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Pseudo-Hermitian description of PT-symmetric systems defined on a complex contour

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Abstract

We describe a method that allows for a practical application of the theory of pseudo-Hermitian operators to PT-symmetric systems defined on a complex contour. We apply this method to study the Hamiltonians $H = p^2 + x^2(\mathrm{i}x)^\nu$ with $\nu \in (-2, \infty)$ that are defined along the corresponding anti-Stokes lines. In particular, we reveal the intrinsic non-Hermiticity of H for the cases that ν is an even integer, so that $H = p^2 \pm x^{2+\nu}$, and give a proof of the discreteness of the spectrum of H for all $\nu \in (-2, \infty)$. Furthermore, we study the consequences of defining a square-well Hamiltonian on a wedge-shaped complex contour. This yields a PT-symmetric system with a finite number of real eigenvalues. We present a comprehensive analysis of this system within the framework of pseudo-Hermitian quantum mechanics. We also outline a direct pseudo-Hermitian treatment of PT-symmetric systems defined on a complex contour which clarifies the underlying mathematical structure of the formulation of PT-symmetric quantum mechanics based on the charge-conjugation operator. Our results provide conclusive evidence that pseudo-Hermitian quantum mechanics provides a complete description of general PT-symmetric systems regardless of whether they are defined along the real line or a complex contour.

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1. Introduction

The notion of a pseudo-Hermitian operator as outlined in [1–3] provides a general framework for understanding the intriguing mathematical properties of PT-symmetric Hamiltonians

[4, 5][1]. It involves an underlying Hilbert space $\mathcal{H}$ in which the operator acts. For PT-symmetric Hamiltonians defined on the real line, $\mathcal{H}$ is the familiar space of square integrable functions. For the PT-symmetric Hamiltonians H defined on a complex contour and having a discrete spectrum, $\mathcal{H}$ is the Hilbert space obtained by Cauchy completing the span of the eigenfunctions of H with respect to an arbitrarily chosen positive-definite inner product [10–12]. The implicit nature of this construction makes a direct application of the theory of pseudo-Hermitian operators for these Hamiltonians intractable. This forms the basis of the view that this theory is incapable of dealing with PT-symmetric Hamiltonians defined on a complex contour. The purpose of this paper is to show that indeed the opposite is true. This is done by an explicit construction that allows for the description of the same system using the information given on the real axis. It reveals the implicit non-Hermiticity of the apparently Hermitian PT-symmetric Hamiltonians, such as $p^2 - x^4$, that are defined along an appropriate complex contour [4, 5]. Furthermore, it leads to a previously unnoticed connection between the spectral properties of the PT-symmetric Hamiltonians of the form

$$H = p^2 + x^2(\mathrm{i}x)^\nu,$$

(defined on an appropriate contour) and those of the Hamiltonians of the form

$$H = p^2 + |x|^{2+\nu},$$

(which are obtained by requiring the eigenfunctions to belong to $L^2(\mathbb{R})$ and satisfy certain boundary conditions at $x = 0$). An important advantage of a pseudo-Hermitian description of PT-symmetric systems defined on a complex contour is that it offers a prescription for computing the physical observables [12–14] of these theories.

In the remainder of this section we include a brief review of the relevant aspects of the theory of pseudo-Hermitian operators. For clarity of presentation, we will only consider Hamiltonian operators that have a discrete nondegenerate spectrum. In particular, we will focus our attention mainly on the cases that the spectrum is not only discrete and nondegenerate but also real (and bounded from below). It is an operator with the latter properties that can serve as the Hamiltonian for a unitary quantum system [15]. If complex eigenvalues are present, we identify the vector space underlying the physical Hilbert space with the span of the eigenfunctions with real eigenvalues and restrict the Hamiltonian to this vector space [10–12].

Let $\mathcal{H}$ be a given separable Hilbert space with inner product $\langle\cdot|\cdot\rangle$ and $H : \mathcal{H} \to \mathcal{H}$ be a linear operator. Then H is called a pseudo-Hermitian operator [1] if there exists a Hermitian invertible operator $\eta : \mathcal{H} \to \mathcal{H}$ satisfying

$$H^\dagger = \eta H \eta^{-1}, \tag{1}$$

where for any linear operator $A : \mathcal{H} \to \mathcal{H}$, $A^\dagger$ stands for the 'adjoint of A', i.e., the unique operator $A^\dagger : \mathcal{H} \to \mathcal{H}$ satisfying $\langle\cdot|A\cdot\rangle = \langle A^\dagger\cdot|\cdot\rangle$. The operator η entering the defining relation (1), which is sometimes referred to as a metric operator, is not unique [16, 17]. In fact, the set $\mathcal{U}_H$ consisting of all metric operators is always an infinite set. A simple property

[1] The term 'pseudo-Hermitian' has been in use within the context of indefinite-metric quantum theories [6] and indefinite-metric linear spaces [7] since the 1940s [8]. In this context, it corresponds to what is termed as 'η-pseudo-Hermitian' in [1], where η is an *a priori* fixed indefinite metric operator. The relevance of the indefinite-metric theories and PT-symmetric systems has been considered in [9]. The definition of a pseudo-Hermitian operator given in [1] (and used below) is slightly different from the one used in earlier publications, e.g., [6, 7, 9]. As explained in detail in [10], this slight difference has important conceptual and technical ramifications. In particular, together with the idea of using biorthonormal systems [1] it opens up the way for the construction of all possible metric operators, leads to the important observation that there is a positive-definite inner product rendering the Hamiltonian Hermitian for the cases that the spectrum is real [2] and reveals the nature of the connection with antilinear symmetries such as PT [3].

of a pseudo-Hermitian operator is that it is Hermitian with respect to the possibly indefinite inner product $\langle\cdot,\cdot\rangle_\eta := \langle\cdot\,|\,\eta\cdot\rangle$, i.e., $\langle\cdot, H\cdot\rangle_\eta = \langle H\cdot,\cdot\rangle_\eta$ [1].

Next, suppose that H has a complete set of eigenvectors $\psi_n \in \mathcal{H}$, i.e., it is diagonalizable. Then one can construct the vectors $\phi_n \in \mathcal{H}$ that together with ψ_n form a biorthonormal system for the Hilbert space, i.e.,

$$\langle\phi_n|\psi_m\rangle = \delta_{mn}, \qquad \sum_n |\psi_n\rangle\langle\phi_n| = 1. \tag{2}$$

Using the properties of such biorthonormal systems, one can prove the following characterization theorem [2].

Theorem. *For a diagonalizable linear operator H with a discrete spectrum the following conditions are equivalent.*

(c1) The spectrum of H is real.
(c2) H is pseudo-Hermitian and the set $\mathcal{U}_H$ includes a positive-definite metric operator η_+.
(c3) H is Hermitian with respect to a positive-definite inner product $\langle\cdot,\cdot\rangle_+$, e.g., $\langle\cdot,\cdot\rangle_{\eta_+} := \langle\cdot\,|\eta_+\cdot\rangle$.
(c4) H can be mapped to a Hermitian operator $h : \mathcal{H}\to\mathcal{H}$ via a similarity transformation, i.e., there is an invertible operator $\rho : \mathcal{H}\to\mathcal{H}$ such that

$$h := \rho H \rho^{-1} \tag{3}$$

is Hermitian.

If one (and therefore all) of these conditions hold, one has the following spectral resolutions for H and $H^\dagger$.

$$H = \sum_n E_n|\psi_n\rangle\langle\phi_n|, \qquad H^\dagger = \sum_n E_n|\phi_n\rangle\langle\psi_n|. \tag{4}$$

Furthermore, a positive-definite metric operator η_+ is given by

$$\eta_+ = \sum_n |\phi_n\rangle\langle\phi_n|, \tag{5}$$

and a canonical example of the invertible operator ρ whose existence is guaranteed by condition (c4) is $\rho = \sqrt{\eta_+}$.[2]

The metric operator η_+ plays the same role in pseudo-Hermitian quantum mechanics [10] as the metric tensor does in general relativity [19]. It allows for the construction of the physical Hilbert space $\mathcal{H}_{\rm phys}$ and the observables of the system. The Hilbert space $\mathcal{H}_{\rm phys}$ has the same vector space structure as $\mathcal{H}$ but its inner product is given by

$$\langle\cdot,\cdot\rangle_+ = \langle\cdot,\cdot\rangle_{\eta_+} := \langle\cdot\,|\eta_+\cdot\rangle. \tag{6}$$

The observables O of the theory are linear Hermitian operators acting in $\mathcal{H}_{\rm phys}$ [13]. They can be obtained from the Hermitian operators o acting in $\mathcal{H}$ according to

$$O = \rho^{-1} o \rho. \tag{7}$$

The formulation of the dynamics and the interpretation of the theory are identical with those of the conventional quantum mechanics. *Pseudo-Hermitian quantum mechanics shares all the postulates of conventional quantum mechanics except that the inner product of the physical Hilbert space $\mathcal{H}_{\rm phys}$ is not a priori fixed but determined by the eigenvalue problem for a linear (Hamiltonian) operator that acts on a reference Hilbert space $\mathcal{H}$.*

[2] For a mathematically rigorous discussion of pseudo-Hermitian operators, see [18].

As we mentioned above, the formulation of the theory does not fix the reference Hilbert space $\mathcal{H}$. For systems with a finite-dimensional state space, one usually identifies $\mathcal{H}$ with the complex Euclidean space, i.e., $\mathbb{C}^N$ with usual Euclidean inner product: $\langle\vec{\psi}|\vec{\phi}\rangle := \vec{\psi}^* \cdot \vec{\phi}$, where a dot means ordinary dot product of vectors [11]. For PT-symmetric theories defined on the real axis, e.g., for $H = p^2 + \mathrm{i}x^3$, the natural choice for $\mathcal{H}$ is $L^2(\mathbb{R})$ [17]. However, for PT-symmetric theories that are defined on a complex contour Γ, such as $H = p^2 - x^4$, a natural and useful choice for the reference Hilbert space $\mathcal{H}$ has not been available. The main purpose of this paper is to offer a satisfactory resolution of this problem by showing how one can formulate and describe the same theories using equivalent PT-symmetric Hamiltonians whose eigenvalue problem is defined in $L^2(\mathbb{R})$. This 'real description' facilitates the understanding of the physical content of these theories. It allows us to use the usual mathematical tools of conventional quantum mechanics and deal with the manifestly non-Hermitian form of the Hamiltonians such as $H = p^2 - x^4$ whose non-Hermiticity stems from their domain of definition rather than their explicit form. An alternative but less practical approach is to develop a pseudo-Hermitian description of PT-symmetric systems that is based on the choice: $\mathcal{H} = L^2(\Gamma)$. This 'complex description' clarifies the underlying mathematical structure of the formulation of PT-symmetric quantum mechanics that is based on the charge-conjugation operator [20–22].

