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Space of state vectors in $\mathcal{PT}$-symmetric quantum mechanics

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Abstract

The space of states of $\mathcal{PT}$-symmetric quantum mechanics is examined. The requirement that eigenstates with different eigenvalues must be orthogonal leads to the conclusion that eigenfunctions belong to a space with an indefinite metric. Self-consistent expressions for the probability amplitude and the average value of operator are suggested. Further specification of the space of state vectors yields a superselection rule, redefining the notion of the superposition principle. An expression for the probability current density, satisfying the equation of continuity and vanishing for the bound state, is proposed.

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1. Introduction

A conjecture of Bessis and Zinn-Justin [1] states that the eigenvalues of the Schrödinger operator with potential $\mathrm{i}x^3$ are real and positive. Bender and Böetcher [2] suggested that the reason for the absence of complex eigenvalues of this non-self-adjoint operator could be the $\mathcal{PT}$ symmetry, where $\mathcal{P}$ is space reflection and $\mathcal{T}$ is time reversal. Using numerical methods and semiclassical approximation, they found that the spectra of the Hamiltonians with the potential $\mathrm{i}x^N$, $N \geqslant 2$ are real. The conjecture [1, 2], and the numerical validation [2] have provoked considerable interest in recent years (see e.g. [3–12]). Lately, the conjecture of Bessis, Zinn-Justin, Bender and Böetcher was justified using interrelations between the theories of ordinary differential equations and integrable models [8]. This approach, based on symmetry considerations, seems highly promising for identification of non-Hermitian Hamiltonians with real spectra.

Although the proof of the conjecture [2] is still lacking, it is reasonable to question whether or not there exists a self-consistent interpretation of the $\mathcal{PT}$ invariant Hamiltonian problem.

Assuming that the spectrum of the Hamiltonian under consideration is real, we shall pursue the problem of interpretation of $\mathcal{PT}$-symmetric quantum mechanics. We shall take for granted that the 'one half of the interpretation', namely that the eigenvalues are real, is already obtained, and shall concentrate on its 'other half'—a probabilistic interpretation in terms of the solutions ψ. We shall not assume that the solutions of the Schrödinger equation are eigenfunctions of $\mathcal{PT}$, i.e. in general $\mathcal{PT}\psi(x) \equiv \psi^\star(-x) \neq e^{i\omega}\psi(x)$.

We shall consider a Schrödinger equation in one dimension with a $\mathcal{PT}$ invariant potential $\mathcal{PT}V(x) \equiv V^\star(-x) = V(x)$ and with a non-vanishing imaginary part—$\mathrm{Im}\, V(x) \neq 0$. We shall assume that the Schrödinger equation with this $V(x)$ can be solved with x on a real line $\mathcal{R}: \ -\infty \leqslant x \leqslant \infty$, i.e. we do not use an analytic continuation in the complex-x plane as done in [13]. For example, this assumption is valid not for potentials of the form $(ix)^{2N+1}$ but for potentials of the form $(ix)^{2N}$ with $N \geqslant 2$ [14].

Average values of operators in a $\mathcal{PT}$ invariant field theory were investigated in [9] using analytic continuation in a complex-$\hat{\phi}$ plane, where $\hat{\phi}$ is a field operator. Since we consider a zero-dimensional counterpart of non-relativistic field theory on a real line, we cannot use an approach based on a Fokker–Planck probability [9].

The paper is organized as follows. In section 2 we shall use the requirement that the state vectors corresponding to the different eigenvalues should be orthogonal to establish that the space of state vectors $\mathcal{F}$ is a space with an indefinite scalar product. Also, as an example of constructing quantum mechanical quantities in $\mathcal{PT}$-symmetric quantum mechanics, we introduce probability current density.

In section 3 we shall review the basics of the theory of indefinite metric spaces and show $\mathcal{F}$ to be a special case. Namely, it turns out that $\mathcal{F}$ is a Krein space, decomposable into an orthogonal sum of two Hilbert spaces with positively and negatively defined scalar products respectively.

The probability amplitude and operator averages are introduced in section 4. It is shown that defining amplitude and average values in terms of vectors belonging to $\mathcal{F}$ is free from inconsistencies and that the Heisenberg operator equations are satisfied.

Results are discussed in section 5.

2. Orthogonality of state vectors: space with an indefinite metric

The combined space reflection and time reversal operator $\theta \equiv \mathcal{PT}$ is defined as [15]

$$\theta\{\, i, \hat{x}, \hat{p}\}\theta^{-1} = \{\, -i, -\hat{x}, \hat{p}\}. \tag{1}$$

An operator $\hat{A}$ is θ invariant if $\theta\hat{A}\theta^{-1} = \hat{A}$, i.e. when $[\hat{\theta}, \hat{A}] = 0$, the latter valid for the vectors of space in which both $\hat{A}$ and $\hat{\theta}$ can be simultaneously defined.

