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CONJECTURE ON THE REALITY OF SPECTRA OF NON-HERMITIAN HAMILTONIANS

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Ordinarily, one demands a Hamiltonian to satisfy $H^\dagger = H$, where $\dagger$ represents the mathematical operation of complex conjugation and matrix transposition. This conventional hermiticity condition ensures that H has a real spectrum. Recently, it was discovered that replacing this mathematical condition by the weaker and more physical requirement $H^\ddagger = H$, where $\ddagger$ represents combined parity reflection and time reversal $\mathcal{PT}$, one obtains new classes of complex Hamiltonians whose spectra are often real and positive. However, the condition of $\mathcal{PT}$ symmetry alone is not strong enough to *guarantee* that the spectrum of H is real. In this paper evidence is presented to support the conjecture that the spectrum of the complex Hamiltonian $H = p^2 + V(x)(ix)^\epsilon$ ($\epsilon > 0$) will be real, positive, and discrete if (1) $V(x)$ is real when x is real; (2) the spectrum of $H = p^2 + V(x)$ is positive and discrete; (3) the function $V(x)$ is even [$V(x) = V(-x)$]; (4) the function $V(x)$ is an *entire* function of complex x. We believe that if these conditions are satisfied then the complex deformation $H = p^2 + V(x)(ix)^\epsilon$ of $H = p^2 + V(x)$ will have a real, positive, and discrete spectrum.

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1 Complex Hamiltonians Having Real Spectra

In a recent letter [1], a class of complex quantum mechanical Hamiltonians

$$H = p^2 + x^2(ix)^\epsilon \quad (\epsilon \text{ real}) \tag{1}$$

was investigated. Despite the lack of hermiticity, the spectrum of H is real and positive for all $\epsilon \geq 0$. As shown in Fig. 1 (and Fig. 1 of Ref. [1]) the spectrum is discrete and each of the energy levels increases with increasing ϵ. The reality of the spectrum is in part a consequence of $\mathcal{PT}$ invariance.

Here, the operators $\mathcal{P}$ and $\mathcal{T}$ represent parity reflection and time reversal. These operators are defined by their action on the position and momentum operators x and p:

$$\begin{aligned} &\mathcal{P}: x \to -x, \quad p \to -p, \\ &\mathcal{T}: x \to x, \quad p \to -p, \quad i \to -i. \end{aligned} \tag{2}$$

When the operators x and p are real, the canonical commutation relation $[x, p] = i$ is invariant under both parity reflection and time reversal. This commutation relation remains invariant under $\mathcal{P}$ and $\mathcal{T}$ even if x and p are complex provided that the above transformations hold [2].

The spectrum of the Hamiltonian (1) is obtained by solving the corresponding Schrödinger equation

$$-\psi''(x) + [x^2(ix)^\epsilon - E]\psi(x) = 0 \tag{3}$$

subject to appropriate boundary conditions imposed in the complex-x plane. These boundary conditions are described in Ref. 1.

Note from Fig. 1 that the spectrum of the Hamiltonian (1) exhibits two regions: When $\epsilon \geq 0$, the energy spectrum of H is real and positive. However, a transition occurs at $\epsilon = 0$. As ϵ goes below 0, the eigenvalues as functions of ϵ pair off and become complex, starting with the highest-energy eigenvalues. For negative ϵ the spectrum contains an infinite number of complex eigenvalues and a finite number of real, positive eigenvalues. As ϵ decreases, there are fewer and fewer real eigenvalues and below approximately $\epsilon = -0.57793$ only one real energy remains. This energy then begins to increase with decreasing ϵ and becomes infinite as ϵ approaches -1.

