Remarks on the $\mathcal{PT}$-pseudo-norm in $\mathcal{PT}$-symmetric quantum mechanics

2005 J. Phys. A: Math. Gen. 38 3665

(http://iopscience.iop.org/0305-4470/38/16/014)

J. Phys. A: Math. Gen. **38** (2005) 3665–3677 doi:10.1088/0305-4470/38/16/014

Remarks on the $\mathcal{PT}$-pseudo-norm in $\mathcal{PT}$-symmetric quantum mechanics

Duc Tai Trinh

Department of Mathematics, Teacher Training College of Dalat, 29 Yersin, Dalat, Vietnam
and
The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, Trieste 34014, Italy

E-mail: tductai@hcm.vnn.vn and tductai@ictp.trieste.it

Received 1 February 2005, in final form 4 March 2005
Published 6 April 2005
Online at stacks.iop.org/JPhysA/38/3665

Abstract
This paper presents an underlying analytical relationship between the $\mathcal{PT}$-pseudo-norm associated with the $\mathcal{PT}$-symmetric Hamiltonian $H = p^2 + V(q)$ and the Stokes multiplier of the differential equation corresponding to this Hamiltonian. We show that the sign alternation of the $\mathcal{PT}$-pseudo-norm, which has been observed as a generic feature of the $\mathcal{PT}$-inner product, is essentially controlled by the derivative of a Stokes multiplier with respect to the eigenparameter.

PACS numbers: 03.65.Ca, 03.65.Ge, 11.30.Er

1. Introduction

Since the late 1990s, the notion of $\mathcal{PT}$-symmetric Hamiltonians in quantum physics has been addressed in many works after its first appearance in a publication of Bender and Boettcher [6] concerning a conjecture of Bessis and Zinn-Justin.

By dropping the requirement of Hermiticity but of course keeping the invariance by the Lorentz group, one opens on a significantly larger class of Hamiltonians satisfying a weaker hypothesis, namely the $\mathcal{PT}$-invariance. This more flexible condition amounts to the commutability of the Hamiltonian H and the composite operator $\mathcal{PT}$ whose components consist of one linear operator $\mathcal{P}$ (for *parity*) and another anti-linear $\mathcal{T}$ (for *time-reversal*).

It has been shown that, despite the lack of Hermiticity, many $\mathcal{PT}$-symmetric Hamiltonians still have a whole real and bounded from below discrete spectrum (see [4, 8, 11, 15, 17, 19, 24, 32]). However, controversy has emerged among researchers due to the fact that the space of states may be no longer a Hilbert space, at variance with traditional quantum mechanics.

Recently, many studies have been devoted to the establishment of a conventional mathematical structure for $\mathcal{PT}$-symmetry quantum mechanics (see [2, 3, 28, 29]). One of the most important considerations is to equip the space of states associated with a given Hamiltonian with a certain inner product, in such a way that the norm induced by this inner product is positive definite.

For Hermitian Hamiltonians on the real axis $\mathbb{R}$, such a space is normally known as the Hilbert space $L^2(\mathbb{R})$, whose inner product is nothing but the usual one. The norm induced from this actually positive definite inner product is interpreted as a probability density in the space of states.

Such an ideal model seems to be no longer available whenever the Hamiltonians are non-Hermitian. However, the specialists in the field have recently succeeded in constructing a consistent physical theory for *unbroken* $\mathcal{PT}$-symmetric Hamiltonians. The most essential aspect in their investigations is the appearance of a linear '*charge*' operator $\mathcal{C}$ whose action enables the so-called $\mathcal{PT}$-pseudo-norm to switch its sign in a suitable way, so that the induced $\mathcal{CPT}$-norm is now positive definite.

This operator $\mathcal{C}$ is nowadays a central subject of interest. Recently, in an attempt to formulate $\mathcal{PT}$-symmetric quantum theories, Bender *et al* obtained many significant results through explicit calculation of the operator $\mathcal{C}$ for some special $\mathcal{PT}$-symmetric Hamiltonians (see [2, 3, 5]). As a rule, the construction relies on the observation of a so-called quasi-parity quantum number [1, 25, 38], so that the $\mathcal{PT}$-pseudo-norm exhibits a generic sign alternation upon the eigenstates of the Hamiltonians.

This paper, which is motivated by these observations, aims mainly to justify the indefiniteness of the $\mathcal{PT}$-inner product for a class of unbroken $\mathcal{PT}$-symmetric Hamiltonians. By using some classical results on Stokes multipliers (see [33], chapters 5 and 6), whose zeros are exactly the eigenvalues of the considered Hamiltonians, we show an analytical relation between the $\mathcal{PT}$-pseudo-norm and the derivative with respect to the eigenparameter of one of these Stokes multipliers, from which the sign alternation occurs as a natural consequence.

This paper is organized as follows. In section 2, we recall some simple notions and facts on the Sturm–Liouville eigenvalue problem associated with a class of complex Hamiltonians. A strong connection between our problem and Sibuya's theory on linear differential equations is formulated for our next purposes. Section 3 contains our main results which allow us to establish a relationship between the $\mathcal{PT}$-pseudo-norm and the derivative in the eigenparameter of a convenient Stokes multiplier. This gives a clear explanation for the indefiniteness of the $\mathcal{PT}$-pseudo-norm, thus justifying what has been observed in various works (e.g., [2]). Finally, in the conclusion we suggest some further considerations and discuss a degenerate case, where the $\mathcal{PT}$-symmetry may be spontaneously broken by the vanishing of the $\mathcal{PT}$-pseudo-norm at some degenerate states.

2. Sturm–Liouville eigenvalue problem associated with a Hamiltonian

We consider a non-Hermitian Hamiltonian

$$H = p^2 + V(q) \tag{1}$$

where p stands for the operator $-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}q}$ and

$$V(q) := -[(\mathrm{i}q)^m + a_1(\mathrm{i}q)^{m-1} + \cdots + a_{m-1}(\mathrm{i}q) + a_m] \tag{2}$$

is a polynomial of degree m in the variable iq with *real* coefficients $a_j \in \mathbb{R}$.

These assumptions induce that the complex-valued potential function $V(q)$ satisfies the following relation:

$$\overline{V(-\overline{q})} = V(q) \tag{3}$$

(where $\overline{q}$ stands for the complex conjugate of q), which is broadly known as the $\mathcal{PT}$-symmetry, or more geometrically as the invariance property of $V(q)$ under the *real* conjugation.

