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General aspects of $\mathcal{PT}$-symmetric and $\mathcal{P}$-self-adjoint quantum theory in a Krein space

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Abstract

In our previous work, we proposed a mathematical framework for $\mathcal{PT}$-symmetric quantum theory, and in particular constructed a Krein space in which $\mathcal{PT}$-symmetric operators would naturally act. In this work, we explore and discuss various general consequences and aspects of the theory defined in the Krein space, not only spectral properties and $\mathcal{PT}$-symmetry breaking but also several issues, crucial for the theory to be physically acceptable, such as time evolution of state vectors, probability interpretation, uncertainty relation, classical–quantum correspondence, completeness, existence of a basis, and so on. In particular, we show that for a given real classical system we can always construct the corresponding $\mathcal{PT}$-symmetric quantum system, which indicates that $\mathcal{PT}$-symmetric theory in the Krein space is another quantization scheme rather than a generalization of the traditional Hermitian one in the Hilbert space. We propose a postulate for an operator to be a physical observable in this framework.

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1. Introduction

More than half a century ago, Dyson conjectured that the perturbation series in the coupling constant e^2 in quantum electrodynamics would be divergent by the physical argument that the theory with $e^2 < 0$ where like charges attract is unstable against the spontaneous pair creation of e^+e^- and thus cannot have a stable vacuum in contrast to the ordinary theory with $e^2 > 0$ [1]. It is well known now that in most quantum systems perturbation series are indeed divergent and at most asymptotic, see e.g. [2]. On the other hand, it might not have been

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duly recognized that Dyson's reasoning itself, which led to the divergence of the perturbation series, is in general invalid.

Immediately after the pioneering semi-classical analysis by Bender and Wu [3, 4], Simon in 1970 clarified with the mathematically rigorous treatment the analytic structure of the energy eigenvalue $E(g)$ of the quantum mechanical quartic anharmonic oscillator [5]

$$(-\partial^2 + x^2 + gx^4)\psi(x; g) = E(g)\psi(x; g). \tag{1.1}$$

Besides the fact that the point $g = 0$ is indeed a singularity of $E(g)$, it was proved that $E(g)$ is analytic in the whole cut plane $|\arg g| < \pi$ and in particular the theory (1.1) is well defined also for $g < 0$. In other words, the system (1.1) with $g < 0$ is *mathematically stable* as an eigenvalue problem although it is *physically unstable* in the sense that the energy eigenvalue $E(g)$ has a non-zero imaginary part besides its apparent unstable shape of the potential. The underlying crucial fact is that the analytic continuation of the system (1.1) with $g > 0$ into the complex g plane inevitably accompanies the rotation of the domain $\mathbb{R}$ into the complex x plane on which the theory is defined. This is because the eigenfunctions $\psi(x; g)$ for $g > 0$ are normalizable in the sector $\left|\arg(\pm x) + \frac{1}{6}\arg g\right| < \frac{\pi}{6}$ when $|x| \to \infty$. As a consequence, the theory (1.1) with $g < 0$ obtained by the analytic continuation from $g > 0$ is defined, e.g., in the sectors $-\frac{4\pi}{3} < \arg x < -\pi$ and $-\frac{\pi}{3} < \arg x < 0$ ($|x| \to \infty$) when $\arg g = \pi$, in the sectors $-\pi < \arg x < -\frac{2\pi}{3}$ and $0 < \arg x < \frac{\pi}{3}$ ($|x| \to \infty$) when $\arg g = -\pi$, and so on. Hence, the important lesson drawn from the above fact is that we must always also take into account the effect on the linear space on which a theory is defined when we change the sign of a parameter involved in the Hamiltonian or Lagrangian.

This lesson was however not duly exercised when in 1973 Symanzik proposed $\lambda\phi^4$-theory with $\lambda < 0$, which is a quantum field theoretical version of the system (1.1) with $g < 0$ in $1+3$ space-time dimension, as the first example of an asymptotically free theory [6]; the majority considered it physically unacceptable based on the intuition that it must be unstable, though the investigation into this controversial model has still persisted, e.g. [7–11] (for a historical survey from a new viewpoint, see [12]).

Recently, it was revealed that the model (1.1) with $g < 0$ admits another novel treatment totally different from the analytic continuation from the sector $g > 0$. In 1998, Bender and Boettcher, motivated by the Bessis–Zinn-Justin conjecture that the spectrum of the Hamiltonian $H = p^2 + x^2 + \mathrm{i}x^3$ is real and positive, found numerically that a family of the system

$$H = p^2 + m^2x^2 + x^2(\mathrm{i}x)^\epsilon \tag{1.2}$$

has indeed a real and positive spectrum for all $\epsilon \geqslant 0$, and argued that it is the underlying $\mathcal{PT}$-symmetry that ensures these spectral properties [13, 14]. Here we note especially the fact that although the latter model, when $\epsilon = 2$, looks the same as the system (1.1) with $g < 0$, their spectral properties are different. The key ingredient underlying the difference is the different boundary conditions. The regions where the eigenfunctions of the latter $\mathcal{PT}$-symmetric model (1.2) are normalizable, when it is defined for $\epsilon > 0$ as the continuation from the harmonic oscillator at $\epsilon = 0$, are given by the following sectors ($|x| \to \infty$) [13]:

$$\arg x = -\pi + \frac{\epsilon\pi}{2(4+\epsilon)} \pm \frac{\pi}{4+\epsilon} \qquad \text{and} \qquad \arg x = -\frac{\epsilon\pi}{2(4+\epsilon)} \pm \frac{\pi}{4+\epsilon}. \tag{1.3}$$

In particular, they are given by $-\pi < \arg x < -\frac{2\pi}{3}$ and $-\frac{\pi}{3} < \arg x < 0$ ($|x| \to \infty$) in the case $\epsilon = 2$, and are different from those for the quartic oscillator (1.1) with $\arg g = \pm\pi$. Hence, the $\mathcal{PT}$-symmetric system (1.2) with $\epsilon = 2$ cannot be obtained by the analytic continuation of the system (1.1) with $g > 0$, a situation anticipated by Symanzik [6].

In addition to the novel spectral properties, it was revealed that the $\mathcal{PT}$-symmetric model (1.2) admits a non-zero vacuum expectation value $\langle 0|x|0\rangle$ even when $m^2 > 0$ and $\epsilon = 2$

[15–17]. All the non-perturbative calculations in these papers indicate that the vacuum expectation value would receive a purely non-perturbative correction in that case irrespective of the space-time dimensions. Hence, the $\mathcal{PT}$-symmetrically formulated $\lambda\phi^4$ theory with $\lambda < 0$ may exhibit a real and positive spectrum, dynamical symmetry breaking and asymptotic freedom (and thus non-triviality), which means in particular that it may be a more suitable candidate for the Higgs sector in the electroweak theory. An important lesson here is again the significance of identifying a linear space on which a given system shall be considered; a single Hamiltonian (or Lagrangian) can admit different theories according to different choices of a linear space.

The $\mathcal{PT}$-symmetric formulation has also shed new light on other quantum field theoretical models. For instance, there have been some attempts to construct an asymptotically free quantum electrodynamics with $e^2 < 0$ [18–20]. The controversial Lee model [21] was reconsidered from a viewpoint of $\mathcal{PT}$-symmetry [22] (see also [23] for some relations between the Lee model and $\mathcal{PT}$-symmetric theory with the extensive references). There are also several non-Hermitian models to which the $\mathcal{PT}$-symmetric approach may apply, from older models such as the $\mathrm{i}\varphi^3$ theory [24, 25] associated with the Lee–Yang edge singularity [26, 27] to newer models such as the timelike Liouville theory [28, 29].

However, the $\mathcal{PT}$-symmetric formulation has not yet reached the level of a physical quantum theory; the emergence of an indefinite metric has been one of the obstacles. Towards the construction of a physical theory, there have been roughly two different approaches, namely, $\mathcal{PT}$-symmetric Hamiltonians with $\mathcal{C}$ operators [30, 31] and pseudo-Hermitian Hamiltonians with positive metric operators [32, 33]. For a brief description of the development in the field, see [34]. The recent progress in the last few years (e.g. [35]) indicates that both the approaches are likely to resolve themselves into classes of the quasi-Hermitian theory proposed in [36], although some disputes have still persisted, e.g. [37, 38]. Besides the disputes, both of them have not so far overcome the following drawbacks sufficiently:

(i) the lack of a systematic prescription independent from domains of operators (see e.g. [39] for a case-by-case treatment);
(ii) the lack of a framework applicable even when $\mathcal{PT}$-symmetry is spontaneously broken, which is serious since ascertaining rigorously unbroken $\mathcal{PT}$-symmetry is extremely difficult (see a rigorous proof in [40]);
(iii) unboundedness of $\mathcal{C}$ or metric operators (see [41]).

In our previous short letter [34], we proposed a unified mathematical framework for $\mathcal{PT}$-symmetric quantum theory defined in a Krein space, which would be able to surmount the above difficulties. There by 'unified' we meant that its applicability does not rely on whether a theory is defined on $\mathbb{R}$ or a complex contour, on whether $\mathcal{PT}$-symmetry is unbroken, and so on; thus it is free from the first and second defects described above. In the context of $\mathcal{PT}$-symmetry, a Krein space was first introduced in [42] and was then employed in e.g. [43, 44]. The Krein space in [34] can be regarded as a generalization of them. Furthermore, our framework can circumvent the third difficulty since it is formulated with a Hilbert space from the beginning and in this sense we need neither another Hilbert space nor any metric operator. We also clarified in particular the relation between $\mathcal{PT}$-symmetry and pseudo-Hermiticity in our framework. However, it has been still nothing more than a mathematical framework; no physics has been involved in it.

In this paper, we therefore explore and discuss various general consequences of $\mathcal{PT}$-symmetric quantum theory defined in the Krein space, putting our emphasis on whether the theory can be acceptable as a physical theory. To this end, we examine not only spectral property and $\mathcal{PT}$-symmetry breaking but also several issues, crucial for the theory to be physically acceptable, such as time evolution of state vectors, probability interpretation, uncertainty relation, classical–quantum correspondence, completeness, existence of a basis, and so on. We find that the several significant properties in ordinary quantum theory can also hold in our case analogously. In particular, we show that for a given real classical system we can always construct the corresponding $\mathcal{PT}$-symmetric quantum system, which indicates that $\mathcal{PT}$-symmetric theory in the Krein space is another quantization scheme rather than a generalization of the traditional Hermitian one in the Hilbert space.

We organize the paper as follows. In the next section, we review the mathematical framework, developed in our previous paper [34], with which we shall discuss various aspects of $\mathcal{PT}$-symmetric quantum theory in this paper. Section 3 is devoted to spectral properties and structure of root and eigenspaces in connection with spontaneous $\mathcal{PT}$-symmetry breaking. In section 4, we investigate the time evolution of state vectors of $\mathcal{PT}$-symmetric Hamiltonians and derive a conserved quantity in time. We then discuss possible ways to a probability interpretation of matrix elements and derive a couple of criteria for $\mathcal{PT}$-symmetric Hamiltonians to be physically acceptable. In section 5, we derive an uncertainty relation hold in $\mathcal{PT}$-symmetric quantum theory. In section 6, we discuss classical-quantum correspondence in $\mathcal{PT}$-symmetric theory. We first derive an alternative to Ehrenfest's theorem in our case, and then discuss its consequences, especially a novel relation to real classical systems. In section 7, we access the problem on completeness and existence of a basis, both of which are inevitable for the theory to be physically acceptable. We show that these requirements together with the criteria derived in section 4 naturally restrict operators to the class $\mathbf{K}(\mathbf{H})$. Finally, we summarize and discuss the results and propose a postulate for an operator to be a physical observable in section 8.

2. $\mathcal{PT}$-symmetric operators in a Krein space

2.1. Preliminaries

To begin with, let us introduce a complex-valued smooth function $\zeta(x)$ on the real line $\zeta : \mathbb{R} \to \mathbb{C}$ satisfying that (i) the real part of $\zeta(x)$ is monotone increasing in x such that $\operatorname{Re}\zeta'(x) > c(> 0)$ for all $x \in \mathbb{R}$ and thus $\operatorname{Re}\zeta(x) \to \pm\infty$ as $x \to \pm\infty$, (ii) the first derivative is bounded, i.e., $(0 <)|\zeta'(x)| < C(< \infty)$ for all $x \in \mathbb{R}$, and (iii) $\zeta(-x) = -\zeta^*(x)$ where $*$ denotes the complex conjugate. The function $\zeta(x)$ defines a complex contour in the complex plane and here we are interested in a family of the following complex contours:

$$\Gamma_a \equiv \{\zeta(x) \mid x \in (-a, a), a > 0\}, \tag{2.1}$$

which has mirror symmetry with respect to the imaginary axis. This family of complex contours would sufficiently cover all the support needed to define $\mathcal{PT}$-symmetric quantum mechanical systems. In particular, we note that Γ_∞ with $\zeta(x) = x$ is just the real line $\mathbb{R}$ on which standard quantum mechanical systems are considered.

Next, we consider a complex vector space $\mathfrak{F}$ of a certain class of complex functions and introduce a sesquilinear Hermitian form $Q_{\Gamma_a}(\cdot,\cdot) : \mathfrak{F} \times \mathfrak{F} \to \mathbb{C}$ on the space $\mathfrak{F}$, with a given $\zeta(x)$, by

$$Q_{\Gamma_a}(\phi, \psi) \equiv \int_{-a}^{a} \mathrm{d}x\, \phi^*(\zeta(x))\psi(\zeta(x)). \tag{2.2}$$

Apparently, it is positive definite, $Q_{\Gamma_a}(\phi, \phi) > 0$ unless $\phi = 0$, and thus defines an inner product on the space $\mathfrak{F}$. With this inner product we define a class of complex functions which satisfy

$$\lim_{a\to\infty} Q_{\Gamma_a}(\phi, \phi) < \infty, \tag{2.3}$$

that is, the class of complex functions which are square integrable (in the Lebesgue sense) in the complex contour Γ_∞ with respect to the *real* integral measure dx. We note that this class is identical with the class of complex functions which are square integrable in Γ_∞ with respect to the complex measure dz along Γ_∞. To see this, suppose first $\phi(z)$ belongs to the former class. Then we have

$$\left|\int_{\Gamma_a} \mathrm{d}z|\phi(z)|^2\right| \leqslant \int_{-a}^{a} \mathrm{d}x|\zeta'(x)||\phi(\zeta(x))|^2 < C\int_{-a}^{a} \mathrm{d}x|\phi(\zeta(x))|^2 < \infty, \tag{2.4}$$

where we use the property (ii) of the function $\zeta(x)$, and thus

$$\left|\int_{\Gamma_\infty} \mathrm{d}z|\phi(z)|^2\right| \leqslant C \lim_{a\to\infty} Q_{\Gamma_a}(\phi,\phi) < \infty, \tag{2.5}$$

that is, $\phi(z)$ also belongs to the latter. Conversely, if $\phi(z)$ belongs to the latter class, then we have

$$\int_{-a}^{a} \mathrm{d}x|\phi(\zeta(x))|^2 < c^{-1}\int_{-a}^{a} \mathrm{d}x\,\mathrm{Re}\,\zeta'(x)|\phi(\zeta(x))|^2 \leqslant c^{-1}\left|\int_{-a}^{a} \mathrm{d}x\,\zeta'(x)|\phi(\zeta(x))|^2\right|, \tag{2.6}$$

where we use the property (i) of the function $\zeta(x)$, and thus

$$\lim_{a\to\infty} Q_{\Gamma_a}(\phi,\phi) \leqslant c^{-1}\left|\int_{\Gamma_\infty} \mathrm{d}z|\phi(z)|^2\right| < \infty, \tag{2.7}$$

that is, $\phi(z)$ also belongs to the former.