In summary, the theory defined by Eq. (1) exhibits two phases, an unbroken-symmetry phase with a purely real energy spectrum when $\epsilon \geq 0$ and a spontaneously-broken-symmetry phase with a partly real and partly

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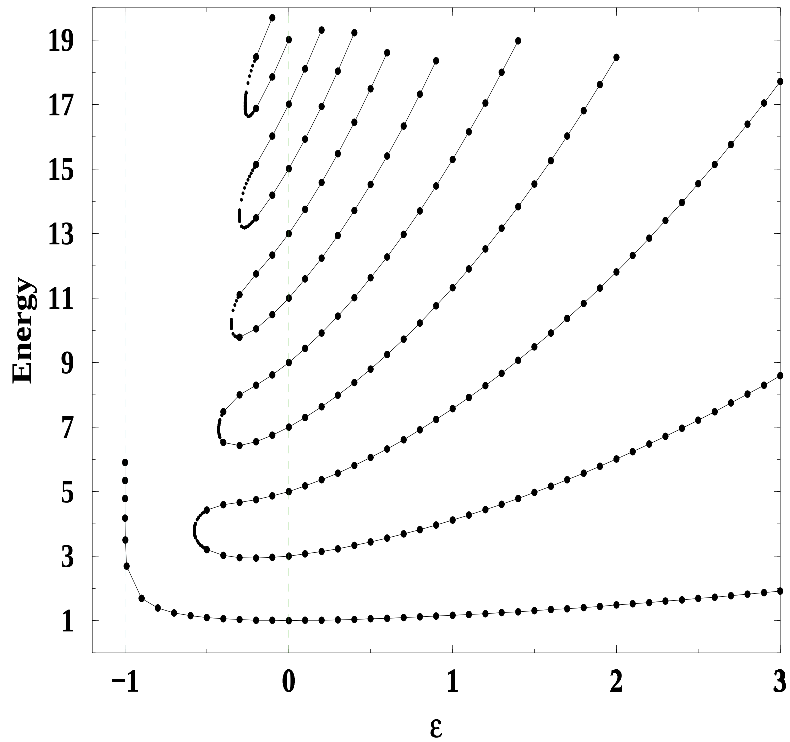

Figure 1. Energy levels of the Hamiltonian $H = p^2 + x^2(ix)^\epsilon$ as a function of the parameter ϵ. When $\epsilon \geq 0$, the spectrum is real and positive and the energy levels rise with increasing ϵ. The lower bound of this region, $\epsilon = 0$, corresponds to the harmonic oscillator, whose energy levels are $E_n = 2n + 1$. When $-1 < \epsilon < 0$, there are a finite number of real positive eigenvalues and an infinite number of complex conjugate pairs of eigenvalues. As ϵ decreases from 0 to -1, the number of real eigenvalues decreases; when $\epsilon \leq -0.57793$, the only real eigenvalue is the ground-state energy. As ϵ approaches -1^+, the ground-state energy diverges. For $\epsilon \leq -1$ there are no real eigenvalues.

complex spectrum when $-1 < \epsilon < 0$, the transition at $\epsilon = 0$ can be seen in both the quantum mechanical system and the underlying classical system [2]. We have numerically verified that the eigenfunctions of H in Eq. (1) are also eigenfunctions of the operator $\mathcal{PT}$ when $\epsilon \geq 0$ [2]. However, when $\epsilon < 0$, the $\mathcal{PT}$ symmetry of the Hamiltonian is spontaneously broken; even though $\mathcal{PT}$ commutes with H, the eigenfunctions of H are *not* all simultaneously eigenfunctions of $\mathcal{PT}$. For these eigenfunctions of H the energies are complex.

Similar qualitative features are exhibited by complex deformations of real

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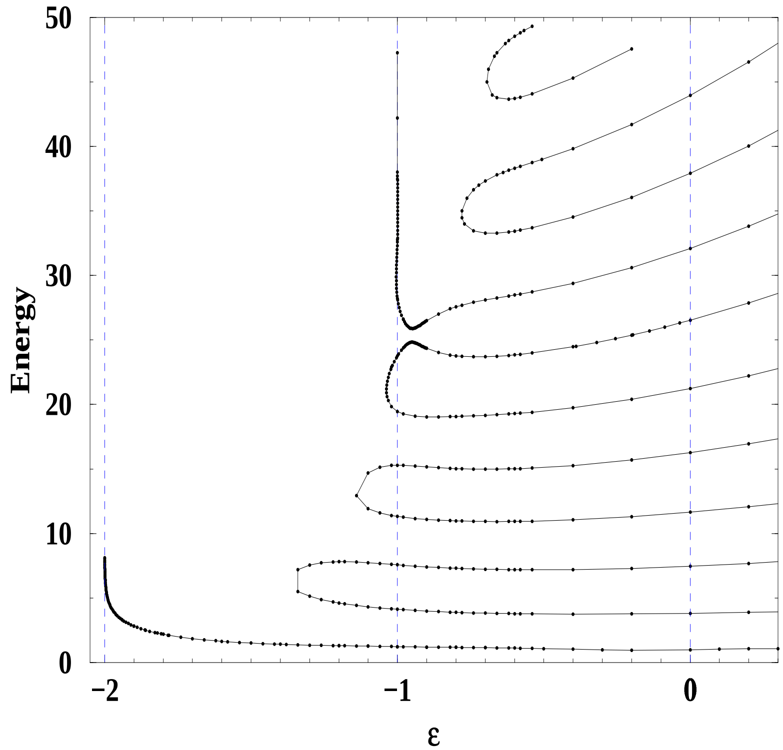