Recall that, as usual, the combination $\mathcal{PT}$ stands for the composite operator of $\mathcal{P}$ (*parity* operator) and $\mathcal{T}$ (*time-reversal* operator) whose actions on the (p, q)-space are generally determined as follows:

$$\mathcal{P} : \begin{cases} q \mapsto -q \\ p \mapsto -p \end{cases} \qquad \text{and} \qquad \mathcal{T} : \begin{cases} q \mapsto \overline{q} \\ p \mapsto -\overline{p}. \end{cases}$$

By definition, $\mathcal{PT}(=\mathcal{TP})$ is not a linear but an anti-linear operator. Its action on a wave function $\phi(q)$ is simply given by

$$\mathcal{PT}\phi(q) = \overline{\phi(-\overline{q})}. \tag{4}$$

Consequently, a function $\phi(q)$ is called $\mathcal{PT}$-*symmetric* if it remains unchanged under the action of the operator $\mathcal{PT}$ in (4). It is obvious that the Hamiltonian H in (1) is $\mathcal{PT}$-symmetric, i.e.

$$\mathcal{PT}H = H\mathcal{PT} \tag{5}$$

provided that $V(q)$ is $\mathcal{PT}$-symmetric. And this is the case when all coefficients a_j in (2) are real.

2.1. $\mathcal{PT}$-inner product and $\mathcal{PT}$-pseudo-norm

In the following, we shall determine a space of functions on which the action of our given Hamiltonian is meaningful. We note that the usual set of functions considered for most (Hermitian) Hamiltonians on the real line is $L^2(\mathbb{R})$, in relation to its useful Hilbert space structure. In the context of non-Hermitian Hamiltonians, defining such a space with an appropriate algebraic structure has not been yet completely settled in general.

Consider the Hamiltonian H in (1) with the assumption that all a_j in (2) are real, so that H is $\mathcal{PT}$-symmetric. For a fixed $m \in \mathbb{N}$, $m \geqslant 2$, we denote by $\mathfrak{H}$ the complex vector space of all entire functions $f(q)$ which are exponentially vanishing at infinity in both of the two open sectors

$$S_l := \left\{ \left| \arg(X) + \frac{\pi}{2} + \frac{2\pi}{m+2} \right| < \frac{\pi}{m+2} \right\}$$

and (6)

$$S_r := \left\{ \left| \arg(X) + \frac{\pi}{2} - \frac{2\pi}{m+2} \right| < \frac{\pi}{m+2} \right\}.$$

This space $\mathfrak{H}$ can be considered as a vector subspace of the space of square integrable functions in both the two neighbourhoods of infinity S_l and S_r. By virtue of the involution of $\mathcal{PT}$ and the definition of $\mathfrak{H}$, we have immediately

$$\mathcal{PT}(\mathfrak{H}) = \mathfrak{H}. \tag{7}$$

The following statement, which can be checked directly, asserts the symmetry of the discrete spectrum of a $\mathcal{PT}$-symmetric Hamiltonian.

Proposition 1. *Let $\mathfrak{G}$ be a certain vector space of functions satisfying $\mathcal{PT}(\mathfrak{G}) \subset \mathfrak{G}$. Then the set of eigenvalues of a $\mathcal{PT}$-symmetry Hamiltonian H acting on $\mathfrak{G}$ is invariant under complex conjugation.*

We are going to introduce a space in which each eigenfunction of the non-Hermitian Hamiltonian H is associated with a real number, usually (but a little abusively) called its $\mathcal{PT}$-pseudo-norm.

Instead of considering the real axis, as is the case for the usual norm in $L^2(\mathbb{R})$, a slightly different curve will be involved in order to be consistent with our goals. Consider an endless curve γ starting from infinity in the sector S_l and ending also at infinity but in the different sector S_r. Note that for a given function $h(q) \in \mathfrak{H}$, which is thus holomorphic and integrable at infinity in $S_l \cup S_r$, the value of the integral $\int_\gamma h(q)\,\mathrm{d}q$ remains unchanged when γ is deformed continuously such that both of its endpoints still lie in S_l and S_r, respectively.

For the sake of simplicity, we shall take γ to be symmetric so that, up to its orientation, the mapping $q \mapsto -\overline{q}$ of the complex plane $\mathbb{C}$, which is nothing but the mirror symmetry with respect to the imaginary axis, leaves γ invariant. Precisely, it will be convenient to define γ by

$$\gamma := \gamma_r - \gamma_l, \tag{8}$$

where γ_r and γ_l (drawn in figure 1) are respectively the rays oriented from the origin to infinity such that

$$\gamma_l = \left\{ q \in \mathbb{C}/\arg(q) = -\frac{\pi}{2} - \frac{2\pi}{m+2} \right\}, \qquad \gamma_r = \left\{ q \in \mathbb{C}/\arg(q) = -\frac{\pi}{2} + \frac{2\pi}{m+2} \right\}.$$

We now introduce a sesquilinear form on $\mathfrak{H}$ as follows. For $f, g \in \mathfrak{H}$, we define

$$\langle\langle f, g\rangle\rangle_\gamma := \int_\gamma f(q)\mathcal{PT}g(q)\,\mathrm{d}q = \int_\gamma f(q)\overline{g(-\overline{q})}\,\mathrm{d}q. \tag{9}$$

By changing the variable of integration $z = -\overline{q}$, one easily checks that for every $f, g \in \mathfrak{H}$,

$$\langle\langle f, g\rangle\rangle_\gamma = \overline{\langle\langle g, f\rangle\rangle}_\gamma. \tag{10}$$

This means that $\langle\langle f, g\rangle\rangle_\gamma$ realizes a Hermitian sesquilinear form on $\mathfrak{H}$.

We naturally define the mapping $\|\cdot\|^2_{\mathcal{PT}} : \mathfrak{H} \to \mathbb{R}$ induced by (10):

$$\|f\|^2_{\mathcal{PT}} := \langle\langle f, f\rangle\rangle_\gamma \tag{11}$$

Here, it is necessary to emphasize that the Hermitian sesquilinear form $\langle\langle .\,, .\rangle\rangle_\gamma$ has no reason to be positive definite. In particular, $\|f\|^2_{\mathcal{PT}}$ can be zero even if $f \not\equiv 0$. Hence, it is deservedly called *$\mathcal{PT}$-pseudo-norm*, while the form $\langle\langle .\,, .\rangle\rangle_\gamma$ will be called *$\mathcal{PT}$-inner product*.