As in the case of $L^2(\mathbb{R})$, we can show that this class of complex functions also constitutes a Hilbert space equipped with the inner product

$$Q_{\Gamma_\infty}(\phi,\psi) \equiv \lim_{a\to\infty} Q_{\Gamma_a}(\phi,\psi), \tag{2.8}$$

which is hereafter denoted by $L^2(\Gamma_\infty)$. A Hilbert space $L^2(\Gamma_a)$ for a finite positive a can be easily defined by imposing a proper boundary condition at $x = \pm a$.

Before entering into the main subject, we shall define another concept for later purposes. For a linear differential operator A acting on a linear function space of a variable x,

$$A = \sum_n \alpha_n(x)\frac{\mathrm{d}^n}{\mathrm{d}x^n}, \tag{2.9}$$

the transposition A^t of the operator A is defined by

$$A^t = \sum_n (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}x^n}\alpha_n(x). \tag{2.10}$$

An operator L is said to have *transposition symmetry* if $L^t = L$. If A acts in a Hilbert space $L^2(\Gamma_\infty)$, namely, $A : L^2(\Gamma_\infty) \to L^2(\Gamma_\infty)$ the following relation holds for all $\phi(z)$, $\psi(z) \in \mathfrak{D}(A) \cap \mathfrak{D}(A^t) \subset L^2(\Gamma_\infty)$:

$$\lim_{a\to\infty}\int_{-a}^{a} \mathrm{d}x\,\phi(\zeta(x))A^t\psi(\zeta(x)) = \lim_{a\to\infty}\int_{-a}^{a} \mathrm{d}x[A\phi(\zeta(x))]\psi(\zeta(x)). \tag{2.11}$$

2.2. $\mathcal{P}$-metric and a Krein space

With these preliminaries, we now introduce the linear parity operator $\mathcal{P}$ which performs spatial reflection $x \to -x$ when it acts on a function of a real spatial variable x as

$$\mathcal{P}f(x) = f(-x). \tag{2.12}$$

We then define another sesquilinear form $Q_{\Gamma_a}(\cdot,\cdot)_{\mathcal{P}} : \mathfrak{F}\times\mathfrak{F}\to\mathbb{C}$ by

$$Q_{\Gamma_a}(\phi,\psi)_{\mathcal{P}} \equiv Q_{\Gamma_a}(\mathcal{P}\phi,\psi). \tag{2.13}$$

We easily see that this new sesquilinear form is also Hermitian since

$$\begin{aligned} Q_{\Gamma_a}(\psi,\phi)_{\mathcal{P}} &= \int_{-a}^{a} \mathrm{d}x [\mathcal{P}\psi(\zeta(x))]^*\phi(\zeta(x)) = \int_{-a}^{a} \mathrm{d}x\, \psi^*(-\zeta^*(x))\phi(\zeta(x)) \\ &= \int_{-a}^{a} \mathrm{d}x'\, \psi^*(-\zeta^*(-x'))\phi(\zeta(-x')) = \int_{-a}^{a} \mathrm{d}x'\, \psi^*(\zeta(x'))\mathcal{P}\phi(\zeta(x')) \\ &= Q_{\Gamma_a}(\psi,\mathcal{P}\phi) = Q^*_{\Gamma_a}(\mathcal{P}\phi,\psi) = Q^*_{\Gamma_a}(\phi,\psi)_{\mathcal{P}}, \end{aligned} \tag{2.14}$$

where we use the Hermiticity of the form (2.2) as well as the property (iii). However, it is evident that the form (2.13) is no longer positive definite in general. We call the indefinite sesquilinear Hermitian form (2.13) $\mathcal{P}$*-metric*.

We are now in a position to introduce the $\mathcal{P}$-metric into the Hilbert space $L^2(\Gamma_\infty)$. For all $\phi(z), \psi(z) \in L^2(\Gamma_\infty)$ it is given by

$$Q_{\Gamma_\infty}(\phi,\psi)_{\mathcal{P}} \equiv \lim_{a\to\infty} Q_{\Gamma_a}(\phi,\psi)_{\mathcal{P}} = \lim_{a\to\infty} \int_{-a}^{a} \mathrm{d}x\, \phi^*(-\zeta^*(x))\psi(\zeta(x)). \tag{2.15}$$

It should be noted that we cannot take the two limits of the integral bounds, $a \to \infty$ and $-a \to -\infty$, independently in order to maintain the Hermiticity of the form given in equation (2.14). Hence, the symbol $\int_{-\infty}^{\infty}\mathrm{d}x$ hereafter employed in this paper is always understood in the following sense:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \equiv \lim_{a\to\infty} \int_{-a}^{a} \mathrm{d}x\, f(x). \tag{2.16}$$

From the definition of $\mathcal{P}$ and the relation (2.14), we easily see that the linear operator $\mathcal{P}$ satisfies $\mathcal{P}^{-1} = \mathcal{P}^\dagger = \mathcal{P}$, where $\dagger$ denotes the adjoint with respect to the inner product $Q_{\Gamma_\infty}(\cdot,\cdot)$, and thus is a *canonical* (or *fundamental*) *symmetry* in the Hilbert space $L^2(\Gamma_\infty)$ (definition 1.3.8 in [45]). Hence, the $\mathcal{P}$-metric turns out to belong to the class of the J-metric and the Hilbert space $L^2(\Gamma_\infty)$ equipped with the $\mathcal{P}$-metric $Q_{\Gamma_\infty}(\cdot,\cdot)_{\mathcal{P}}$ is a Krein space, which is hereafter denoted by $L^2_{\mathcal{P}}(\Gamma_\infty)$. Similarly, a Hilbert space $L^2(\Gamma_a)$ with $Q_{\Gamma_a}(\cdot,\cdot)_{\mathcal{P}}$ is also a Krein space $L^2_{\mathcal{P}}(\Gamma_a)$.

A generalization of the framework to many-body systems (described by M spatial variables x_i) would be straightforward by introducing M complex-valued functions $\zeta_i(x_i)$ which satisfy similar properties of (i)–(iii) with respect to each variable x_i $(i = 1,\ldots,M)$. An inner product on a vector space $\mathfrak{F}$ of complex functions of M variables is introduced by

$$Q_{\Gamma^M_{\{a_i\}}}(\phi,\psi) = \int_{-a_1}^{a_1} \mathrm{d}x_1 \cdots \int_{-a_M}^{a_M} \mathrm{d}x_M\, \phi^*(\zeta_1(x_1),\ldots,\zeta_M(x_M))\psi(\zeta_1(x_1),\ldots,\zeta_M(x_M)), \tag{2.17}$$

where $\Gamma^M_{\{a_i\}} = \Gamma_{a_1}\times\cdots\times\Gamma_{a_M}$ with each Γ_{a_i} given by equation (2.1). Then, we can easily follow a similar procedure in the previous and this subsection to construct a Hilbert space L^2 and a Krein space $L^2_{\mathcal{P}}$ in the case of many-body systems.

A canonical decomposition of the Krein space $L^2_{\mathcal{P}}$ is easily obtained by introducing the canonical orthoprojectors

$$P^\pm = \tfrac{1}{2}(I \pm \mathcal{P}). \tag{2.18}$$

With them we have

$$L^2_{\mathcal{P}} = L^2_{\mathcal{P}+}[\dot{+}]L^2_{\mathcal{P}-}, \qquad L^2_{\mathcal{P}\pm} \equiv P^\pm L^2_{\mathcal{P}} = \left\{\phi \in L^2_{\mathcal{P}} \middle| \mathcal{P}\phi = \pm\phi\right\}, \tag{2.19}$$

where $[\dot{+}]$ denotes the $\mathcal{P}$-orthogonal direct sum. That is, the positive (negative) subspace $L^2_{\mathcal{P}+}$ $\left(L^2_{\mathcal{P}-}\right)$ is composed of all the $\mathcal{P}$-even ($\mathcal{P}$-odd) vectors in $L^2_{\mathcal{P}}$, respectively.

2.3. $\mathcal{P}$-Hermiticity and $\mathcal{PT}$ symmetry

Let us next consider a linear operator A acting in the Krein space $L^2_{\mathcal{P}}$, namely, $A : \mathfrak{D}(A) \subset L^2_{\mathcal{P}} \to \mathfrak{R}(A) \subset L^2_{\mathcal{P}}$ with non-trivial $\mathfrak{D}(A)$ and $\mathfrak{R}(A)$. The $\mathcal{P}$-adjoint of the operator A is such an operator A^c that satisfies for all $\phi \in \mathfrak{D}(A)$

$$Q_{\Gamma_\infty}(\phi, A^c\psi)_{\mathcal{P}} = Q_{\Gamma_\infty}(A\phi, \psi)_{\mathcal{P}}, \qquad \psi \in \mathfrak{D}(A^c), \tag{2.20}$$

where the domain $\mathfrak{D}(A^c)$ of A^c is determined by the existence of $A^c\psi \in L^2_{\mathcal{P}}$. By the definitions (2.15) and (2.20) the $\mathcal{P}$-adjoint operator A^c satisfies

$$Q_{\Gamma_\infty}(\phi, A^c\psi)_{\mathcal{P}} = Q_{\Gamma_\infty}(\mathcal{P}A\phi, \psi) = Q_{\Gamma_\infty}(\phi, A^\dagger\mathcal{P}\psi) = Q_{\Gamma_\infty}(\phi, \mathcal{P}A^\dagger\mathcal{P}\psi)_{\mathcal{P}}, \tag{2.21}$$

that is, it is related to the adjoint operator $A^\dagger$ in the corresponding Hilbert space L^2 by

$$A^c = \mathcal{P}A^\dagger\mathcal{P}, \qquad \mathfrak{D}(A^c) = \mathfrak{D}(A^\dagger). \tag{2.22}$$

A linear operator A is called *$\mathcal{P}$-Hermitian* if $A^c = A$ in $\mathfrak{D}(A) \subset L^2_{\mathcal{P}}$, and is called *$\mathcal{P}$-self-adjoint* if $\overline{\mathfrak{D}(A)} = L^2_{\mathcal{P}}$ and $A^c = A$. Here we note that the concept of *η-pseudo-Hermiticity* introduced in [32] is essentially equivalent to what the mathematicians have long called *G-Hermiticity* (with $G = \eta$) among the numerous related concepts in the field (cf sections 1.6 and 2.3 in [45]). Therefore, in this paper we exclusively employ the latter mathematicians' terminology to avoid confusion. Unless specifically stated, we follow the terminology after the book [45] supplemented by the one employed in the book [46].[2]

We now consider so-called $\mathcal{PT}$-symmetric operators in the Krein space $L^2_{\mathcal{P}}$. The action of the anti-linear time-reversal operator $\mathcal{T}$ on a function of a real spatial variable x is defined by

$$\mathcal{T} f(x) = f^*(x), \tag{2.23}$$

and thus $\mathcal{T}^2 = 1$ and $\mathcal{PT} = \mathcal{TP}$ follow. Then an operator A acting on a linear function space $\mathfrak{F}$ is said to be *$\mathcal{PT}$-symmetric* if it commutes with $\mathcal{PT}$:[3]

$$[\mathcal{PT}, A] = \mathcal{PT}A - A\mathcal{PT} = 0. \tag{2.24}$$

To investigate the property of $\mathcal{PT}$-symmetric operators in the Krein space $L^2_{\mathcal{P}}$, we first note that the $\mathcal{P}$-metric can be expressed as

$$Q_{\Gamma_a}(\phi, \psi)_{\mathcal{P}} = \int_{-a}^{a} \mathrm{d}x[\mathcal{P}\phi(\zeta(x))]^*\psi(\zeta(x)) = \int_{-a}^{a} \mathrm{d}x[\mathcal{PT}\phi(\zeta(x))]\psi(\zeta(x)). \tag{2.25}$$

It is similar to but is slightly different from the (indefinite) $\mathcal{PT}$ inner product in [30]. Furthermore, if $\zeta(x) = x$ with finite a or $a \to \infty$, it reduces to the one considered in [42–44, 47] and is essentially equivalent to the indefinite metric introduced (without the notion of $\mathcal{PT}$) by Pauli in 1943 [48].

Let A be a $\mathcal{PT}$-symmetric operator in the Krein space $L^2_{\mathcal{P}}$. By the definitions (2.20) and (2.24), and equations (2.11) and (2.25), the $\mathcal{P}$-adjoint of A reads

$$\begin{aligned} Q_{\Gamma_\infty}(\phi, A^c\psi)_{\mathcal{P}} &= \int_{-\infty}^{\infty} \mathrm{d}x[\mathcal{PT}A\phi(\zeta(x))]\psi(\zeta(x)) = \int_{-\infty}^{\infty} \mathrm{d}x[A\mathcal{PT}\phi(\zeta(x))]\psi(\zeta(x)) \\ &= \int_{-\infty}^{\infty} \mathrm{d}x[\mathcal{PT}\phi(\zeta(x))]A^t\psi(\zeta(x)) = Q_{\Gamma_\infty}(\phi, A^t\psi)_{\mathcal{P}}, \end{aligned} \tag{2.26}$$

[2] Some of the terms are different between them. In particular, the notations and terms regarding the relation between a positive definite Hilbert space inner product and indefinite metrics are opposite.

[3] There exists the notion of *G-symmetry* which lies in an intermediate position between G-Hermiticity and G-self-adjointness (cf definitions 2.3.1 and 2.3.2 in [45]). But $\mathcal{PT}$ is anti-linear and is not a Gram operator (cf definition 1.6.3 in [45]). Thus confusion would not arise.

that is, $A^c = A^t$ in $\mathfrak{D}(A^c)$ for an arbitrary $\mathcal{PT}$-symmetric operator A. Hence, a $\mathcal{PT}$-symmetric operator is $\mathcal{P}$-Hermitian in $L^2_{\mathcal{P}}$ if and only if it has transposition symmetry as well. In particular, since any Schrödinger operator $H = -\mathrm{d}^2/\mathrm{d}x^2 + V(x)$ has transposition symmetry, $\mathcal{PT}$-symmetric Schrödinger operators are always $\mathcal{P}$-Hermitian in $L^2_{\mathcal{P}}$. The latter fact naturally explains the characteristic properties of the $\mathcal{PT}$-symmetric quantum systems found in the literature; indeed they are completely consistent with the well-established mathematical consequences of J-Hermitian (more precisely, J-self-adjoint) operators in a Krein space [45] with $J = \mathcal{P}$. Therefore, we can naturally consider any $\mathcal{PT}$-symmetric quantum system in the Krein space $L^2_{\mathcal{P}}$, regardless of whether the support Γ_∞ is $\mathbb{R}$ or not, and of whether $\mathcal{PT}$-symmetry is spontaneously broken or not. It should be noted, however, that the relation between $\mathcal{PT}$-symmetry and J-Hermiticity (more generally G-Hermiticity) varies according to in what kind of Hilbert space we consider operators. This is due to the different characters of the two concepts; any kind of Hermiticity is defined in terms of a given inner product while $\mathcal{PT}$-symmetry is not [49].

Finally, we note that it would be to some extent restrictive to consider only operators with transposition symmetry although we are mostly interested in Schrödinger operators. For operators without transposition symmetry, $\mathcal{PT}$-symmetry does not guarantee $\mathcal{P}$-Hermiticity. Hence, the requirement of $\mathcal{PT}$-symmetry alone would be less restrictive as an alternative to the postulate of self-adjointness in ordinary quantum mechanics. Furthermore, as we will see later on, even the stronger condition of $\mathcal{P}$-self-adjointness turns to be unsatisfactory from the viewpoint of physical requirements.

3. Spectral properties and $\mathcal{PT}$-symmetry breaking

In this section, we first review some significant mathematical properties regarding eigenvectors and spectrum of J-Hermitian operators, and then discuss $\mathcal{PT}$-symmetry breaking. For this purpose, let us first summarize the mathematical definitions which are indispensable for understanding the characteristic features of the spectral properties in indefinite metric spaces.