Figure 2. Energy levels of the Hamiltonian $H = p^2 + x^4(ix)^\epsilon$ as a function of the parameter ϵ. This figure is similar to Fig. 1, but now there are four regions. When $\epsilon \geq 0$, the spectrum is real and positive and it rises monotonically with increasing ϵ. Below $\epsilon = 0$ there are complex eigenvalues (except at $\epsilon = -1$).

Hamiltonians other than the harmonic oscillator. The class of Hamiltonians

$$H = p^2 + x^{2N}(ix)^\epsilon \tag{4}$$

have the same qualitative properties as H in Eq. (1). As ϵ decreases below 0, all of these theories exhibit a transition from an unbroken $\mathcal{PT}$-symmetric regime to a regime in which $\mathcal{PT}$ symmetry is spontaneously broken. Each of these $\mathcal{PT}$-symmetric theories may be viewed as analytic continuations of conventional Hermitian theories from real to complex phase space [2].

Consider, for example, the spectrum of an $x^4(ix)^\epsilon$ theory ($N = 2$), which is displayed in Fig. 2. This figure resembles Fig. 1 for the case $N = 1$ except that now there are four regions: When $\epsilon \geq 0$, the spectrum is discrete, real, and positive and it rises monotonically with increasing ϵ. The lower

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bound $\epsilon = 0$ of this $\mathcal{PT}$-symmetric region corresponds to the pure quartic anharmonic oscillator, whose Hamiltonian is $H = p^2 + x^4$. When $-1 < \epsilon < 0$, $\mathcal{PT}$ symmetry is spontaneously broken. There are a finite number of real positive eigenvalues and an infinite number of complex conjugate pairs of eigenvalues; as a function of ϵ the eigenvalues pinch off in pairs and move into the complex plane. As ϵ approaches -1 from above only eight real eigenvalues remain. Just as ϵ reaches -1 the entire spectrum reemerges from the complex plane and becomes real. Note that at $\epsilon = -1$ the entire spectrum agrees with the entire spectrum in Fig. 1 at $\epsilon = 1$. This reemergence is difficult to see in this figure. Just below $\epsilon = -1$, the eigenvalues once again begin to pinch off and disappear in pairs into the complex plane. However, this pairing is different from the pairing in the region $-1 < \epsilon < 0$. Above $\epsilon = -1$ the lower member of a pinching pair is even and the upper member is odd (that is, E_8 and E_9 combine, E_{10} and E_{11} combine, and so on); below $\epsilon = -1$ this pattern reverses (that is, E_7 combines with E_8, E_9 combines with E_{10}, and so on). As ϵ decreases from -1 to -2, the number of real eigenvalues continues to decrease until the only real eigenvalue is the ground-state energy. Then, as ϵ approaches -2^+, the ground-state energy diverges logarithmically. For $\epsilon \leq -2$ there are no real eigenvalues.