Proposition 2. *The $\mathcal{PT}$-symmetric Hamiltonian H is symmetric under the $\mathcal{PT}$-inner product:*

$$\langle\langle H\phi, \psi\rangle\rangle_\gamma = \langle\langle \phi, H\psi\rangle\rangle_\gamma \qquad \forall \phi, \psi \in \mathfrak{H}.$$

Proof. We note that if ϕ belongs to $\mathfrak{H}$, then $H\phi \in \mathfrak{H}$ also. Now by definition we have

$$\langle\langle H\phi, \psi\rangle\rangle_\gamma = \int_\gamma H\phi\mathcal{PT}\psi\,\mathrm{d}q = \int_\gamma (-\phi'' + V(q)\phi)\mathcal{PT}\psi\,\mathrm{d}q.$$

Integrating the right-hand side by parts twice yields

$$\begin{aligned}\langle\langle H\phi, \psi\rangle\rangle_\gamma &= \int_\gamma \phi(-(\mathcal{PT}\psi)'' + V(q)\mathcal{PT}\psi)\,\mathrm{d}q \\ &= \int_\gamma \phi H\mathcal{PT}\psi\,\mathrm{d}q = \int_\gamma \phi\mathcal{PT}H\psi\,\mathrm{d}q = \langle\langle \phi, H\psi\rangle\rangle_\gamma.\end{aligned}$$

This completes the proof. □

This proposition induces the following two direct consequences.

Corollary 2.1. *Two eigenfunctions corresponding to distinguish real eigenvalues are orthogonal with respect to $\langle\langle\cdot\,,\cdot\rangle\rangle_\gamma$.*

Corollary 2.2. *If ϕ_E is an eigenfunction corresponding to a complex eigenvalue E then $\|\phi_E\|^2_{\mathcal{PT}} = 0$.*

2.2. Stokes multipliers

In what follows, we briefly recall some important results of Sibuya [33] on complex second-order linear differential equations. We consider in the complex plane the following equation:

$$-\Phi''(X) + W(X)\Phi(X) = 0 \tag{12}$$

where $W(X) = X^m + a_1 X^{m-1} + \cdots + a_m$ is a monic polynomial function of degree $m \in \mathbb{N}$, with coefficients $a_1, a_2, \ldots, a_m \in \mathbb{C}$.

The following theorem, which is due to Sibuya, asserts the existence and uniqueness of a solution characterized by its asymptotic behaviour at infinity.

Theorem 3. *Equation (12) admits a unique solution* $\Phi_0(X, a) := \Phi_0(X; a_1, a_2, \ldots, a_m)$ *such that*

1. $\Phi_0(X, a)$ *is an entire function in* $(X; a_1, a_2, \ldots, a_m)$*,*
2. $\Phi_0(X, a)$ *and its derivative* $\Phi_0'(X, a)$ *admit the following asymptotic behaviours:*

$$\Phi_0(X) \simeq X^{r_m}\, \mathrm{e}^{-S(X,a)}[1 + O(X^{-1/2})] \tag{13}$$

$$\Phi_0'(X) \simeq X^{\frac{m}{2}+r_m}\, \mathrm{e}^{-S(X,a)}[-1 + O(X^{-1/2})] \tag{14}$$

when $X \to \infty$ *in each sub-sector strictly contained in the sector*

$$\Sigma_0 = \left\{ |\arg(X)| < \frac{3\pi}{m+2} \right\}$$

and the asymptotic regimes occur uniformly with respect to $a = (a_1, a_2, \ldots, a_m)$ *in any compact of* $\mathbb{C}^m$*.*

In the above theorem r_m and $S(X, a)$ can be determined explicitly from $W(X)$. As $X \to \infty$, one can write

$$\begin{aligned} \sqrt{W(X)} &= X^{\frac{m}{2}}\{1 + a_1 X^{-1} + \cdots + a_m X^{-m}\}^{1/2} \\ &= X^{\frac{m}{2}}\left\{1 + \textstyle\sum_{k=1}^{\infty} b_k(a) X^{-k}\right\} \end{aligned} \tag{15}$$

where, obviously, $b_k(a)$ are quasi-homogeneous polynomials in $a_1, \ldots, a_m$ with real coefficients.

By integrating term by term the series on the right-hand side, we get a primitive of $\sqrt{W(X)}$. The function $S(X, a)$ is associated with the 'principal part' of this primitive

$$S(X, a) = \frac{2}{m+2} X^{\frac{m+2}{2}} + \cdots$$

that only contains terms with strictly positive powers of X. And $r_m = r_m(a)$ is given by

$$r_m(a) = \begin{cases} -m/4 & \text{for } m \text{ odd} \\ -m/4 - b_{1+m/2}(a) & \text{for } m \text{ even.} \end{cases} \tag{16}$$

We should note that for $m > 2$, $r_m(a)$ does not depend on the last coefficient a_m and if all a_j (possibly except a_m) are equal to zero then $r_m = -m/4$.

We shall define other solutions of (12) by introducing a rotation of the complex plan. Let us denote

$$\omega := \exp\left\{-\frac{\mathrm{i}2\pi}{m+2}\right\} \qquad \text{and} \qquad \omega_k(a) := (\omega^k a_1, \omega^{2k} a_2, \ldots, \omega^{km} a_m); \qquad (k \in \mathbb{Z}).$$

For each $k \in \mathbb{Z}$, we construct functions $\Phi_k(X; a)$ by setting

$$\Phi_k(X; a) := \Phi_0(\omega^k X; \omega_k(a)). \tag{17}$$

It is not difficult to check that $\Phi_k(X; a)$ are indeed solutions of (12) and exponentially vanishing at infinity in the corresponding sector

$$S_k := \left\{ \left| \arg(X) - k\frac{2\pi}{m+2} \right| < \frac{\pi}{m+2} \right\}. \tag{18}$$

The following lemma, which can be verified in a straightforward way (see [18, 33]), implies the linear independence of two consecutive solutions Φ_k and Φ_{k+1}.