Let λ be an eigenvalue of a linear operator A in a linear space $\mathfrak{F}$, namely, $\lambda \in \sigma_p(A)$. The vector ϕ ($\neq 0$) is a *root* (or *principal*) vector of A belonging to λ if there is a natural number n such that $\phi \in \mathfrak{D}(A^n)$ and $(A - \lambda I)^n \phi = 0$. The span of all the root vectors of A belonging to λ is the root subspace denoted by $\mathfrak{S}_\lambda(A)$, namely,

$$\mathfrak{S}_\lambda(A) = \bigcup_{n=0}^{\infty} \mathrm{Ker}((A - \lambda I)^n). \tag{3.1}$$

The algebraic and geometric multiplicities of λ, denoted by $m^{(a)}_\lambda(A)$ and $m^{(g)}_\lambda(A)$, respectively, are defined by

$$m^{(a)}_\lambda(T) = \dim \mathfrak{S}_\lambda(A), \qquad m^{(g)}_\lambda(T) = \dim \mathrm{Ker}(A - \lambda I). \tag{3.2}$$

It is evident that $m^{(a)}_\lambda \geqslant m^{(g)}_\lambda$ for all λ. An eigenvalue λ is called *semi-simple* if $m^{(a)}_\lambda = m^{(g)}_\lambda$, that is, if $\mathfrak{S}_\lambda(A) = \mathrm{Ker}(A - \lambda I)$. Furthermore, a (semi-simple) eigenvalue λ is called *simple* if $m^{(a)}_\lambda \big(= m^{(g)}_\lambda\big) = 1$.

Let $\mathfrak{H}_J$ be a Krein space equipped with a J-metric $Q(\cdot,\cdot)_J$. Vectors $\phi, \psi \in \mathfrak{H}_J$ are said to be *J-orthogonal* and denoted by $\phi[\perp]\psi$ if $Q(\phi,\psi)_J = 0$. Similarly, subspaces $\mathfrak{L}_1, \mathfrak{L}_2 \subset \mathfrak{H}_J$ are said to be J-orthogonal and denoted by $\mathfrak{L}_1[\perp]\mathfrak{L}_2$ if $\phi[\perp]\psi$ for all $\phi \in \mathfrak{L}_1$ and $\psi \in \mathfrak{L}_2$. The *J-orthogonal complement* of a set $\mathfrak{L} \subset \mathfrak{H}_J$ is the subspace $\mathfrak{L}^{[\perp]} \subset \mathfrak{H}_J$ defined by

$$\mathfrak{L}^{[\perp]} = \{\psi \in \mathfrak{H}_J \mid \psi[\perp]\mathfrak{L}\}. \tag{3.3}$$

A vector $\phi \in \mathfrak{H}_J$ is said to be *neutral* if $\phi[\perp]\phi$. Similarly, a subspace $\mathfrak{L}$ is said to be neutral if $\phi[\perp]\phi$ for all $\phi \in \mathfrak{L}$. It follows from the Cauchy–Schwarz inequality (cf equation (4.12)), which holds in any neutral space, that every neutral subspace $\mathfrak{L}$ is J-orthogonal to itself and thus $\mathfrak{L} \subset \mathfrak{L}^{[\perp]}$ (cf proposition 1.4.17 in [45]). The *isotropic part* $\mathfrak{L}_0$ of a subspace $\mathfrak{L} \subset \mathfrak{H}_J$ is defined by $\mathfrak{L}_0 = \mathfrak{L} \cap \mathfrak{L}^{[\perp]}$ and its (non-zero) elements are called *isotropic vectors* of $\mathfrak{L}$. In other words, $\psi_0 \in \mathfrak{L}$ is an isotropic vector of $\mathfrak{L}$ if $(0 \neq)\psi_0[\perp]\mathfrak{L}$. It is evident that the isotropic part of any subspace is neutral. A subspace $\mathfrak{L}$ is said to be *non-degenerate* if its isotropic part is trivial, $\mathfrak{L}_0 = \{0\}$. Otherwise, it is called *degenerate*.

With these preliminaries, let us review some relevant mathematical theorems on the structure of root subspaces of a J-self-adjoint operator. One of the most notable ones in our context is the following (theorem II.3.3 in [46]):

Theorem 1. *Let A be a J-Hermitian operator. If λ and μ are eigenvalues of A such that $\lambda \neq \mu^*$, then $\mathfrak{S}_\lambda(A)[\perp]\mathfrak{S}_\mu(A)$.*

The $\mathcal{P}$-orthogonal relations on $\mathbb{R}$ found in [42, 47] are just a special case of theorem 1 when both the eigenvalues λ and μ are semi-simple. As a consequence of theorem 1, we have the following:

Corollary 2. *Any root subspace belonging to a non-real eigenvalue of a J-Hermitian operator is neutral.*

However, it does not guarantee that every root vector belonging to a real eigenvalue of a J-Hermitian operator is non-degenerate. To see this, suppose λ is a non-semi-simple real eigenvalue of a J-Hermitian operator A, and let $Q(\cdot,\cdot)_J$ be the J-metric. Then there exists a natural number $n \geqslant 2$ and a vector $\phi_n \in \mathfrak{D}(A^n)$ which satisfies $(A-\lambda I)^n\phi_n = 0$ and $(A-\lambda I)^{n-1}\phi_n \equiv \phi_1 \neq 0$. By definition ϕ_1 is an eigenvector belonging to λ, namely, $\phi_1 \in \mathrm{Ker}(A-\lambda I)$. On the other hand, from the J-Hermiticity of A and the reality of λ we have, for all $\psi \in \mathrm{Ker}(A-\lambda I)$

$$\begin{aligned} Q(\phi_1,\psi)_J &= Q((A-\lambda I)^{n-1}\phi_n,\psi)_J \\ &= Q((A-\lambda I)^{n-2}\phi_n,(A-\lambda I)\psi)_J = 0. \end{aligned} \tag{3.4}$$

That is, $\phi_1[\perp]\mathrm{Ker}(A-\lambda I)$ and thus ϕ_1 is an isotropic eigenvector of $\mathrm{Ker}(A-\lambda I)$. Hence we have,

Proposition 3. *If a real eigenvalue λ of a J-Hermitian operator is not semi-simple, the corresponding eigenspace* $\mathrm{Ker}(A-\lambda I)$ *is degenerate.*

It is important to note that the existence of isotropic eigenvectors of $\mathrm{Ker}(A-\lambda I)$ does not immediately imply the degeneracy of $\mathfrak{S}_\lambda(A)$ since there can exist vectors of $\mathfrak{S}_\lambda(A)\backslash\mathrm{Ker}(A-\lambda I)$ which are *not* J-orthogonal to each isotropic vector of $\mathrm{Ker}(A-\lambda I)$. As a simple example, let us consider a two-dimensional vector space $\mathbb{C}^2$ with an ordinary inner product $(\phi,\psi) = a_1^*b_1 + a_2^*b_2$ for $\phi = (a_1,a_2)^t$ and $\psi = (b_1,b_2)^t$, and let A and J be operators in $\mathbb{C}^2$ and e_i $(i = 1,2)$ be a basis of $\mathbb{C}^2$ as the followings:

$$A = \begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}, \qquad J = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{3.5}$$

where $\lambda \in \mathbb{R}$. Then, it is easy to see that A is J-Hermitian, $JA^\dagger J = A$, that λ is a non-semi-simple real eigenvalue of A, and that $\mathrm{Ker}(A-\lambda I) = \langle e_1\rangle$ and $\mathfrak{S}_\lambda(A) = \mathbb{C}^2$. On the other hand, $(e_1, Je_1) = 0$ and $(e_1, Je_2) = 1$, that is, $\mathrm{Ker}(A-\lambda I)$ is neutral but $\mathfrak{S}_\lambda(A)$ is non-degenerate with respect to the J-metric $(\cdot, J\cdot)$.

Regarding the non-degeneracy of the root subspaces, the concept of normality of eigenvalues plays a key role. An eigenvalue λ of a closed linear operator A in a Hilbert space $\mathfrak{H}$ is said to be *normal* if $(0 <)m_\lambda^{(a)}(A) < \infty$, $\mathfrak{H} = \mathfrak{S}_\lambda(A) \dotplus \mathfrak{L}$ where $\mathfrak{L}$ is closed, $A\mathfrak{L} \subset \mathfrak{L}$, and $\lambda \in \rho(A|_\mathfrak{L})$. Then the following theorem holds (theorem VI.7.5 in [46]):

Theorem 4. *Let A be a J-self-adjoint operator with $\rho(A) \neq \emptyset$. If λ is a normal eigenvalue of A, so is λ^*, and the root subspaces $\mathfrak{S}_\lambda(A)$ and $\mathfrak{S}_{\lambda^*}(A)$ are skewly linked (or dual companions), namely, $\mathfrak{S}_\lambda(A) \cap \mathfrak{S}_{\lambda^*}(A)^{[\perp]} = \mathfrak{S}_\lambda(A)^{[\perp]} \cap \mathfrak{S}_{\lambda^*}(A) = \{0\}$, the relation being denoted by $\mathfrak{S}_\lambda(A)\#\mathfrak{S}_{\lambda^*}(A)$.*[4]

When λ in the above is real, the consequence that $\mathfrak{S}_\lambda$ is skewly linked with itself apparently means that it is non-degenerate. On the other hand, when λ is non-real, we first note that from corollary 2 $\mathfrak{S}_{\lambda^*}$ is neutral and thus $\mathfrak{S}_{\lambda^*} \subset \mathfrak{S}_{\lambda^*}^{[\perp]}$. Suppose $\psi = \phi + \varphi$ ($\phi \in \mathfrak{S}_\lambda$, $\varphi \in \mathfrak{S}_{\lambda^*}$) is an isotropic vector of $\mathfrak{S}_\lambda \dotplus \mathfrak{S}_{\lambda^*}$. Then, we have $\psi \in (\mathfrak{S}_\lambda \dotplus \mathfrak{S}_{\lambda^*})^{[\perp]} \subset \mathfrak{S}_{\lambda^*}^{[\perp]}$ on one hand and $\varphi \in \mathfrak{S}_{\lambda^*}^{[\perp]}$ on the other hand. Hence, $\phi \in \mathfrak{S}_\lambda \cap \mathfrak{S}_{\lambda^*}^{[\perp]}$, but the latter subspace is trivial from $\mathfrak{S}_\lambda\#\mathfrak{S}_{\lambda^*}$ and thus $\phi = 0$. As a result, $\psi = \varphi \in (\mathfrak{S}_\lambda \dotplus \mathfrak{S}_{\lambda^*})^{[\perp]} \subset \mathfrak{S}_\lambda^{[\perp]}$ and hence $\varphi \in \mathfrak{S}_\lambda^{[\perp]} \cap \mathfrak{S}_{\lambda^*}$. But the latter space is again trivial from $\mathfrak{S}_\lambda\#\mathfrak{S}_{\lambda^*}$ and thus we finally have $\psi = 0$, that is, the isotropic part of $\mathfrak{S}_\lambda \dotplus \mathfrak{S}_{\lambda^*}$ is trivial (cf lemma I.10.1 in [46]). Summarizing the above results, we have the following:

Corollary 5. *Let λ be a normal eigenvalue of a J-self-adjoint operator A with $\rho(A) \neq \emptyset$. If λ is real, then the root subspace $\mathfrak{S}_\lambda(A)$ is non-degenerate. If λ is non-real, then $\mathfrak{S}_\lambda(A) \cap \mathfrak{S}_{\lambda^*}(A) = \{0\}$ and the subspace $\mathfrak{S}_\lambda(A) \dotplus \mathfrak{S}_{\lambda^*}(A)$ is non-degenerate.*

Since every finite-dimensional non-degenerate subspace $\mathfrak{L}$ of a Krein space $\mathfrak{H}_J$ is *projectively complete*, namely, $\mathfrak{L}[\dotplus]\mathfrak{L}^{[\perp]} = \mathfrak{H}_J$ (corollary 1.7.18 in [45]), corollary 5 implies that for each normal eigenvalue λ we can decompose the space as $\mathfrak{H}_J = \mathfrak{S}_\lambda[\dotplus]\mathfrak{H}'_J$ when $\lambda \in \mathbb{R}$ and as $\mathfrak{H}_J = (\mathfrak{S}_\lambda \dotplus \mathfrak{S}_{\lambda^*})[\dotplus]\mathfrak{H}'_J$ when $\lambda \notin \mathbb{R}$. From theorem 1 we can proceed with the J-orthogonal decomposition until the remaining subspace contains no root vectors corresponding to the normal eigenvalues. Hence we have,

Proposition 6. *Let A be a J-self-adjoint operator in a Krein space $\mathfrak{H}_J$ with $\rho(A) \neq \emptyset$, and suppose the spectrum $\sigma(A)$ consists of only normal eigenvalues. Then $\mathfrak{H}_J$ admits the J-orthogonal decomposition as*

$$\mathfrak{H}_J = \underset{\lambda\subset\mathbb{C}^+}{[\dotplus]}\,[\mathfrak{S}_\lambda(A) \dotplus \mathfrak{S}_{\lambda^*}(A)]\,\underset{\lambda\subset\mathbb{R}}{[\dotplus]}\,\mathfrak{S}_\lambda(A)[\dotplus]\mathfrak{H}'_J, \tag{3.6}$$

where $\mathbb{C}^+$ is the set of complex numbers λ with $\Im\lambda > 0$ and $\sigma(A|_{\mathfrak{H}'_J}) = \emptyset$.

Next, we consider spontaneous $\mathcal{PT}$-symmetry breaking. Let H be a $\mathcal{PT}$-symmetric and $\mathcal{P}$-self-adjoint operator in $L^2_\mathcal{P}$, and let $\phi \in L^2_\mathcal{P}$ be an eigenvector of H belonging to an eigenvalue λ. It immediately follows from $\mathcal{PT}$-symmetry of H that

$$H\phi = \lambda\phi \quad\Longrightarrow\quad H\mathcal{PT}\phi = \lambda^*\mathcal{PT}\phi. \tag{3.7}$$

We note that $\mathcal{PT}\phi \in L^2_\mathcal{P}$ since

$$\begin{aligned} Q_{\Gamma_\infty}(\mathcal{PT}\phi, \mathcal{PT}\phi)_\mathcal{P} &= \int_{-\infty}^{\infty} \mathrm{d}x[\mathcal{PTPT}\phi(\zeta(x))]\mathcal{PT}\phi(\zeta(x)) \\ &= \int_{-\infty}^{\infty} \mathrm{d}x\,\phi(\zeta(x))\mathcal{PT}\phi(\zeta(x)) = Q_{\Gamma_\infty}(\phi, \phi)_\mathcal{P}. \end{aligned} \tag{3.8}$$

[4] In this case, the dimensions of $\mathfrak{S}_\lambda$ and $\mathfrak{S}_{\lambda^*}$ are finite and thus they admit a J-biorthogonal basis (cf lemma 1.1.31 in [45]). Note, however, that it is different from the biorthogonal basis employed in, e.g., Mostafazadeh's pseudo-Hermitian formulation [32]; the former is J-biorthogonal with respect to an indefinite J-metric while the latter is biorthogonal with respect to a positive definite inner product.

