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LETTER TO THE EDITOR

Complex WKB analysis of energy-level degeneracies of non-Hermitian Hamiltonians

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Abstract

The Hamiltonian $H = p^2+x^4+\mathrm{i}Ax$, where A is a real parameter, is investigated. The spectrum of H is discrete and entirely real and positive for $|A| < 3.169$. As $|A|$ increases past this point, adjacent pairs of energy levels coalesce and then become complex, starting with the lowest-lying energy levels. For large energies, the values of A at which this merging occurs scale as the three-quarters power of the energy. That is, as $|A| \to \infty$ and $E \to \infty$, at the points of coalescence the ratio $a = |A|E^{-3/4}$ approaches a constant whose numerical value is $a_{\mathrm{crit}} = 1.1838363072914\cdots$. Conventional WKB theory determines the high-lying energy levels but cannot be used to calculate a_{crit}. This critical value is predicted exactly by complex WKB theory.

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In this Letter we examine the Hamiltonian

$$H = p^2 + x^4 + \mathrm{i}Ax, \tag{1}$$

where A is a real parameter. This Hamiltonian is an additive complex deformation of the conventional Hermitian Hamiltonian $H = p^2+x^4$, which represents the pure quartic oscillator. This Hamiltonian is a special case of a slightly more general Hamiltonian previously examined by Delabaere and Pham [1][5].

This Hamiltonian is of interest because, while the Hamiltonian H is complex for all $A \neq 0$, its entire spectrum is discrete, real, and positive for $|A| < 3.169$ (see figure 1). The reality of the spectrum is apparently due to the $\mathcal{PT}$ invariance of the Hamiltonian. However, not all

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[5] Very recently, an oscillator problem like that in (1) except with x^4 replaced by x^3 was studied by Delabaere and Trinh [2].

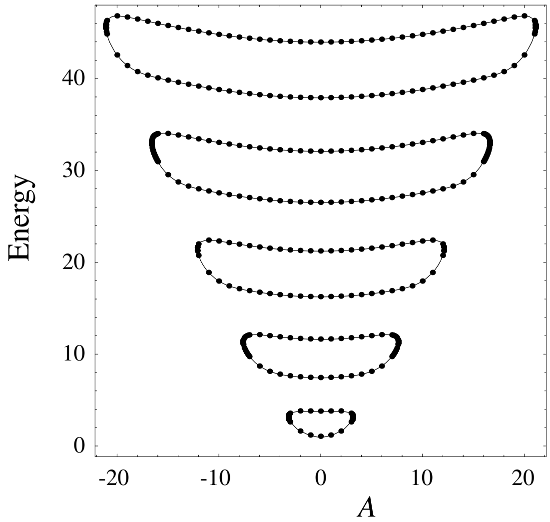

Figure 1. First ten energy levels of the Hamiltonian $H = p^2 + x^4 + \mathrm{i}Ax$ as a function of the real parameter A as represented by dots. All of the energy levels are real for $|A| < 3.169$. As $|A|$ increases past this value, the two lowest eigenvalues become degenerate and move off into the complex plane. If A were pure imaginary there would be no such degeneracy because a Hermitian perturbation causes energy levels to repel. When $|A|$ passes the value 7.625, the next two energy levels coalesce and then become complex. This pairing-off process continues as $|A|$ increases; the subsequent values of $|A|$ at which pairs of energy levels are degenerate are 12.110, 16.609, 21.109, and so on (see table 1). The continuous curves represent the energy levels given by the WKB quantization formula (13).

$\mathcal{PT}$-symmetric Hamiltonians have entirely real spectra. Indeed, figure 1 shows that as $|A|$ increases past the points 3.169, 7.625, 12.110, 16.609, 21.109, $\cdots$, pairs of adjacent energy levels merge and become complex, starting with the lowest two eigenvalues. Note that for any finite value of A there are always a finite number of complex eigenvalues and an infinite number of real eigenvalues[6].

This pairwise coalescence of eigenvalues exhibits scaling behaviour: The values of A at which adjacent energy levels become degenerate grow as the three-quarters power of the energy. That is, as $|A| \to \infty$ and $E \to \infty$, at the points of coalescence the ratio $a = |A|E^{-3/4}$ approaches a constant whose numerical value is $a_{\rm crit} = 1.1838363072914\cdots$. The purpose of this paper is to use the methods of complex WKB theory [3] to calculate $a_{\rm crit}$.