Lemma 4. *For any $k \in \mathbb{Z}$, the Wronskian of Φ_k and Φ_{k+1} is given by the formula*

$$\mathsf{Wr}(\Phi_k, \Phi_{k+1}) = 2(-1)^k \omega^{-\frac{km}{2} + r_m(\omega_{k+1}(a))}. \tag{19}$$

From this observation, together with classical results on the structure of solutions of linear differential equations, we can infer that $\{\Phi_k, \Phi_{k+1}\}$ constitutes a basis for the vector space of the solutions of equation (12). Therefore, every solution can be expressed as a linear combination of Φ_k, Φ_{k+1}. In particular, for each $k \in \mathbb{Z}$, we have

$$\Phi_{k-1} = C_k(a)\Phi_k + \widetilde{C}_k(a)\Phi_{k+1}. \tag{20}$$

The multipliers $C_k(a)$ and $\widetilde{C}_k(a)$ are called the *Stokes multipliers* of Φ_{k-1} with respect to Φ_k and Φ_{k+1}. Further studies on these objects are addressed in [18, 30, 33]. By definition, it is evident that

$$C_k(a) = \frac{\mathsf{Wr}(\Phi_{k-1}, \Phi_{k+1})}{\mathsf{Wr}(\Phi_k, \Phi_{k+1})} \qquad \text{and} \qquad \widetilde{C}_k(a) = \frac{\mathsf{Wr}(\Phi_{k-1}, \Phi_k)}{\mathsf{Wr}(\Phi_{k+1}, \Phi_k)}.$$

Since $\Phi_k(X; a)$ are entire functions in a, it follows immediately from these equalities and lemma 4 that $C_k(a)$ and $\widetilde{C}_k(a)$ are also entire functions in a. Furthermore, we also get an explicit expression for $\widetilde{C}_k(a)$

$$\widetilde{C}_k(a) = \omega^{m+2r_m(\omega_k(a))}.$$

We emphasize that $\widetilde{C}_k(a)$ is never vanishing. Thus, this coefficient can be reduced to 1 by a suitable renormalization of the Φ_k's. For instance, when $k = 0$, (20) reads

$$\Phi_{-1} = C_0(a)\Phi_0 + \omega^{m+2r_m(a)}\Phi_1. \tag{21}$$

By setting

$$Y_1 := \omega^{m/2+r_m(a)}\Phi_1 = \omega^{m/2+r_m(a)}\Phi_0(\omega X; \omega(a))$$

and (22)

$$Y_{-1} := \omega^{-m/2-r_m(a)}\Phi_{-1} = \omega^{-m/2-r_m(a)}\Phi_0(\omega^{-1}X; \omega_{-1}(a))$$

we can write (21) under a slightly symmetric form,

$$Y_{-1} = C(a)Y_0 + Y_1, \tag{23}$$

where Y_0 stands for Φ_0 and $C(a) := \omega^{-m/2-r_m(a)}C_0(a)$ is also called the *Stokes multiplier* of Y_{-1} with respect to Y_0.

With these conventions, we get a very simple expression for the Wronskian of Y_0 and Y_1, namely,

$$\mathsf{Wr}(Y_0, Y_1) = 2. \tag{24}$$

Concerning the (sole) Stokes multiplier $C(a)$ in (23), which plays a very important role for our purposes, we have

Proposition 5. *For any $a \in \mathbb{C}^m$,*

$$\overline{C(a)} + C(\overline{a}) = 0. \tag{25}$$

Proof. By virtue of the quasi-homogeneity of equation (12), we can see that $\overline{\Phi_0(\overline{X}, \overline{a})}$ is also one of its solutions whose asymptotic behaviour at ∞ in the sector S_0 is the same as $\Phi_0(X, a)$.

The uniqueness of the canonical solution in theorem 3 implies immediately that

$$\overline{\Phi_0(X, a)} = \Phi_0(\overline{X}, \overline{a}). \tag{26}$$

Taking into account the above definitions of Y_{-1} and Y_1, we can check without difficulty that

$$Y_{-1}(\overline{X}, \overline{a}) = \overline{Y_1(X, a)} \tag{27}$$

for any $X \in \mathbb{C}$ and any $a \in \mathbb{C}^m$.

Putting these relations in (23) leads to the desired identity. □

2.3. Eigenvalues as zeros of the Stokes multiplier

We now consider the complex Sturm–Liouville eigenvalue problem associated with the Hamiltonian H in (1):

$$\begin{cases} -\phi''(q) + V(q)\phi(q) = E\phi(q) \\ \lim\limits_{q \to -i\infty \cdot \mathrm{e}^{\mathrm{i}\theta}} \phi(q) = 0 \quad \text{and} \quad \lim\limits_{q \to -i\infty \cdot \mathrm{e}^{-\mathrm{i}\theta}} \phi(q) = 0 \end{cases} \tag{28}$$

where $\theta := \frac{2\pi}{m+2}$.

It is necessary to note that the boundary condition ($\lim \phi(q) = 0$) in (28) is equivalent to the fact that $\phi(q)$ is exponentially vanishing at infinity in both of the two sectors S_l and S_r.

For our purposes, we prefer to consider the problem (28) in a new variable, introducing the rotation $q \mapsto X := \mathrm{i}q$. This transforms the differential equation in (28) into the following one[1]:

$$-\Phi''(X) + (X^m + a_1 X^{m-1} + \cdots + a_{m-1}X + E)\Phi(X) = 0, \tag{29}$$

where $\Phi(X)$ stands for $\phi(q)$.

The boundary value conditions in (28) turn into the requirement that the solution $\Phi(X)$ vanishes exponentially in both of the two sectors S_{-1} and S_1, which are defined in (18), see also figure 1.

With the notation of the previous subsection and writing $C(a, E) := C(a_1, \ldots, a_{m-1}, E)$ for the Stokes multiplier, we have

Lemma 6. *E_{eigen} is an eigenvalue of the problem (28) if and only if $C(a, E_{\mathrm{eigen}}) = 0$.*

Proof. Let $\phi_{\mathrm{eigen}}(q)$ be an eigenfunction corresponding to the eigenvalue E_{eigen}. Then $Y_{\mathrm{eigen}}(X) := \phi_{\mathrm{eigen}}(-\mathrm{i}X)$ solves (29) and vanishes exponentially at infinity in both S_{-1} and S_1 in the X-plane. This fact, together with the observation that $Y_0(X)$ growths exponentially in $S_{\pm1}$, implies that $Y_{\mathrm{eigen}}(X)$ is proportional to $Y_{\pm1}(X)$ in $S_{\pm1}$, respectively. By virtue of (23), this is only possible if $C(a, E_{\mathrm{eigen}}) = 0$.