Thus, $\mathcal{PT}\phi$ is also an eigenvector of H belonging to the eigenvalue λ^*. It is evident that $\lambda^* = \lambda$ if ϕ is $\mathcal{PT}$-symmetric, namely, if $\mathcal{PT}\phi \propto \phi$. In particular, every eigenvector belonging to a simple real eigenvalue $\left(m_\lambda^{(g)} = 1\right)$, must be $\mathcal{PT}$-symmetric. On the other hand, $\lambda^* \neq \lambda$ implies $\mathcal{PT}\phi \not\propto \phi$, that is, a system exhibits spontaneous $\mathcal{PT}$-symmetry breaking whenever a non-real eigenvalue exists. Then, subtlety can emerge only when *simultaneously* $\mathcal{PT}\phi \not\propto \phi$ *and* $\lambda^* = \lambda$ for a degenerate[5] real eigenvalue λ $\left(m_\lambda^{(g)} > 1\right)$.[6] But in the latter case we can always choose the two linearly independent eigenvectors to be $\mathcal{PT}$-symmetric. In fact, we easily see

$$H\psi_\pm = \lambda\psi_\pm, \qquad \mathcal{PT}\psi_\pm = \pm\psi_\pm, \qquad \psi_\pm \equiv \tfrac{1}{2}(I \pm \mathcal{PT})\phi \in L^2_{\mathcal{P}}. \tag{3.9}$$

Hence, for an arbitrary real eigenvalue we can always have $\mathcal{PT}$-symmetric eigenvectors irrespective of the existence of that kind of spectral degeneracy. We note, however, that the $\mathcal{PT}$-symmetrically chosen eigenvectors (3.9) belonging to the same real eigenvalue are not $\mathcal{P}$-orthogonal unless $Q_{\Gamma_\infty}(\mathcal{PT}\phi, \phi)_{\mathcal{P}} \in \mathbb{R}$ since (cf, equation (3.8))

$$\begin{aligned} Q_{\Gamma_\infty}(\psi_+, \psi_-)_{\mathcal{P}} &= \frac{1}{4} Q_{\Gamma_\infty}(\phi + \mathcal{PT}\phi, \phi - \mathcal{PT}\phi)_{\mathcal{P}} \\ &= \frac{1}{2}\Im Q_{\Gamma_\infty}(\mathcal{PT}\phi, \phi)_{\mathcal{P}} = \frac{1}{2}\Im \int_{-\infty}^{\infty} \mathrm{d}x\, \phi(\zeta(x))^2. \end{aligned} \tag{3.10}$$

Conversely, if we choose the two linearly independent eigenvectors belonging to the same real eigenvalue to be $\mathcal{P}$-orthogonal, they are no longer eigenstates of $\mathcal{PT}$ in general. Hence, we should say $\mathcal{PT}$-symmetry is *ill defined* if there is a degenerate real eigenvalue for which $\mathcal{PT}$-symmetry and $\mathcal{P}$-orthogonality of the corresponding eigenvectors are incompatible. If a $\mathcal{PT}$-symmetric system A has not only a real spectrum $\sigma(A) \subset \mathbb{R}$ but also the entirely well-defined $\mathcal{PT}$-symmetry, that is, all the eigenvectors are $\mathcal{PT}$-symmetric and $\mathcal{P}$-orthogonal with each other, we shall say $\mathcal{PT}$-symmetry is unbroken *in the strong sense*. If, on the other hand, only the reality of the spectrum is ascertained, we shall say $\mathcal{PT}$-symmetry is unbroken *in the weak sense*.

It is interesting to note that the last integral expression of equation (3.10) is reminiscent of the one appeared in the context of the non-analyticity condition of eigenvalues in the coupling constant of the anharmonic oscillator [3–5]:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \psi(x; E)^2 = 0, \tag{3.11}$$

which is also the necessary and sufficient condition of the non-semi-simpleness of the eigenvalues in the case. As we shall briefly discuss in what follows, there is indeed an indication of some relationship. Although the theorems in [5] strongly rely on the parity symmetry of the anharmonic oscillator, they can be generalized to a certain extent under a more general assumption, suitable for the application to our present case. Let H be a linear differential operator in L^2 with transposition symmetry, and let λ be an eigenvalue and $\phi(\zeta(x)) \in L^2$ be the corresponding eigenvector of H. Suppose there is a unique (up to a multiplicative constant) solution $\varphi(\zeta(x); \Lambda)$ to the equation

$$(H - \Lambda)\varphi(\zeta(x); \Lambda) = 0, \tag{3.12}$$

[5] Here we note the two different meanings of *degenerate* used in this paper; the one refers to the non-triviality of the isotropic part of subspaces and the other to the multiplicity of eigenvalues.

[6] It cannot be the case for Schrödinger operators of a single variable by a similar argument leading to the no-go theorem in ordinary quantum mechanics which prohibits the existence of spectral degeneracy in one-dimensional bound-state problems.

Table 1. Aspects of root spaces and $\mathcal{PT}$-symmetry relative to the (non-)reality of eigenvalues of an arbitrary $\mathcal{PT}$-symmetric and $\mathcal{P}$-self-adjoint operator A.

Eigenvalue λ	Conditions	Root space	$\mathcal{PT}$-symmetry
Non-real		Neutral $\mathfrak{S}_\lambda$	Broken
	Normal, $\rho(A) \neq \emptyset$	Non-degenerate $\mathfrak{S}_\lambda \dot{+} \mathfrak{S}_{\lambda^*}$	
Real	Normal, $\rho(A) \neq \emptyset$	Non-degenerate $\mathfrak{S}_\lambda$	
	$m_\lambda^{(a)} > m_\lambda^{(g)} (\geqslant 1)$	Degenerate $\operatorname{Ker}(A - \lambda I)$	Possibly unbroken
	$m_\lambda^{(a)} = m_\lambda^{(g)} > 1$		Possibly ill defined
	$m_\lambda^{(g)} = 1$		Unbroken

in a neighbourhood $\mathfrak{N}_\lambda$ of λ such that $\varphi(\zeta(x); \Lambda)$ is analytic with respect to Λ in $\mathfrak{N}_\lambda$ and $\varphi(\zeta(x); \lambda) = \phi(\zeta(x))$. Differentiating equation (3.12) with respect to Λ in $\mathfrak{N}_\lambda$ we obtain

$$(H - \Lambda)\chi(\zeta(x); \Lambda) = \varphi(\zeta(x); \Lambda), \qquad \chi(\zeta(x); \Lambda) \equiv \frac{\partial \varphi(\zeta(x); \Lambda)}{\partial \Lambda}. \tag{3.13}$$

Then, if $\chi(\zeta(x); \lambda) \in L^2$, the eigenvalue λ is not semi-simple on one hand, since by virtue of equation (3.13)

$$(H - \lambda)^2 \chi(\zeta(x); \lambda) = (H - \lambda)\phi(\zeta(x)) = 0, \tag{3.14}$$

which means that $\chi(\zeta(x); \lambda)$ is an *associated* vector (namely, a root vector which is not an eigenvector) belonging to λ. On the other hand, if $\chi(\zeta(x); \lambda) \in L^2$ we have

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}x\, \phi(\zeta(x))^2 &= \int_{-\infty}^{\infty} \mathrm{d}x\, \phi(x)(H - \lambda)\chi(\zeta(x); \lambda) \\ &= \int_{-\infty}^{\infty} \mathrm{d}x [(H - \lambda)\phi(\zeta(x))]\chi(\zeta(x); \lambda) = 0, \end{aligned} \tag{3.15}$$

where we use the transposition symmetry of H, equations (2.11) and (3.13). Thus under the same condition $\chi \in L^2$, Jordan anomalous behaviour and the vanishing of the integral (3.15) take place simultaneously.

The above analysis suggests that the eigenvectors belonging to a real eigenvalue λ with $m_\lambda^{(a)} > m_\lambda^{(g)} > 1$ can be simultaneously $\mathcal{PT}$-symmetric and $\mathcal{P}$-orthogonal; the neutral eigenvector ϕ in equation (3.15) belonging to a non-semi-simple eigenvalue automatically satisfies the $\mathcal{P}$-orthogonality $Q_{\Gamma_\infty}(\psi_+, \psi_-) = 0$ from equation (3.10). Thus, in this case $\mathcal{PT}$-symmetry may be well defined and unbroken even if $\mathcal{PT}\phi \not\propto \phi$. We further note that when λ is a simple real eigenvalue $\big(m_\lambda^{(g)} = 1\big)$ and thus the corresponding eigenvector ϕ must be $\mathcal{PT}$-symmetric $\mathcal{PT}\phi \propto \phi$, the vanishing of the integral (3.15) is equivalent to the neutrality of ϕ since

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \phi(\zeta(x))^2 \propto \int_{-\infty}^{\infty} \mathrm{d}x [\mathcal{PT}\phi(\zeta(x))]\phi(\zeta(x)) = Q_{\Gamma_\infty}(\phi, \phi)_{\mathcal{P}} = 0. \tag{3.16}$$

Hence, the emergence of a neutral eigenvector in the real sector of the spectrum does not necessarily mean spontaneous $\mathcal{PT}$-symmetry breaking. Instead, it can imply Jordan anomalous behaviour as we have just discussed (the converse is always true as proposition 3 states). This kind of possibility when the algebraic multiplicity of a real eigenvalue is greater than 1 was also indicated by the analysis of Stokes multiplier in [50].

Finally, we summarize in table 1 the consequences regarding the structure of root spaces and $\mathcal{PT}$-symmetry breaking relative to the (non-)reality of eigenvalues of $\mathcal{PT}$-symmetric and $\mathcal{P}$-self-adjoint operators discussed in this section. In the fourth column of table 1 'possibly' means that more rigorous case-by-case studies would be needed for ascertaining the statement.

4. Time evolution and probability interpretation

Next, we shall examine the time evolution of quantum state vectors of a $\mathcal{PT}$-symmetric Hamiltonian. It is determined by the time-dependent Schrödinger equation:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\zeta(x),t) = H\Psi(\zeta(x),t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(\zeta(x),t), \qquad (4.1)$$

where $\Psi(z,t) \in L^2_{\mathcal{P}}$ and the Hamiltonian H is an operator acting in $L^2_{\mathcal{P}}$ and satisfying $\mathcal{PT}H = H\mathcal{PT}$. Here we note a novel feature of our framework. In the conventional treatment, we consider a Schrödinger operator of a complex variable z along a contour Γ_∞ which has mirror symmetry with respect to the imaginary axis:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(z,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V(z)\right]\Psi(z,t). \qquad (4.2)$$

Hence, if we parametrize the path as $z = \zeta(x)$ in terms of a real variable x, we have in the conventional approach

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\zeta(x),t) = \left[-\frac{\hbar^2}{2m}\frac{1}{\zeta'(x)}\frac{\partial}{\partial x}\frac{1}{\zeta'(x)}\frac{\partial}{\partial x} + V(\zeta(x))\right]\Psi(\zeta(x),t). \qquad (4.3)$$

This difference (when $\zeta(x) \neq x$) is related with the different choices of a metric. In our Krein space $L^2_{\mathcal{P}}$ the $\mathcal{P}$-metric is defined with respect to the real measure $\mathrm{d}x$ irrespective of the choice of $\zeta(x)$ and linear operators we have been considering in the space are differential operators of a real variable x, equation (2.9). In the conventional treatment, on the other hand, we consider Schrödinger operators of a complex variable $z = \zeta(x)$ and the naturally induced metric is defined in terms of the complex measure $\mathrm{d}z$, e.g. [30, 31].[7] Mathematically, this difference is just different settings of eigenvalue problems. But as we will show, our framework provides us with a natural way to construct a physically acceptable theory.

Acting the operator $\mathcal{PT}$ to the time-dependent Schrödinger equation (4.1), we have

$$-\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi^*(-\zeta^*(x),t) = H\Psi^*(-\zeta^*(x),t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi^*(-\zeta^*(x),t), \qquad (4.4)$$

where $\mathcal{PT}$-symmetry of H and the property (iii) of ζ are used. For a given initial state at $t = t_0$, $\Psi(\zeta(x),t_0)$, a formal solution to equation (4.1) is given by

$$\Psi(\zeta(x),t) = U(t,t_0)\Psi(\zeta(x),t_0), \qquad U(t,t_0) = \mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar}. \qquad (4.5)$$

In contrast to ordinary quantum theory, the Hamiltonian H is non-Hermitian in the Hilbert space L^2 but is $\mathcal{P}$-Hermitian in the Krein space $L^2_{\mathcal{P}}$. Hence, the time-evolution operator $U(t,t_0)$ is non-unitary in L^2 but would be $\mathcal{P}$-*isometric* (possibly $\mathcal{P}$-*unitary* when H is $\mathcal{P}$-self-adjoint) in $L^2_{\mathcal{P}}$ (cf definition 2.5.1 in [45]). To show the latter formally, we first note that for a $\mathcal{PT}$-symmetric Hamiltonian H we have

$$\mathcal{PT}U(t,t_0) = \mathcal{PT}\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n(t-t_0)^n}{\hbar^n n!}H^n = \sum_{n=0}^{\infty}\frac{\mathrm{i}^n(t-t_0)^n}{\hbar^n n!}H^n\mathcal{PT} = U(t_0,t)\mathcal{PT}. \qquad (4.6)$$

The transposition of $U(t,t_0)$ reads

$$U(t,t_0)^t = \left(\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n(t-t_0)^n}{\hbar^n n!}H^n\right)^t = \sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n(t-t_0)^n}{\hbar^n n!}H^n = U(t,t_0), \qquad (4.7)$$

[7] As a set of square integrable complex functions with respect to each metric they are identical as has been shown in equations (2.4)–(2.7). Hence, every wavefunction $\Psi(z,t)$ in the conventional framework (4.2) also belongs to $L^2_{\mathcal{P}}(\Gamma_\infty)$. But we note that the latter metric is not Hermitian in general.

that is, the time-evolution operator has transposition symmetry so long as the Hamiltonian has. Thus, for an arbitrary $\Psi = \Psi(\zeta(x), t_0) \in \mathfrak{D}(U)$ and a time t we obtain

$$\begin{aligned} Q_{\Gamma_\infty}(U\Psi, U\Psi)_{\mathcal{P}} &= \int_{-\infty}^{\infty} \mathrm{d}x\, [\mathcal{PT}U(t,t_0)\Psi(\zeta(x),t_0)]\, U(t,t_0)\Psi(\zeta(x),t_0) \\ &= \int_{-\infty}^{\infty} \mathrm{d}x\, [U(t_0,t)\mathcal{PT}\Psi(\zeta(x),t_0)]\, U(t,t_0)\Psi(\zeta(x),t_0) \\ &= \int_{-\infty}^{\infty} \mathrm{d}x\, [\mathcal{PT}\Psi(\zeta(x),t_0)]\, U(t_0,t)U(t,t_0)\Psi(\zeta(x),t_0) \\ &= Q_{\Gamma_\infty}(\Psi,\Psi)_{\mathcal{P}}, \end{aligned} \tag{4.8}$$

which shows the $\mathcal{P}$-isometric property of $U(t, t_0)$. Putting mathematical rigour aside, the above result indicates that we should replace the requirement of unitarity, of S matrix for instance, imposed in ordinary quantum theory by that of $\mathcal{P}$-unitarity in the case of $\mathcal{PT}$-symmetric quantum theory. For a more rigorous treatment, namely, a counterpart of Stone's theorem in indefinite metric spaces, see [51].