2. Moving back to the real line

Suppose $\mathcal{F}$ is the set of real-analytic functions[3] $\psi : \mathbb{R} \to \mathbb{C}$ and $H : \mathcal{F} \to \mathcal{F}$ is a linear operator of the form

$$H = [p - A(x)]^2 + V(x), \tag{8}$$

where $A, V : \mathbb{R} \to \mathbb{C}$ are piecewise real-analytic functions, $p\psi(x) := -\mathrm{i}\psi'(x)$ for all $\psi \in \mathcal{F}$, and a prime stands for a derivative. A particularly well-studied example is

$$H = p^2 + x^2(\mathrm{i}x)^\nu, \qquad \nu \in (-2, \infty). \tag{9}$$

The main observation that has led to the current interest in PT-symmetric quantum mechanics is that for certain non-real choices of V (and $A = 0$), for example (9) with $\nu \geqslant 0$, the operator H has a real and discrete spectrum provided that its eigenvalue problem is solved along an appropriate contour Γ in the complex plane [4][4]. This was a rather intriguing observation because generically the operator H, which we will call the Hamiltonian, is manifestly non-Hermitian with respect to the L^2-inner product.

A typical physicist who is not familiar with the subject would immediately reject the statement that '$H = p^2 - x^4$ has a discrete spectrum'[5]. Indeed, this statement is neither true nor false, because the eigenvalue problem for a linear operator defined on an infinite-dimensional vector space is well posed only for specific choices of the domain of the operator. In the case of differential operators such as (8), in particular (9), the determination of the domain is related to the choice of the asymptotic boundary conditions. A nontrivial observation made in [4] is that one obtains a discrete spectrum for (9) provided that one imposes the asymptotic boundary conditions along an appropriate contour Γ in the complex plane[6]. This means that

[3] Note that $\mathcal{F} \cap L^2(\mathbb{R})$ is a dense subset of $L^2(\mathbb{R})$.
[4] A mathematically rigorous proof of this statement is given in [23, 24].
[5] This Hamiltonian corresponds to the choice $\nu = 2$ in (9).
[6] For the cases that ν is an integer greater than -2, so that the potential term in (9) is a monomial, this was known to mathematicians [26]. We will give a proof of the discreteness of the spectrum for all $\nu \in (-2, \infty)$ in the appendix.

one has to identify the eigenvalue equation for (8) with its complex (holomorphic) extension [25, 26]

$$\left\{-\left[\frac{\mathrm{d}}{\mathrm{d}z}-\mathrm{i}A(z)\right]^2+V(z)\right\}\Psi_n(z)=E_n\Psi_n(z), \tag{10}$$

and seek for solutions Ψ_n such that

$$|\Psi_n(z)|\to 0 \quad \text{exponentially as } z \text{ moves off to infinity along } \Gamma. \tag{11}$$

Note that the contour Γ is generally the graph of a (continuous piecewise) regular curve [27] parametrized by $s\in\mathbb{R}$, i.e., there is a (continuous piecewise) differentiable function $\zeta:\mathbb{R}\to\mathbb{C}$ with non-vanishing first derivative such that

$$\Gamma=\{\zeta(s)|s\in\mathbb{R}\}, \tag{12}$$

and that $\lim_{s\to\pm\infty}\mathrm{Re}[\zeta(s)]=\pm\infty$. Here and in what follows Re and Im, respectively, mean 'real' and 'imaginary part of'. Clearly, we may state the boundary condition (11) as

$$|\Psi_n(\zeta(s))|\to 0 \quad \text{exponentially as } s\to\pm\infty. \tag{13}$$

For the Hamiltonians (9), it is the choice of an appropriate contour Γ and the imposition of the boundary conditions (11) that lead to a discrete set of nontrivial solutions for (10). The same holds for various generalizations of (9) [5, 28]. In general, the contour Γ is not uniquely determined by the mathematical considerations, though it is required to stay in the so-called Stokes wedges in the asymptotic region, i.e., where $s\to\pm\infty$. In particular, there is a preferred choice for the asymptotic shape of Γ that maximizes the decay rate of the solutions of (10). This corresponds to the bisector of the appropriate Stokes wedge. Making this choice for the Hamiltonians (9), we have [4]

$$\lim_{s\to\pm\infty}\arg[\zeta(s)]=-\theta_\nu^\pm, \tag{14}$$

where 'arg' abbreviates 'argument of' and

$$\theta_\nu^+=\theta_\nu:=\frac{\pi\nu}{2(\nu+4)}, \qquad \theta_\nu^-:=\pi-\theta_\nu. \tag{15}$$

Next, we identify the real and imaginary axes of $\mathbb{C}$ with the x- and y-axes of the usual Cartesian coordinate system on $\mathbb{R}^2=\mathbb{C}$, so that $z=x+\mathrm{i}y$, and consider a general smooth contour Γ such that $\mathrm{Re}[\Gamma(x+\mathrm{i}y)]$ is an increasing function of $x:=\mathrm{Re}(z)$.[7] Then we can express the function ζ in terms of a differentiable real-valued function $f:\mathbb{R}\to\mathbb{R}$ according to

$$\zeta(x)=x+\mathrm{i}f(x). \tag{16}$$

The condition that ζ is a regular curve is also satisfied, because $|\zeta'(x)|^2=1+f'(x)^2\neq 0$.

Now, we wish to restrict the complex differential equation (10) to the contour Γ, and obtain an equivalent real differential equation with generally complex coefficients. Along Γ we have $z=\zeta(x)=x+\mathrm{i}f(x)$. A simple change of variable $z\to x+\mathrm{i}f(x)$ in (10) yields

$$\left\{-g(x)^2\left[\frac{\mathrm{d}}{\mathrm{d}x}-\mathrm{i}a(x)\right]^2+\mathrm{i}g(x)^3f''(x)\left[\frac{\mathrm{d}}{\mathrm{d}x}-\mathrm{i}a(x)\right]+v(x)\right\}\psi_n(x)=E_n\psi_n(x), \tag{17}$$

where

$$g(x):=[\zeta'(x)]^{-1}=[1+\mathrm{i}f'(x)]^{-1}, \qquad a(x):=g(x)^{-1}A[x+\mathrm{i}f(x)], \tag{18}$$

[7] This is not a strong condition. One can always choose such a contour for the purpose of defining boundary conditions (11).

$$v(x) := V[x + \mathrm{i}f(x)], \qquad \psi_n(x) := \Psi_n[x + \mathrm{i}f(x)]. \tag{19}$$

The complex differential equation (10) together with the boundary condition (11) (alternatively (13)) is clearly equivalent to real differential equation (17) together with the boundary condition

$$|\psi(x)| \to 0 \quad \text{exponentially as } |x| \to \infty. \tag{20}$$

The analyticity properties [25] of Ψ_n and consequently of ψ_n together with condition (20) implies that $\psi_n \in L^2(\mathbb{R})$. In other words, the eigenvalue problem for the Hamiltonian (8) defined by equation (10) is equivalent to the eigenvalue problem for the Hamiltonian

$$H' := g(x)^2[p - a(x)]^2 - g(x)^3 f''(x)[p - a(x)] + v(x), \tag{21}$$

viewed as an operator acting in $L^2(\mathbb{R})$.

3. Consequences of imposing PT-symmetry

Let $\xi : \mathbb{R} \to \mathbb{C}$ be a function. Then under the joint action of the parity P and time-reversal T operators, $\xi(x) \to PT\xi(x)PT = \xi(-x)^*$. Applying this rule to the Hamiltonian (21) and using $PTpPT = p$, we find

$$PTH'PT = g(-x)^{*2}[p - a(-x)^*]^2 - g(-x)^{*3} f''(-x)^*[p - a(-x)^*] + v(-x)^*. \tag{22}$$

In particular, demanding H' to be PT-symmetric yields

$$g(-x)^{*2} = g(x)^2, \qquad g(-x)^* f''(-x)^* = g(-x)^* f''(x), \tag{23}$$

$$a(-x)^* = a(x), \qquad v(-x)^* = v(x). \tag{24}$$

In view of equations (18), (19), (23) and (24), the fact that f is a real-valued function, and x takes zero as a value, we have

$$\begin{aligned} &f(x) = f(-x), \qquad A(u)^*|_{u=-[x+\mathrm{i}f(x)]} = A[x + \mathrm{i}f(x)], \\ &V(u)^*|_{u=-[x+\mathrm{i}f(x)]} = V[x + \mathrm{i}f(x)]. \end{aligned} \tag{25}$$

The first of these equations imply that along the contour Γ, $z(-x)^* = -z(x)$. Therefore, the condition that H' be PT-symmetric implies that Γ has reflection symmetry about the y- (or imaginary-) axis. The second and third equations in (25) and the assumption that A and V can be analytically continued onto the contour Γ indicate that they are separately PT-symmetric, i.e.,

$$PTA(x)PT = A(x), \qquad PTV(x)PT = V(x). \tag{26}$$

These are equivalent to requirement that the original Hamiltonian (8) be PT-symmetric.

In summary, the Hamiltonian (8) and the contour Γ are PT-symmetric if and only if the Hamiltonian (21) is PT-symmetric. In the following we will only consider the cases that these conditions hold.