Conversely, if $E_{\mathrm{eigen}} = E_{\mathrm{eigen}}(a)$ is a zero of $C(a, E)$ then $Y_{\mathrm{eigen}}(X) := Y_{-1}(X, E_{\mathrm{eigen}}) \equiv Y_1(X, E_{\mathrm{eigen}})$ exponentially vanishes at ∞ in both of $S_{\pm1}$. Replacing $X = \mathrm{i}q$, we obtain a solution for (28). □

Remark 7. We note that by construction, $C(a, E)$ is a non-constant entire function in both a and E. For each fixed $a \in \mathbb{C}^{m-1}$, as an entire function of E, $C(a, E)$ has the order of $\frac{1}{2} + \frac{1}{m}$ (see [33]). Since the order is a non-integral positive number for $m > 2$, $C(a, E)$ must have infinitely many zeros $E_n = E_n(a)$. By estimating the asymptotic behaviour of $C(a, E)$ as

[1] We can always drop a_m by adding it in E.

$E \to \infty$, Sibuya proved that, except possibly for a finite number, these zeros are *simple* (i.e. the derivative $\frac{\partial}{\partial E} C(a, E) \neq 0$ at those points). Furthermore, the large zeros are known to be close to the positive real half-axis and satisfy the following estimate:

$$E_n = \left(\frac{(2n-1)\pi}{2K \sin(2\pi/m)} \right)^{\frac{2m}{m+2}} [1 + \nu_n] \tag{30}$$

where $K := \int_0^{+\infty} \left(\sqrt{1+t^m} - \sqrt{t^m} \right) \mathrm{d}t > 0$ and $\nu_n \to 0, n \to \infty$.

The most interesting thing here is that the first terms in this asymptotic estimate do not depend on a.

Under the assumption that all coefficients a_j in (2) are real, the eigenvalues E_n of the Hamiltonian H are real or complex conjugate in pairs according to lemma 6, as already mentioned in proposition 1. Some intensive studies on the reality of all the eigenvalues could be found in [19, 32].

3. Indefiniteness of the $\mathcal{PT}$-pseudo-norm

In what follows we shall assume that all the coefficients a_j are real, so that the Hamiltonian H defined in (1) is $\mathcal{PT}$-symmetric and as a consequence all the eigenvalues E_n of the problem (28) are real or complex conjugate in pairs.

In the following, for the sake of simplicity, we do not always mention the parameter a in the notation, for instance $C(E)$ will be written in place of $C(a, E)$.

Let E_n be an eigenvalue of the problem (28). Then we have $C(E_n) = 0$ and also $Y_1(X, E_n) \equiv Y_{-1}(X, E_n) =: Y_{E_n}(X)$. Let L be any endless oriented path in the X-plane, starting from infinity in S_{-1} and then going back to infinity, but in S_1. The following theorem will result from a quite simple proof [2].

Theorem 8. *With the above assumptions, we have*

$$\int_L Y_{E_n}^2(X)\,\mathrm{d}X = -2C'(E_n)$$

where the prime denotes for the derivation with respect to the eigenparameter E.

Proof. We start with $Y_1(X, E)$ which solves the equation

$$-Y_1'' + (X^m + a_1 X^{m-1} + \cdots + a_{m-1}X + E)Y_1 = 0. \tag{31}$$

Making E varying, and taking the derivative with respect to E, we immediately deduce that $Z_1(X, E) := \frac{\partial Y_1}{\partial E}(X, E)$ satisfies

$$-(Z_1)''_{XX} + (X^m + a_1 X^{m-1} + \cdots + a_{m-1}X + E)Z_1 + Y_1 = 0. \tag{32}$$

Combining these equalities together yields

$$-((Z_1)'_X Y_1 - Z_1 (Y_1)'_X)'_X + Y_1^2 = 0. \tag{33}$$

Next, by fixing an arbitrary point $X_0 \in L$, we can decompose

$$L = L_1 - L_{-1},$$

where $L_{\pm 1}$ are oriented path starting from X_0 and ending at infinity in $S_{\pm 1}$, respectively.

Note that both of Y_1 and Z_1 are exponentially vanishing as $X \to \infty$ along L_1. Therefore, by integrating (33) on the path L_1, we obtain

$$\int_{L_1} Y_1^2(X, E)\,\mathrm{d}X = ((Z_1)'_X Y_1 - Z_1 (Y_1)'_X)\Big|_{X_0}^{\infty \in L_1} = \mathsf{Wr}_X(Z_1, Y_1)\Big|_{X = X_0}. \tag{34}$$

[2] We refer the reader to Sibuya's book ([33], chapter 6) for a comparison.

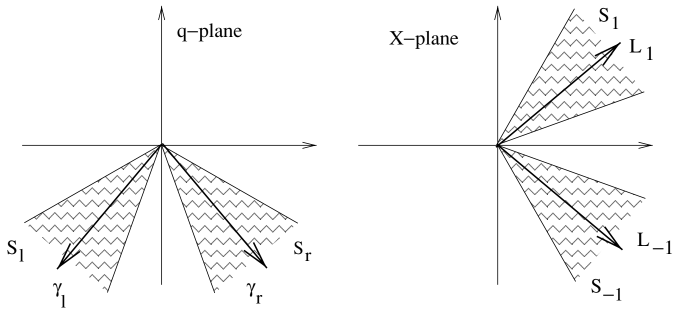

Figure 1. The $\gamma := \gamma_r - \gamma_l$ and $L := L_1 - L_{-1}$ in the q-plane and X-plane, respectively.