Next, we shall address the issue of the probability interpretation. From the time-dependent Schrödinger equation (4.1) and its $\mathcal{P}$-adjoint version (4.4), the following continuity equation, which is a generalization of the one derived in [47], holds for arbitrary solutions $\Psi_i \in L^2_{\mathcal{P}}$ $(i = 1, 2)$ of equation (4.1):

$$\frac{\partial}{\partial t}[\Psi_1^*(-\zeta^*(x),t)\Psi_2(\zeta(x),t)] = -\frac{\partial}{\partial x}\mathcal{J}(\zeta(x),t), \tag{4.9}$$

where the current density $\mathcal{J}$ is defined by

$$\mathcal{J}(\zeta(x),t) = \frac{\hbar}{2m\mathrm{i}}\left[\Psi_1^*(-\zeta^*(x),t)\frac{\partial}{\partial x}\Psi_2(\zeta(x),t) - \Psi_2(\zeta(x),t)\frac{\partial}{\partial x}\Psi_1^*(-\zeta^*(x),t)\right]. \tag{4.10}$$

Integrating both sides of the continuity equation (4.9) with respect to $x \in (-\infty, \infty)$ we obtain the conservation law of the $\mathcal{P}$-metric:

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty}\mathrm{d}x\,\Psi_1^*(-\zeta^*(x),t)\Psi_2(\zeta(x),t) = \frac{\partial}{\partial t}Q_{\Gamma_\infty}(\Psi_1,\Psi_2)_{\mathcal{P}} = 0. \tag{4.11}$$

This means that though the $\mathcal{P}$-metric is indefinite, the character of each state vector, namely, positivity, negativity, or neutrality, remains unchanged in the time evolution. The conservation law of this kind is indispensable for the probability interpretation. To examine further the possibility of it in our framework, we first note that the emergence of negative norm itself would not immediately mean the inability of it since probabilities of physical process are eventually given by the *absolute value* of a certain metric (matrix element) but not by its complex value itself. Thus, we should here stress the fact that the true obstacle is the violation of the Cauchy–Schwarz inequality

$$|Q(\phi,\psi)|^2 \leqslant Q(\phi,\phi)Q(\psi,\psi), \tag{4.12}$$

in indefinite spaces, where $Q(\cdot,\cdot)$ is a sesquilinear Hermitian form $\mathfrak{F}\times\mathfrak{F} \to \mathbb{C}$. The inequality ensures that the absolute value of an arbitrary matrix element $Q(\phi,\psi)$ is less than or equal to 1 so long as every vector in $\mathfrak{F}$ is normalized with respect to $Q(\cdot,\cdot)$, from which we can assign probability to the quantity $|Q(\phi,\psi)|^2$. To see the violation of the inequality (4.12) in an indefinite space, let us consider a two-dimensional vector space $\mathbb{C}^2$ equipped with an indefinite metric Q defined by $Q(\phi,\psi) = a_1^*b_1 - a_2^*b_2$ for $\phi = (a_1, a_2)^t$ and $\psi = (b_1, b_2)^t$. The two vectors $e_+ = (\sqrt{2}, -1)^t$ and $e_- = (1, \sqrt{2})^t$ are normalized in the sense of $|Q(e_\pm, e_\pm)| = 1$, but $|Q(e_-, e_+)| = 2\sqrt{2} \nleqslant 1$. Hence, the fact that the Cauchy–Schwarz inequality holds at most in semi-definite spaces (cf proposition 1.1.16 in [45]) indicates that we must always restrict ourselves to considering quantum process in a semi-definite subspace in order to make a probability interpretation in any kind of quantum-like theory with an indefinite metric.

This observation naturally leads us to consider a pair of subspaces $(\mathfrak{L}_+, \mathfrak{L}_-)$ of the Krein space $L^2_{\mathcal{P}}$ where $\mathfrak{L}_+$ (respectively, $\mathfrak{L}_-$) is a non-negative (respectively, a non-positive) subspace of $L^2_{\mathcal{P}}$ and $\mathfrak{L}_+[\perp]\mathfrak{L}_-$. This kind of pair corresponds to what is called a *dual pair* (definition 1.10.1 in [45]). Then, in each semi-definite subspace $\mathfrak{L}_+$ or $\mathfrak{L}_-$, the inequality (4.12) with $Q(\cdot,\cdot) = Q_{\Gamma_\infty}(\cdot,\cdot)_{\mathcal{P}}$ certainly holds. However, the situation is not yet satisfactory. To see this, suppose, at the initial time t_0, we have a normalized positive physical state $\Psi_{t_0} \equiv \Psi(\zeta(x), t_0) \in \mathfrak{L}_+$. After the time evolution determined by equation (4.5), the state $\Psi_t \equiv \Psi(\zeta(x), t)$ at $t > t_0$ remains positive by virtue of the conservation law (4.11). However, it does not necessarily mean $\Psi_t \in \mathfrak{L}_+$; in general we have

$$\Psi_t = \Psi_t^+ + \Psi_t^-, \qquad \Psi_t^+ \in \mathfrak{L}_+, \qquad \Psi_t^- \in L^2_{\mathcal{P}} \backslash \mathfrak{L}_+, \qquad Q_{\Gamma_\infty}(\Psi_t, \Psi_t)_{\mathcal{P}} > 0, \tag{4.13}$$

with a non-zero $\Psi_t^- \in L^2_{\mathcal{P}} \backslash \mathfrak{L}_+$. As a consequence, we cannot consider the matrix element $Q_{\Gamma_\infty}(\Psi_t, \Psi_{t_0})_{\mathcal{P}}$ in the initially prepared positive semi-definite subspace $\mathfrak{L}_+$. This situation would be hardly acceptable since we cannot choose and fix beforehand a semi-definite subspace where we should consider a physical process. This difficulty would not arise only when the Hamiltonian H, and thus the time-evolution operator U, preserves the initial semi-definite subspaces $\mathfrak{L}_+$ and $\mathfrak{L}_-$ separately, namely, $\overline{\mathfrak{D}(H) \cap \mathfrak{L}_\pm} = \mathfrak{L}_\pm$ and $H(\mathfrak{D}(H) \cap \mathfrak{L}_\pm) \subset \mathfrak{L}_\pm$. If the latter is the case, the state vector Ψ_t at every time $t > t_0$ stays in the semi-definite subspace $\mathfrak{L}_+$ or $\mathfrak{L}_-$ if the initial state Ψ_{t_0} is an element of $\mathfrak{L}_+$ or $\mathfrak{L}_-$, respectively, and it makes sense to regard the quantity $Q_{\Gamma_\infty}(\Psi_t, \Psi_{t_0})_{\mathcal{P}}$ in the corresponding subspace as a transition amplitude, as in ordinary quantum theory. Furthermore, for arbitrary $\Psi_{t_1}^+ \equiv \Psi^+(\zeta(x), t_1) \in \mathfrak{L}_+$ and $\Psi_{t_2}^- \equiv \Psi^-(\zeta(x), t_2) \in \mathfrak{L}_-$ we have $Q_{\Gamma_\infty}\big(\Psi_{t_1}^+, \Psi_{t_2}^-\big)_{\mathcal{P}} = 0$, that is, there is no transition between states in $\mathfrak{L}_+$ and $\mathfrak{L}_-$. But both $\mathfrak{L}_+$ and $\mathfrak{L}_-$ should be wide enough such that every element of $L^2_{\mathcal{P}}$ can contribute dynamics. This naturally leads to the requirement that $\mathfrak{L}_+ \in \mathfrak{M}^+\big(L^2_{\mathcal{P}}\big)$ and $\mathfrak{L}_- \in \mathfrak{M}^-\big(L^2_{\mathcal{P}}\big)$ where $\mathfrak{M}^+(\mathfrak{H}_J)$ $(\mathfrak{M}^-(\mathfrak{H}_J))$ is the set of all *maximal* non-negative (non-positive) subspaces of a Krein space $\mathfrak{H}_J$, respectively. That is, $P^\pm \mathfrak{L}_\pm = L^2_{\mathcal{P}\pm}$ where $P^\pm$ and $L^2_{\mathcal{P}\pm}$ are defined by equations (2.18) and (2.19), respectively (cf theorem 1.4.5 in [45]). However, operators in a Krein space do not always have such a pair of invariant maximal semi-definite subspaces, and thus we now arrive at a criterion for a given Hamiltonian acting in $L^2_{\mathcal{P}}$ to be physically acceptable:

Criterion 1. A $\mathcal{P}$-self-adjoint Hamiltonian H can be physically acceptable if and only if it admits an invariant maximal dual pair $(\mathfrak{L}_+, \mathfrak{L}_-)$, and thus, so does the one-parameter family of $\mathcal{P}$-unitary operators $U = \mathrm{e}^{-\mathrm{i}tH}$.

An immediate consequence of the inequality (4.12), which now holds in each invariant semi-definite subspace $\mathfrak{L}_\pm$, is that every neutral vector $\psi_\pm^{(0)} \in \mathfrak{L}_\pm$ is isotropic in each $\mathfrak{L}_\pm$, namely, $\psi_\pm^{(0)}[\perp]\mathfrak{L}_\pm$. Hence, every transition amplitude with initial or final neutral state is identically zero. So, it is natural to consider a decomposition of each semi-definite sector $\mathfrak{L}_\pm$ into its isotropic part $\mathfrak{L}_\pm^0$ and a definite part $\mathfrak{L}_{\pm\pm}$:

$$\mathfrak{L}_\pm = \mathfrak{L}_\pm^0[\dot{+}]\mathfrak{L}_{\pm\pm}, \qquad \mathfrak{L}_\pm^0 = \mathfrak{L}_\pm \cap \mathfrak{L}_\pm^{[\perp]}, \tag{4.14}$$

where $\mathfrak{L}_{++}$ $(\mathfrak{L}_{--})$ is a positive (negative) definite subspace, respectively. It is now apparent that the $\mathcal{P}$-metric restricted in each $\mathfrak{L}_{\pm\pm}$, namely, $\pm Q_{\Gamma_\infty}(\phi, \psi)_{\mathcal{P}}$ $(\phi, \psi \in \mathfrak{L}_{\pm\pm})$ is positive definite. Therefore, we can finally make a probability interpretation in each definite subspace $\mathfrak{L}_{\pm\pm}$ separately, provided that every vector $\psi_\pm$ in $\mathfrak{L}_{\pm\pm}$ is normalized with respect to the *intrinsic $\mathcal{P}$-norm* $|\cdot|_{\mathfrak{L}_{\pm\pm}}$ on $\mathfrak{L}_{\pm\pm}$ such that

$$|\psi_\pm|_{\mathfrak{L}_{\pm\pm}} \equiv \sqrt{|Q_{\Gamma_\infty}(\psi_\pm, \psi_\pm)_{\mathcal{P}}|} = 1. \tag{4.15}$$

Considering mathematical subtleties such as the continuity of the $\mathcal{P}$-metric restricted on to $\mathfrak{L}_{\pm\pm}$, we would conclude that $\mathfrak{L}_{\pm\pm}$ should be *uniformly* definite, which in our case means the equivalence between the intrinsic $\mathcal{P}$-norm $|\psi_\pm|_{\mathfrak{L}_{\pm\pm}}$ and the Hilbert space norm $\|\psi_\pm\| \equiv \sqrt{Q_{\Gamma_\infty}(\psi_\pm, \psi_\pm)}$ defined in L^2 for all $\psi_\pm \in \mathfrak{L}_{\pm\pm}$, respectively (cf section 1.5 in [45]). Hence, we arrive at the second criterion:

Criterion 2. Each of the subspaces $\mathfrak{L}_\pm$ in criterion 1 should admit a decomposition $\mathfrak{L}_\pm = \mathfrak{L}_\pm^0[\dot{+}]\mathfrak{L}_{\pm\pm}$ into a $\mathcal{P}$-orthogonal direct sum of its isotropic part $\mathfrak{L}_\pm^0$ and a uniformly definite subspace $\mathfrak{L}_{\pm\pm}$, respectively.

The subspaces $\mathfrak{L}_{\pm\pm}$ are then complete relative to the intrinsic $\mathcal{P}$-norm $|\cdot|_{\mathfrak{L}_{\pm\pm}}$, respectively (proposition 1.5.6 in [45]). Thus $\mathfrak{L}_{\pm\pm}$ with the positive definite *intrinsic $\mathcal{P}$-metric* $\pm Q_{\Gamma_\infty}(\cdot,\cdot)_{\mathcal{P}}|_{\mathfrak{L}_{\pm\pm}}$ are Hilbert spaces, respectively. In particular, the time-evolution operator in equation (4.5) restricted on to $\mathfrak{L}_{\pm\pm}$, $U(t, t_0)|_{\mathfrak{L}_{\pm\pm}}$ is unitary in each of the Hilbert spaces $\mathfrak{L}_{\pm\pm}$.

A natural way to construct physical spaces is to consider the quotient spaces $\tilde{\mathfrak{L}}_\pm = \mathfrak{L}_\pm \big/ \mathfrak{L}_\pm^0$ in each of the sectors. An element $\tilde{\psi}_\pm \in \tilde{\mathfrak{L}}_\pm$ is defined by the formula $\tilde{\psi}_\pm = \psi_\pm + \mathfrak{L}_\pm^0$ for each $\psi_\pm \in \mathfrak{L}_{\pm\pm}$, respectively. An induced positive definite metric $\tilde{Q}_\pm(\cdot,\cdot)$ is respectively given by

$$\tilde{Q}_\pm(\tilde{\phi}_\pm, \tilde{\psi}_\pm) = \pm Q_{\Gamma_\infty}(\phi_\pm, \psi_\pm)_{\mathcal{P}}, \qquad \phi_\pm, \psi_\pm \in \mathfrak{L}_{\pm\pm}. \tag{4.16}$$

Then, the quotient space $\tilde{\mathfrak{L}}_+$ ($\tilde{\mathfrak{L}}_-$) is isometrically (skew-symmetrically) isomorphic to the positive (negative) definite subspace $\mathfrak{L}_{++}$ ($\mathfrak{L}_{--}$), respectively (proposition 1.1.23 in [45]). This kind of prescription was already employed, e.g., in the BRST quantization of non-Abelian gauge theories; the whole state vector space of the latter systems is also indefinite and the positive definite physical space is given by the quotient space $\mathrm{Ker}\mathcal{Q}_B/\mathrm{Im}\mathcal{Q}_B$, where $\mathcal{Q}_B$ is a nilpotent BRST charge [52] and $\mathrm{Im}\mathcal{Q}_B$ is the BRST-exact neutral subspace of the BRST-closed non-negative state vector space $\mathrm{Ker}\mathcal{Q}_B$ [53] (for a review see, e.g. [54]).

Finally, we can classify the set of the systems which satisfy criteria 1 and 2 according to the dimension of the subspaces $\mathfrak{L}_\pm^0$ and $\mathfrak{L}_{\pm\pm}$:

Case 1. $\dim \mathfrak{L}_\pm^0 < \infty$ and $\dim \mathfrak{L}_{\pm\pm} = \infty$, respectively.

Case 2. $\dim \mathfrak{L}_\pm^0 = \infty$ and $\dim \mathfrak{L}_{\pm\pm} = \infty$, respectively.

Case 3. $\dim \mathfrak{L}_\pm^0 = \infty$ and $\dim \mathfrak{L}_{\pm\pm} < \infty$, respectively.

In case 3, the physically relevant space $\mathfrak{L}_{++}$ or $\mathfrak{L}_{--}$ is finite dimensional and thus the system, at least as physical, would be less interesting. So, our main concern would be for systems corresponding to cases 1 and 2. In connection with case 1, we recall a special class of semi-definite subspaces of a Krein space. A non-negative (non-positive) subspace $\mathfrak{L}$ of a Krein space $\mathfrak{H}_J$ is called a subspace of *class* h^+ (*class* h^-) if it admits a decomposition $\mathfrak{L} = \mathfrak{L}^0[\dot{+}]\mathfrak{L}^+$ ($\mathfrak{L} = \mathfrak{L}^0[\dot{+}]\mathfrak{L}^-$) into a direct J-orthogonal sum of a *finite-dimensional isotropic* subspace $\mathfrak{L}^0$ ($\dim \mathfrak{L}^0 < \infty$) and a *uniformly positive* (*uniformly negative*) subspace $\mathfrak{L}^+$ ($\mathfrak{L}^-$) [55]. We easily see that in case 1 the semi-definite subspace $\mathfrak{L}_+$ ($\mathfrak{L}_-$) belongs to the class h^+ (h^-), respectively. We will later see in section 7 that there exists a class of $\mathcal{P}$-self-adjoint operators which satisfies criteria 1 and 2 corresponding to case 1.

