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FAST TRACK COMMUNICATION

Conjecture on the analyticity of $\mathcal{PT}$-symmetric potentials and the reality of their spectra

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Abstract
The spectrum of the Hermitian Hamiltonian $H = p^2 + V(x)$ is real and discrete if the potential $V(x) \to \infty$ as $x \to \pm\infty$. However, if $V(x)$ is complex and $\mathcal{PT}$-symmetric, it is conjectured that, except in rare special cases, $V(x)$ must be analytic in order to have a real spectrum. This conjecture is demonstrated by using the potential $V(x) = (\mathrm{i}x)^a|x|^b$, where a, b are real.

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1. Introduction

The field of $\mathcal{PT}$ quantum mechanics [1] has attracted significant interest in recent years and a large community of active researchers has developed. This area of study began with the observation that the complex $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian

$$H = p^2 + x^2(\mathrm{i}x)^\epsilon \qquad (\epsilon \geqslant 0) \tag{1}$$

has a positive real discrete eigenspectrum [2, 3]. The property of $\mathcal{PT}$ symmetry is not sufficient to guarantee that the eigenvalues of a non-Hermitian Hamiltonian are real; $\mathcal{PT}$ symmetry merely ensures that the *secular determinant* $\det(H - \mathbb{1}E)$ is a real function of E [5]. The eigenvalues of H are the roots of

$$\det(H - \mathbb{1}E) = 0, \tag{2}$$

and thus the condition of $\mathcal{PT}$ symmetry implies that the eigenvalues are either real or come in complex-conjugate pairs. If the eigenvalues of a $\mathcal{PT}$-symmetric Hamiltonian are all real, we say that the Hamiltonian has an *unbroken* $\mathcal{PT}$ symmetry, but if there are any complex eigenvalues, we say that the $\mathcal{PT}$ symmetry of H is *broken*.

Lacking further information, one would expect (2) to have some complex roots. Thus, it was surprising to find that the class of $\mathcal{PT}$-symmetric Hamiltonians (1) has an entirely real spectrum. In [2–4] numerical evidence and detailed perturbative asymptotic analysis was presented to show that the eigenvalues of the Hamiltonian (1) are real when $\epsilon \geqslant 0$. A rigorous proof that these eigenvalues are all real was given by Dorey *et al* [6, 7].

Using the WKB quantization condition

$$\int_{x_1}^{x_2} \mathrm{d}x \sqrt{E - V(x)} = \left(n + \frac{1}{2}\right)\pi, \tag{3}$$

where x_1 and x_2 are the *turning points* (roots of $V(x) - E = 0$), one can understand heuristically why the eigenvalues of H in (1) cease to be real when $\epsilon < 0$. The quantization condition (3) requires that there be a continuous integration contour from x_1 to x_2. Such a contour exists for $\epsilon \geqslant 0$, but as soon as ϵ goes below 0, the contour joining x_1 and x_2 is broken by the existence of a branch cut in the complex-x plane and there is no longer a finite-length path connecting the turning points.

The discovery that the eigenvalues of H in (1) are real led to a search for and subsequent study of other non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians whose spectra are also real [8–20]. We emphasize that the reality of the eigenspectrum is an unusual property of a complex Hamiltonian and that many $\mathcal{PT}$-symmetric Hamiltonians do not have entirely real spectra. For example, while the $\mathrm{i}x^2y$ potential studied in [21, 22] has a real ground-state energy, it has recently been found that some of the other eigenvalues are complex [23].

In this paper we conjecture that analyticity of the potential is a necessary (but not sufficient) criterion for a non-Dirac-Hermitian Hamiltonian to have real eigenvalues. This conjecture is based on extensive numerical studies in which we have found that, except in rare cases, a $\mathcal{PT}$-symmetric Hamiltonian $H = p^2 + V(x)$ does not have a real spectrum if its potential $V(x)$ is not an analytic function of x. An example of such a nonanalytic $\mathcal{PT}$-symmetric potential, which is discussed in section 2, is

$$V(x) = \mathrm{i}x|x|. \tag{4}$$

We show in section 2 that this potential has only one real eigenvalue.