Similarly, by denoting $Z_{-1}(X, E) := \frac{\partial Y_{-1}}{\partial E}(X, E)$, we also have

$$\int_{L_{-1}} Y_{-1}^2(X, E)\,\mathrm{d}X = \mathsf{Wr}_X(Z_{-1}, Y_{-1})\Big|_{X=X_0}. \tag{35}$$

Substituting $E = E_n$ into (23) and its derivative with respect to E yields

$$Y_1(X, E_n) = Y_{-1}(X, E_n)$$

and

$$Z_{-1}(X, E_n) = Z_1(X, E_n) + C'(E_n)Y_0(X, E_n).$$

Now, combining these equalities with (34) and (35), one gets

$$\begin{aligned}\int_L Y_{E_n}^2(X)\,\mathrm{d}X &= \int_{L_1} Y_1^2(X, E_n)\,\mathrm{d}X - \int_{L_{-1}} Y_{-1}^2(X, E_n)\,\mathrm{d}X \\ &= \mathsf{Wr}_X\big(Z_1(X, E_n) - Z_{-1}(X, E_n), Y_1(X, E_n)\big)\Big|_{X=X_0} \\ &= -C'(E_n)\mathsf{Wr}(Y_0(X, E_n), Y_1(X, E_n)).\end{aligned}$$

Taking into account (24), we get the conclusion. □

As a consequence, we now can derive the sign of the $\mathcal{PT}$-pseudo-norm from the sign of the derivative of the Stokes multiplier. Indeed, let E_n be a real eigenvalue and $\phi_n(q)$ be an eigenfunction corresponding to E_n. We emphasize that, by the reality of E_n, $\phi_n(q)$ can be chosen to be $\mathcal{PT}$-symmetric.

$$\mathcal{PT}\phi_n(q) = \phi_n(q). \tag{36}$$

We now have

Theorem 9.

$$\|\phi_n\|_{\mathcal{PT}}^2 = \langle\langle\phi_n, \phi_n\rangle\rangle_\gamma = \mathrm{i}K_n C'(E_n),$$

where K_n is a positive real number.

Proof. Assume that γ has been chosen as in (8). By changing the integral variable $\mathrm{i}q = X$, we obtain

$$\|\phi_n\|_{\mathcal{PT}}^2 = \int_\gamma \phi_n^2(q)\,\mathrm{d}q = -\mathrm{i}\int_L \phi_n^2(-\mathrm{i}X)\,\mathrm{d}X,$$

where L is the image of γ under the mapping $q \mapsto \mathrm{i}q =: X$ (see figure 1).

Since $\phi_n(q)$ is an eigenfunction, $\phi_n(-\mathrm{i}X)$ must vanish exponentially at infinity in both $S_{\pm 1}$. So, there exists a non-zero constant α_n such that

$$\phi_n(-\mathrm{i}X) = \alpha_n Y_1(X, E_n) = \alpha_n Y_{-1}(X, E_n).$$

When X take real values, we can deduce from (27) and (36) that $Y_{\pm 1}(X, E_n)$ and $\phi_n(-\mathrm{i}X)$ are all real. Hence, $\alpha_n \in \mathbb{R}$.

By theorem 8, we have

$$\|\phi_n\|^2_{\mathcal{PT}} = \mathrm{i}2\alpha_n^2 C'(E_n).$$

The proof is complete by setting $K_n := 2\alpha_n^2$. □

The following result is a direct consequence of the theorem.

Corollary 9.1. *Assume that E_n is a real eigenvalue of H, then $\|\phi_n\|^2_{\mathcal{PT}} = 0$ if the multiplicity of E_n is greater than 1.*

We now recall a classical result from real analysis.

Lemma 10. *Suppose that a real-valued function $f(x)$ is continuously differentiable on (a, b) and $x_1, x_2 \in (a, b)$ are its two consecutive zeros. Then $f'(x_1) f'(x_2) \leqslant 0$.*

Proof. Assume conversely that $f'(x_1) f'(x_2) > 0$; for instance $f'(x_1) > 0$ and $f'(x_2) > 0$. We deduce from this assumption that $f(x)$ increases strictly in sufficiently small neighbourhoods of x_1 and x_2. This implies that $f(x_1 + \epsilon) > 0$ and $f(x_2 - \epsilon) < 0$ for a sufficiently small $\epsilon > 0$. By its continuity, $f(x)$ must vanish at least once in the interval $(x_1 + \epsilon, x_2 - \epsilon)$. This is contrary to the hypothesis. □

This lemma asserts that if all zeros x_n of $f(x)$ are simple then $f'(x_n)$ changes its sign alternately. Hence, a switch like $(-1)^n$. This is exactly what we describe in the next theorem.

Theorem 11. *Assume that all eigenvalues E_n of the problem (28) are real and simple. Then, up to a normalization, the set of the corresponding eigenfunctions $\{\phi_n\}, n \geqslant 0$, is $\mathcal{PT}$-orthonormal in the sense that*

$$\langle\langle \phi_n, \phi_m \rangle\rangle_{\mathcal{PT}} = \pm(-1)^n \delta_{mn} \tag{37}$$

where $\pm 1 = \langle\langle \phi_0, \phi_0 \rangle\rangle_{\mathcal{PT}}$.

Proof. We first note that the reality of the whole set of eigenvalues $\{E_n\}$ enables us to treat $C(E) := C(a, E)$ as a function of the real variable E (for each fixed $a \in \mathbb{R}^{m-1}$). This function is purely imaginary because of (25). Hence, $-\mathrm{i}C(E) = \operatorname{Im} C(E)$ is a real-valued function of $E \in \mathbb{R}$. So also is $-\mathrm{i}C'(E)$.

For $m \neq n$, the equality (37) is a direct consequence of corollary 2.1. We should note that, as $m = n$, the sign of $\|\phi_n\|^2_{\mathcal{PT}}$ does not change when multiplying ϕ_n by a non-zero constant. Therefore, by applying lemma 10 to $-\mathrm{i}C(E)$ and normalizing ϕ_n, we get the conclusion. □

We emphasize that the hypothesis on the simpleness of all eigenvalues in this theorem is crucially necessary. Nevertheless, this requirement is not always satisfied, especially in cases of Hamiltonians involving parameters.

To end this section, we now detail the striking case when all $a_j = 0$ and $m \geqslant 2$. The Hamiltonian then becomes $H = p^2 + q^2(\mathrm{i}q)^{m-2}$, whose whole eigenvalues have been proved to be real and positive using several different methods (see [6, 7, 15, 17, 19, 32]).

In their recent papers [2, 3], Bender *et al* showed that for some unbroken $\mathcal{PT}$-symmetric Hamiltonians, the charge operator $\mathcal{C}$ can be computed explicitly using perturbative techniques. They also provided numerical evidence on the sign alternation of $\|\phi_n\|^2_{\mathcal{PT}}$. We can now explain this phenomenon quite simply.