4. Wedge-shaped contours

The simplest possible PT-symmetric choices for the contour Γ are the wedge-shaped contours:

$$\Gamma(x) = x[1 - \mathrm{i}\,\mathrm{sign}(x)\tan\theta], \tag{27}$$

where $\mathrm{sign}(x) := x/|x|$ for $x \neq 0$, $\mathrm{sign}(0) := 0$ and $\theta \in [0, \pi/2)$. Clearly, Γ is not a regular curve at $x = 0$. Therefore, we will smoothen it in a small neighbourhood of $x = 0$, say

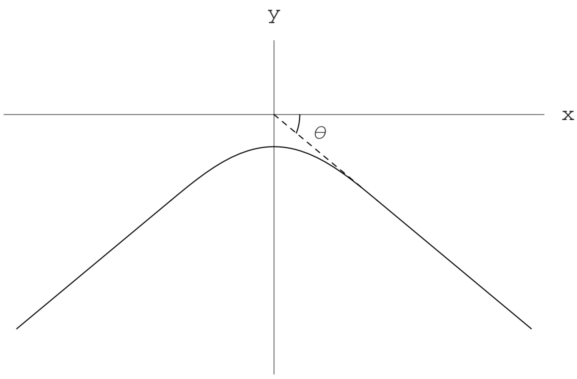

Figure 1. Plot of $y = f_\epsilon(x)$. f_ϵ has a maximum at $x = 0$ with value $f_\epsilon(0) = -3\epsilon\tan\theta/8$. The angle θ is also displayed.

according to $\Gamma \to \Gamma_\epsilon$, where

$$\Gamma_\epsilon(x) := x + \mathrm{i}\, f_\epsilon(x), \tag{28}$$

$$f_\epsilon(x) := \begin{cases} -|x|\tan\theta & \text{for} \quad |x| \geqslant \epsilon \\ \varphi_\epsilon(x) & \text{for} \quad |x| \leqslant \epsilon, \end{cases} \tag{29}$$

$$\varphi_\epsilon(x) := \frac{\epsilon\tan\theta}{8}\left[\left(\frac{x}{\epsilon}\right)^4 - 6\left(\frac{x}{\epsilon}\right)^2 - 3\right], \tag{30}$$

and $\epsilon \in \mathbb{R}^+$ is an arbitrary constant. Note that f_ϵ is a twice-differentiable function that can be substituted for f in expression (21) for the Hamiltonian H' and that its maximum value is $f_\epsilon(0) = -3\epsilon\tan\theta/8$. Figure 1 shows a plot of f_ϵ. Furthermore, in view of (28) and (29), we have

$$\Gamma_\epsilon(x) = \begin{cases} \sec(\theta)\, \mathrm{e}^{-\mathrm{i}\theta\, \mathrm{sign}(x)} x & \text{for} \quad |x| \geqslant \epsilon \\ x + \mathrm{i}\varphi_\epsilon(x) & \text{for} \quad |x| \leqslant \epsilon. \end{cases} \tag{31}$$

In what follows we shall consider the contours of the form (31) which yield the wedge-shaped contours (27) in the limit $\epsilon \to 0$.

Setting $f = f_\epsilon$ in (18) and using (29), we obtain

$$\text{for} \quad |x| \geqslant \epsilon: \quad f'(x) = -\tan(\theta)\,\mathrm{sign}(x), \qquad f''(x) = 0,$$
$$g(x) = \cos(\theta)\, \mathrm{e}^{\mathrm{i}\theta\, \mathrm{sign}(x)}, \tag{32}$$

$$\text{for} \quad |x| \leqslant \epsilon: \quad f'(x) = \varphi'_\epsilon(x), \qquad f''(x) = \varphi''_\epsilon(x), \qquad g(x) = \gamma_\epsilon(x), \tag{33}$$

where

$$\varphi'_\epsilon(x) := \frac{\tan\theta}{2}\left[\left(\frac{x}{\epsilon}\right)^3 - 3\left(\frac{x}{\epsilon}\right)\right], \tag{34}$$

$$\varphi''_\epsilon(x) := \frac{3\tan\theta}{2\epsilon}\left[\left(\frac{x}{\epsilon}\right)^2 - 1\right], \tag{35}$$

$$\gamma_\epsilon(x) := \left\{1 + \frac{\mathrm{i}\tan\theta}{2}\left[\left(\frac{x}{\epsilon}\right)^3 - 3\left(\frac{x}{\epsilon}\right)\right]\right\}^{-1}. \tag{36}$$

These relations together with (18), (19) and (21) then yield

$$H' = H_-^{(\epsilon)} + H'_\epsilon + H_+^{(\epsilon)}, \qquad H_\pm^{(\epsilon)} := \Lambda_\pm^{(\epsilon)} H_\pm \Lambda_\pm^{(\epsilon)}, \qquad H'_\epsilon := \Lambda_\epsilon H_\epsilon \Lambda_\epsilon, \tag{37}$$

where

$$\Lambda_+^{(\epsilon)} := \int_\epsilon^\infty \mathrm{d}x |x\rangle\langle x|, \qquad \Lambda_-^{(\epsilon)} := \int_{-\infty}^{-\epsilon} \mathrm{d}x\, |x\rangle\langle x|, \qquad \Lambda_\epsilon := \int_{-\epsilon}^{\epsilon} \mathrm{d}x\, |x\rangle\langle x|, \tag{38}$$

$$H_\pm := \cos^2(\theta)\,\mathrm{e}^{\pm 2\mathrm{i}\theta}\{p - \sec(\theta)\,\mathrm{e}^{\mp\mathrm{i}\theta} A[\sec(\theta)\,\mathrm{e}^{\mp\mathrm{i}\theta} x]\}^2 + V[\sec(\theta)\,\mathrm{e}^{\mp\mathrm{i}\theta} x], \tag{39}$$

$$H_\epsilon := \gamma_\epsilon(x)^2[p - a_\epsilon(x)]^2 - \gamma_\epsilon(x)^3\varphi''_\epsilon(x)[p - a_\epsilon(x)] + v_\epsilon(x), \tag{40}$$

$$a_\epsilon(x) := \gamma_\epsilon(x)^{-1} A[x + \mathrm{i}\varphi_\epsilon(x)], \qquad v_\epsilon(x) := V[x + \mathrm{i}\varphi_\epsilon(x)]. \tag{41}$$

Note that $\mathcal{PT}\Lambda_+^{(\epsilon)}\mathcal{PT} = \Lambda_-^{(\epsilon)}$ and $\mathcal{PT}\Lambda_\epsilon\mathcal{PT} = \Lambda_\epsilon$. These together with (26) and (30)–(41) yield the following relations that are clearly consistent with the $\mathcal{PT}$-symmetry of H'.

$$\mathcal{PT}\; H_+^{(\epsilon)}\; \mathcal{PT} = H_-^{(\epsilon)}, \qquad \mathcal{PT}\; H_\epsilon\; \mathcal{PT} = H_\epsilon. \tag{42}$$

In practice, to solve the eigenvalue problem for H', we may solve the corresponding differential equation for $|x| \geqslant \epsilon$ in the limit $\epsilon \to 0$ and match the solution at $x = 0$ by enforcing appropriate continuity requirements. As we shall see below, the latter yield a pair of boundary conditions at $x = 0$. It is the Hamiltonians $H_\pm$ together with these boundary conditions at $x = 0$ and the requirement $\psi_n \in L^2(\mathbb{R})$ that determine the eigenvalues E_n.

The Hamiltonians $H_\pm$ take a simpler form in terms of the scaled position and momentum operators:

$$\mathrm{x} := \frac{x}{\cos\theta}, \qquad \mathrm{p} := \cos\theta p. \tag{43}$$

The classical analogue of x corresponds to the arc-length parametrization of the contour Γ [27]. Using (39) and (43), we have

$$H_\pm := \mathrm{e}^{\pm 2\mathrm{i}\theta}[\mathrm{p} - \mathrm{e}^{\mp\mathrm{i}\theta} A(\mathrm{e}^{\mp\mathrm{i}\theta}\mathrm{x})]^2 + V(\mathrm{e}^{\mp\mathrm{i}\theta}\mathrm{x}). \tag{44}$$

The boundary conditions at $x = 0$ can be obtained by integrating both sides of the eigenvalue equation for H' over the interval $[-\epsilon, \epsilon]$ and taking the limit $\epsilon \to 0$ in the resulting expression. Doing an integration by parts, using the fact that A and V are continuous functions, noting that

$$\varphi_\epsilon(\pm\epsilon) = \varphi''_\epsilon(\pm\epsilon) = 0, \qquad \varphi'_\epsilon(\pm\epsilon) = 1, \qquad \gamma_\epsilon(\pm\epsilon) = (1 \mp \mathrm{i}\tan\theta)^{-1},$$

and introducing the notation

$$\psi_n(0^\pm) := \lim_{x\to 0^\pm} \psi_n(x), \qquad \psi'_n(0^\pm) := \lim_{x\to 0^\pm} \psi'_n(x),$$

we find the following boundary condition at $x = 0$.

$$\frac{\psi'_n(0^+)}{(1 - \mathrm{i}\tan\theta)^2} - \frac{\psi'_n(0^-)}{(1 + \mathrm{i}\tan\theta)^2} = 2\mathrm{i}\, A(0)[\psi(0^+) - \psi(0^-)]. \tag{45}$$

Imposing the condition that ψ_n be continuous at $x = 0$, i.e.,

$$\psi(0^\pm) = \psi(0), \tag{46}$$

reduces (45) to

$$\mathrm{e}^{-2\mathrm{i}\theta}\psi'_n(0^-) = \mathrm{e}^{2\mathrm{i}\theta}\psi'_n(0^+), \tag{47}$$

or equivalently to

$$|\psi_n'(0^-)| = |\psi_n'(0^+)| \tag{48}$$

and

$$\arg[\psi_n'(0^-)] = \arg[\psi_n'(0^-)] + 4\theta \qquad \text{if} \quad \psi_n'(0^\pm) \neq 0. \tag{49}$$

Therefore, for ψ_n to be differentiable at $x = 0$ either $\theta = 0$ or $\psi_n'(0) = 0$.

For a PT-invariant eigenfunction ψ_n, where

$$\psi_n(-x) = \psi_n(x)^*, \qquad \psi_n'(-x) = -\psi_n'(x)^*, \tag{50}$$

and in particular

$$\psi_n(0^-) = \psi_n(0^+) = \psi_n(0) \in \mathbb{R} \tag{51}$$

$$\psi_n'(0^-) = -\psi_n'(0^+)^*, \tag{52}$$

(49) implies that

$$\text{either} \quad \psi_n'(0^-) = \psi_n'(0^+) = 0 \qquad \text{or} \qquad \arg[\psi_n'(0^\pm)] = \frac{\pi}{2} \mp 2\theta. \tag{53}$$

As a result ψ_n is differentiable at $x = 0$ if at least one of the following conditions hold: (1) $\psi'(0) = 0$; (2) $\theta = 0$ and $\psi'(0)$ is imaginary[8].

Having derived the explicit expression for the boundary conditions at $x = 0$ we can identify the eigenvalue problem for the initial Hamiltonian H and the contour (27) with that of

$$H' = \Lambda_-^{(0)} H_- \Lambda_-^{(0)} + \Lambda_+^{(0)} H_+ \Lambda_+^{(0)} \tag{54}$$

and the requirement that the eigenfunctions belong to $L^2(\mathbb{R})$ and satisfy the boundary conditions (46) and (47). For real eigenvalues, where we may choose to work with the PT-invariant eigenfunctions, we have the boundary conditions (51), (48), and (53).