A heuristic explanation of the role played by analyticity can be based on the WKB contour integral in (3). For complex $\mathcal{PT}$-symmetric potentials the derivation and application of this integral makes explicit use of the analyticity of the potential. Of course, the potential of a Hermitian Hamiltonian need not be analytic because its turning points lie on the real axis. Here, the integral for the WKB quantization condition is unambiguously taken along the real axis and does not need to be deformed into the complex plane. By contrast, the turning points for a complex potential are likely to be complex, and thus the contour for the WKB integral necessarily lies off the real axis. Giving up Hermiticity forces the quantization condition (3) into the complex plane and thus introduces the requirement of path independence and hence analyticity.

The square-well potential studied by Znojil in [8] is a rare example of a complex nonanalytic $\mathcal{PT}$-symmetric potential having a real spectrum. This potential evades the conjecture above simply because there are no turning points at all; for the square-well potential there is no solution to the equation $V(x) = E$.

This paper is organized very simply. In section 2 we examine the exactly solvable nonanalytic potential in (4) and in section 3 we present numerical results for the class of nonanalytic $\mathcal{PT}$-symmetric potentials

$$V(x) = (\mathrm{i}x)^a|x|^b \qquad (a, b \text{ real}). \tag{5}$$

In section 4 we make some brief concluding remarks.

2. An exactly solvable nonanalytic potential

In this section we consider the $\mathcal{PT}$-symmetric Hamiltonian

$$H = p^2 + \mathrm{i}x|x|, \tag{6}$$

whose potential is a nonanalytic function of x. The Schrödinger eigenvalue differential equation associated with this Hamiltonian is

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathrm{i}x|x| - E\right)\psi(x) = 0, \tag{7}$$

where x is real and where the eigenfunction $\psi(x)$ is required to obey the boundary conditions that $\psi \to 0$ as $x \to \pm\infty$.

To solve this differential equation, we partition the real axis into two regions. In the region $x > 0$ the differential equation (7) takes the form

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathrm{i}x^2 - E\right)\psi(x) = 0 \tag{8}$$

and the exact solution is

$$\psi(x) = c_1 D_\nu(x\,\mathrm{e}^{\mathrm{i}\pi/8}\sqrt{2}) + c_2 D_\nu(-x\,\mathrm{e}^{\mathrm{i}\pi/8}\sqrt{2}). \tag{9}$$

Here, D_ν is the parabolic cylinder function with

$$\nu = \tfrac{1}{2}E\,\mathrm{e}^{-\mathrm{i}\pi/4} - \tfrac{1}{2}, \tag{10}$$

and c_1 and c_2 are arbitrary constants. The boundary condition $\lim_{x\to+\infty}\psi(x) = 0$ implies that $c_2 = 0$. Thus, for $x > 0$ we have

$$\psi(x) = c_1 D_\nu(x\,\mathrm{e}^{\mathrm{i}\pi/8}\sqrt{2}). \tag{11}$$

Similarly, in the region $x < 0$ the differential equation (7) becomes

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \mathrm{i}x^2 - E\right)\psi(x) = 0, \tag{12}$$

whose exact solution is

$$\psi(x) = d_1 D_\mu(x\,\mathrm{e}^{-\mathrm{i}\pi/8}\sqrt{2}) + d_2 D_\mu(-x\,\mathrm{e}^{-\mathrm{i}\pi/8}\sqrt{2}). \tag{13}$$