The spectrum for $H = p^2 + x^6(ix)^\epsilon$ $(N = 3)$ is displayed in Fig. 3. This figure resembles Fig. 2 for the case $N = 2$. However, now there are transitions at both $\epsilon = -1$ and $\epsilon = -2$. The spectrum is discrete, real, and positive when $\epsilon \geq 0$ and the energy levels rise monotonically with increasing ϵ. The lower bound $\epsilon = 0$ of this $\mathcal{PT}$-symmetric region corresponds to the sextic anharmonic oscillator, whose Hamiltonian is $H = p^2 + x^6$. The other four regions are $-1 < \epsilon < 0$, $-2 < \epsilon < -1$, $-3 < \epsilon < -2$, and $\epsilon < -3$. The $\mathcal{PT}$ symmetry is spontaneously broken when ϵ is negative, and the number of real eigenvalues decreases as ϵ becomes more negative. However, at the boundaries $\epsilon = -1, \ -2$ there is a complete real positive spectrum. When $\epsilon = -1$, the eigenspectrum is identical to the eigenspectrum in Fig. 2 at $\epsilon = 1$. For $\epsilon \leq -3$ there are no real eigenvalues.

While there is as yet no proof that the spectrum of H in Eq. (1) is real, it is possible to gain insight regarding the reality and positivity of the spectrum of a $\mathcal{PT}$-invariant Hamiltonian H by calculating the spectral zeta function. An exact calculation of the zeta function was done for the case $\epsilon = 3$ by Mezincescu [3] and this work was generalized to arbitrary $\epsilon > 0$ by Bender and Wang [4]. Other work has been done by Delabaere *et al.* [5]

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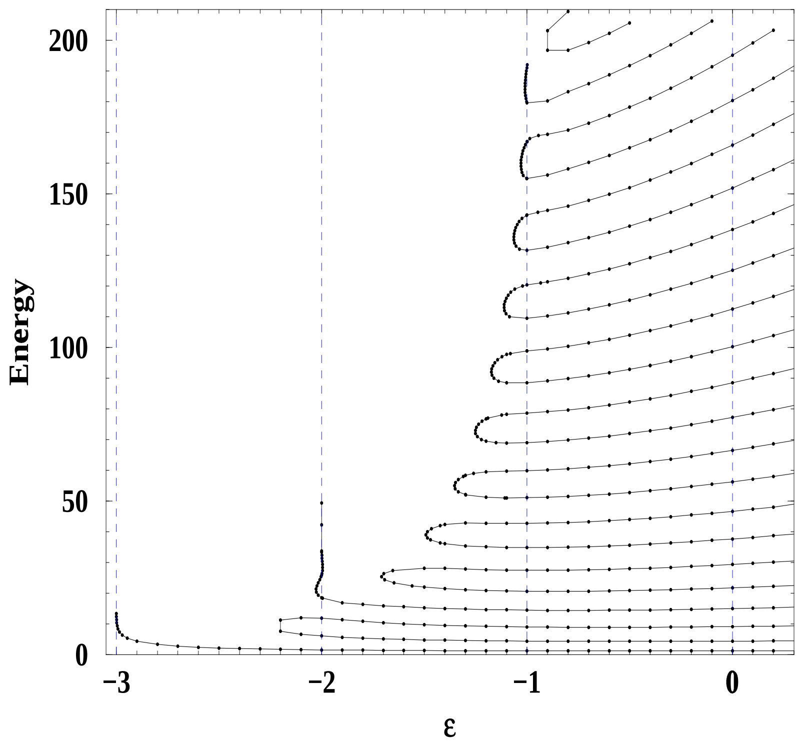

Figure 3. Energy levels of the Hamiltonian $H = p^2 + x^6(ix)^\epsilon$ as a function of the parameter ϵ. This figure is similar to Fig. 2, but now there are five regions. When $\epsilon \geq 0$, the spectrum is real and positive and it rises monotonically with increasing ϵ. Below $\epsilon = 0$ the spectrum is complex except when $\epsilon = -1$ and $\epsilon = -2$.

2 Complex Deformations of Nonanalytic Potentials

$\mathcal{PT}$ symmetry alone is not sufficient to guarantee that the spectrum of a Hamiltonian is real. We conjecture that analyticity of the underlying real potential is also required. To illustrate this, we study complex deformations of some nonanalytic potentials. In our discussion so far we have considered complex deformations of the potentials x^{2N}, which are entire functions of x. Let us now consider deformations of the *nonanalytic* potentials $|x|^P$ (P real). We will see that the eigenvalues of the potentials $|x|^P(ix)^\epsilon$ are real only when $\epsilon = 0$ (and sometimes at other isolated values of ϵ). Thus, it appears that deforming a nonanalytic potential destroys a crucial property of the theory; namely, that the spectrum be real.