5. Application to $H = p^2 + x^2(ix)^\nu$

For the Hamiltonians (9), we have

$$A(x) = 0, \qquad V(x) = \mathrm{i}^\nu x^{\nu+2}, \qquad \theta = \theta_\nu := \frac{\pi\nu}{2(\nu+4)}. \tag{55}$$

Inserting these in (44), we are led to the following remarkable result:

$$H_\pm = \mathrm{e}^{\pm 2\mathrm{i}\theta_\nu} H_{\nu+2}, \tag{56}$$

where

$$H_N := \mathrm{p}^2 + |\mathrm{x}|^N \qquad \text{for} \quad N \in \mathbb{R}. \tag{57}$$

Therefore, in view of (54), we have

$$H' = \mathrm{e}^{-2\mathrm{i}\theta_\nu} \Lambda_-^{(0)} \, H_{\nu+2} \, \Lambda_-^{(0)} + \mathrm{e}^{2\mathrm{i}\theta_\nu} \Lambda_+^{(0)} \, H_{\nu+2} \, \Lambda_+^{(0)}. \tag{58}$$

The eigenvalue problem for the Hamiltonian (9) that is defined by the contour (27) with θ given by (55) is equivalent to the eigenvalue equation

$$\mathrm{e}^{2\mathrm{i}\theta_\nu \mathrm{sign(x)}}[-\psi_n''(\mathrm{x}) + |\mathrm{x}|^{\nu+2}\psi_n(\mathrm{x})] = E\psi_n(\mathrm{x}) \qquad \text{for} \quad \mathrm{x} \neq 0, \tag{59}$$

[8] In conventional quantum mechanics, where $\theta = 0$, the PT-symmetric eigenfunctions of a PT-symmetric Hamiltonian of the standard form $p^2 + V(x)$ are either real and even (where condition (1) holds) or imaginary and odd (where condition (2) holds). For an example, see [13].

where ψ_n are required to be continuous elements of $L^2(\mathbb{R})$ satisfying

$$e^{-2i\theta_\nu}\psi_n'(0^-) = e^{2i\theta_\nu}\psi_n'(0^+). \tag{60}$$

Next, we show that the eigenfunctions ψ_n never vanish at $x = 0$ and they are necessarily non-differentiable at this point[9].

Lemma. *Let $\psi_n \in L^2(R)$ be a continuous solution of (59) and (60) with $\nu > -2$ and $\nu \neq 0$ and $\psi_{n\pm} : \mathbb{R}^\pm \cup \{0\} \to \mathbb{C}$ be its restrictions: $\psi_{n\pm}(\mathrm{x}) := \psi_n(\mathrm{x})$ for all $\pm\mathrm{x} \in \mathbb{R}^+$, $\psi_{n\pm}(0) := \psi_n(0)$, and $\psi_{n\pm}'(0) := \psi_n'(0^\pm)$. Then,*

$$\psi_n(0) \neq 0 \neq \psi'(0^\pm). \tag{61}$$

Proof. Clearly (59) and (60) are, respectively, equivalent to

$$-\psi_{n\pm}''(\mathrm{x}) + |\mathrm{x}|^{\nu+2}\psi_{n\pm}(\mathrm{x}) = e^{\mp 2i\theta_\nu}E_n\psi_{n\pm}(\mathrm{x}) \qquad \text{for} \quad \pm\mathrm{x} \in \mathbb{R}^\pm, \tag{62}$$

$$e^{-2i\theta_\nu}\psi_{n-}'(0) = e^{2i\theta_\nu}\psi_{n+}'(0). \tag{63}$$

Multiplying both sides of (62) by $\psi_{n\pm}^*$, integrating over $\mathbb{R}^\pm \cup \{0\}$, and performing an integration by parts yield

$$\pm\psi_{n\pm}(0)^*\psi_{n\pm}'(0) + \|\psi_{n\pm}'\|_\pm^2 + \||\mathrm{x}|^{\nu/2+1}\psi_{n\pm}\|_\pm^2 = e^{\mp 2i\theta_\nu}E_n\|\psi_{n\pm}\|_\pm^2, \tag{64}$$

where for all $\xi_\pm : \mathbb{R}^\pm \to \mathbb{C}$, $\|\xi_\pm\|_\pm^2 := \int_{\mathbb{R}^\pm}|\xi_\pm(\mathrm{x})|^2\,\mathrm{dx}$. [10] Now, if at least one of $\psi(0)$, $\psi'(0^+)$ and $\psi'(0^-)$ vanishes, then so is the first term in (64). This implies that $e^{\mp 2i\theta_\nu}E_n$ must be real for both choices of the sign. For $\nu > -2$ and $\nu \neq 0$, this is only possible if $E_n = 0$. But then the right-hand side of (64) vanishes, while its left-hand side is strictly positive. This is a contradiction proving (61). □

A direct implication of (61) is that if $\nu > -2$ and $\nu \neq 0$, then for all n, ψ_n fails to be differentiable at $\mathrm{x} = 0$ and that we can always normalize ψ_n so that $\psi_n(0) = 1$.

For real eigenvalues E_n we can take ψ_n to be PT-invariant and for the cases of interest, namely $\nu > 0$, the boundary conditions on the eigenvalue equation (59) take the form

$$\psi_n(0^-) = \psi_n(0^+) \in \mathbb{R}, \tag{65}$$

$$|\psi_n'(0^-)| = |\psi_n'(0^+)|, \tag{66}$$

$$\arg[\psi_n'(0^\pm)] = \frac{\pi}{2}\left(\frac{4 + (1 \mp 2)\nu}{4 + \nu}\right). \tag{67}$$

An interesting particular example is the Hamiltonian

$$H = p^2 - x^4, \tag{68}$$

which corresponds to $\nu = 2$ and

$$H_\pm = e^{\pm\frac{i\pi}{3}}[\mathrm{p}^2 + \mathrm{x}^4], \tag{69}$$

with eigenvalue equation

$$e^{\frac{i\pi}{3}\,\mathrm{sign(x)}}[-\psi_n''(\mathrm{x}) + \mathrm{x}^4\psi_n(\mathrm{x})] = E_n\psi_n(\mathrm{x}) \qquad \text{for} \quad \mathrm{x} \neq 0, \tag{70}$$

and boundary conditions (65), (66) and

$$\arg[\psi_n'(0^\pm)] = \frac{(3 \mp 2)\pi}{6}. \tag{71}$$

[9] ψ_n is necessarily twice differentiable at all $x \neq 0$.

[10] Note that because $|\mathrm{x}|^{2+\nu}$ is bounded from below, $\|\psi_{n\pm}'\|_\pm^2$ and $\||\mathrm{x}|^{\nu/2+1}\psi_{n\pm}\|_\pm^2$ are finite numbers [25, section 10.1].

The switching of the sign of the potential term from minus in (68) to plus in (69) and (70) is quite remarkable. As seen from (57)–(59), this is a characteristic feature of the Hamiltonians H of the form (9). In view of the discreteness of the spectrum of the Hamiltonians H_N for $N > 0$ [29], this phenomenon provides invaluable insight in the origin of the discreteness of the spectrum of H. Indeed, as we shall show below, it leads to a rigorous proof of the fact that for all $\nu \in (-2, \infty)$ the spectrum of H is discrete. Note that here and in what follows the spectra of H_N, H' and H are, respectively, defined by the exponentially vanishing boundary condition at $\pm\infty$ along $\mathbb{R}$, the latter together with the boundary conditions (65)–(67) at $x = 0$ and exponentially vanishing boundary condition at $\pm\infty$ along the contour (31) with $\theta = \theta_\nu$.

To establish the discreteness of the spectrum of H' (and consequently H), we use the equivalence of the eigenvalue problem for H' with equations (62) and (63), and note that in terms of the functions $y_\pm : [0, \infty) \to \mathbb{C}$ defined by

$$y_\pm(\mathrm{x}) := \psi_{n\pm}(\pm\mathrm{x}), \tag{72}$$

(62) takes the form

$$-y''_\pm(\mathrm{x}) + \mathrm{x}^{\nu+2} y_\pm(\mathrm{x}) = \lambda_\pm y_\pm(\mathrm{x}), \qquad \text{for} \quad \mathrm{x} \in [0, \infty), \tag{73}$$

where

$$\lambda_\pm = \mathrm{e}^{\mp 2\mathrm{i}\theta_\nu} E_n = \mathrm{e}^{\mp \frac{\mathrm{i}\pi\nu}{\nu+4}} E_n. \tag{74}$$

The eigenvalue problem for H' is equivalent to finding the solutions $y_\pm$ of (73) that belong to $L^2[0, \infty)$ and satisfy

$$y_-(0) = y_+(0) \neq 0, \tag{75}$$

$$y'_-(0) = -\mathrm{e}^{4\mathrm{i}\theta_\nu} y'_+(0) \neq 0. \tag{76}$$

This problem can be treated using the classical theory of singular boundary-value problems developed mainly by Weyl [25, section 10]. In the appendix, we will use some basic results of this theory to give a proof of the discreteness of spectrum of H for all $\nu \in (-2, \infty)$.

We close this section by pointing out that the formulation of the eigenvalue problem for H as the differential equations (73) with boundary conditions (75) and (76) is also of practical importance because it allows for the immediate application of the known numerical, perturbative and variational methods that are tailored to deal with functions of a real variable [30]. It should also be interesting to see if one can obtain an alternative proof of the reality of the spectrum using this formulation.