5. Uncertainty relation

In the previous section, we have derived the criteria for a quantum-like theory with an indefinite metric to be physically acceptable from the viewpoint of the probability interpretation. They are, of course, not sufficient at all. One of the most crucial criteria is the existence of a secure correspondence to classical theory. In this and the next sections, we shall discuss in detail the correspondence between our $\mathcal{PT}$-symmetric theory in the Krein space $L^2_{\mathcal{P}}$ and classical mechanics. Two principal issues shall be addressed, namely, uncertainty relation in this section, and classical equations of motion in the next section.

The results in the preceding section indicate that the $\mathcal{P}$-metric in the Krein space $L^2_{\mathcal{P}}$ rather than the inner product (2.2) in the Hilbert space L^2 plays a central role in $\mathcal{PT}$-symmetric quantum theory. Hence, we define the expectation value of an operator $\hat{O}$ in the Krein space $L^2_{\mathcal{P}}$ by

$$\langle \hat{O} \rangle_{\mathcal{P}} \equiv Q_{\Gamma_\infty}(\Psi, O\Psi)_{\mathcal{P}} = \int_{-\infty}^{\infty} \mathrm{d}x\, \Psi^*(-\zeta^*(x), t) O \Psi(\zeta(x), t), \tag{5.1}$$

where O denotes the x-representation of the operator $\hat{O}$ and $\Psi \in L^2_{\mathcal{P}}$ is a solution of the time-dependent Schrödinger equation (4.1). We shall call the quantity defined by equation (5.1) *$\mathcal{P}$-expectation value*. It reduces to the one considered in e.g. [42] when $\Gamma_\infty = \mathbb{R}$.

We first examine $\mathcal{P}$-adjoint operators relevant in both classical and quantum theories, namely, scalar multiplication, position and momentum operators. From the relation (2.22) we immediately have

$$\lambda^c = \mathcal{P}\lambda^\dagger \mathcal{P} = \lambda^* \qquad (\lambda \in \mathbb{C}), \tag{5.2}$$

$$\hat{x}^c = \mathcal{P}\hat{x}^\dagger \mathcal{P} = -\hat{x}, \tag{5.3}$$

$$\hat{p}^c = \mathcal{P}\hat{p}^\dagger \mathcal{P} = -\hat{p}. \tag{5.4}$$

The last two relations show that both the position and momentum operators are *anti-$\mathcal{P}$-Hermitian* in the Krein space $L^2_{\mathcal{P}}$. Since physical quantities are usually expressed as functions of position and momentum, we shall mainly consider anti-$\mathcal{P}$-Hermitian operators as well as $\mathcal{P}$-Hermitian operators.

It follows from the Hermiticity (2.14) of the $\mathcal{P}$-metric that $\mathcal{P}$-expectation values (5.1) of (anti-)$\mathcal{P}$-Hermitian operators are all real (purely imaginary), respectively:

$$\begin{aligned} \langle \hat{A} \rangle_{\mathcal{P}}^* &= Q^*_{\Gamma_\infty}(\Psi, A\Psi)_{\mathcal{P}} = Q_{\Gamma_\infty}(A\Psi, \Psi)_{\mathcal{P}} \\ &= Q_{\Gamma_\infty}(\Psi, A^c\Psi)_{\mathcal{P}} = \pm Q_{\Gamma_\infty}(\Psi, A\Psi)_{\mathcal{P}} \\ &= \pm\langle \hat{A} \rangle_{\mathcal{P}} \qquad \text{for} \quad \hat{A}^c = \pm \hat{A}. \end{aligned} \tag{5.5}$$

Next, we shall consider a commutation relation between two linear operators

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = \mathrm{i}\hbar \hat{C}. \tag{5.6}$$

It is easy to see that the operator $\hat{C}$ is $\mathcal{P}$-Hermitian when both $\hat{A}$ and $\hat{B}$ are simultaneously either $\mathcal{P}$-Hermitian or anti-$\mathcal{P}$-Hermitian, and that $\hat{C}$ is anti-$\mathcal{P}$-Hermitian when one of $\hat{A}$ and $\hat{B}$ is $\mathcal{P}$-Hermitian and the other is anti-$\mathcal{P}$-Hermitian.

As in the case of ordinary quantum mechanics, we introduce the *deviation* operator $\Delta\hat{A}$ of $\hat{A}$ by

$$\Delta\hat{A} = \langle \hat{A} \rangle_{\mathcal{P}} - \hat{A}. \tag{5.7}$$

The deviation operator $\Delta\hat{A}$ is (anti-)$\mathcal{P}$-Hermitian when $\hat{A}$ is (anti-)$\mathcal{P}$-Hermitian, respectively; for from equations (5.2) and (5.5),

$$\begin{aligned} (\Delta\hat{A})^c &= \langle \hat{A} \rangle_{\mathcal{P}}^* - \hat{A}^c = \pm\langle \hat{A} \rangle_{\mathcal{P}} \mp \hat{A} \\ &= \pm\Delta\hat{A} \qquad \text{for} \quad \hat{A}^c = \pm\hat{A} \end{aligned} \tag{5.8}$$

follows. For two operators $\hat{A}$ and $\hat{B}$ satisfying the commutation relation (5.6), the corresponding deviation operators $\Delta\hat{A}$ and $\Delta\hat{B}$ satisfy the same relation:

$$[\Delta\hat{A}, \Delta\hat{B}] = \mathrm{i}\hbar\hat{C}. \tag{5.9}$$

We are now in a position to discuss the uncertainty relation in $\mathcal{PT}$-symmetric quantum theory. Due to the indefiniteness of the $\mathcal{P}$-metric, however, it would be difficult to establish a certain inequality in the whole Krein space; we recall the violation of the inequality (4.12). But the discussion in the previous section shows that we must always consider physics in a semi-definite subspace $\mathfrak{L}_-$ or $\mathfrak{L}_+$. In this sense, we would satisfy ourselves by establishing an uncertainty relation which holds only in semi-definite subspaces $\mathfrak{L}_\pm$.

Let us suppose that $\hat{A}$ and $\hat{B}$ are respectively either $\mathcal{P}$-Hermitian or anti-$\mathcal{P}$-Hermitian, and that both the vectors $\Delta A\Psi$ and $\Delta B\Psi$ are simultaneously elements of a given semi-definite subspace $\mathfrak{L}_+$ or $\mathfrak{L}_-$. Under these assumptions, we first note that

$$\begin{aligned} |Q_{\Gamma_\infty}(\Psi, [\Delta A, \Delta B]\Psi)_{\mathcal{P}}| &\leqslant |Q_{\Gamma_\infty}(\Psi, \Delta A\Delta B\Psi)_{\mathcal{P}}| + |Q_{\Gamma_\infty}(\Psi, \Delta B\Delta A\Psi)_{\mathcal{P}}| \\ &= |Q_{\Gamma_\infty}(\Delta A\Psi, \Delta B\Psi)_{\mathcal{P}}| + |Q_{\Gamma_\infty}(\Delta B\Psi, \Delta A\Psi)_{\mathcal{P}}| \\ &= 2|Q_{\Gamma_\infty}(\Delta A\Psi, \Delta B\Psi)_{\mathcal{P}}|. \end{aligned} \tag{5.10}$$

Taking square of the above and applying the inequality (4.12) with $\phi = \Delta A\Psi$ and $\psi = \Delta B\Psi$ we obtain

$$\begin{aligned} |Q_{\Gamma_\infty}(\Psi, [\Delta A, \Delta B]\Psi)_{\mathcal{P}}|^2 &\leqslant 4|Q_{\Gamma_\infty}(\Delta A\Psi, \Delta B\Psi)_{\mathcal{P}}|^2 \\ &\leqslant 4Q_{\Gamma_\infty}(\Delta A\Psi, \Delta A\Psi)_{\mathcal{P}} Q_{\Gamma_\infty}(\Delta B\Psi, \Delta B\Psi)_{\mathcal{P}} \\ &= 4Q_{\Gamma_\infty}(\Psi, (\Delta A)^2\Psi)_{\mathcal{P}} Q_{\Gamma_\infty}(\Psi, (\Delta B)^2\Psi)_{\mathcal{P}}. \end{aligned} \tag{5.11}$$

By the definition of $\mathcal{P}$-expectation value (5.1) and the commutation relation (5.9), we finally obtain

$$\langle(\Delta\hat{A})^2\rangle_{\mathcal{P}}\langle(\Delta\hat{B})^2\rangle_{\mathcal{P}} \geqslant \frac{\hbar}{4}|\langle\hat{C}\rangle_{\mathcal{P}}|^2, \qquad \Delta A\Psi, \Delta B\Psi \in \mathfrak{L}_+ \text{ or } \mathfrak{L}_-, \tag{5.12}$$

which can be regarded as an uncertainty relation in $\mathcal{PT}$-symmetric quantum theory.

6. Classical–quantum correspondence

In this section, we shall investigate and discuss classical–quantum correspondence in the $\mathcal{PT}$-symmetric theory. The classical equations of motion subjected to $\mathcal{PT}$-symmetric potentials were analysed in detail in [14, 56, 57]. Since $\mathcal{PT}$-symmetric potentials are generally non-real, the classical motion were considered in a complex plane. The results indicate a strong correlation between classical and quantum systems especially from the viewpoint of $\mathcal{PT}$-symmetry breaking though up to now no correspondence principle between them in $\mathcal{PT}$-symmetric theory has been explicitly established. The purposes of this section are first to establish the $\mathcal{PT}$-symmetric version of Ehrenfest's theorem and then to discuss its consequences. As we will see, it provides a novel correspondence to classical systems completely different from the conventional one in the literature.

Let us first examine the time derivative of the $\mathcal{P}$-expectation value of the position operator $\hat{x}$:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle_{\mathcal{P}} &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\mathrm{d}x\,\Psi^*(-\zeta^*(x), t)x\Psi(\zeta(x), t) \\ &= \int_{-\infty}^{\infty}\mathrm{d}x\left[\frac{\partial\Psi^*(-\zeta^*(x), t)}{\partial t}x\Psi(\zeta(x), t) + \Psi^*(\zeta^*(x), t)x\frac{\partial\Psi(\zeta(x), t)}{\partial t}\right]. \end{aligned} \tag{6.1}$$

Applying equations (4.1) and (4.4), and integrating by parts, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle_{\mathcal{P}} = \frac{\hbar}{2m\mathrm{i}}\int_{-\infty}^{\infty}\mathrm{d}x\left[\frac{\partial^2\Psi^*(-\zeta^*(x), t)}{\partial x^2}x\Psi(\zeta(x), t) - \Psi^*(-\zeta^*(x), t)x\frac{\partial^2\Psi(\zeta(x), t)}{\partial x^2}\right]$$

$$
\begin{aligned}
&= -\frac{\hbar}{2m\mathrm{i}} \int_{-\infty}^{\infty} \mathrm{d}x \left[\frac{\partial \Psi^*(-\zeta^*(x), t)}{\partial x} \Psi(\zeta(x), t) - \Psi^*(-\zeta^*(x), t) \frac{\partial \Psi(\zeta(x), t)}{\partial x} \right] \\
&= \frac{\hbar}{m\mathrm{i}} \int_{-\infty}^{\infty} \mathrm{d}x\, \Psi^*(-\zeta^*(x), t) \frac{\partial \Psi(\zeta(x), t)}{\partial x}.
\end{aligned} \tag{6.2}
$$

Next, the time derivative of the $\mathcal{P}$-expectation value of the momentum operator $\hat{p}$ reads

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{p} \rangle_{\mathcal{P}} &= -\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \int_{-\infty}^{\infty} \mathrm{d}x\, \Psi^*(-\zeta^*(x), t) \frac{\partial \Psi(\zeta(x), t)}{\partial x} \\
&= \mathrm{i}\hbar \int_{-\infty}^{\infty} \mathrm{d}x \left[\frac{\partial \Psi^*(-\zeta^*(x), t)}{\partial x} \frac{\partial \Psi(\zeta(x), t)}{\partial t} - \frac{\partial \Psi^*(-\zeta^*(x), t)}{\partial t} \frac{\partial \Psi(\zeta(x), t)}{\partial x} \right].
\end{aligned} \tag{6.3}
$$

Again, applying equations (4.1) and (4.4), and integrating by parts we obtain

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{p} \rangle_{\mathcal{P}} &= \int_{-\infty}^{\infty} \mathrm{d}x \left[\frac{\partial \Psi^*(-\zeta^*(x), t)}{\partial x} V(x) \Psi(\zeta(x), t) + \Psi^*(-\zeta^*(x), t) V(x) \frac{\partial \Psi(\zeta(x), t)}{\partial x} \right] \\
&= -\int_{-\infty}^{\infty} \mathrm{d}x\, \Psi^*(-\zeta^*(x), t) \frac{\mathrm{d}V(x)}{\mathrm{d}x} \Psi(\zeta(x), t).
\end{aligned} \tag{6.4}
$$

Hence from equations (6.2) and (6.4) we obtain a set of equations of motion:

$$
m \frac{\mathrm{d}\langle \hat{x} \rangle_{\mathcal{P}}}{\mathrm{d}t} = \langle \hat{p} \rangle_{\mathcal{P}}, \qquad \frac{\mathrm{d}\langle \hat{p} \rangle_{\mathcal{P}}}{\mathrm{d}t} = -\langle V'(\hat{x}) \rangle_{\mathcal{P}}, \tag{6.5}
$$

which can be regarded as an alternative to *Ehrenfest's theorem* in the ordinary Hermitian quantum mechanics. The most important point is that in the case of $\mathcal{PT}$-symmetric systems it holds for the expectation values with respect to the indefinite $\mathcal{P}$-metric in $L^2_{\mathcal{P}}$ but not with respect to the positive definite metric in L^2. As we will show in what follows, it leads to novel consequences and features of the classical-quantum correspondence in $\mathcal{PT}$-symmetric theory.

First of all, we recall the fact that both the position and momentum operators are anti-$\mathcal{P}$-Hermitian in the Krein space, (5.3) and (5.4). We can easily check that for any $\mathcal{PT}$-symmetric Hamiltonian the first derivative of the potential $V'(x)$ is also anti-$\mathcal{P}$-Hermitian:

$$
\begin{aligned}
Q_{\Gamma_\infty}(\phi, V'(x)^c \psi)_{\mathcal{P}} &= \int_{-\infty}^{\infty} \mathrm{d}x \frac{\mathrm{d}V^*(-x)}{\mathrm{d}(-x)} \phi^*(-\zeta^*(x)) \psi(\zeta(x)) \\
&= -\int_{-\infty}^{\infty} \mathrm{d}x\, \phi^*(-\zeta^*(x)) \frac{\mathrm{d}V(x)}{\mathrm{d}x} \psi(\zeta(x)) \\
&= -Q_{\Gamma_\infty}(\phi, V'(x)\psi)_{\mathcal{P}}.
\end{aligned} \tag{6.6}
$$

Thus, all the $\mathcal{P}$-expectation values appeared in the equations of motion (6.5), which should correspond to the classical quantities, are purely imaginary, cf equation (5.5).