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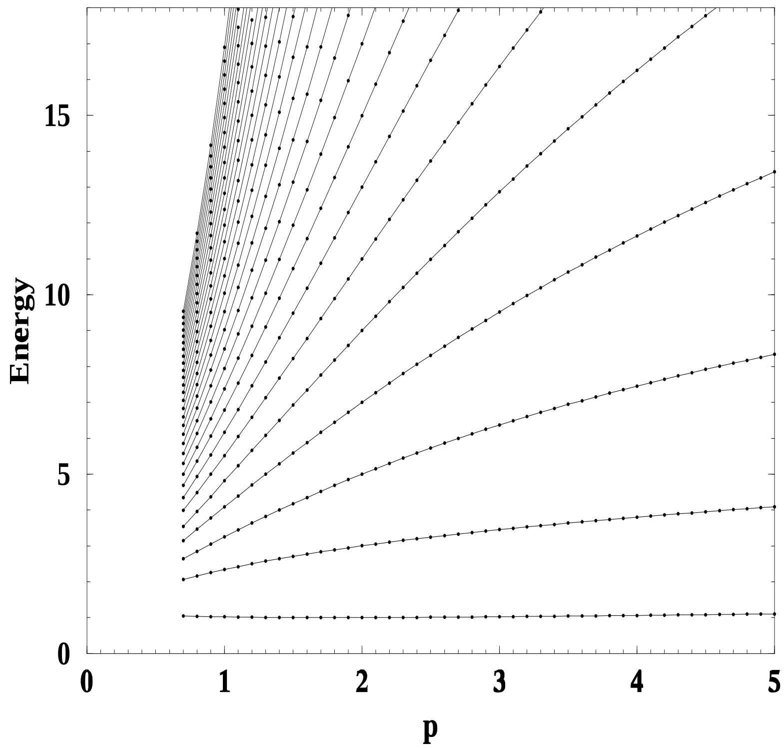

Figure 4. Energy levels of the Hamiltonian $H = p^2 + |x|^P$ as a function of the parameter P. This figure is similar to Fig. 1, but the eigenvalues do not pinch off and go into the complex plane because H is Hermitian (instead, the spectrum becomes denser as P approaches 0).

We begin by examining the spectrum of the $|x|^P$ potential. The eigenvalues of this potential are displayed as a function of P in Fig. 4 (see Ref. [6]). The spectrum of this potential is similar to that of the $x^2(ix)^\epsilon$ potential for positive ϵ (see Fig. 1). The difference between the spectra of these two potentials becomes apparent when ϵ is large: As $\epsilon \to \infty$, the spectrum of $|x|^{2+\epsilon}$ approaches that of the square-well potential [$E_n = (n+1)^2\pi^2/4$], while the energies of the $x^2(ix)^\epsilon$ potential diverge [7].

WKB theory gives an excellent approximation to the spectrum of both real and complex potentials and thus provides an interesting comparison. For the $x^2(ix)^\epsilon$ potential, when $\epsilon \geq 0$, the WKB calculation must be performed in the complex plane [8]. The turning points $x_\pm$ are the roots of $E - x^2(ix)^\epsilon = 0$

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that *analytically continue* off the real axis as ϵ moves away from zero:

$$x_- = E^{\frac{1}{2+\epsilon}} e^{i\pi\frac{4+3\epsilon}{4+2\epsilon}}, \quad x_+ = E^{\frac{1}{2+\epsilon}} e^{-i\pi\frac{\epsilon}{4+2\epsilon}}. \tag{5}$$

These turning points lie in the lower-half (upper-half) x-plane when $\epsilon > 0$ ($\epsilon < 0$).

The WKB phase-integral quantization condition to leading order is $(n+1/2)\,\pi = \int_{x_-}^{x_+} dx\,\sqrt{E - x^2(ix)^\epsilon}$. It is crucial that this integral follows a path along which the *integral is real.* When $\epsilon > 0$, this path lies entirely in the lower-half x-plane and when $\epsilon = 0$ the path lies on the real axis. But, when $\epsilon < 0$ the path is in the upper-half x-plane; it crosses the cut on the positive imaginary axis and thus is *not a continuous path joining the turning points.* Hence, WKB fails when $\epsilon < 0$.