6. Square well placed on a wedge-shaped contour

Consider the Hamiltonian $H = p^2 + V(x)$ for the ordinary Hermitian infinite square-well potential

$$V(x) := \begin{cases} 0 & \text{for} \quad |x| < \frac{L}{2} \\ \infty & \text{for} \quad |x| \geqslant \frac{L}{2}, \end{cases} \tag{77}$$

where $L \in \mathbb{R}^+$. If one solves the eigenvalue problem for this Hamiltonian on the real axis one finds an infinite discrete set of eigenvalues

$$E_n^{(0)} = \frac{\pi^2 n^2}{L^2}, \qquad n \in \mathbb{Z}^+. \tag{78}$$

As this Hamiltonian is both Hermitian and PT-symmetric, one may choose to work with normalized PT-invariant eigenfunctions which are given, up to an arbitrary sign, by [13]

$$\psi_n^{(0)}(x) = \frac{\mathrm{i}^{\mu_n}}{\sqrt{L}} \sin\left[\pi n\left(\frac{x}{L}+\frac{1}{2}\right)\right], \qquad \mu_n := \frac{1+(-1)^n}{2}. \tag{79}$$

We wish to explore the consequences of defining the eigenvalue problem for the square-well Hamiltonian using a wedge-shaped contour (27) with arbitrary angle $\theta \in (0, \pi/2)$.[11]

Pursuing the approach of section 4, we find that the eigenvalue problem for this system is equivalent to the following boundary-value problem:

$$-\psi''_{n\pm}(\mathrm{x}) = \mathrm{e}^{\mp 2\mathrm{i}\theta} E_n \psi_{n\pm}(\mathrm{x}) \qquad \text{for} \quad \pm\,\mathrm{x} \in \left[0, \frac{L}{2}\right], \tag{80}$$

$$\psi_{n-}(0) = \psi_{n+}(0), \qquad \mathrm{e}^{-2\mathrm{i}\theta}\psi'_{n-}(0) = \mathrm{e}^{+2\mathrm{i}\theta}\psi'_{n+}(0), \tag{81}$$

$$\psi_{n\pm}\left(\pm\frac{L}{2}\right) = 0. \tag{82}$$

Clearly, $\psi_{n\pm}$ determine the eigenfunctions ψ_n of the system according to

$$\psi_n(\mathrm{x}) = \psi_{n\pm}(\mathrm{x}), \qquad \text{if} \quad \pm\mathrm{x} \in \left[0, \frac{L}{2}\right]. \tag{83}$$

They belong to

$$\mathcal{H}' := \left\{\psi \in L^2\left[-\frac{L}{2}, \frac{L}{2}\right] \middle| \psi\left(\pm\frac{L}{2}\right) = 0\right\}. \tag{84}$$

The eigenvalue problems (80)–(82) can be easily solved: zero is an acceptable eigenvalue only for $\theta = \pi/4$. The corresponding PT-invariant eigenfunction is given by

$$\psi(\mathrm{x}) = \pm c\left(\mathrm{x} \mp \frac{L}{2}\right) \qquad \text{for} \quad \pm\mathrm{x} \in \left[0, \frac{L}{2}\right], \tag{85}$$

where c is a real normalization constant. The eigenfunctions with nonzero eigenvalues have the form

$$\psi_{n\pm}(\mathrm{x}) = c_\pm\,\mathrm{e}^{\mathrm{i}\omega_{n\pm}\mathrm{x}} + d_\pm\,\mathrm{e}^{-\mathrm{i}\omega_{n\pm}\mathrm{x}}, \tag{86}$$

where $\omega_{n\pm} := \mathrm{e}^{\mp\mathrm{i}\theta}\sqrt{E_n}$ and

$$c_- = \tfrac{1}{2}[(1+\mathrm{e}^{2\mathrm{i}\theta})c_+ + (1-\mathrm{e}^{2\mathrm{i}\theta})d_+], \qquad d_- = \tfrac{1}{2}[(1-\mathrm{e}^{2\mathrm{i}\theta})c_+ + (1+\mathrm{e}^{2\mathrm{i}\theta})d_+], \tag{87}$$

$$c_+\,\mathrm{e}^{\mathrm{i}\omega_{n+}L/2} + d_+\,\mathrm{e}^{-\mathrm{i}\omega_{n+}L/2} = 0, \qquad c_-\,\mathrm{e}^{-\mathrm{i}\omega_{n+}L/2} + d_-\,\mathrm{e}^{\mathrm{i}\omega_{n+}L/2} = 0. \tag{88}$$

Equations (87) and (88) follow from the boundary conditions (81) and (82), respectively. They have a nontrivial solution provided that the eigenvalues E_n satisfy a transcendental equation that takes the following simple form in terms of the variable $u_n := \cos(\theta)L\sqrt{E_n}$:

$$\tan(\theta)\sinh[\tan(\theta)u_n] = \sin(u_n). \tag{89}$$

For $\theta = 0$ it reduces to $\sin(u_n) = 0$, and one recovers $E_n = E_n^{(0)}$. But for $\theta > 0$, it has a finite number $N(\theta)$ of real solutions where N is a decreasing function of θ. In particular, for

[11] Taking the $\nu \to \infty$ limit of (9) one obtains a similar square-well Hamiltonian (with $L = 2$ and $\theta = \theta_\nu \to \pi/2$) [31]. For large but finite value of ν this Hamiltonian has an infinite number of positive real eigenvalues all of which are proportional to ν^2. Therefore in the limit $\nu \to \infty$, real part of the spectrum is mapped to (the point at) infinity. The spectral problem considered in this section is different from the one treated in [31], for we view the potential (77) as given and take θ as a free parameter. We will see that for large θ ($\theta > \pi/4$) the spectrum is entirely complex.

Table 1. The first five exceptional points $\mathcal{E}_\ell$ and the corresponding exceptional values θ_ℓ of θ.

ℓ	1	2	3	4	5
$\mathcal{E}_\ell$	0	$61.58L^{-2}$	$200.9L^{-2}$	$418.9L^{-2}$	$715.7L^{-2}$
θ_ℓ	45.00°	14.81°	9.88°	7.59°	6.23°

$\theta > \pi/4$, $N(\theta) = 0$ and there is no real solution. As one decreases the value of θ from $\pi/2$ down to zero one encounters an infinite strictly increasing sequence $\{\mathcal{E}_\ell\}$ of exceptional points [32]. The angles θ for the corresponding wedge-shaped contours form a strictly decreasing sequence $\{\theta_\ell\}$ that converges to zero. Table 1 lists the values of the first five exceptional points and the corresponding angles θ_ℓ.

In general, the number of real eigenvalues are given by

$$N(\theta) = \begin{cases} 2\ell - 1 & \text{for} \quad \theta \in (\theta_{\ell+1}, \theta_\ell) \quad \text{with} \quad \ell \geqslant 1 \\ 2\ell - 2 & \text{for} \quad \theta = \theta_\ell \quad \text{with} \quad \ell \geqslant 2 \\ 1 & \text{for} \quad \theta = \theta_1 = \pi/4. \end{cases} \tag{90}$$

Because the eigenvalues are nondegenerate, the dimension of the invariant subspace spanned by the eigenfunctions with a real eigenvalue is $N(\theta)$. This $N(\theta)$-dimensional subspace is the underlying vector space $\mathcal{V}$ for both the reference Hilbert space $(\mathcal{H})$ and the physical Hilbert space $(\mathcal{H}_{\text{phys}})$ of the system. For $\theta = 0$, $N(\theta) = \infty$ and $\mathcal{H}$, $\mathcal{H}_{\text{phys}}$ and $\mathcal{H}'$ coincide. But for $\theta > 0$, $\mathcal{V}$ is finite dimensional. In particular, for $\theta > \theta_1 = \pi/4$ the vector space $\mathcal{V}$ is zero dimensional and the system does not admit a unitary quantum description.

Another peculiar feature of this system is that the dimension of the physical Hilbert space takes even values only for the exceptional values θ_ℓ of θ with $\ell \geqslant 2$. As these constitute a measure zero subset of $[0, \pi/4)$, the physical Hilbert space is generically odd dimensional!

Three comments are in order.

1. If one defines the eigenvalue problem using the Neumann boundary conditions at $x = \pm L/2$, i.e., requires $\psi'_{n\pm}(\pm L/2) = 0$, the (nonzero) eigenvalues are given by equation (89) with the sign of the right-hand side changed. The corresponding pseudo-Hermitian quantum system shares the general features of the square-well system discussed above. The only difference is that for all values of θ, zero is an eigenvalue with a constant eigenfunction. In particular, the physical Hilbert space is finite dimensional for $0 < \theta \leqslant \pi/2$, infinite dimensional for $\theta = 0$ and one dimensional for $\pi/4 \leqslant \theta < \pi/2$.
2. The quantum system corresponding to the square-well Hamiltonian placed on a wedge-shaped contour defines a PT-symmetric quantum system which is fundamentally different from the PT-symmetric square well studied in [13, 33, 34]. The latter system involves a non-Hermiticity parameter $Z \in [0, \infty)$. As one increases the value of Z (starting from zero), one encounters an infinite sequence of exceptional points which correspond to a strictly increasing sequence $\{Z_\ell\}$ of exceptional values of Z. As a result unlike the system introduced above, the physical Hilbert space is always infinite dimensional. In particular, for $0 \leqslant Z < Z_1$ the reference Hilbert space $\mathcal{H}$ coincides with $\mathcal{H}'$.
3. For the square-well system defined on a wedge-shaped contour, $\theta = 0$—which corresponds to the Hermitian limit of the problem—is an accumulation point of the exceptional values θ_ℓ of θ. This is the reason why for all positive values of θ the physical Hilbert space is finite dimensional[12]. This observation shows that changing the domain of the definition of a Hamiltonian from the real line to a complex contour can lead to

[12] It is not difficult to see that the same holds for negative θ.

completely different quantum systems. For example, for $\theta = \theta_2$ the physical Hilbert space is two dimensional. Therefore, it describes the interaction of a spin-half particle with a magnetic field [35]. In contrast, for $\theta = 0$, the system describes the one-dimensional motion of a particle that is trapped between two impenetrable walls.

7. Application of pseudo-Hermitian QM for square well along the wedge-shaped contour with $\theta = \theta_2$

The largest value of the angle θ that corresponds to a nontrivial unitary quantum system is $\theta = \theta_2 \approx 14.81°$. For this choice of θ, the Hamiltonian has two real eigenvalues. They are $E_1 \approx 9.09L^{-2}$ and $E_2 = \mathcal{E}_2 \approx 61.6L^{-2}$. The corresponding eigenfunctions ψ_1 and ψ_2 are given by (83) and (86) where

$$c_{n\pm} = c_\pm(E_n), \qquad d_{n\pm} = d_\pm(E_n), \tag{91}$$

$$c_\pm(E) := \frac{\mathcal{N}(E)}{1 - \mathrm{e}^{\pm \mathrm{i}\Omega_\pm(E)}}, \qquad d_\pm(E) := \frac{\mathcal{N}(E)}{1 - \mathrm{e}^{\mp \mathrm{i}\Omega_\pm(E)}}, \tag{92}$$

$$\Omega_\pm(E) := \mathrm{e}^{\mp\mathrm{i}\theta} L\sqrt{E}, \tag{93}$$

and $\mathcal{N}(E)$ is an arbitrary real normalization constant. Substituting (91) and (92) in (86) and using (83), we have

$$\psi_n(\mathrm{x}) = \psi_{n\pm}(\mathrm{x}) = \frac{\mathcal{N}_n \sin\left[\Omega_\pm(E_n)\left(\frac{1}{2} \mp \frac{\mathrm{x}}{L}\right)\right]}{\sin\left[\frac{\Omega_\pm(E_n)}{2}\right]} \qquad \text{for} \quad \pm\mathrm{x} \in \left[0, \frac{L}{2}\right], \tag{94}$$

where $\mathcal{N}_n \in \mathbb{R}^+$ are normalization constants and $n = 1, 2$.