This consequence naturally let us consider the real quantities x_I and p_I as classical 'canonical' coordinates defined by

$$
x(t) = -\mathrm{i}x_I(t) \in \mathrm{i}\mathbb{R}, \qquad p(t) = -\mathrm{i}p_I(t) \in \mathrm{i}\mathbb{R}. \tag{6.7}
$$

Regarding the potential term, we first note that any $\mathcal{PT}$-symmetric potential satisfying $V^*(-x) = V(x)$ $(x \in \mathbb{R})$ can be expressed as

$$
V(x) = -U(\mathrm{i}x), \tag{6.8}
$$

where U is a real-valued function on $\mathbb{R}$, namely, $U : \mathbb{R} \to \mathbb{R}$. To show this, we begin with the Laurant expansion of the potential function:

$$
V(z) = \sum_{n=-\infty}^{\infty} a_n z^n, \qquad a_n, z \in \mathbb{C}. \tag{6.9}
$$

Then $\mathcal{PT}$-symmetry of V on $\mathbb{R}$ is equivalent to

$$a_n^* = (-1)^n a_n, \qquad \forall n \in \mathbb{Z}, \tag{6.10}$$

that is, a_n is real (purely imaginary) for all even (odd) integer n. Thus, without loss of generality we can put for all n

$$a_n = \mathrm{i}^n b_n, \qquad b_n \in \mathbb{R}. \tag{6.11}$$

Hence, the $\mathcal{PT}$-symmetric potential reads

$$V(x) = \sum_{n=-\infty}^{\infty} b_n (\mathrm{i}x)^n \equiv -U(\mathrm{i}x), \tag{6.12}$$

where $U(y) = -\sum_n b_n y^n$ is in fact a real-valued function on $\mathbb{R}$. As a result, we have in particular

$$\frac{\mathrm{d}V(x)}{\mathrm{d}x} = -\frac{\mathrm{d}U(\mathrm{i}x)}{\mathrm{d}x} = -\mathrm{i}U'(\mathrm{i}x). \tag{6.13}$$

Therefore, if we assume the classical–quantum correspondence for the purely imaginary quantities as

$$\langle\hat{x}\rangle_{\mathcal{P}} \longleftrightarrow x(t) = -\mathrm{i}x_I(t), \qquad \langle\hat{p}\rangle_{\mathcal{P}} \longleftrightarrow p(t) = -\mathrm{i}p_I(t), \tag{6.14}$$

the equations of motion for the real 'canonical' coordinates x_I and p_I, which correspond to equation (6.5), read[8]

$$m\frac{\mathrm{d}x_I(t)}{\mathrm{d}t} = p_I(t), \qquad \frac{\mathrm{d}p_I(t)}{\mathrm{d}t} = -U'(x_I). \tag{6.15}$$

That is, they constitute a real dynamical system subject to the real-valued potential U.

This consequence is quite striking. Although $\mathcal{PT}$-symmetric quantum potentials are complex and supports of square integrable wavefunctions are complex contours in general, we can establish a correspondence of such a $\mathcal{PT}$-symmetric quantum system to a real classical system. Conversely, for every classical dynamical system described by a real potential $U(x)$, we can construct the corresponding $\mathcal{PT}$-symmetric quantum potential $V(x)$ through the relation (6.12). In what follows, we exhibit several $\mathcal{PT}$-symmetric quantum potentials V in the literature and the corresponding classical potentials U as examples.

- Example 1 in [14]:

$$V(x) = x^{2K}(\mathrm{i}x)^{\epsilon}. \tag{6.16}$$

$$U(x) = (-1)^{K+1}x^{2K+\epsilon}. \tag{6.17}$$

- Example 2 in [40]:

$$V(x) = -(\mathrm{i}x)^{2M} - \alpha(\mathrm{i}x)^{M-1} + \frac{l(l+1)}{x^2}. \tag{6.18}$$

$$U(x) = x^{2M} + \alpha x^{M-1} + \frac{l(l+1)}{x^2}. \tag{6.19}$$

[8] We can choose x_I and p_I by, e.g., putting $p(t) = \mathrm{i}p_I(t)$ instead of the second one in (6.7) and (6.14) so that their corresponding quantum operators maintain the canonical commutation relation $[\hat{x}_I, \hat{p}_I] = \mathrm{i}\hbar$. In this case, each of the equations of motion in (6.15) holds with the reversed sign. But the combined form $m(\mathrm{d}^2x_I/\mathrm{d}t^2) = -U'(x_I)$ is invariant.

- Example 3 in [58]:

$$V(x) = -\omega^2\,\mathrm{e}^{4\mathrm{i}x} - D\,\mathrm{e}^{2\mathrm{i}x}. \tag{6.20}$$

$$U(x) = \omega^2\,\mathrm{e}^{4x} + D\,\mathrm{e}^{2x}. \tag{6.21}$$

- Example 4 in [59]:

$$V(x) = -(\mathrm{i}\sinh x)^{\alpha}(\cosh x)^{\beta}. \tag{6.22}$$

$$U(x) = (\sin x)^{\alpha}(\cos x)^{\beta}. \tag{6.23}$$

- Example 5 in [60]:

$$V(x) = \mathrm{i}(\sin x)^{2N+1}. \tag{6.24}$$

$$U(x) = (-1)^{N+1}(\sinh x)^{2N+1}. \tag{6.25}$$

For an arbitrary operator $\hat{O}(t)$ which can have explicit dependence on the time variable t, we can also establish the correspondence. We consider the time derivative of the $\mathcal{P}$-expectation value of $\hat{O}$:

$$\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{O}(t)\rangle_{\mathcal{P}} &= \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\mathrm{d}x\,\Psi^*(-\zeta^*(x),t)O(t)\Psi(\zeta(x),t)\\
&= \mathrm{i}\hbar\int_{-\infty}^{\infty}\mathrm{d}x\left[\Psi^*(-\zeta^*(x),t)O(t)\frac{\partial\Psi(\zeta(x),t)}{\partial t} + \frac{\partial\Psi^*(-\zeta^*(x),t)}{\partial t}O(t)\Psi(\zeta(x),t)\right]\\
&\quad + \mathrm{i}\hbar\int_{-\infty}^{\infty}\mathrm{d}x\,\Psi^*(-\zeta^*(x),t)\frac{\partial\hat{O}(t)}{\partial t}\Psi(\zeta(x),t).
\end{aligned} \tag{6.26}$$

By virtue of equations (4.1) and (4.4), and the transposition symmetry of the Hamiltonian and the relation (2.11), the term in the second line of equation (6.26) reads

$$\begin{aligned}
&\int_{-\infty}^{\infty}\mathrm{d}x\{\Psi^*(-\zeta^*(x),t)O(t)H\Psi(\zeta(x),t) - [H\Psi^*(-\zeta^*(x),t)]O(t)\Psi(\zeta(x),t)\}\\
&\quad = \int_{-\infty}^{\infty}\mathrm{d}x\,\Psi^*(-\zeta^*(x),t)(O(t)H - HO(t))\Psi(\zeta(x),t).
\end{aligned} \tag{6.27}$$

Hence, we obtain the generalized Ehrenfest's theorem in $\mathcal{PT}$-symmetric quantum theory:

$$\mathrm{i}\hbar\frac{\mathrm{d}\langle\hat{O}(t)\rangle_{\mathcal{P}}}{\mathrm{d}t} = \langle[\hat{O}(t),\hat{H}]\rangle_{\mathcal{P}} + \mathrm{i}\hbar\left\langle\frac{\partial\hat{O}(t)}{\partial t}\right\rangle_{\mathcal{P}}, \tag{6.28}$$

where we note again that the formula relates the quantities defined in terms of the $\mathcal{P}$-expectation values.

7. Additional restrictions on $\mathcal{P}$-self-adjointness

Although we have now established the classical–quantum correspondence in our framework, it is not yet sufficient for the theory to be physically acceptable. To see this, we shall first review the roles of self-adjointness in ordinary quantum theory, and then come back to consider our case. Completeness of eigenvectors is the central issue in this section. For the later discussions, we introduce the following notation:

$$\mathfrak{E}(A) = \overline{\langle\mathfrak{S}_{\lambda}(A)\mid\lambda\in\sigma_p(A)\rangle}, \tag{7.1}$$

$$\mathfrak{E}_0(A) = \overline{\langle \mathrm{Ker}(A - \lambda I) \mid \lambda \in \sigma_p(A) \rangle}. \tag{7.2}$$

That is, $\mathfrak{E}(A)$ ($\mathfrak{E}_0(A)$) is the completion of the vector space spanned by all the root vectors (eigenvectors) of the operator A, respectively. By definition, $\mathfrak{E}_0(A) \subset \mathfrak{E}(A)$.

In ordinary quantum theory, it is crucial that any state vector in the Hilbert space L^2 can be expressed as a linear combination of the eigenstates of the Hamiltonian or physical observables under consideration. However, this property, called *completeness*, is so frequently employed in vast areas of applications without any doubt that one may forget the fact that it is guaranteed by the self-adjointness of the operators. The mathematical theorem which ensures the completeness of the eigenvectors of a self-adjoint operator and the existence of an eigenbasis is the following (lemma 4.2.7 in [45]):

Theorem 7. *If A is a self-adjoint operator in a Hilbert space $\mathfrak{H}$ with a spectrum having no more than a countable set of points of condensation, then $\mathfrak{E}_0(A) = \mathfrak{H}$, and in $\mathfrak{H}$ there is an orthonormalized basis composed of the eigenvectors of the operator A.*

We thus emphasize that the postulate of self-adjointness of physical observable operators in ordinary quantum theory is crucial not only for the reality of their spectrum but also for the completeness of their eigenvectors and the existence of a basis composed of them. Reminded by this important fact, we shall next consider the situation of $\mathcal{PT}$-symmetric quantum theory defined in the Krein space.

Unfortunately, it has been known that the system of even the root vectors of a J-self-adjoint operator does not generally span a dense set of the whole Krein space, and more strikingly, that completeness of the system of the eigenvectors does not guarantee the existence of a basis composed of such vectors (cf section 4.2 in [45]). Therefore, that the completeness of the eigenvectors (or at worst, of root vectors) and the existence of a basis composed of them in the Krein space $L^2_{\mathcal{P}}$ would be inevitable for the theory to be physically acceptable leads to the following:

Criterion 3. Every physically acceptable $\mathcal{P}$-self-adjoint operator must admit a complete basis composed of its eigenvectors, or at worst, of its root vectors.

Fortunately, we have found that there exists (at least) one, among subclasses of J-self-adjoint operators, which can fulfil criteria 1–3, namely, the so-called class $\mathbf{K}(\mathbf{H})$ [55]. For the preciseness, we shall present in what follows the mathematical definitions (cf definitions 2.4.2, 2.4.18, 3.5.1 and 3.5.10 in [45]). To define the class $\mathbf{K}(\mathbf{H})$, we first need the following classes of operators:

Definition 8. *An operator V in a Krein space $\mathfrak{H}_J$ with a J-metric $Q(\cdot,\cdot)_J$ is said to be J-non-contractive if $Q(V\phi, V\phi)_J \geqslant Q(\phi,\phi)_J$ for all $\phi \in \mathfrak{D}(V)$. A continuous J-non-contractive operator V with $\mathfrak{D}(V) = \mathfrak{H}_J$ is said to be J-bi-non-contractive if V^c is also J-non-contractive.*

Definition 9. *A bounded operator T is said to belong to the class* $\mathbf{H}$*, if it has at least one pair of invariant maximal non-negative and non-positive subspaces $\mathfrak{L}_+ \in \mathfrak{M}^+$ and $\mathfrak{L}_- \in \mathfrak{M}^-$, and if every maximal semi-definite subspace $\mathfrak{L}_\pm \in \mathfrak{M}^\pm$ invariant to T belongs to the class $h^\pm$ respectively.*

With these concepts, the class $\mathbf{K}(\mathbf{H})$ is defined as

Definition 10. *A family of operators $\mathcal{A} = \{A\}$ is said to belong to the class* $\mathbf{K}(\mathbf{H})$ *if every operator $A \in \mathcal{A}$ with $\rho(A) \cap \mathbb{C}^+ \neq \emptyset$ commutes with a J-bi-non-contractive operator V_0 of the class* $\mathbf{H}$.

An important consequence of these definitions can be roughly described as follows. By virtue of the commutativity with V_0, the structure of invariant subspaces of each $A \in \mathbf{K}(\mathbf{H})$ is mostly inherited from that of V_0, and when A is J-self-adjoint also from that of V_0^c. On the other hand, both of V_0 and V_0^c are J-bi-non-contractive and belong to the class $\mathbf{H}$. In particular, if $\mathfrak{L}_+ \in \mathfrak{M}^+ \cap h^+$ ($\mathfrak{L}_- \in \mathfrak{M}^- \cap h^-$) is an invariant maximal semi-definite subspace of V_0, then $\mathfrak{L}_+^{[\perp]} \in \mathfrak{M}^- \cap h^-$ $\left(\mathfrak{L}_-^{[\perp]} \in \mathfrak{M}^+ \cap h^+\right)$ is an invariant maximal semi-definite subspace of V_0^c, respectively. Hence, a J-self-adjoint operator $A \in \mathbf{K}(\mathbf{H})$ can have an invariant maximal dual pair $\left(\mathfrak{L}_+, \mathfrak{L}_+^{[\perp]}\right)$ or $\left(\mathfrak{L}_-^{[\perp]}, \mathfrak{L}_-\right)$ with $\mathfrak{L}_\pm, \mathfrak{L}_\mp^{[\perp]} \in \mathfrak{M}^\pm \cap h^\pm$. Therefore, a $\mathcal{P}$-self-adjoint Hamiltonian of the class $\mathbf{K}(\mathbf{H})$ in particular can meet criteria 1 and 2 corresponding to case 1 in section 4. For a more rigorous understanding, trace related mathematical theorems in the literature.

Another important consequence is that every neutral invariant subspace of $A \in \mathbf{K}(\mathbf{H})$ can have at most a *finite* dimensionality. Then, for every J-self-adjoint operator A of the class $\mathbf{K}(\mathbf{H})$ the Krein space $\mathfrak{H}_J$ admits a J-orthogonal decomposition into invariant subspaces of A as (cf section 3.5.6 in [45])

$$\mathfrak{H}_J = \mathop{[\dot{+}]}_{i=1}^{\kappa_1} \left[\mathfrak{S}_{\lambda_i}(A) \dot{+} \mathfrak{S}_{\lambda_i^*}(A)\right] [\dot{+}] \mathfrak{H}'_J, \tag{7.3}$$

where κ_1 is a *finite* number, and $\lambda_i \notin \mathbb{R}$ are normal non-real eigenvalues of A. Relative to the above decomposition of the space, the operator A has block diagonal form:

$$A = \begin{pmatrix} A_1 & & & \\ & \ddots & & \\ & & A_{\kappa_1} & \\ & & & A' \end{pmatrix}, \tag{7.4}$$

where $A_i = A|_{\mathfrak{S}_{\lambda_i} \dot{+} \mathfrak{S}_{\lambda_i^*}}$ and $A' = A|_{\mathfrak{H}'_J}$. The spectrum of the operator A' is real, $\sigma(A') \subset \mathbb{R}$, and there is at most a *finite* number k of real eigenvalues μ_i for which the eigenspaces $\mathrm{Ker}(A^{(\prime)} - \mu_i I)$ are degenerate. The set of such points $\{\mu_i\}_1^k$ is called the *set of critical points* and denoted by $s(A)$. In particular, the number κ_2 of non-semi-simple real eigenvalues is also finite with $\kappa_2 \leqslant k$ (cf proposition 3).

It is evident that when $\kappa_1 = 0$, the operator A has no non-real eigenvalues and thus $\mathcal{PT}$-symmetry is unbroken (in the weak sense). However, as we have discussed in section 3 the existence of neutral eigenvectors in the real sector, and thus the value of k, has no direct relation to the ill definiteness and breakdown of $\mathcal{PT}$-symmetry. In particular, we should note that $\kappa_1 = k = 0$ does not guarantee unbroken $\mathcal{PT}$-symmetry in the strong sense; for a degenerate real semi-simple eigenvalue λ $\left(m_\lambda^{(a)} = m_\lambda^{(g)} > 1\right)$ the corresponding eigenspace can be non-degenerate (hence it does not contribute to the values of either κ_1 and k) but $\mathcal{PT}$-symmetry can be ill defined (cf table 1). Hence, the class $\mathbf{K}(\mathbf{H})$ cannot characterize unbroken $\mathcal{PT}$-symmetry perfectly, but it can certainly exclude a pathological case where an infinite number of neutral eigenvectors emerge.