When $\epsilon \geq 0$, we deform the phase-integral contour so that it follows the rays from x_- to 0 and from 0 to x_+:

$$\left(n+\frac{1}{2}\right)\pi = 2\sin[\pi/(2+\epsilon)]E^{\frac{4+\epsilon}{4+2\epsilon}} \int_0^1 ds\,\sqrt{1-s^{2+\epsilon}}.$$

We then solve for E_n:

$$E_n \sim \left[\frac{\Gamma\left(\frac{8+3\epsilon}{4+2\epsilon}\right)\sqrt{\pi}(n+1/2)}{\sin\left(\frac{\pi}{2+\epsilon}\right)\Gamma\left(\frac{3+\epsilon}{2+\epsilon}\right)}\right]^{\frac{4+2\epsilon}{4+\epsilon}} \qquad (n \to \infty). \tag{6}$$

To perform a higher-order WKB calculation we replace the phase integral by a *closed contour* that encircles the path connecting the two turning points (see Ref. 9). With $Q(x) = x^2(ix)^\epsilon - E$, the next-to-leading-order WKB quantization condition is

$$\left(n+\frac{1}{2}\right)\pi = \frac{1}{2i}\oint_C dx\,\sqrt{Q(x)} + \frac{1}{2i}\oint_C dx\,\frac{Q''(x)}{48Q(x)^{\frac{3}{2}}}, \tag{7}$$

where the contour C encircles the turning points x_+ and x_- in a counter-clockwise direction. Assuming that n is large, we obtain

$$E_n \sim \left[\frac{\Gamma\left(\frac{8+3\epsilon}{4+2\epsilon}\right)\sqrt{\pi}(n+1/2)}{\sin\left(\frac{\pi}{2+\epsilon}\right)\Gamma\left(\frac{3+\epsilon}{2+\epsilon}\right)}\right]^{\frac{4+2\epsilon}{4+\epsilon}} \left[1 + \frac{(2+\epsilon)(1+\epsilon)\sin\left(\frac{2\pi}{2+\epsilon}\right)}{6\pi\left(n+\frac{1}{2}\right)^2(4+\epsilon)^2}\right]. \tag{8}$$

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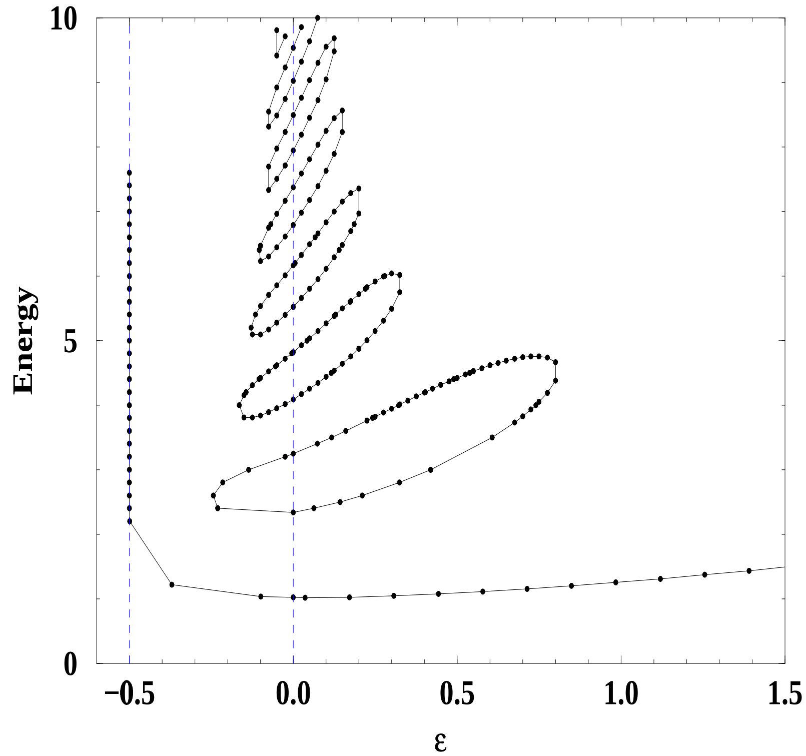

Figure 5. Energy levels of the Hamiltonian $H = p^2 + |x|(ix)^\epsilon$ as a function of the parameter ϵ. The spectrum is entirely real only when $\epsilon = 0$.

