a positive Hermitian operator. This means that the operator

$$T = (e^{Q} - I)(e^{Q} + I)^{-1} = \frac{e^{Q/2} - e^{-Q/2}}{2} \left( \frac{e^{Q/2} + e^{-Q/2}}{2} \right)^{-1} = \frac{\sinh(Q/2)}{\cosh(Q/2)} = \tanh \frac{Q}{2}$$

is a Hermitian strong contraction defined on $L_2(\mathbb{R})$. Moreover, $T$ anticommutes with $P$ and $T$ since $[Q, P] = [Q, T] = 0$. With the help of $T$ and (A.2), we determine the maximal positive (negative) subspaces $\mathcal{L}_\pm$ in the direct sum (8). The subspaces $\mathcal{L}_\pm$ are $PT$ invariant. The operator $C$ corresponding to (8) is determined by (A.4); that is,

$$C = (I - T)^{-1}(I + T)P = \left( I - \tanh \frac{Q}{2} \right)^{-1} \left( I + \tanh \frac{Q}{2} \right)P = e^{Q}P.$$ 

Therefore, the domain of definition $\mathcal{D}(C)$ is determined by (8) and $C = e^{Q}P$ acts as the identity operator on elements of $\mathcal{L}_\pm$.

Using (A.4) again we establish (10):

$$\frac{1}{2} (I \pm C)\mathcal{D}(C) = \frac{1}{2} (I \pm (P_+ - P_-))\mathcal{D}(C) = P_\pm \mathcal{D}(C) = \mathcal{L}_\pm.$$

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