Let us agree on the simpleness of all eigenvalues E_n, which will be the matter of a forthcoming paper, so that each $-\mathrm{i}C'(E_n)$ possesses a sign. Note that by construction, the entire function $Y_0(X, E)$ is the solution (unique by its asymptotic behaviour at infinity) of equation (29) which vanishes exponentially at $+\infty$ and takes only real values whenever X and E are real. It is not hard to verify that $Y_0(0, 0) \neq 0$. Therefore, substituting $X = 0$ and $E = 0$ in (27) yields

$$\omega^{-m/4} Y_0(0, 0) = C(0) Y_0(0, 0) + \omega^{m/4} Y_0(0, 0).$$

This implies immediately that

$$-\mathrm{i}C(0) = \frac{\omega^{-m/4} - \omega^{m/4}}{\mathrm{i}} = 2 \sin\left(\frac{m\pi}{2(m+2)}\right) > 0.$$

One can regard $-\mathrm{i}C(E)$ now as a (real-valued) function of $E \in \mathbb{R}$ with only simple zeros $0 < E_0 < E_1 < \cdots$ and starting with a positive value $-\mathrm{i}C(0) > 0$. As a direct consequence of lemma 10, we obtain

$$\mathrm{sign}(-\mathrm{i}C'(E_n)) = (-1)^{n+1}; \qquad \forall n \in \mathbb{N}.$$

Then after normalizing ϕ_n, we finally find out

$$\|\phi_n\|^2_{\mathcal{PT}} = (-1)^n, \qquad \text{for} \quad n = 0, 1, 2, 3, \ldots.$$

4. Conclusion

In this paper, we have established an explicit relation between the $\mathcal{PT}$-pseudo-norm and the derivative of the Stokes multiplier $C(E)$ with respect to the eigenparameter. In this formulation, the indefiniteness of the $\mathcal{PT}$-pseudo-norm associated with a non-Hermitian but $\mathcal{PT}$-symmetric Hamiltonian is interpreted as a natural sign alternation of the derivative of an entire function at its zeros. This relation also supplies us with a simple criterion to recognize degenerate eigenstates in the sense that their $\mathcal{PT}$-pseudo-norms are vanishing.

By corollary 9.1, one has to acknowledge the unavoidable occurrence of such degenerate eigenstates, even if the corresponding eigenvalues are real. The reality of the whole spectral set of a $\mathcal{PT}$-symmetric Hamiltonian does not completely ensure the non-degeneracy of its eigenstates. This observation indicates that the unbroken $\mathcal{PT}$-symmetry is not exactly equivalent to the reality of the whole set of eigenvalues of a $\mathcal{PT}$-symmetric Hamiltonian.

To strengthen our arguments on this point, we should refer to an earlier joint work with Delabaere [17], where the spectrum of the Hamiltonian $H_\alpha = p^2 + \mathrm{i}(q^3 + \alpha q)$ is investigated by means of (exact) semiclassical analysis. This Hamiltonian exhibits a version of a degeneracy of its eigenvalues $E_n = E_n(\alpha)$ for negative real α. More precisely, when α goes to $-\infty$, some pairs of real eigenvalues gradually turn into complex conjugate. For the first critical value of α where this phenomenon occurs, the corresponding pairs of eigenvalues are nothing but double zeros of $C(E)$, which means that $C'(E) = 0$ at these zeros. Such a critical value has been computed in [22] $\alpha_{\mathrm{crit}} \simeq -2.6118094$, and the eigenvalues becoming complex conjugate are the two lowest ones (see [17], figure 1). We should note that in this situation, the eigenvalues of $H_{\alpha_{\mathrm{crit}}}$ are still all real.

Obviously, the action of the charge operator $\mathcal{C}$ (if any exists) on eigenfunctions in the case of degeneracy may not be merely to switch signs by multiplying ϕ_n by $(-1)^n$ as in [3, 5].

Nevertheless, since there are at most a finite number of such degenerate eigenfunctions, we believe that an analogous method such as those in the above citations could be still applicable to define the charge operator $\mathcal{C}$.

Findings on the indefiniteness of $\mathcal{PT}$-pseudo-norm enable us to keep on constructing the mathematical apparatus for $\mathcal{PT}$-symmetric quantum mechanics. In this study, the structure of a Krein space may be involved.

Moreover, there seems to exist some hidden relations between the Stokes multiplier $C(E)$ and the calculation of the charge operator $\mathcal{C}$. At least as we indicated, the simpleness and the reality of all the zeros of $C(E)$ first lead to the non-degeneracy of $\mathcal{PT}$-pseudo-norm, which is a necessary condition to construct this operator.

Acknowledgments

The author is indebted to Professor F Pham for introducing him to this topic. He thanks Professor E Delabaere for suggesting the problem and for several helpful discussions during the preparation of this paper. This work was supported by the Abdus Salam International Centre for Theoretical Physics (ICTP) in the framework of Post-doctoral Fellowship. The author is grateful to Professor Le Dung Trang and the staff of the Mathematics Section for their warm hospitality. He also thanks Professors Nguyen Huu Duc and Ta Le Loi for their spiritual support.

Note added in proof. The authors of [19] kindly reminded us that the first complete proof of the reality of the spectrum of the Bender–Boettcher Hamiltonians is contained in appendix B of [19]. We would like to add that reference [20] is also an interesting introductory work for applying spectral determinants to $\mathcal{PT}$-symmetric problems.