This is the next-to-leading-order WKB result for the energy. The corresponding WKB result for the $|x|^{2+\epsilon}$ ($\epsilon > -2$) potential is quite similar:

$$E_n \sim \left[\frac{\Gamma\left(\frac{8+3\epsilon}{4+2\epsilon}\right)\sqrt{\pi}(n+1/2)}{\Gamma\left(\frac{3+\epsilon}{2+\epsilon}\right)}\right]^{\frac{4+2\epsilon}{4+\epsilon}} \left[1 + \frac{(2+\epsilon)(1+\epsilon)\cot\left(\frac{\pi}{2+\epsilon}\right)}{3\pi\left(n+\frac{1}{2}\right)^2(4+\epsilon)^2}\right]. \quad (9)$$

Now we perform a complex deformation of the $|x|^P$ potential. That is, we consider an $|x|^P(ix)^\epsilon$ potential. Of course, since $|x|$ is not an analytic function, we cannot define an analytic continuation of the Schrödinger eigenvalue problem

$$-\psi''(x) + |x|^p(ix)^\epsilon\psi(x) = E\psi(x) \quad (10)$$

into the complex x-plane. However, for sufficiently small ϵ we can allow x

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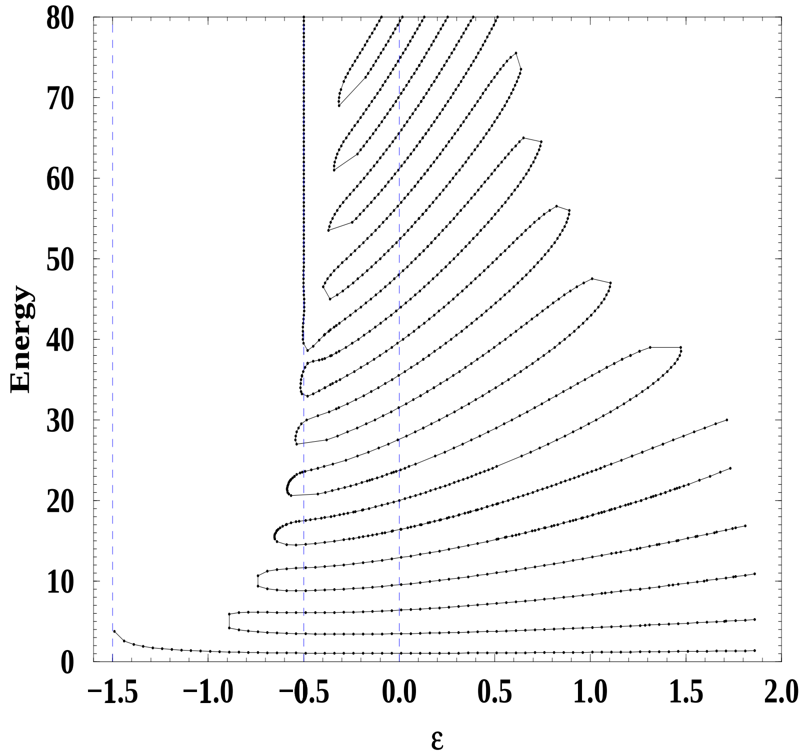

Figure 6. Energy levels as a function of the parameter ϵ for the Hamiltonian $H = p^2 + |x|^3(ix)^\epsilon$. The spectrum is real when $\epsilon = 0$ and $\epsilon = -0.5$.

to remain *real* and we can impose the boundary condition that $\psi(x) \to 0$ for $x \to \pm\infty$. Specifically, we have the condition for *all* P that if $|\epsilon| < 2$, then this boundary condition on the real x-axis may be consistently imposed to define the eigenspectrum.

Let us consider two cases: $P = 1$ (Fig. 5) and $P = 3$ (Fig. 6). Figure 5 is quite similar to Fig. 1, and Fig. 6 resembles Fig. 2. The key features of these figures are that (1) the lowest energy level diverges at $\epsilon = -P/2$, and that (2) the energy levels pinch off and move into the complex plane on *both* sides of $\epsilon = 0$. Thus, the spectrum is entirely real only when $\epsilon = 0$.

Acknowledgments

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