Here,

$$\mu = \tfrac{1}{2}\,\mathrm{e}^{\mathrm{i}\pi/4}E - \tfrac{1}{2}, \tag{14}$$

and d_1 and d_2 are arbitrary constants. The boundary condition $\lim_{x\to-\infty}\psi(x) = 0$ implies that $d_1 = 0$. Thus, for $x < 0$ we have

$$\psi(x) = d_2 D_\mu(-x\,\mathrm{e}^{-\mathrm{i}\pi/8}\sqrt{2}). \tag{15}$$

We must patch the two solutions (11) and (15) together at the origin $x = 0$. Continuity of $\psi(x)$ at $x = 0$ implies that

$$c_1 D_\nu(0) = d_2 D_\mu(0), \tag{16}$$

and continuity of $\psi'(x)$ at $x = 0$ implies that

$$c_1\,\mathrm{e}^{\mathrm{i}\pi/8}D'_\nu(0) = -d_2\,\mathrm{e}^{-\mathrm{i}\pi/8}D'_\mu(0). \tag{17}$$

Taking the ratio of (17) and (16) eliminates the constants c_1 and d_2 and gives the following exact equation for the eigenvalues:

$$\frac{\mathrm{e}^{\mathrm{i}\pi/8}D'_\nu(0)}{D_\nu(0)} = -\frac{\mathrm{e}^{-\mathrm{i}\pi/8}D'_\mu(0)}{D_\mu(0)}. \tag{18}$$

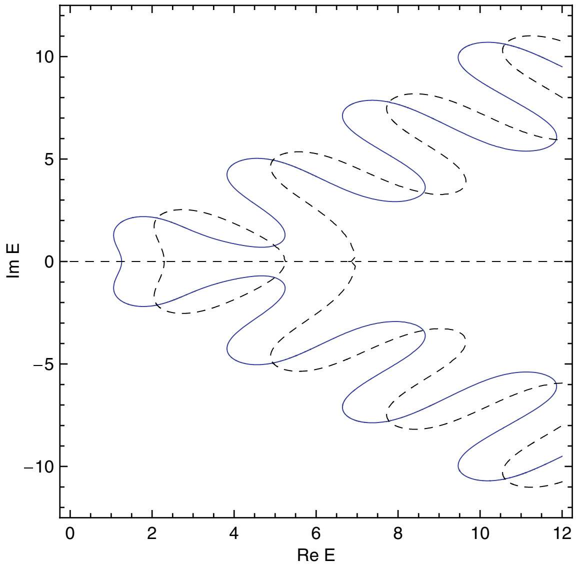

Figure 1. Numerical solution to the secular equation (19) for the eigenvalues of the Hamiltonian $H = p^2 + \mathrm{i}x|x|$. The solid line is the region in the complex-E plane where the real part of the secular determinant vanishes. The dotted line indicates where the imaginary part of the secular equation vanishes. The intersections of the solid and dotted lines are the eigenvalues. There is one real eigenvalue, which is located at $E = 1.258\,092$. All other eigenvalues come in complex-conjugate pairs.

(This figure is in colour only in the electronic version)

This condition can be rewritten simply in terms of Gamma functions as

$$\mathrm{e}^{\mathrm{i}\pi/8}\frac{\Gamma\left(\frac{3}{4} - \frac{1}{4}E\,\mathrm{e}^{-\mathrm{i}\pi/4}\right)}{\Gamma\left(\frac{1}{4} - \frac{1}{4}E\,\mathrm{e}^{-\mathrm{i}\pi/4}\right)} + \mathrm{e}^{-\mathrm{i}\pi/8}\frac{\Gamma\left(\frac{3}{4} - \frac{1}{4}E\,\mathrm{e}^{\mathrm{i}\pi/4}\right)}{\Gamma\left(\frac{1}{4} - \frac{1}{4}E\,\mathrm{e}^{\mathrm{i}\pi/4}\right)} = 0. \tag{19}$$

As required by $\mathcal{PT}$ symmetry, the secular equation (19) is a *real* function of E. This is so because it is the sum of two terms that are complex conjugates of each other.