References

[1] Bagchi B, Quesne C and Znojil M 2001 Generalized continuity equation and modified normalization in $\mathcal{PT}$-symmetric quantum mechanics *Mod. Phys. Lett.* A **16** 2047–57

[2] Bender C M, Brody D C and Jones H F 2003 Must a Hamiltonian be Hermitian? *Am. J. Phys.* **71** 1095–102

[3] Bender C M, Brod J, Refig A and Reuter M E 2004 The operator $\mathcal{C}$ in $\mathcal{PT}$-symmetric quantum theories *J. Phys. A: Math. Gen.* **37** 10139–65

[4] Bender C M, Berry M and Mandilara A 2002 Generalized $\mathcal{PT}$ symmetry and real spectra *J. Phys. A: Math. Gen.* **35** L467–71

[5] Bender C M, Meisinger P N and Wang Q 2003 Calculation of the hidden symmetry operator in $\mathcal{PT}$-symmetric quantum mechanics *J. Phys. A: Math. Gen.* **36** 1973–83

[6] Bender C M and Boettcher S 1998 Real spectra in non-Hermitian Hamiltonians having $\mathcal{PT}$-symmetry *Phys. Rev. Lett.* **80** 5243

[7] Bender C M, Boettcher S and Meisinger P N 1999 $\mathcal{PT}$-symmetric quantum mechanics *J. Math. Phys.* **40** 2201

[8] Bender C M and Milton K A 1998 Model of supersymmetric quantum field theory with broken parity symmetry *Phys. Rev.* D **57** 3595–608

[9] Bender C M and Wu T T 1969 Anharmonic oscillator *Phys. Rev.* **184** 1231–60

[10] Boas R Ph Jr 1954 *Entire Functions* (New York: Academic)

[11] Caliceti E, Graffi S and Maioli M 1980 Perturbation theory of odd anharmonic oscillators *Commun. Math. Phys.* **75** 51–66

[12] Cannata F, Junker G and Trost J 1998 Schrödinger operators with complex potential but real spectrum *Phys. Lett.* A **246** 219–26

[13] Delabaere E and Pham F 1997 Unfolding the quartic oscillator *Ann. Phys.* **261** 180–218

[14] Delabaere E, Dillinger H and Pham F 1997 Exact semi-classical expansions for one dimensional quantum oscillators *J. Math. Phys.* **38** 6126–84

[15] Delabaere E and Pham F 1998 Eigenvalues of complex Hamiltonians with $\mathcal{PT}$-symmetry I *Phys. Lett.* A **250** 25

[16] Delabaere E and Pham F 1998 Eigenvalues of complex Hamiltonians with $\mathcal{PT}$-symmetry II *Phys. Lett.* A **250** 29

[17] Delabaere E and Trinh D T 2000 Spectral analysis of the complex cubic oscillator *J. Phys. A: Math. Gen.* **33** 8771–96

[18] Delabaere E and Rasoamanana J-M Resurgent deformations for an ordinary differential equation of order 2 *Preprint* math.CA/0403085 (*Pac. J. Math.* at press)

[19] Dorey P, Dunning C and Tateo R 2001 Spectral equivalences, Bethe ansatz equations, and reality properties in $\mathcal{PT}$-symmetric quantum mechanics *J. Phys. A: Math. Gen.* **34** 5679–704

[20] Dorey P and Tateo R 1999 On the relation between Stokes multipliers and the T-Q systems of conformal field theory *Nucl. Phys.* B **563** 573–602

[21] Fernández F M, Guardiola R, Ros J and Znojil M 1999 A family of complex potentials with real spectrum *J. Phys. A: Math. Gen.* **32** 3105–16

[22] Handy C R 2001 Generating converging bounds to the (complex) discrete states of the $P^2 + iX^3 + i\alpha X$ Hamiltonian *J. Phys. A: Math. Gen.* **34** 5065–81

[23] Japaridze G S 2002 Space of state vectors in $\mathcal{PT}$ symmetrical quantum mechanics *J. Phys. A: Math. Gen.* **35** 1709–18

[24] Lévai G and Znojil M 2001 Conditions for complex spectra in a class of $\mathcal{PT}$-symmetric potentials *Mod. Phys. Lett.* A **16** 1973–81

[25] Lévai G, Cannata F and Ventura A 2002 $\mathcal{PT}$-symmetry breaking and explicit expressions for the pseudo-norm in the Scarf II potential *Phys. Lett.* A **300** 271–81

[26] Mezincescu G A 2000 Some properties of eigenvalues and eigenfunctions of the cubic oscillator with imaginary coupling constant *J. Phys. A: Math. Gen.* **33**

[27] Mostafazadeh A 2002 Pseudo-Hermiticity versus $\mathcal{PT}$ symmetry: the necessary condition for the reality of the spectrum of a non-Hermitian Hamiltonian *J. Math. Phys.* **43** 205–14

[28] Mostafazadeh A 2003 Exact $\mathcal{PT}$-symmetry is equivalent to Hermiticity *J. Phys. A: Math. Gen.* **36** 7081–709

[29] Mostafazadeh A and Batal A 2004 Physical aspects of pseudo-Hermitian and $\mathcal{PT}$-symmetric quantum mechanics *J. Phys. A: Math. Gen.* **37** 11645–79

[30] Pham F 1996 Confluence of turning points in exact WKB analysis *The Stokes Phenomenon and Hilbert's 16th Problem (Groningen, 1995)* (River Edge, NJ: World Scientific) pp 215–35

[31] Pham F 2000 Multiple turning points in exact WKB analysis (variations on a theme of Stokes) *Toward the Exact WKB Analysis of Differential Equations Linear or Non-Linear* ed C Howls, T Kawai and Y Takei (Kyoto: Kyoto University Press) pp 71–85

[32] Shin K C 2002 On the reality of the eigenvalues for a class of $\mathcal{PT}$-symmetric oscillators *Commun. Math. Phys.* **229** 543–64

[33] Sibuya Y 1975 *Global Theory of a Second Order Linear Differential Equation with a Polynomial Coefficient Mathematics Studies* vol 18 (Amsterdam: North-Holland)

[34] Tai T D 2002 Asymptotique et analyse spectrale de l'oscillateur cubique *Thèse* Université de Nice

[35] Tai T D 2004 On the Sturm–Liouville problem for the complex cubic oscillator *Asymptotic Anal.* **40** 211–34

[36] Voros A 1983 The return of the quartic oscillator. The complex WKB method *Ann. Inst. H Poincaré Phys. Théor.* **39** 211–338

[37] Voros A 1999 Exact resolution method for general 1D polynomial Schrödinger equation *J. Phys. A: Math. Gen.* **32** 5993–6007

[38] Znojil M 2004 Conservation of pseudo-norm in $\mathcal{PT}$ symmetric quantum mechanics *Rend. Circ. Mat. Palermo (2) Suppl.* **72** 211–8

[39] Znojil M 2001 $\mathcal{PT}$-symmetrized supersymmetric quantum mechanics *DI-CRM Workshop on Mathematical Physics (Prague, 2000) Czech. J. Phys.* **51** 420–8