Let us now come back to the central problems in this section. Regarding the completeness and existence of a basis, the following theorem has been proved[9]:

Theorem 11 (Azizov [45, 61]). *Let A be a continuous J-self-adjoint operator of the class* $\mathbf{K}(\mathbf{H})$ *in a Krein space $\mathfrak{H}_J$, and let $\sigma(A)$ have no more than a countable set of points of condensation. Then,*

(i) $\dim \mathfrak{H}_J/\mathfrak{E}(A) \leqslant \dim \mathfrak{H}_J/\mathfrak{E}_0(A) < \infty$*;*

[9] Here we omit the assertion on the existence of a p-basis in the original for simplicity.

(ii) $\mathfrak{E}_0(A) = \mathfrak{H}_J$ *if and only if* $s(A) = \emptyset$ *and* $\mathfrak{S}_\lambda(A) = \mathrm{Ker}(A - \lambda I)$ *when* $\lambda \neq \lambda^*$*;*

(iii) $\mathfrak{E}(A) = \mathfrak{H}_J$ *if and only if* $\langle \mathfrak{S}_\lambda(A) \mid \lambda \in s(A)\rangle$ *is a non-degenerate subspace;*

(iv) if $\mathfrak{E}_0(A) = \mathfrak{H}_J$ *(respectively,* $\mathfrak{E}(A) = \mathfrak{H}_J$*), then there is in* $\mathfrak{H}_J$ *an almost* J*-orthonormalized (Riesz) basis composed of eigenvectors (respectively, root vectors) of the operator* A*;*

(v) if $\mathfrak{E}_0(A) = \mathfrak{H}_J$*, then there is in* $\mathfrak{H}_J$ *a* J*-orthonormalized (Riesz) basis composed of eigenvectors of the operator* A *if and only if* $\sigma(A) \subset \mathbb{R}$.

Comparing theorems 7 and 11, one easily recognizes the complicated situation in the case of Krein spaces, and, in particular, the fact that even the restriction to the class **K**(**H**) does not automatically guarantee the completeness of the system of eigenvectors or root vectors.

Let us first discuss consequences of the theorem for the case $\mathfrak{E}(A) = \mathfrak{H}_J$. By virtue of corollary 5 and the third assertion in theorem 11, one of the sufficient conditions for $\mathfrak{E}(A) = \mathfrak{H}_J$ is that all the real eigenvalues μ_i belonging to $s(A)$ are normal. In this case, they must not be semi-simple; otherwise, $\mathfrak{S}_{\mu_i}(A) = \mathrm{Ker}(A - \mu_i I)$ is non-degenerate, which contradicts $\mu_i \in s(A)$. Hence, we have $k = \kappa_2$ and can further decompose the space (7.3) as

$$\mathfrak{H}_J = \overset{\kappa_1}{\underset{i=1}{[\dot{+}]}} \left[\mathfrak{S}_{\lambda_i}(A) \dot{+} \mathfrak{S}_{\lambda_i^*}(A)\right] \overset{\kappa_2}{\underset{i=1}{[\dot{+}]}} \mathfrak{S}_{\mu_i}(A)[\dot{+}]\mathfrak{H}_J'', \tag{7.5}$$

where $\mu_i \in s(A)$ and thus each $\mathfrak{S}_{\mu_i}$ contains at least one neutral eigenvector, and the spectrum of $A'' \equiv A|_{\mathfrak{H}_J''}$ is real $\sigma(A'') \subset \mathbb{R}$, and in particular, all the eigenvalues of A'' are real and semi-simple with non-degenerate eigenspaces. Then the fourth assertion guarantees that the system of the root vectors can always constitute an almost J-orthonormalized basis, that is, it is the union of a finite subset of vectors $\{f_i\}_1^n$ and a J-orthonormalized subset $\{e_i\}_1^\infty$ satisfying $Q(e_i, e_j)_J = \delta_{ij}$ or $-\delta_{ij}$, these two subsets being J-orthogonal to one another (definition 4.2.10 in [45]) such that

$$\mathfrak{H}_J = \overline{\langle f_1, \ldots, f_n\rangle [\dot{+}] \langle e_1, e_2, \ldots\rangle}. \tag{7.6}$$

Next, we shall consider the most desirable case $\mathfrak{E}_0(A) = \mathfrak{H}_J$ where eigenvectors of A span a dense subset of the whole space $\mathfrak{H}_J$. The second assertion in theorem 11 means that it is the case if and only if all the eigenvalues of A are semi-simple with no degenerate eigenspaces. But a degenerate eigenspace belonging to a real semi-simple eigenvalue can exist only when the eigenvalue is not normal; from corollary 5 for every normal real semi-simple eigenvalue λ the corresponding eigenspace $\mathrm{Ker}(A - \lambda I) = \mathfrak{S}_\lambda(A)$ is always non-degenerate. Hence, so long as all the real eigenvalues are normal in this case, we always have

$$\mathfrak{H}_J = \mathfrak{E}_0(A) = \overline{\overset{\kappa_1}{\underset{i=1}{[\dot{+}]}} [\mathrm{Ker}(A - \lambda_i I) \dot{+} \mathrm{Ker}(A - \lambda_i^* I)] \underset{\lambda \subset \mathbb{R}}{[\dot{+}]} \mathrm{Ker}(A - \lambda I)}, \tag{7.7}$$

which can be regarded as a special case of equation (3.6) in proposition 6. Here we recall the fact that all the eigenvectors corresponding to non-real eigenvalues are neutral and thus cannot be elements of a J-orthonormalized basis $\{e_i\}$ satisfying $Q(e_i, e_j)_J = \delta_{ij}$ or $-\delta_{ij}$. Thus, in the case of equation (7.7), the number n in equation (7.6) is given by

$$n = \sum_{i=1}^{\kappa_1} \left[m_{\lambda_i}^{(a)}(A) + m_{\lambda_i^*}^{(a)}(A)\right] = 2\sum_{i=1}^{\kappa_1} m_{\lambda_i}^{(g)}(A). \tag{7.8}$$

Hence, if furthermore all the eigenvalues are real, namely, $\kappa_1 = 0$, we have $n = 0$ and thus the system of eigenvectors can form a J-orthonormalized basis, as is indeed ensured by the fifth assertion.

We now understand that for an arbitrary continuous $\mathcal{P}$-self-adjoint operator A of the class **K**(**H**) the completeness $\mathfrak{E}_0(A) = L^2_{\mathcal{P}}$ and the existence of a basis composed of the eigenvectors of A in $L^2_{\mathcal{P}}$ are guaranteed if and only if all the eigenvalues are semi-simple and there is no degenerate eigenspaces in the real sector, irrespective of the existence of non-real eigenvalues, or in other words, irrespective of whether $\mathcal{PT}$-symmetry is spontaneously broken. But the latter condition of the non-degeneracy is always guaranteed unless there appears a non-normal real eigenvalue, as we have just discussed. Thus, in most of the cases we would not need to resort to the quotient-space prescription proposed in the previous paper [34]. Therefore, a remaining problem is how to deal with neutral eigenvectors belonging to non-real eigenvalues when $\mathcal{PT}$-symmetry is spontaneously broken. In our previous paper [34], we have proposed the possibility of interpreting them as physical states describing unstable decaying states (and their 'spacetime-reversal' states). Until now we have not found any active reason to discard it. However, the fact that we must always restrict ourselves to a semi-definite subspace for the probability interpretation would make the role of these neutral vectors quite restrictive (cf section 4).

8. Discussion and summary

In this work, we have revealed the various general aspects of $\mathcal{PT}$-symmetric quantum theory defined in the Krein space $L^2_{\mathcal{P}}$, previously proposed by us in [34]. The fact that $\mathcal{P}$-self-adjoint Hamiltonians 'favour' the Krein space $L^2_{\mathcal{P}}$ rather than the Hilbert space L^2 inevitably led us to formulate a quantum theory in a space with an indefinite metric. Attempts to quantize a physical system in an indefinite metric space are traced back to Dirac's work in 1942 [62]. Since then, there have appeared numerous attempts of this kind in various contexts (see references cited in [23], and [54] for non-Abelian gauge theories). The significant feature in our case is the conservation law (4.11), which ensures that the character (positivity etc.) of every state vectors remains unchanged in the time evolution. This, together with the fact that the probability interpretation is possible only in a semi-definite space, naturally led us to criteria 1 and 2. Here we note that they would be valid not only in our present case but also in any case one would like to quantize a system in a Krein space. Criterion 3 would be indispensable in any kind of quantum theory. We have found that there exists a class of J-self-adjoint operators, called the class $\mathbf{K}(\mathbf{H})$, which can satisfy those 3 criteria.

We note that our quantization scheme of $\mathcal{PT}$-symmetric theory turns to be completely different from the existing approaches such as the use of $\mathcal{C}$ or positive metric operators. The origin of the difference is twofold. The first reason comes from the different settings of eigenvalue problems, equations (4.1) and (4.2). Our setting may seem to be strange especially to those who are familiar with the conventional one. But it is the conventional setting that makes the physical interpretation of, e.g., the complex position and momentum quite difficult when a system cannot be defined on the real line. It is evident that this difficulty cannot be overcome even if we express a Hamiltonian in terms of a real variable as equation (4.3); the 'Hamiltonian' which determines the time evolution of state vectors is no longer a Schrödinger operator and it is almost impossible to establish any correspondence with Newtonian classical dynamical systems and any reasonable interpretation of physical observables even for the most fundamental ones such as position and momentum. The second reason comes from the different choices of linear spaces where one would like to make a probability interpretation. In the conventional approaches, we must transform a given Hamiltonian to another operator acting in a positive definite Hilbert space. But the transformed operator is in general not a Schrödinger operator and thus they suffer from the same problem as the one just mentioned above (besides the problem of unboundedness of metric operators), cf [35, 63, 64]. This difficulty is in fact the central origin of the disputes found in e.g. [37, 38].

In this respect, we would like to emphasize first that reality of spectrum, existence of a positive-definite norm, and so on, are neither sufficient nor necessary conditions for a quantum-like theory to be physically acceptable. Crucial viewpoints must be put on the possibility whether we can assign a reasonable physical interpretation for each consequence of the theory and on the consistency of the interpretation with experimental results. Regarding the former point of view, we have not detected so far any difficulty in physical interpretations, apparent breakdown or fatal inconsistency in our framework, and the investigations presented in this paper indicates that it can stand as another consistent quantum theory. Therefore, among the different mathematical settings of the eigenvalue problems for $\mathcal{PT}$-symmetric Hamiltonians in the literature, our formulation has been shown to possess the most desirable property as a physical quantum theory, though the others are still quite interesting as purely mathematical problems. But we should regard the present results as a necessary minimum and explore further extensive studies to see whether the theory would be certainly free from any insurmountable discrepancy.

The classical-quantum correspondence in $\mathcal{PT}$-symmetric theory we have established in section 6 suggests that we should regard $\mathcal{PT}$-symmetric quantum theory as another quantization scheme rather than a generalization of traditional Hermitian quantum theory. That is, for a given real classical potential $U(x)$ we associate the real Hermitian operator $U(\hat{x})$ acting in the Hilbert space L^2 in the traditional scheme, while we associate the complex $\mathcal{P}$-Hermitian operator $V(\hat{x})$, obtained through the relation (6.12), acting in the Krein space $L^2_{\mathcal{P}}$ in the $\mathcal{PT}$-symmetric scheme. But certainly some classical potentials $U(x)$ would only admit a $\mathcal{PT}$-symmetric quantization but not a Hermitian one due to the lack of normalizable eigenfunctions for $U(x)$ on $x \in \mathbb{R}$. An intriguing situation can arise when a given classical potential admits both quantization schemes. As a physical theory, which of them we should take must be of course determined by the comparison between theoretical prediction and experiment. From this point of view, it is quite interesting to examine the cases where the two different quantum models constructed from a single classical system predict different physical consequences.

The classical systems obtained from the classical-quantum correspondence are completely real. On the other hand, the $\mathcal{PT}$-symmetric complex classical systems investigated in [14, 56, 57] have (at least until now) no correspondence principle which relates them to the $\mathcal{PT}$-symmetric quantum systems. Nevertheless, the results in the latter references strongly indicate an intimate relation between complex classical and quantum systems especially in view of spontaneous $\mathcal{PT}$-symmetry breaking. We can easily expect that the corresponding real classical systems in our framework would be insensitive to $\mathcal{PT}$-symmetry breaking at the quantum level since $\mathcal{P}$-expectation value of $\mathcal{P}$-Hermitian Hamiltonians are always real, and in particular zero for every eigenstates belonging to non-real energy eigenvalues. Therefore, it is still quite important to reveal and understand underlying dynamical relations between $\mathcal{PT}$-symmetric complex classical and quantum systems.

We have shown in section 2.3 that the concept of transposition symmetry plays a key role in connecting $\mathcal{PT}$-symmetry with $\mathcal{P}$-Hermiticity. On the other hand, as was pointed out in [5], this symmetry underlies the intimate relation between level crossing phenomena and Jordan anomalous behaviour. The fact that these two significant aspects rely on the same property would not be accidental. In fact, several $\mathcal{PT}$-symmetric Hamiltonians characterized by a set of parameters have non-trivial phase diagrams [13, 14, 65], that is, they have both the symmetric and broken phases of $\mathcal{PT}$-symmetry in the parameter-space and at the boundary a level crossing takes place; a pair of different real eigenvalues in the symmetric phase degenerates at the boundary and then splits into a complex-conjugate pair in the broken phase. Hence, the underlying mechanism of the emergence of a non-trivial phase diagram of $\mathcal{PT}$-symmetry and that of the Bender–Wu singularities [3–5] would be essentially the same. In this respect, it is also interesting to note that, the structure of the energy levels of the potential (6.16) shown in [14] indicates that $\epsilon = 0$ would be an accumulation point of the spectral singularity in the ϵ-plane, which also resembles the structure of the Bender–Wu singularities despite the totally different roles of the parameters between them. We further recall the analogous situation in the Lee model. It was already shown by Heisenberg in 1957 that at the critical point where the 'dipole-ghost' state emerges, the system exhibits a level crossing and admits an associated state vector and a zero-norm eigenstate [66].

The restriction $\Delta A\Psi, \Delta B\Psi \in \mathfrak{L}_+$ or $\mathfrak{L}_-$ for the uncertainty relation in equation (5.12) suggests that every operator O corresponding to a physical observable should also preserve the invariant maximal semi-definite subspaces $\mathfrak{L}_\pm$ relative to the Hamiltonian H. It would be possible if each operator O commutes with the operator $V_0 \in \mathbf{H}$ which characterizes the class $\mathbf{K}(\mathbf{H})$ to which the Hamiltonian H belongs. From this observation, we reach the following postulate for an operator O to be a physical observable:

Postulate. *A set of physical observables $\mathcal{O} = \{O\}$ for a given Hamiltonian $H \in \mathbf{K}(\mathbf{H})$ is a family of $\mathcal{P}$-self-adjoint or anti-$\mathcal{P}$-self-adjoint operators belonging to the same class $\mathbf{K}(\mathbf{H})$ characterized by the same V_0, namely, $H \cup \mathcal{O} \in \mathbf{K}(\mathbf{H}, V_0)$.*

Then, a natural question is whether we can make a sensible physical interpretation of the operator V_0. If it turns out that it is indeed possible, it might provide a physical reason why we should restrict ourselves to $\mathcal{P}$-self-adjoint operators of the class $\mathbf{K}(\mathbf{H})$. Mathematically, the class $\mathbf{K}(\mathbf{H})$ would not be a necessary condition for satisfying criteria 1 and 2. Thus, it is possible that another class of J-self-adjoint operators which is more suitable for a physical application could be found in the future.

Regarding Azizov's theorem in section 7, we note the fact that rigorously speaking it applies only to continuous operators. On the other hand, physical Hamiltonians we are interested in are usually unbounded. To the best of our knowledge, an extension of the theorem to unbounded operators has not been established. We expect most of the assertions would remain valid also for unbounded operators under a relatively small number of additional assumptions. We hope this paper will interest and motivate some mathematicians to study the issue.

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