To solve (19) for E, we substitute $E = \mathrm{Re}\,E + \mathrm{i}\,\mathrm{Im}\,E$ and take the real and imaginary parts of the resulting equation. We then plot in figure 1 the curves in the complex-E plane along which the real part of (19) vanishes (solid line) and the imaginary part of (19) vanishes (dotted line). (Of course, the condition of $\mathcal{PT}$ symmetry requires that the dotted line lie along the real-E axis. However, note that the real-E axis is not the only curve along which the imaginary part of (19) vanishes.)

The intersections of the solid and dotted lines in figure 1 are the eigenvalues of H in (6). Note that there is only one real eigenvalue; all other intersections occur in complex-conjugate pairs. The numerical value of the real eigenvalue is

$$E_0 = 1.258\,092\ldots. \tag{20}$$

Note that for this real value of the energy the eigenfunction is $\mathcal{PT}$ symmetric. This can be seen immediately by examination of the eigenfunction in (11) and (15). Thus, if we reverse the sign of x and simultaneously take the complex conjugate, the eigenfunction remains unchanged.

Table 1. Real eigenvalues for the Hamiltonian $H = p^2 + (\mathrm{i}x)^a|x|^b$ in (21), where $a = 0$. The symbol . . . indicates that the spectrum is entirely real and that the list of real eigenvalues is infinite.

E_i	$b = 1/2$	$b = 1$	$b = 3/2$	$b = 2$	$b = 5/2$	$b = 3$
$a = 0$	1.059617	1.01879	1.00118	1	1.00859	1.02295
	1.833394	2.33811	2.70809	3	3.24223	3.45056
	2.210015	3.24820	4.17714	5	5.72682	6.37029
	2.550647	4.08795	5.58566	7	8.31328	9.52208
	3.051182	4.82010	6.92282	9	10.9916	12.8703
	3.253157	5.52056	8.22687	11	13.7342	16.3694
	3.452132	6.16331	9.49059	13	16.5353	20.0009
	3.623138	7.37218	10.7317	15	19.3837	23.7455
	3.793400	8.48849	11.9453	17	22.2757	27.5924
	3.943821	9.53546	13.1419	19	25.2052	31.5308
	...	...	...	21	28.1698	35.5535
				23	31.1655	39.6536
				25	34.1908	43.8258
				27	37.2428	48.0654
				29	40.3203	52.3684
				31	43.4214	56.7311
				33	46.5449	61.1507
				35	49.6894	65.6241
				37	52.8541	70.1491
				39	56.0377	74.7232
				41	...	79.3445
				43		84.0112
				45		88.7215
				...		93.4738
						98.2668
						...

3. Numerical study of a class of nonanalytic potentials

In this section we examine numerically the eigenvalue differential equation for the complex $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian

$$H = p^2 + (\mathrm{i}x)^a|x|^b, \tag{21}$$

where a and b are real parameters.

We begin by determining the appropriate $\mathcal{PT}$-symmetric boundary conditions to be imposed on the eigenfunctions of H in (21). Using WKB analysis, we find the possible asymptotic behaviors of the eigenfunction $\psi(x)$ satisfying the time-independent Schrödinger equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (\mathrm{i}x)^a|x|^b - E\right)\psi(x) = 0. \tag{22}$$

For example, when $x > 0$, the controlling factor of the asymptotic behavior of $\psi(x)$ as $x \to +\infty$ is

$$\exp\left[\pm\frac{2}{a+b+2}\mathrm{i}^{a/2}x^{(a+b+2)/2}\right]. \tag{23}$$

Table 2. Real eigenvalues for the Hamiltonian $H = p^2 + (\mathrm{i}x)^a |x|^b$ in (21), where $a = 1/2$. The eigenvalues in bold type are the largest of all the real eigenvalues; when an eigenvalue is given in bold type all of the real eigenvalues are listed. As in table 1, the symbol ... indicates that the spectrum is entirely real and infinite.