The underlying vector space $\mathcal{V}$ for the reference and the physical Hilbert spaces is the two-dimensional subspace of $\mathcal{H}'$ spanned by ψ_1 and ψ_2. The reference Hilbert space $\mathcal{H}$ is obtained by endowing $\mathcal{V}$ with the subspace inner product $\langle\cdot|\cdot\rangle$ induced from $\mathcal{H}'$. Choosing the normalization constants as $\mathcal{N}_1 \approx 1.226L^{-1/2}\kappa$ and $\mathcal{N}_2 \approx 0.717L^{-1/2}\kappa$, for some $\kappa \in \mathbb{R}^+$, we have

$$\langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = \kappa^2, \qquad \langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle = r\kappa^2, \tag{95}$$

where

$$r \approx 0.068. \tag{96}$$

Clearly, $\{\psi_1, \psi_2\}$ form a non-orthogonal basis of $\mathcal{H}$. We can use the Gram–Schmidt procedure [36] to construct an orthonormal basis $\{\varepsilon_1, \varepsilon_2\}$ according to

$$\varepsilon_1 := \kappa^{-1}\psi_1, \qquad \varepsilon_2 := \frac{\psi_2 - r\psi_1}{\kappa\sqrt{1-r^2}}. \tag{97}$$

In this basis, the Hamiltonian is represented by the following manifestly non-Hermitian 2×2 matrix:

$$\tilde{H} = \begin{pmatrix} E_1 & \frac{r(E_2-E_1)}{\sqrt{1-r^2}} \\ 0 & E_2 \end{pmatrix} \approx L^{-2}\begin{pmatrix} 9.09 & 3.56 \\ 0 & 61.6 \end{pmatrix}. \tag{98}$$

We can compute the adjoint of H using its matrix representation (98) and determine its eigenvectors ϕ_n that together with ψ_n form a biorthonormal system for $\mathcal{H}$. This yields

$$\phi_1 = \kappa^{-1}\left(\varepsilon_1 - \frac{r}{\sqrt{1-r^2}}\varepsilon_2\right) = \frac{\psi_1 - r\psi_2}{\kappa^2(1-r^2)}, \qquad \phi_2 = \frac{\varepsilon_2}{\kappa\sqrt{1-r^2}} = \frac{\psi_2 - r\psi_1}{\kappa^2(1-r^2)}. \tag{99}$$

Now, we are in a position to compute the metric operator η_+. In view of (5) and (99), it has the following matrix representation in the orthonormal basis $\{\varepsilon_1, \varepsilon_2\}$:

$$\tilde{\eta}_+ = \kappa^{-2} \begin{pmatrix} 1 & -\frac{r}{\sqrt{1-r^2}} \\ -\frac{r}{\sqrt{1-r^2}} & \frac{1+r^2}{1-r^2} \end{pmatrix} \approx \kappa^{-2} \begin{pmatrix} 1 & -0.068 \\ -0.068 & 1.009 \end{pmatrix}. \tag{100}$$

In view of this relation, we have, for all $\xi, \zeta \in \mathcal{V}$,

$$\begin{aligned}\langle \xi, \zeta \rangle_+ := \langle \xi | \eta_+ \zeta \rangle &= \kappa^{-2} \left[\xi_1^* \zeta_1 - \frac{r(\xi_1^* \zeta_2 + \xi_2^* \zeta_1)}{\sqrt{1-r^2}} + \frac{(1+r^2)\xi_2^* \zeta_2}{1-r^2} \right] \\ &\approx \kappa^{-2} [\xi_1^* \zeta_1 - 0.068 (\xi_1^* \zeta_2 + \xi_2^* \zeta_1) + 1.009 \xi_2^* \zeta_2],\end{aligned} \tag{101}$$

where $\xi_n = \langle \varepsilon_n | \xi \rangle$, $\zeta_n = \langle \varepsilon_n | \zeta \rangle$ and $n = 1, 2$. Note that the coefficient κ^{-2} is a trivial scaling of the inner product.

If we use (101) to compute the inner product of the eigenvectors ψ_n, we find that as expected $\{\psi_1, \psi_2\}$ form an orthonormal basis of the physical Hilbert space, $\langle \psi_n, \psi_m \rangle_+ = \delta_{mn}$ for $m, n = 1, 2$. This also shows that the Hamiltonian viewed as acting in $\mathcal{H}_{\rm phys}$ is a Hermitian operator.

Next, we construct the physical observables O of the system. This requires the computation of $\rho = \sqrt{\eta_+}$. The matrix representation of ρ in the basis $\{\varepsilon_1, \varepsilon_2\}$ has the form

$$\tilde{\rho} = \sqrt{\tilde{\eta}_+} \approx \kappa^{-1} \begin{pmatrix} 0.999 & -0.034 \\ -0.034 & 1.004 \end{pmatrix}. \tag{102}$$

According to (7), the physical observables are given by $O = \sum_{\ell=0}^{3} \omega_\ell \Sigma_\ell$ where $\omega_\ell \in \mathbb{R}$ are arbitrary constants, Σ_0 is the identity operator acting in $\mathcal{H}$, for $\ell = 1, 2, 3$, Σ_ℓ are defined through their matrix representations in the basis $\{\varepsilon_1, \varepsilon_2\}$ according to

$$\tilde{\Sigma}_\ell = \tilde{\rho}^{-1} \sigma_\ell \tilde{\rho}, \tag{103}$$

and σ_ℓ are Pauli matrices. Specifically,

$$\tilde{\Sigma}_0 = \sigma_0 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \tilde{\Sigma}_1 \approx \begin{pmatrix} 0 & 1.005 \\ 0.995 & 0 \end{pmatrix},$$

$$\tilde{\Sigma}_2 \approx \mathrm{i} \begin{pmatrix} 0.068 & -1.007 \\ 0.998 & -0.068 \end{pmatrix}, \qquad \tilde{\Sigma}_3 \approx \begin{pmatrix} 1.002 & -0.068 \\ 0.068 & -1.002 \end{pmatrix}.$$

Using these relations and (98), we can show that indeed

$$H \approx L^{-2} (35.5\, \Sigma_0 + 1.78\, \Sigma_1 - 26.2\, \Sigma_3). \tag{104}$$

Next, we compute the Hermitian Hamiltonian h of (3) that is associated with H. We can obtain the matrix representation $\tilde{h}$ of h in the basis $\{\varepsilon_1, \varepsilon_2\}$ using either of (102) and (98) or (103) and (3). Both yield

$$\tilde{h} \approx L^{-2} \begin{pmatrix} 9.15 & 1.78 \\ 1.78 & 61.5 \end{pmatrix} = L^{-2} (35.5\, \sigma_0 + 1.78\, \sigma_1 - 26.2\, \sigma_3). \tag{105}$$

Therefore,

$$h \approx L^{-2} (9.15 |\varepsilon_1\rangle\langle\varepsilon_1| + 1.78 (|\varepsilon_1\rangle\langle\varepsilon_2| + |\varepsilon_2\rangle\langle\varepsilon_1|) + 61.5 |\varepsilon_2\rangle\langle\varepsilon_2|).$$

Having obtained the biorthonormal system $\{|\psi_n\rangle, |\phi_n\rangle\}$, we can also compute the generalized parity $\mathcal{P}$, time-reversal $\mathcal{T}$ and charge-conjugation $\mathcal{C}$ operators of [17], namely[13]

[13] See also [37].

$$\mathcal{P} := |\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2|, \tag{106}$$

$$\mathcal{T} := |\phi_1\rangle \star \langle\phi_1| - |\phi_2\rangle \star \langle\phi_2|, \tag{107}$$

$$\mathcal{C} := |\psi_1\rangle\langle\phi_1| - |\psi_2\rangle\langle\phi_2|, \tag{108}$$

where $\star$ is the complex conjugation defined by

$$\star\,|\zeta\rangle := \sum_{n=1}^{2} \langle\varepsilon_n|\zeta\rangle^*|\varepsilon_n\rangle = \sum_{n=1}^{2} \langle\zeta|\varepsilon_n\rangle\,|\varepsilon_n\rangle, \qquad \text{for all} \quad \zeta \in \mathcal{H}. \tag{109}$$

In particular, in the basis $\{\varepsilon_1, \varepsilon_2\}$, $\star$ is represented by ordinary complex conjugation '$*$' of complex vectors,

$$*\,\vec{z} := \vec{z}^*, \qquad \text{where} \quad \vec{z} = \begin{pmatrix} \langle\varepsilon_1|\zeta\rangle \\ \langle\varepsilon_2|\zeta\rangle \end{pmatrix} \in \mathbb{C}^2, \quad \zeta \in \mathcal{H}. \tag{110}$$

As explained in [17], unlike $\mathcal{C}$ which is always an involution ($\mathcal{C}^2 = 1$), $\mathcal{P}$ and $\mathcal{T}$ need not be involutions. Requiring them to be involutions restricts the choice of the biorthonormal system. In the case at hand, this restriction amounts to fixing the normalization constant for the eigenvectors ψ_n as

$$\kappa = (1 - r^2)^{-1/4} \approx 1.001. \tag{111}$$

Making this choice, we find that the matrix representations of $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{C}$, in the basis $\{\varepsilon_1, \varepsilon_2\}$, are respectively given by

$$\tilde{\mathcal{P}} = \begin{pmatrix} \sqrt{1-r^2} & -r \\ -r & -\sqrt{1-r^2} \end{pmatrix} \approx \begin{pmatrix} 0.998 & -0.068 \\ -0.068 & -0.998 \end{pmatrix}, \tag{112}$$

$$\tilde{\mathcal{T}} = \tilde{\mathcal{P}}*, \qquad \tilde{\mathcal{C}} = \begin{pmatrix} 1 & -\frac{2r}{\sqrt{1-r^2}} \\ 0 & -1 \end{pmatrix} \approx \begin{pmatrix} 1 & -0.136 \\ 0 & -1 \end{pmatrix}. \tag{113}$$

Using these relations we can directly check that indeed

$$\mathcal{P}^2 = \mathcal{T}^2 = \mathcal{C}^2 = 1, \qquad \mathcal{C} = \eta_+^{-1}\mathcal{P}, \qquad [H, \mathcal{C}] = [H, \mathcal{PT}] = 0. \tag{114}$$

In view of the identity $\mathcal{PT} = \star$, the $\mathcal{PT}$-symmetry of H corresponds to the fact that H is a real operator with respect to the complex conjugation (109), i.e., $\star H \star = H$. An explicit manifestation of the latter relation is that $\tilde{H}$ is a real matrix[14].