We consider a Schrödinger equation on a real line:

$$\hat{\mathcal{H}}\psi(x) = \left(-\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x) = E\psi(x) \tag{2}$$

with $V^\star(-x) = V(x)$, $\mathrm{Im}\, V(x) \neq 0$ and $\mathrm{Im}\, E = 0$. Let us address the question about the nature of the space of state vectors $\mathcal{F} \ni \psi$ and the existence of a satisfactory interpretation in terms of ψ.

As a starting point in analysing $\mathcal{F}$ we consider the eigenvalue equations $\mathcal{H}\psi_\alpha = E_\alpha\psi_\alpha$, $\mathcal{H}\psi_\beta = E_\beta\psi_\beta$. From $\theta V(x) \equiv V^\star(-x) = V(x)$ it follows that the solutions of (2) are $\psi(x)$ and $\psi^\star(-x)$ which, in turn, leads to the relation

$$(E_\alpha - E_\beta)\int_{\mathcal{R}} \mathrm{d}x\, \psi_\alpha(x)\psi_\beta^\star(-x) = 0. \tag{3}$$

In (3) it is already assumed that $\mathrm{Im}\, E = 0$; if eigenvalues are complex, $E_\alpha - E_\beta$ has to be replaced by $E_\alpha - E_\beta^\star$.

One of the cornerstones of the interpretation is that it is impossible to measure two different eigenvalues for the same state [15]. Therefore, probability is defined in accordance with the requirement that there is no transition between the eigenstates with different eigenvalues [15]. In order to maintain in θ-symmetric quantum mechanics the feature that the transition probability between the eigenstates with different eigenvalues vanishes, let us suggest that the transition probability amplitude in θ-symmetric quantum mechanics is

$$(\psi_\alpha|\psi_\beta) \equiv \int_{\mathcal{R}} \mathrm{d}x\ \psi_\alpha(x)(\theta\psi_\beta(x)) = \int_{\mathcal{R}} \mathrm{d}x\ \psi_\alpha(x)\psi_\beta^\star(-x); \tag{4}$$

in other words, we postulate that $\mathcal{F}$ is a linear space with the scalar product (4). Relations (3) and (4) imply that $(\psi_\alpha|\psi_\beta) = 0$ when $E_\alpha \neq E_\beta$.

Another way to introduce the scalar product (4) is as follows. Let both the Sturm–Liouville operator $\hat{\mathcal{H}}$ and the eigenvalue E be invariant under arbitrary transformation Ω, i.e. let $\Omega\hat{\mathcal{H}}(x)\Omega^{-1} = \hat{\mathcal{H}}(x)$ and $\Omega E = E$. Then, instead of starting from (4), one could postulate that the scalar product in $\mathcal{F}$ is defined by

$$(\psi_\alpha|\psi_\beta) = \int_{\mathcal{R}} \mathrm{d}x\ \psi_\alpha(x)(\Omega\psi_\beta(x)). \tag{5}$$

When the Hamiltonian is Hermitian ($\mathrm{Im}\, V(x) = 0$), definition (5) leads to the familiar expression for the scalar product in a Hilbert space: $(\psi_\alpha|\psi_\beta)_H = \int_{\mathcal{R}} \mathrm{d}x\ \psi_\alpha(x)\psi_\beta^\star(x) \equiv \langle\psi_\alpha|\psi_\beta\rangle$. The difference between $\langle\psi_\alpha|\psi_\beta\rangle$ and $(\psi_\alpha|\psi_\beta)$ is determined by the symmetry properties of the Hamiltonian: from the hermiticity of the Hamiltonian it follows that the scalar product is $\langle\psi_\alpha|\psi_\beta\rangle$, and for a θ invariant Hamiltonian the scalar product, satisfying the requirement of orthogonality for ψ_α and ψ_β, is defined as in (4).

When $V(x)$ is θ invariant and $\mathrm{Im}\, V(x) \neq 0$, $\psi^\star(x)$ is not the solution of (2) and as a result $\langle\psi_\alpha|\psi_\beta\rangle$ is no longer orthogonal:

$$(\psi_\alpha|\psi_\beta)_H \equiv \langle\psi_\alpha|\psi_\beta\rangle = \int_{\mathcal{R}} \mathrm{d}x\ \psi(x)_\alpha\psi_\beta^\star(x) \neq 0. \tag{6}$$

This relation is an evident consequence of $V(x) \neq V^\star(x)$.

Since in the case of θ invariant Hamiltonian ψ_α and ψ_β are orthogonal with respect to the scalar product (4), $(\psi_\alpha|\psi_\beta) = 0$ for $E_\alpha \neq E_\beta$, one is tempted to interpret the scalar product (4) as the transition probability amplitude between the two states described by the vectors ψ_α and ψ_β. This will lead to a satisfactory result—the transition probability between the states ψ_α and ψ_β (for $E_\alpha \neq E_\beta$) is zero, as it should be for a physical state [15].