E_i	$b = 1/2$	$b = 1$	$b = 3/2$	$b = 2$	$b = 5/2$	$b = 3$
$a = 1/2$	**1.180777**	1.08693	1.05583	1.04896	1.05404	1.06568
		3.19578	3.27843	3.43454	3.59460	3.74791
		4.4220	5.36421	6.05174	6.64515	7.17496
			7.67568	8.79101	9.91884	10.9735
			9.53919	11.6207	13.4256	15.1112
				14.5219	17.0514	19.4889
				17.4829	20.8691	24.1139
				20.4952	24.7239	28.9111
				23.5529	28.8137	33.9218
				26.6504	32.7868	39.0482
				29.7848	37.2141	44.3936
				32.9526	41.0803	49.7770
				36.1511	**46.2256**	55.4476
				39.3784		60.9963
				42.6321		67.0561
				45.9112		72.5848
				...		79.2958
						84.3126
						92.7345

Table 3. Same as in tables 1 and 2 except that $a = 1$ and $a = 3/2$.

E_i	$b = 1/2$	$b = 1$	$b = 3/2$	$b = 2$	$b = 5/2$	$b = 3$
$a = 1$	**1.446448**	**1.25809**	1.18627	1.15627	1.14615	1.14685
			4.21683	4.10923	4.13051	4.19436
			6.93323	7.56227	7.95153	8.30206
				11.3144	12.0844	12.9101
				15.2916	16.8072	18.1062
				19.4515	21.3065	23.5322
				23.7667	27.4779	29.6147
				28.2175	**30.3268**	35.3873
				32.7891		42.9034
				37.4698		**47.4048**
				42.2504		
				...		
$a = 3/2$	**1.791941**	**1.48873**	1.36338	1.30151	1.26993	1.2550
			5.52801	4.96979	4.80096	4.7494
			8.50818	9.48003	9.60759	9.7042
				14.5305	14.6672	15.2406
				19.9977	21.7069	21.8910
				25.8103	**24.9567**	**28.1147**
				31.9205		
				38.2938		
				44.9038		
				...		