8. Formulation based on the $\mathcal{CPT}$ inner product, discussion and conclusion

In this paper, we have presented a formulation of PT-symmetric theories defined along a complex contour in which the state vectors belong to the familiar Hilbert space of square integrable functions. This formulation has a number of advantages. Firstly, it yields the necessary means for a straightforward application of the results of the theory of pseudo-Hermitian operators. Secondly, it provides a novel description of the Hamiltonians of the form (9) that reveals the origin of the discreteness of their spectrum. Finally, it is practically appealing as it allows for a direct application of the standard approximation schemes developed for solving differential equations on the real line [30].

[14] Because the matrix representation $\tilde{H}$ of the Hamiltonian is not symmetric, the definition of observables proposed in [38] cannot be employed [39].

In order to elucidate the practical aspects of our method we have considered the PT-symmetric system obtained by placing an infinite square-well potential on a wedge-shaped contour Γ. We have conducted a comprehensive study of this model showing that as soon as one makes the characteristic angle θ of the contour Γ different from zero (i.e., moves off the real axis), the physical Hilbert space of the system becomes finite dimensional. The dimension of this space depends on θ. It changes at certain critical values of θ that correspond to the exceptional spectral points associated with the system. The simplest nontrivial case occurs at the second exceptional point where $\theta \approx 14.81^\circ$ and the physical Hilbert space is two dimensional. For this case, we showed how one could employ the constructions developed in the framework of pseudo-Hermitian quantum mechanics to determine the explicit form of the inner product of the physical Hilbert space, the physical observables and the corresponding Hermitian Hamiltonian.

The results reported in this paper show that PT-symmetric quantum mechanics is indeed a special case of pseudo-Hermitian quantum mechanics. In order to apply the pseudo-Hermitian quantum mechanics to PT-symmetric systems defined on a complex contour, one may employ the fact that these systems admit a convenient description in terms of PT-symmetric Hamiltonians defined on the real line. The latter can be treated most perspicuously within the framework of pseudo-Hermitian quantum mechanics. In particular, one can compute the observables of the theory and explore its classical limit as outlined in [13, 14].

There is also a more direct, but less practical, pseudo-Hermitian description of PT-symmetric systems defined on a complex contour Γ. This is also suggested by the analysis of section 2.[15] It involves identifying the reference Hilbert space $\mathcal{H}$ with $L^2(\Gamma)$, where the contour Γ is viewed as a one-dimensional real submanifold of $\mathbb{R}^2 = \mathbb{C}$, i.e., a continuous (piecewise regular) plane curve. The relationship between this 'complex pseudo-Hermitian description' and the 'real pseudo-Hermitian description' that is based on transforming the system onto the real line can be reduced to the action of a diffeomorphism $\mathcal{G}$ of the complex plane that maps the real axis onto the contour Γ. This mapping maybe identified with the arc-length parametrization of Γ. In view of (16), we can parametrize Γ by the x-coordinate. We can use this parametrization to define the arc-length parameter: $\mathrm{x} = \mathcal{F}(x) := \int_0^x \sqrt{1+f'(s)^2}\,\mathrm{d}s$. Note that for the contours of interest $\mathcal{F} : \mathbb{R} \to \mathbb{R}$ is a diffeomorphism. The restriction of $\mathcal{G}$ onto the real axis defines the following mapping of $\mathbb{R}$ onto Γ:

$$\mathcal{G}(\mathrm{x}) := x + \mathrm{i}f(x) = \mathcal{F}^{-1}(\mathrm{x}) + \mathrm{i}f(\mathcal{F}^{-1}(\mathrm{x})), \qquad \text{for all} \quad \mathrm{x} \in \mathbb{R}. \tag{115}$$

This in turn induces a unitary operator $u_{\mathcal{G}} : L^2(\mathbb{R}) \to L^2(\Gamma)$ defined by[16]

$$(u_{\mathcal{G}}\psi)(z) := \psi(\mathcal{G}^{-1}(z)), \qquad \text{for all} \quad \psi \in L^2(\mathbb{R}), \quad z \in \Gamma. \tag{116}$$

Alternatively, setting $\Psi := u_{\mathcal{G}}\psi$ we have

$$\Psi(z) = \psi(\mathrm{x}) \qquad \text{if and only if} \quad z = \mathcal{G}(\mathrm{x}). \tag{117}$$

The statement that $u_{\mathcal{G}}$ is a unitary operator means that for all $\psi, \phi \in L^2(\mathbb{R})$

$$\langle u_{\mathcal{G}}\psi | u_{\mathcal{G}}\phi\rangle_\Gamma = \langle\psi|\phi\rangle, \tag{118}$$

where $\langle\cdot|\cdot\rangle_\Gamma$ is the inner product of $L^2(\Gamma)$, i.e.,

$$\langle\Psi|\Phi\rangle_\Gamma := \int_\Gamma \Psi(z)^*\Phi(z)\,\mathrm{d}z. \tag{119}$$

[15] See also [23].
[16] One might try to express $u_{\mathcal{G}}$ in the form $\mathrm{e}^{\mathrm{i}\{G(\mathrm{x}),\mathrm{p}\}/2}$ for some complex-valued function G by extending the results of [40].

The validity of equation (118) becomes obvious once we identify Γ with a plane curve and view the right-hand side of (119) as a line integral. Letting $\Psi := u_{\mathcal{G}}\psi$ and $\Phi := u_{\mathcal{G}}\phi$ and using (115) and (116), we have

$$\langle u_{\mathcal{G}}\psi|u_{\mathcal{G}}\phi\rangle_\Gamma = \langle\Psi|\Phi\rangle_\Gamma = \int_{\mathbb{R}} \Psi(\mathcal{G}(\mathrm{x}))^*\Phi(\mathcal{G}(\mathrm{x}))\,\mathrm{dx} = \int_{\mathbb{R}} \psi(\mathrm{x})^*\phi(\mathrm{x})\,\mathrm{dx} = \langle\psi|\phi\rangle.$$

An important property of $u_{\mathcal{G}}$ is that it establishes a one-to-one correspondence between the ingredients of the two pseudo-Hermitian descriptions of the system; to each linear operator A acting in $L^2(\mathbb{R})$ it associated a linear operator $\mathcal{A} := u_{\mathcal{G}}Au_{\mathcal{G}}^{-1}$ acting in $L^2(\Gamma)$. In particular, it maps the charge-conjugation operator $C := \eta^{-1}P$ of the real description to the charge-conjugation operator $\mathcal{C} : L^2(\Gamma) \to L^2(\Gamma)$ of the complex description according to

$$\mathcal{C} := u_{\mathcal{G}}Cu_{\mathcal{G}}^{-1}. \tag{120}$$

In view of the results of [17], for the Hamiltonians (9) with $\nu \geqslant 0$, the operator $\mathcal{C}$ is nothing but the charge-conjugation operator introduced in [20]. In fact, what the authors of [20] do is to define C on the real line (though they use the same symbol for both C and $\mathcal{C}$), perform the diffeomorphism $u_{\mathcal{G}}$ to obtain $\mathcal{C}$ and then use it in a contour integral along Γ to define their $\mathcal{CPT}$ inner product:

$$\langle\Psi,\Phi\rangle_{\mathcal{CPT}} := \int_\Gamma [\mathcal{CPT}\Psi(z)]\Phi(z)\,\mathrm{d}z \qquad \text{for} \quad \Psi,\Phi \in L^2(\Gamma). \tag{121}$$

Note that in the real description [17],

$$\langle\psi,\phi\rangle_{\mathcal{CPT}} := \int_{\mathbb{R}} [\mathcal{CPT}\psi(\mathrm{x})]\phi(\mathrm{x})\,\mathrm{dx} = \langle\psi|\eta_+|\phi\rangle = \langle\psi,\phi\rangle_+ \qquad \text{for} \quad \psi,\phi \in L^2(\mathbb{R}). \tag{122}$$

Moreover, the eigenfunctions Ψ_n (respectively ψ_n)[17] form an orthonormal set with respect to $\langle\cdot,\cdot\rangle_{\mathcal{CPT}}$ (respectively $\langle\cdot,\cdot\rangle_+$),

$$\langle\Psi_m,\Psi_n\rangle_{\mathcal{CPT}} = \delta_{mn} = \langle\psi_m,\psi_n\rangle_+ = \langle\psi_m|\eta_+|\psi_n\rangle. \tag{123}$$

Next, we introduce a metric operator $\eta_+^{\mathbb{C}} : L^2(\Gamma) \to L^2(\Gamma)$ and the corresponding inner product $\langle\cdot,\cdot\rangle_+^{\mathbb{C}} : L^2(\Gamma)\times L^2(\Gamma) \to \mathbb{C}$ according to

$$\eta_+^{\mathbb{C}} := u_{\mathcal{G}}\eta_+u_{\mathcal{G}}^{-1}, \qquad \langle\cdot,\cdot\rangle_+^{\mathbb{C}} := \langle\,\cdot\,|\eta_+^{\mathbb{C}}\cdot\rangle_\Gamma. \tag{124}$$

In view of the identity $\Psi_n = u_{\mathcal{G}}\psi_n$ and the fact that $u_{\mathcal{G}}$ is unitary, we then find

$$\delta_{mn} = \langle\psi_m|\eta_+|\psi_n\rangle = \left\langle u_{\mathcal{G}}^{-1}\Psi_m\middle|\eta_+\middle|u_{\mathcal{G}}^{-1}\psi_n\right\rangle = \langle\Psi_m|\eta_+^{\mathbb{C}}|\Psi_n\rangle. \tag{125}$$

Equations (123) and (125) show that Ψ_n, which are supposed to form a complete set, are orthonormal with respect to both the $\mathcal{CPT}$ inner product (121) and the inner product $\langle\cdot,\cdot\rangle_+^{\mathbb{C}}$. This proves that these two inner products are identical. Therefore, the formulation of PT-symmetric quantum mechanics based on the $\mathcal{CPT}$ inner product, as outlined in [20], admits a complete description in terms of the theory of pseudo-Hermitian operators.