Scalar product (4), respecting orthogonality for the different eigenvalues, is defined in terms of $\psi(x)$ and $\psi^\star(-x)$. As an example of using $(|)$ instead of the one defined in Hilbert space, $\langle|\rangle$, let us consider the diagonal form $(\psi|V|\psi)$. Note that when V is a θ invariant operator, $(\psi|V|\psi)$ is real:

$$\begin{aligned}
\mathrm{Im}\,(\psi|V|\psi) &= \mathrm{Im} \int_{\mathcal{R}} \mathrm{d}x\ \psi(x)V(x)\psi^\star(-x) \\
&= \int_{\mathcal{R}} \mathrm{d}x\ ([\mathrm{Re}\,\psi(x)\mathrm{Re}\,\psi(-x) + \mathrm{Im}\,\psi(x)\mathrm{Im}\,\psi(-x)]\mathrm{Im}\,V(x) \\
&\quad +[\mathrm{Re}\,\psi(-x)\mathrm{Im}\,\psi(x) - \mathrm{Re}\,\psi(x)\mathrm{Im}\,\psi(-x)]\mathrm{Re}\,V(x)) = 0
\end{aligned} \tag{7}$$

which follows from $\mathrm{Re}\,V(x) = \mathrm{Re}\,V(-x)$, $\mathrm{Im}\,V(x) = -\mathrm{Im}\,V(-x)$. The relation (7) resembles the one used in quantum mechanics: $\mathrm{Im}\,\langle\psi|V|\psi\rangle = 0$ for self-adjoint $V^\dagger = V$ [15].

As another example let us consider the following expression:

$$j(x) = \psi(x)\frac{\partial\theta\psi(x)}{\partial x} - \theta\psi(x)\frac{\partial\psi(x)}{\partial x}. \tag{8}$$

It is straightforward to verify that when $\theta V(x) \equiv V^\star(-x) = V(x)$, equation (2) leads to a continuity equation for j:

$$\frac{\partial j(x)}{\partial x} = 0. \tag{9}$$

If one uses $\psi^\star(x)$ instead of $\theta\psi(x)$, the continuity equation fails: $\partial j(x)/\partial x \sim \mathrm{Im}\ V(x) \neq 0$ (since it is assumed that $\mathrm{Im}\, E = 0$, we do not consider unstable states). Symmetry of the Hamiltonian suggests that $j(x)$ should be defined as a bilinear form of $\psi(x)$ and $\theta\psi(x)$.

If $j(x)$ represents the probability current density, it has to satisfy the condition that for the bound state $j(x) = 0$. Let us impose on a θ-symmetric problem (2) the boundary condition, similar to the bound state condition for the Hermitian case,

$$\psi(\pm\infty) = 0. \tag{10}$$

Note that the well known feature of non-degeneracy of a one-dimensional motion [15] is retained—if $\psi_\alpha(x)$ and $\psi_\beta(x)$ satisfy equation (2) and boundary condition (10) with the same eigenvalue, then $\psi_\alpha(x) = c\psi_\beta(x)$ with c constant (at this point it is not necessary for eigenvalues to be real). When $\mathrm{Im}\, V \neq 0$, the real and imaginary parts of ψ do not satisfy the same equation; therefore, non-degeneracy does not lead to $\mathrm{Im}\,\psi(x) = c\mathrm{Re}\,\psi(x)$. In other words, it is not necessary that $\psi = \mathrm{Re}\,\psi + \mathrm{i}\mathrm{Im}\,\psi = (1+\mathrm{i}c)\mathrm{Re}\,\psi$: a solution of the Schrödinger equation with a θ invariant Hamiltonian, satisfying boundary condition (10), can have a non-vanishing imaginary part. Since it is $\theta\psi(x)$, and not $\psi^\star(x)$, which satisfies the Schrödinger equation, non-degeneracy implies that $\psi_{Bound}(x)$, satisfying (10), is an eigenfunction of $\mathcal{PT}$[1]:

$$\theta\psi_{Bound}(x) \equiv \psi^\star_{Bound}(-x) = \mathrm{e}^{\mathrm{i}\omega}\psi_{Bound}(x). \tag{11}$$

From the definition (8) and equation (11) we find that for a bound state $j(x)$ vanishes:

$$j_{Bound}(x) = 0. \tag{12}$$

Equations (9) and (12) indicate that $j(x)$ could serve as a probability current density: $j(x)$ is conserved, and $j_{Bound}(x) = 0$, as one would expect [15].

Thus, the scalar product (4) leads to a results similar to those of conventional quantum mechanics, and one could consider (4) as a necessary ingredient for describing and interpreting quantum mechanical problems with $\mathcal{PT}$ invariant Hamiltonians.