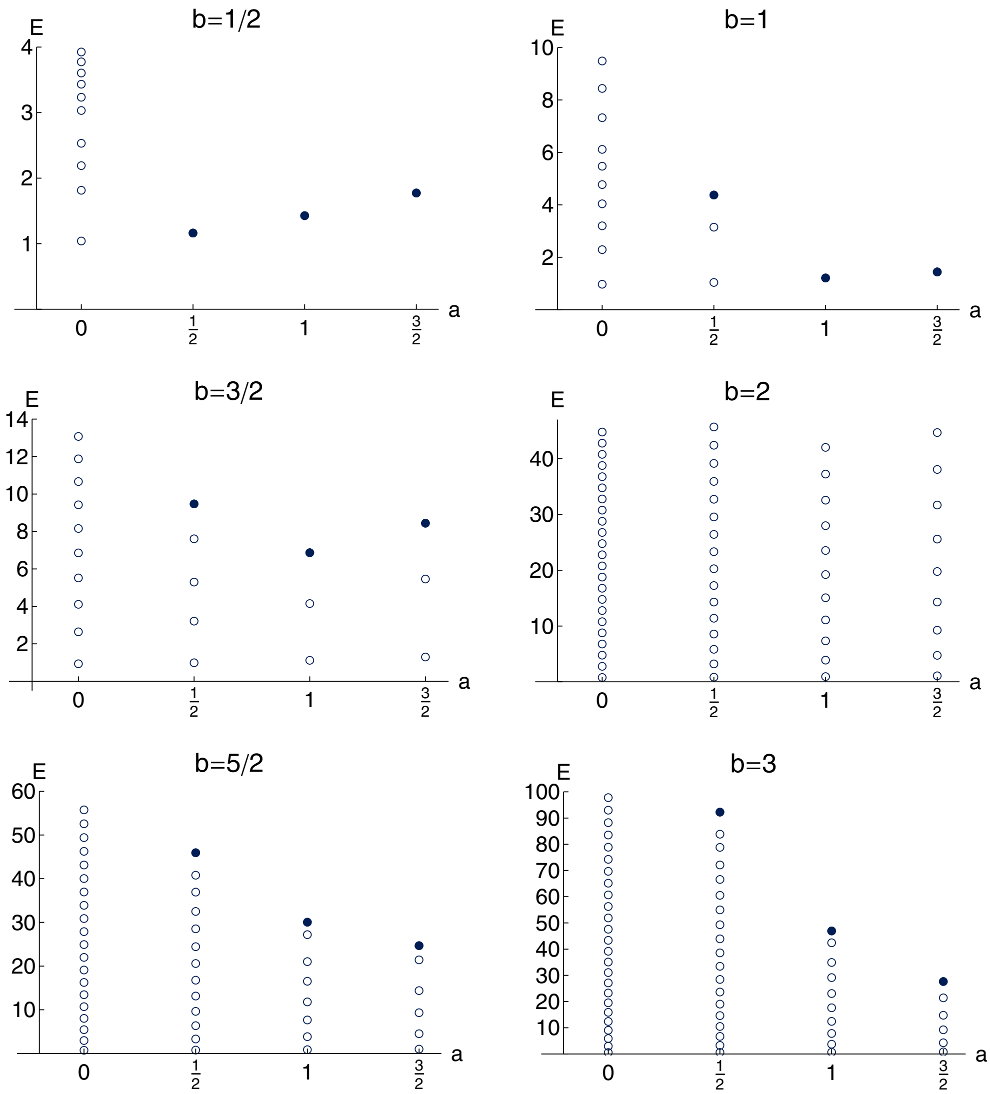

Figure 2. Real eigenvalues, indicated by circles, for the Hamiltonian $H = p^2 + (ix)^a|x|^b$ in (21). The data for this figure is taken from tables 1–3. When a circle representing an eigenvalue is filled, this indicates that there are no more real eigenvalues in the tower. Notice that the number of real eigenvalues increases with increasing b and decreases with increasing a.

Thus, for $a < 2$ there exists a solution that grows exponentially and another that decays exponentially for large positive x. The same is true for large negative x so long as $a < 2$. To determine the eigenvalues for $a < 2$ we impose the boundary conditions that $\psi(x) \to 0$ as $|x| \to \infty$ on the real-x axis. Note that because the potential is not an analytic function of x, the notion of Stokes' wedges in the complex-x plane in which the boundary conditions are imposed is not applicable.

We have calculated the eigenvalues for various values of a and b and our results are listed in tables 1 and 2 and plotted in figure 2. Clearly, when b is an even integer, the Hamiltonian in (21) reduces to that in (1) and it has an entirely real spectrum. However, for other values of b, when $a \neq 0$ there are only a finite number of real eigenvalues. The number of real eigenvalues decreases as a increases, and increases as b increases. It is not clear from figure 2 that this behavior holds when a is small and $b = \frac{1}{2}$, so we have calculated the real eigenvalues for some additional values of a: when $a = \frac{1}{4}$ there is still only one real eigenvalue, but when $a = \frac{1}{8}$ there are *two* real eigenvalues at 1.064 07 and 2.058 27. When $a = \frac{1}{16}$, there are *three* eigenvalues: 1.0582, 2.3488, 3.4132. As a continues to decrease, the number of real eigenvalues grows until at $a = 0$ there are an infinite number of real eigenvalues.

4. Concluding remarks

Most $\mathcal{PT}$-symmetric potentials $V(x)$ studied so far in the literature are special because they are analytic. In this paper we have explored a new class of nonanalytic $\mathcal{PT}$-symmetric potentials of the form $V(x) = (\mathrm{i}x)^a|x|^b$, and on the basis of numerical and theoretical calculations we are led to conjecture that, except in rare cases, analyticity is an essential feature that is necessary for the Hamiltonian to have a real spectrum.

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