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Note added. After the completion of this project, I discovered a preprint of Znojil [41] where he considers the analytic continuation of the *PT*-symmetric square well of [33] onto a smooth complex contour. The spectral properties of this system is similar to the one considered in section 6. In both cases, the spectrum is determined through a set of boundary conditions at the intersection point of the contour and the imaginary axis. The main difference between the two systems is that the defining boundary conditions used in [41] are postulated whereas those used in section 6 are derived. As explained in section 4, the latter are the general boundary conditions associated with the wedge-shaped contours.

[17] Recall that according to the analysis of section 5, the eigenfunctions ψ_n and Ψ_n are related via $\Psi_n(\mathcal{G}(\mathrm{x})) = \psi_n(\mathrm{x})$.

Appendix. Discreteness of the spectrum of (9)

Theorem. *The spectrum of the Hamiltonians* $H = p^2 + x^2(\mathrm{i}x)^\nu$ *defined by the contour (27) with* $\theta = \theta_\nu := \pi\nu/[2(\nu+4)]$ *is discrete for all* $\nu \in (-2, \infty)$.

Proof. For $\nu = 0$ this statement is well known to hold [29]. To prove it for $\nu \neq 0$, we prove the equivalent statement that for all $\nu \in (-2, \infty)$ the following boundary-value problem has a solution only for a discrete set of values of E_n.[18]

$$-y''_\pm(\mathrm{x}) + \mathrm{x}^{\nu+2} y_\pm(\mathrm{x}) = \lambda_\pm y_\pm(\mathrm{x}) \qquad \text{for} \quad \mathrm{x} \in [0, \infty), \tag{A.1}$$

$$\lambda_\pm = \mathrm{e}^{\mp 2\mathrm{i}\theta_\nu} E_n \in \mathbb{C}, \tag{A.2}$$

$$y_\pm \in L^2[0, \infty), \tag{A.3}$$

$$y_-(0) = y_+(0) \neq 0, \tag{A.4}$$

$$y'_-(0) = -\mathrm{e}^{4\mathrm{i}\theta_\nu} y'_+(0) \neq 0. \tag{A.5}$$

Let $\lambda \in \mathbb{C}$ be arbitrary, and consider finding solutions $y(\cdot; \lambda)$ of

$$-y''(\mathrm{x}) + \mathrm{x}^{\nu+2} y(\mathrm{x}) = \lambda y(\mathrm{x}), \qquad \text{with} \quad \nu > -2, \quad \mathrm{x} \in [0, \infty), \tag{A.6}$$

that belong to $L^2[0, \infty)$. Then because $\mathrm{x}^{\nu+2}$ is bounded below by zero, one has the so-called limit point case [25, section 10.1] where there is at most one linearly independent L^2-solution and such a solution exists for all non-real λ and has the form

$$y(\mathrm{x}; \lambda) = C(\lambda)[y_1(\mathrm{x}; \lambda) + m(\lambda) y_2(\mathrm{x}; \lambda)], \tag{A.7}$$

where $C(\lambda) \in \mathbb{C} - \{0\}$ is a constant, y_1 and y_2 are the fundamental solutions of (A.6) satisfying

$$y_1(0; \lambda) = 0, \qquad y'_1(0; \lambda) = -1, \qquad y_2(0; \lambda) = 1, \qquad y'_1(0; \lambda) = 0, \tag{A.8}$$

and $m : \mathbb{C} \to \mathbb{C}$ is a function having the property [25, section 10.2]

$$m(\lambda^*) = m(\lambda)^*. \tag{A.9}$$

Now, consider the boundary-value problem: (A.6), $y'(0) = 0$ and $y \in L^2[0, \infty)$. Because $\mathrm{x}^{\nu+2} \to \infty$ as $\mathrm{x} \to \infty$, this problem defines a discrete (pure point) spectrum $\mathcal{S} := \{\lambda_k | k \in \mathbb{Z}^+\}$ which is real and unbounded [25, section 10.3]. Furthermore, the eigenfunction associated with λ_k is, up to a multiplicative constant, $y_2(\cdot; \lambda_k)$, and the function m has the following spectral resolution:

$$m(\lambda) = \sum_{k=1}^{\infty} \frac{\sigma_k}{\lambda_k - \lambda}, \tag{A.10}$$

where $\sigma_k = \left[\int_0^\infty |y_2(\mathrm{x}; \lambda_k)|^2 \, \mathrm{dx}\right]^{-1} \in \mathbb{R}$. In particular, m is a holomorphic function in $\mathbb{C} - \mathcal{S}$ and λ_k are the poles of m which are all simple[19].

Next, consider the following two possibilities:

1. $\lambda_+ \in \mathbb{R}$ or $\lambda_- \in \mathbb{R}$: first suppose $\lambda_+ \in \mathbb{R}$, then $\lambda_- \notin \mathbb{R}$ and we have

$$y_-(\mathrm{x}; \lambda_-) = C(\lambda_-)[y_1(\mathrm{x}; \lambda_-) + m(\lambda_-) y_2(\mathrm{x}; \lambda_-)], \tag{A.11}$$

where m is given by (A.10). Equations (A.4), (A.5) and (A.11) imply

$$y_+(0) = y_-(0) = C(\lambda_-) m(\lambda_-), \qquad y'_+(0) = -\mathrm{e}^{-4\mathrm{i}\theta_\nu} y'_-(0) = \mathrm{e}^{-4\mathrm{i}\theta_\nu} C(\lambda_-), \tag{A.12}$$

[18] The equivalence of this statement with that of the above theorem is established in section 5. E_n are the eigenvalues of H.

[19] Note that $\lambda_k > 0$ for all $k \in \mathbb{Z}^+$ and that $\mathcal{S}$ has no accumulation (cluster) point.

and consequently

$$y_+(0) - e^{4i\theta_\nu} m(\lambda_-) y_+'(0) = 0. \tag{A.13}$$

In view of (A.2), which implies $\lambda_+ = e^{-4i\theta_\nu}\lambda_-$, and (A.10) we can express (A.13) as

$$y_+(0) + \chi(\lambda_+) y_+'(0) = 0, \tag{A.14}$$

where

$$\chi(\lambda) := \sum_{k=1}^{\infty} \frac{\sigma_k}{\lambda - e^{-4i\theta_\nu}\lambda_k}, \tag{A.15}$$

Next, consider a fixed $\lambda_+ \in \mathbb{R}$. Then because we have the limit point case there is at most one linearly independent L^2-solution y_+ of

$$-\, y_+''(x) + x^{\nu+2} y_+(x) = \lambda_+ y_+(x). \tag{A.16}$$

This implies that y_+^*, which also belongs to $L^2[0,\infty)$ and solves (A.16), satisfies $y_+(x)^* = e^{i\gamma} y_+(x)$ for some $\gamma \in [0, 2\pi)$. Inserting this equation in the one obtained by taking the complex conjugate of both sides of (A.14) and using $y_+(0) \neq 0 \neq y_+'(0)$, we have $\chi(\lambda_+)^* = \chi(\lambda_+)$. In view of (A.15), the latter relation reads $\Phi_1(\lambda_+) = 0$ where

$$\Phi_1(\lambda) := \sum_{k=1}^{\infty} \left(\frac{1}{\lambda - e^{4i\theta_\nu}\lambda_k} - \frac{1}{\lambda - e^{-4i\theta_\nu}\lambda_k} \right) \sigma_k. \tag{A.17}$$

Hence, λ_+ is a real zero of Φ_1. Clearly, Φ_1 is a holomorphic function in $\mathbb{C} - \mathcal{S}_1^- \cup \mathcal{S}_1^+$ where $\mathcal{S}_1^\pm := \{e^{\pm 4i\theta_\nu}\lambda_k \mid k \in \mathbb{Z}^+\}$. Therefore, its zeros (if exist) form a discrete set. This in turn means that λ_+ and consequently the eigenvalues $E_n = e^{2i\theta_\nu}\lambda_+$ (associated with this case, if there are any) belong to discrete sets. The same argument applies for the case $\lambda_- \in \mathbb{R}$. In summary, the eigenvalues that lie on the rays: $\arg(z) = \pm 2i\theta_\nu$ form a possibly empty discrete subset of $\mathbb{C}$. Next, we show that the same holds for the eigenvalues lying outside these rays.

2. $\lambda_+ \notin \mathbb{R}$ and $\lambda_- \notin \mathbb{R}$: in this case, we can use (A.7) to express $y_\pm$ as

$$y_\pm(x) = C(\lambda_\pm)[y_1(x;\lambda_\pm) + m(\lambda_\pm) y_2(x;\lambda_\pm)]. \tag{A.18}$$

Substituting this relation in (A.4) and (A.5), we obtain

$$C(\lambda_+) m(\lambda_+) = C(\lambda_-) m(\lambda_-), \qquad C(\lambda_-) = -e^{4i\theta_\nu} C(\lambda_+).$$

These together with (A.2), (A.10) and $C(\lambda_\pm) \neq 0$ yield

$$\Phi_2(E_n) = e^{2i\theta_\nu} m(e^{2i\theta_\nu} E_n) + e^{-2i\theta_\nu} m(e^{-2i\theta_\nu} E_n) = 0, \tag{A.19}$$

where

$$\Phi_2(\lambda) := -\sum_{k=1}^{\infty} \left(\frac{1}{\lambda - e^{2i\theta_\nu}\lambda_k} + \frac{1}{\lambda - e^{-2i\theta_\nu}\lambda_k} \right) \sigma_k. \tag{A.20}$$

Therefore, the eigenvalues E_n are the zeros of Φ_2.[20] Clearly, Φ_2 is a holomorphic function in $\mathbb{C} - \left(\mathcal{S}_2^- \cup \mathcal{S}_2^+\right)$ where $\mathcal{S}_2^\pm := \{e^{\pm 2i\theta_\nu}\lambda_k \mid k \in \mathbb{Z}^+\}$. This implies that the zeros E_n of Φ_2

[20] Note that in light of (A.9) we have $\Phi_2(\lambda^*) = \Phi_2(\lambda)^* = \Phi_2(\lambda)$. Hence, the complex conjugate of every zero of Φ_2 is also a zero of Φ_2. This is consistent with the fact that the eigenvalues of H are either real or come in complex-conjugate pairs [1, 4, 5].

form a discrete set. Hence, the eigenvalues that do not lie on the rays $\arg(z) = \pm 2i\theta_\nu$ also form a discrete set.

This completes the proof that the set of all the eigenvalues E_n is discrete. □

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