The subtlety appears when one address the question of normalization. Let us examine the diagonal form:

$$(\psi|\psi) = \int_{\mathcal{R}} \mathrm{d}x\ \psi(x)\theta\psi(x) = \int_{\mathcal{R}} \mathrm{d}x\ \psi(x)\psi^\star(-x) \equiv \int_{\mathcal{R}} \mathrm{d}x\ \rho(x). \tag{13}$$

If $(\psi_\alpha|\psi_\beta)$ is understood as the transition probability amplitude between the states ψ_α and ψ_β the expression (13) is the transition amplitude from ψ into the same state, and the physical requirement is $(\psi|\psi) = 1$.

The integrand in (13) has a non-zero imaginary part but since $\mathrm{Im}\,\rho(-x) = -\mathrm{Im}\,\rho(x)$ we readily obtain that $(\psi|\psi)$ is real:

$$(\psi|\psi) = \int_{\mathcal{R}} \mathrm{d}x\ (\mathrm{Re}\,\psi(x)\mathrm{Re}\,\psi(-x) + \mathrm{Im}\,\psi(x)\mathrm{Im}\,\psi(-x)). \tag{14}$$

The distinctive feature is that the expressions (13), (14) are not positively defined, and thus $(\psi|\psi)$ cannot be normalized to unity. A positively defined expression is achieved only when ψ is an even function, $\psi_{ev}(-x) = \psi_{ev}(x)$:

$$(\psi_{ev}|\psi_{ev}) = \int_{\mathcal{R}} \mathrm{d}x\ \psi_{ev}(x)\psi^\star_{ev}(x) \geqslant 0 \tag{15}$$

[1] Numerical solution for $V(x) = \mathrm{i}x^3$ shows that for bound as well as for excited states $\mathrm{Re}\,\psi(x) = \mathrm{Re}\,\psi(-x)$ and $\mathrm{Im}\,\psi(x) = -\mathrm{Im}\,\psi(-x)$, i.e. in this case $\theta\psi(x) = \psi(x)$ [17].

but in general, the diagonal form (13) can be positive, negative or zero. For example, when ψ_ω is an eigenfunction, i.e. $\theta\psi_\omega(x) \equiv \psi^\star_\omega(-x) = \mathrm{e}^{\mathrm{i}\omega}\psi_\omega(x)$, we have

$$(\psi_\omega|\psi_\omega) = \int_{\mathcal{R}} \mathrm{d}x\,(\cos\omega[\mathrm{Re}^2\psi_\omega(x) - \mathrm{Im}^2\psi_\omega(x)] - 2\sin\omega\mathrm{Re}\,\psi_\omega(x)\mathrm{Im}\,\psi_\omega(x)). \tag{16}$$

Therefore, $\mathcal{F}$ is a linear space with an indefinite metric; in particular, $(\psi|\psi) = 0$ does not imply $\psi = 0$.

In [16] it was suggested that the norm (in a complex x-plane) is given by

$$\int_C \mathrm{d}x\,\psi^2(x) \tag{17}$$

and it was conjectured that in the momentum space this norm could be positively defined. Since we are considering motion on a real line $\mathcal{R}$, using the Fourier transform it is straightforward to demonstrate that

$$(\psi|\psi) = \int_{\mathcal{R}_p} \mathrm{d}p\,\tilde{\psi}(p)\tilde{\psi}^\star(-p) \tag{18}$$

i.e. the expressions (13) and (17) ((17) is the special case of (13), realized when $\theta\psi(x) = \psi(x)$) are not positively defined on the momentum real line either.

Thus, $\mathcal{F} \in \psi$ is a space with an indefinite metric and we need to specify a space where a scalar product is defined via (4), and at the same time, it is possible to realize the probabilistic interpretation of a θ-symmetric quantum mechanical problem. To do so, let us recall some basic statements and theorems from the theory of spaces with an indefinite metric [18].

3. Normalization of state vectors: Krein space

For any element ψ of an indefinite metric space $\mathcal{F}$ there are three possibilities: the vector ψ is positive, $\{\psi^+ \in \mathcal{F}^{++} : (\psi^+|\psi^+) > 0\}$, or negative, $\{\psi^- \in \mathcal{F}^{--} : (\psi^-|\psi^-) < 0\}$, or neutral $\{\psi^0 \in \mathcal{F}^0,\ \psi^0 \neq 0 : (\psi^0|\psi^0) = 0\}$ (clearly the zero vector $\psi = 0$ is neutral). In general, $\mathcal{F}$ contains all three subspaces. The semidefinite subspaces $\mathcal{F}^+$ and $\mathcal{F}^-$ are defined as those with non-negative and non-positive scalar products: $\{\psi^+ \in \mathcal{F}^+ : (\psi^+|\psi^+) \geqslant 0\}$ and $\{\psi^- \in \mathcal{F}^- : (\psi^-|\psi^-) \leqslant 0\}$.

In the semidefinite subspace the scalar product $(\psi_\alpha|\psi_\beta)$ is insensitive to ψ^0. To see this, let us use the Schwarz inequality, valid in $\mathcal{F}^\pm$ [18]:

$$|(\psi^0|\psi^{\pm,\,0})|^2 \leqslant (\psi^0|\psi^0)(\psi^{\pm,\,0}|\psi^{\pm,\,0}). \tag{19}$$

From (19) it follows that ψ^0 is orthogonal to any $\psi \in \mathcal{F}$: $(\psi^0|\psi^{\pm,\,0}) = 0$. Therefore, a neutral vector does not affect the value of the scalar product: $(\psi_\alpha + a\psi^0|\psi_\beta + b\psi^0) = (\psi_\alpha|\psi_\beta)$. Since $(\psi^0|\mathcal{F}^\pm) = 0$ and $(\psi^0|\psi^0) = 0$, below we shall consider $\psi^+ \in \mathcal{F}^+$ and $\psi^- \in \mathcal{F}^-$, excluding the subspace $\mathcal{F}^0$ from the space of states $\mathcal{F}$. Therefore, the first constraint we impose on the space of state vectors is that $\mathcal{F}$ is an indefinite metric space not containing neutral vectors ψ^0.

A second constraint originates from the fact that, in general, $\mathcal{F}$ might be not decomposable as an orthogonal sum of $\mathcal{F}^+$ and $\mathcal{F}^-$ [18], and for this reason it is impossible to introduce the norm into the whole space $\mathcal{F}$. A space with an indefinite metric $\mathcal{F}$ can be decomposed as an orthogonal sum of $\mathcal{F}^+$ and $\mathcal{F}^-$ when $\mathcal{F}^+$ and $\mathcal{F}^-$ are orthogonal with regard to the scalar product defined into the whole $\mathcal{F}$:

$$(\mathcal{F}^+|\mathcal{F}^-) = 0. \tag{20}$$

In this case, i.e. when $\mathcal{F} = \mathcal{F}^+ \oplus \mathcal{F}^-$, subspaces $\mathcal{F}^\pm$ can be completed to Hilbert spaces with the norms $\|\psi\| = \sqrt{(\psi|\psi)}$ when $\psi \in \mathcal{F}^+$, and $\|\psi\| = \sqrt{-(\psi|\psi)}$ when $\psi \in \mathcal{F}^-$.

This is a definition of a Krein space, an indefinite metric space which admits an orthogonal decomposition in which $\mathcal{F}^{\pm}$ are complete, and where the positively defined norm can be introduced [18]. Based on these properties, we suggest that the space of states of θ-symmetric quantum mechanics is a Krein space.

Let us describe the prescription for introducing a norm in the Krein space [18]. Define projection operators $\Pi^{\pm}$ satisfying relations

$$\Pi^{\pm}\mathcal{F} = \mathcal{F}^{\pm} \qquad \Pi^{+} + \Pi^{-} = 1 \qquad \Pi^{+}\Pi^{-} = 0. \tag{21}$$

Operators $\Pi^{\pm}$, $\Pi^{\pm}\psi = \psi^{\pm}$ cannot be introduced in just any space with an indefinite metric: the necessary condition is equation (20), i.e. $\mathcal{F}$ has to be the Krein space (it can be proved that any space with an indefinite metric and positively defined norm can be mapped to a Krein space [18]).

The next step is to consider a linear unitary operator J which maps $\mathcal{F}$ onto itself, $\mathcal{F} \xrightarrow{J} \mathcal{F}$:

$$J \equiv \Pi^{+} - \Pi^{-}. \tag{22}$$

It can be demonstrated that J is a bounded self-adjoint operator, and $\mathcal{F}^{\pm}$ is the eigenspace of J with eigenvalues ± 1.

The operator J enables us to introduce a (positively defined) scalar product $(\psi|\phi)_{\mathcal{F}}$ into the whole Krein space (i.e. for all $\psi, \phi \in \mathcal{F}$) according to the formula

$$(\psi|\phi)_{\mathcal{F}} \equiv (J\psi|\phi) = (\psi^{+}|\phi^{+}) - (\psi^{-}|\phi^{-}). \tag{23}$$

Note that when $\psi \in \mathcal{F}^{+}$ and $\phi \in \mathcal{F}^{-}$, i.e. when $(\psi|\phi) = 0$ (see equation (20)), it follows from (23) that $(\psi|\phi)_{\mathcal{F}} = (\psi|0) - (0|\phi) = 0$.

Let us now apply the prescription (23) to an indefinite metric space where the scalar product is given by (4):

$$(\psi|\phi) = \int_{\mathcal{R}} \mathrm{d}x\, \psi(x)(\theta\phi(x)) = \int_{\mathcal{R}} \mathrm{d}x\, \psi(x)\phi^{\star}(-x) \tag{24}$$

and $\mathcal{F} = \mathcal{F}^{+} \oplus \mathcal{F}^{-}$.

To find the operator J and thus to find out the norm, we introduce

$$K^{\pm} \equiv \frac{1 \pm \mathcal{P}}{2} \tag{25}$$

where $\mathcal{P}$ is the space reflection operator: $\mathcal{P}\psi(x) = \psi(-x)$. From $\mathcal{P}(K^{+}\psi(x)) = K^{+}\psi(x)$ we obtain

$$\begin{aligned} (K^{+}\psi|K^{+}\psi) &= \int_{\mathcal{R}} \mathrm{d}x\, K^{+}\psi(x)(K^{+}\psi(-x))^{\star} \\ &= \int_{\mathcal{R}} \mathrm{d}x\, K^{+}\psi(x)(\mathcal{P}(K^{+}\psi(x)))^{\star} = \int_{\mathcal{R}} \mathrm{d}x\, K^{+}\psi(x)(K^{+}\psi(x))^{\star} > 0 \end{aligned} \tag{26}$$

i.e. when the scalar product is given by (4), it follows that the positive vector ψ^{+} is $\psi^{+} = K^{+}\psi$, and the comparison with (21) gives

$$\Pi^{+} = K^{+}. \tag{27}$$

Arguments similar to those leading to (27) result in $\Pi^{-} = K^{-}$, and from (22) and (25) we obtain that in our case J is the space reflection operator:

$$J = \Pi^{+} - \Pi^{-} = K^{+} - K^{-} = \mathcal{P}. \tag{28}$$

Now from (23), (24) and (28) it follows that the positively defined scalar product into the whole Krein space $\mathcal{F} = \mathcal{F}^{+} \oplus \mathcal{F}^{-}$ is

$$(\psi|\phi)_{\mathcal{F}} \equiv (J\psi|\phi) = (\psi|\mathcal{P}\phi) = \int_{\mathcal{R}} \mathrm{d}x\, \psi(x)(\mathcal{P}\phi(-x))^{\star} = \int_{\mathcal{R}} \mathrm{d}x\, \psi(x)\phi^{\star}(x) \equiv \langle\psi|\phi\rangle \tag{29}$$

i.e. the Hilbert space scalar product is reproduced. The norm in a Krein space with the scalar product (4) is therefore given by

$$\|\psi\|^2 = (\psi|J\psi) = (\psi|\mathcal{P}\psi) = \int_{\mathcal{R}} \mathrm{d}x\, \psi(x)\psi^\star(x) \equiv \langle\psi|\psi\rangle \geqslant 0. \tag{30}$$

Expression (30) satisfies the renormalizability requirement for a vector of physical state ψ—since $\|\psi\| = \sqrt{\|\psi\|^2} \geqslant 0$, one can always renormalize: $\psi \to \psi'$ where $\|\psi'\|^2 = 1$. Note that 'moving backwards', i.e. suggesting that according to (30) the amplitude of transition from ψ_α to ψ_β is given by $\langle\psi_\alpha|\psi_\beta\rangle = \int \mathrm{d}x \psi_\alpha \psi_\beta^\star(x)$, will lead to a wrong result as the vectors corresponding to different eigenvalues will no longer be orthogonal (see equation (6)).

4. Probability and average value in θ-symmetric quantum mechanics

We shall not consider the case when the Krein space reduces to $\mathcal{F}^+$ or to $\mathcal{F}^-$, i.e. when the space of states is a Hilbert space. In other words we assume that Im $V(x)$ cannot be removed by a similarity transformation. The case when a quantum mechanical system with non-Hermitian Hamiltonian can be mapped onto the one defined in a Hilbert space with a positively defined scalar product is discussed in [10].

We suggest the following expression for the amplitude describing the transition from the state ψ_α^j to the state $\psi_\beta^{j'}$:

$$A_{\alpha\beta}^{jj'} = \theta A_{\beta\alpha}^{j'j} = \frac{(\psi_\alpha^j|\psi_\beta^{j'})}{\sqrt{(\psi_\alpha^j|\psi_\alpha^j)}\sqrt{(\psi_\beta^{j'}|\psi_\beta^{j'})}} \tag{31}$$

where α, β label eigenstates of the Hamiltonian, and $j, j' = \pm 1$ are the eigenvalues of the operator J (see (22)).

For $j \neq j'$, from the definition of the Krein space as an orthogonal sum, $(\mathcal{F}^+|\mathcal{F}^-) = 0$ implies that $A_{\alpha\beta}^{+-} = 0$. Note that if we define $A_{\alpha\beta}^{jj'}$ not via the scalar product (4) but by the scalar product in the Hilbert space, the '$\pm$ orthogonality' is still valid, since we have $(\mathcal{F}^+|\mathcal{F}^-) = 0$ as well as $\langle\mathcal{F}^+|\mathcal{F}^-\rangle = 0$. However, if both ψ_α and ψ_β belong only to $\mathcal{F}^+$, or only to $\mathcal{F}^-$, an amplitude written in terms of $\langle\psi_\alpha^j|\psi_\beta^{j'}\rangle$ will not vanish. The reason for choosing amplitude as in (31) is that $(\psi_\alpha^j|\psi_\beta^{j'})$ guarantees orthogonality when ψ_α^j and $\psi_\beta^{j'}$ belong to the same as well as to different subspaces of $\mathcal{F}$.

The fact that the space of state vectors does not contain the neutral vector leads to a superselection rule in θ-symmetric quantum mechanics: if ψ_α^+ is a state vector and ψ_β^- is a state vector, $\phi = c_\alpha\psi_\alpha^+ + c_\beta\psi_\beta^-$ does not correspond to any physical system. Since the equation $(\phi|\phi) = c_\alpha c_\alpha^\star(\psi_\alpha^+|\psi_\alpha^+) + c_\beta c_\beta^\star(\psi_\beta^-|\psi_\beta^-) = 0$ can have a non-trivial solution, ϕ cannot belong to $\mathcal{F}$. Unlike in the Hilbert space, the superposition principle acts separately in subspaces $\psi \in \mathcal{F}^+$ and $\psi \in \mathcal{F}^-$. A linear superposition of ψ^+ and ψ^- is not an element of $\mathcal{F}$. This superselection rule resembles the one in quantum field theory, where a linear superposition of states with the different quantum numbers (e.g. $\Psi_{proton} + \Psi_{electron}$), or superposition of different representations of the Poincaré group (e.g. $\Psi_{spin\ 1} + \Psi_{spin\ 1/2}$) is not a state vector [19]. We interpret the eigenvalues ± 1 of the operator J as (conserved) quantum numbers in θ-symmetric quantum mechanics; consequently, one can describe θ-symmetric quantum mechanics as a conventional quantum mechanics in a J-invariant space (for a description of J-invariant space see [18]).

Using the inequality (19) we obtain that the amplitude $A_{\alpha\beta}^{jj'}$ satisfies conditions similar to those in quantum mechanics [15]:

$$|A_{\alpha\beta}^{jj'}| \leqslant 1 \qquad A_{\alpha\alpha}^{jj} = 1. \tag{32}$$

Thus, although the space of states contains negative vectors, definition (31) does not lead to inconsistencies caused by an indefinite metric.

Another point of interest is the average values. In analogy with quantum mechanics we suggest that an average value of the operator $\hat{\mathcal{O}}$ in a state ψ^j is

$$Av(\hat{\mathcal{O}}) = \frac{(\psi^j|\hat{\mathcal{O}}\psi^j)}{(\psi^j|\psi^j)}. \tag{33}$$

Let us consider the time derivative of the average value (since $\psi^0 \notin \mathcal{F}$, the denominator in (33) can always be normalized to 1, or -1; the derivation below is valid for either sign):

$$\frac{\mathrm{d}}{\mathrm{d}t}Av(\hat{\mathcal{O}}) = \int_{\mathcal{R}} \mathrm{d}x \left(\frac{\partial(\theta\psi(x,t))}{\partial t}\hat{\mathcal{O}}\psi(x,t) + (\theta\psi(x,t))\hat{\mathcal{O}}\frac{\partial\psi(x,t)}{\partial t} \right). \tag{34}$$

Using the time-dependent Schrödinger equation with a θ invariant Hamiltonian

$$\mathrm{i}\frac{\partial\psi^j(x,t)}{\partial t} = \hat{\mathcal{H}}\psi^j(x,t) \qquad -\mathrm{i}\frac{\partial(\theta\psi^j(x,t))}{\partial t} = \hat{\mathcal{H}}(\theta\psi^j(x,t)) \tag{35}$$

it is straightforward to demonstrate that

$$\frac{\mathrm{d}}{\mathrm{d}t}Av(\hat{\mathcal{O}}) = \mathrm{i}Av(\hat{\mathcal{H}}\hat{\mathcal{O}} - \hat{\mathcal{O}}\hat{\mathcal{H}}). \tag{36}$$

Therefore, in a θ-symmetric quantum mechanics the Heisenberg equation

$$\mathrm{i}\frac{\mathrm{d}\hat{\mathcal{O}}}{\mathrm{d}t} = \hat{\mathcal{O}}\hat{\mathcal{H}} - \hat{\mathcal{H}}\hat{\mathcal{O}} \tag{37}$$

is satisfied. Of course, operator equation (37) is defined in space $\mathcal{F}$ with the scalar product (4).

Note that the scalar product (4) satisfies the relation $(\psi|\hat{\mathcal{O}}\phi) = (\theta\hat{\mathcal{O}}\theta^{-1}\psi|\phi)$, the analogy of which in a Hilbert space is $\langle\psi|\hat{\mathcal{O}}\phi\rangle = \langle\hat{\mathcal{O}}^{\dagger}\psi|\phi\rangle$. Since a self-adjoint operator in a Hilbert space may be not self-adjoint in a Krein space, expression (33) can be related to observables only when $\hat{\mathcal{O}}$ is θ invariant, as are the Hamiltonian, the momentum or the operator $\mathrm{i}\hat{x}$. In connection with the notion of self-adjoint operators in Krein space we refer to the following theorem: the spectrum of an operator $\hat{\mathcal{O}}$ which is symmetric (i.e. $(\hat{\mathcal{O}}\psi|\phi) = (\psi|\hat{\mathcal{O}}\phi)$ for every $\psi,\ \phi \in \mathcal{F}$), and positive (i.e. $(\hat{\mathcal{O}}\psi|\psi) \geqslant 0$ for every $\psi \in \mathcal{F}$), is real [18]. According to this theorem, the necessary condition for $\hat{\mathcal{O}}$ to have a real spectrum is that $\hat{\mathcal{O}}$ is a symmetric, i.e. θ invariant operator. The spectrum will be real if a θ invariant operator $\hat{\mathcal{O}}$ is positive, the case necessary to investigate separately for every given operator. This problem lies beyond the scope of the present paper.

5. Discussion

We have considered a quantum mechanical problem with a $\theta \equiv \mathcal{PT}$ invariant Hamiltonian $\hat{\mathcal{H}} = -\partial^2 + V(x)$, $\theta V(x) \equiv V^{\star}(-x) = V(x)$, $\operatorname{Im} V(x) \neq 0$. Requiring orthogonality and using the symmetry of the Hamiltonian we found that the scalar product in the space of state vectors $\mathcal{F}$ is given by (4), which, in turn, leads to the conclusion that $\mathcal{F}$ is a space with an indefinite metric. The requirement of normalizability leads to the further constraints on the space of state vectors and as a result, $\mathcal{F}$ can be identified with the Krein space. The latter can be (loosely) defined as the orthogonal sum of two Hilbert spaces, with positively and negatively defined scalar products respectively. Excluding neutral vector $\psi^0 \neq 0 : (\psi^0|\psi^0) = 0$ from physical states we have arrived at a superselection rule in $\mathcal{F}$: not every superposition of state vectors belongs to $\mathcal{F}$. The transition amplitude (31), and the average value (33) can be defined in a self-consistent way in $\mathcal{F}$.

The superselection rule often occurs in quantum field theory, where, unlike in quantum mechanics, there is no one-to-one correspondence between the pure states and the rays of space where the algebra of field operators is realized [19]. In other words, the space of states in quantum field theory is not a linear space, but rather an orthogonal sum of linear spaces [19]: the same is true in the θ-symmetric quantum mechanics.

Another aspect of θ-symmetric quantum mechanics, not realized in conventional quantum mechanics, is the space with an indefinite metric. Again, this feature appears in certain field-theoretical models: the two well established examples are quantum electrodynamics [19], and the exactly solvable field theoretical model of Lee [20]. The indefinite metric occurring in quantum field theory is in a sense 'fictitious', since it corresponds to the dynamics of the redundant degrees of freedom, and the requirement that the dynamics should be realizable in the space of physical degrees of freedom leads to the reduction of the space of all (physical and non-physical) states to the space of physical states with positively defined scalar product. The space of physical states is complete with respect to this scalar product [19, 20]. In a θ-symmetric quantum mechanics there are no 'extra, non-physical' degrees of freedom, therefore it is impossible to introduce an auxiliary condition allowing us to eliminate a subspace with a non-positively defined scalar product. In general, the complete set of basis vectors in spaces with an indefinite metric consists of vectors belonging to $\mathcal{F}^+$ as well as to $\mathcal{F}^-$, and $\mathcal{F}$ is complete, i.e. it is a Hilbert space relative to the norm $\langle\psi|\psi\rangle$ [18]. The reduction of space of states can result in an incomplete set (the problem of completeness for the potentials $\mathrm{i}x^3$ and $-x^4$ is discussed in [21]) which would make interpretation impossible.

To conclude, it is possible to give a self-consistent interpretation for a $\mathcal{PT}$-symmetric version of quantum mechanics. The price one has to pay is to abandon the Hilbert space and to switch to Krein space with an indefinite metric. This feature, as well as the superselection rule, are not present in formulation of the Hermitian quantum mechanics. Nevertheless, they do not violate the general requirements of the probabilistic interpretation. The results presented are valid when Im $V(x)$ is not vanishing. Therefore there cannot be a smooth transition to the Hermitian case: from the very beginning, depending on the symmetry of the Hamiltonian, the scalar product is defined either as $(|)$ (Krein space), or as $\langle|\rangle$ (Hilbert space).

Needless to say, the discovery of a dynamical system, described in terms of a non-Hermitian and $\mathcal{PT}$ invariant Hamiltonian, will be more than welcome.

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While this manuscript was under revision, the authors of [22] arrived at the same probability current as expression (8) of the present paper.

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