Many examples of complex $\mathcal{PT}$-symmetric Hamiltonians have been studied recently. These remarkable Hamiltonians, whose spectra are often entirely real and positive, are all complex deformations of conventional Hermitian Hamiltonians. However, in most cases the deformations are *multiplicative* rather than *additive* as in (1). For example, the non-Hermitian Hamiltonian

$$H_N = p^2 - (\mathrm{i}x)^N \tag{2}$$

is a complex multiplicative deformation of $H_2 = p^2 + x^2$, the Hermitian harmonic oscillator Hamiltonian[7]. Although it has not yet been proved rigorously, it is believed that for $N \geqslant 2$

[6] The Hamiltonian (1) is one member of a large class of Hamiltonians that arise from the study of $\mathcal{PCT}$-symmetric two-component Dirac equations.

[7] Other examples of multiplicative deformations of Hermitian Hamiltonians are $H = p^2 + x^{2K}(\mathrm{i}x)^\epsilon$, where $K = 1, 2, 3, \cdots$ and $\epsilon \geqslant 0$. All such Hamiltonians are $\mathcal{PT}$ symmetric and appear to have entirely real, positive spectra [5].

the entire spectrum of H_N is discrete, real, and positive [4, 5]. A transition occurs at $N = 2$. When $1 < N < 2$, a finite number of eigenvalues (the lowest-lying eigenvalues) are real and the remaining infinite number of eigenvalues are complex[8].

Direct numerical evidence for the reality and positivity of the spectrum of H_N ($N \geqslant 2$) can be found by performing a Runge–Kutta integration of the complex Schrödinger equation associated with H_N [4]. Alternatively, the large-energy eigenvalues of the spectrum can be calculated with great accuracy by using conventional WKB techniques [6]. To do so, we find the turning points $x_\pm$, which are the roots of $E + (\mathrm{i}x)^N = 0$ that analytically continue off the real axis as N increases from 2:

$$x_- = E^{\frac{1}{N}} e^{-\mathrm{i}\pi\frac{N+2}{2N}} \qquad x_+ = E^{\frac{1}{N}} e^{-\mathrm{i}\pi\frac{N-2}{2N}}. \tag{3}$$

These turning points lie in the lower-half complex-x plane when $N > 2$. The WKB phase-integral quantization condition to leading order is

$$\left(n + \frac{1}{2}\right)\pi = \int_{x_-}^{x_+} \mathrm{d}x\, \sqrt{E + (\mathrm{i}x)^N}.$$

It is crucial that this integral follows a path along which the integral is *real*. When $N = 2$, this path lies on the real axis and when $N > 2$, the path lies in the lower-half x plane. To evaluate the integral we deform the contour of integration so that it follows the rays from x_- to 0 and from 0 to x_+, yielding

$$\left(n + \frac{1}{2}\right)\pi = 2\sin\left(\frac{\pi}{N}\right) E^{\frac{2+N}{2N}} \int_0^1 \mathrm{d}s\, \sqrt{1 - s^N}.$$

We then solve for E_n:

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

These energies are all real and positive.

Additional evidence for the reality and positivity of the spectrum can be obtained by calculating the spectral zeta function Z_N (the sum the inverses of the eigenvalues) of the Hamiltonian H_N. This was done for the case $N = 3$ by Mezincescu [7] and for the case of arbitrary $N > 2$ by Bender and Wang [8]. The exact result for arbitrary $N > 2$ is

$$Z_N = \frac{4\sin^2\left(\frac{\pi}{N+2}\right)\Gamma\left(\frac{1}{N+2}\right)\Gamma\left(\frac{2}{N+2}\right)\Gamma\left(\frac{N-2}{N+2}\right)}{(N+2)^{\frac{2N}{N+2}}\Gamma\left(\frac{N-1}{N+2}\right)\Gamma\left(\frac{N}{N+2}\right)}. \tag{5}$$

Using the numerical values for the first few eigenvalues and the WKB formula (4) for the high eigenvalues, one can conclude that any complex eigenvalues must be larger in magnitude than about 10^{18}.

Rigorous results regarding the reality of the eigenvalues of H_N have been obtained by Shin [9], who showed that the entire spectrum of H_N must lie in a narrow wedge containing the positive-real axis. Other results have been obtained by Delabaere *et al* (see [2, 10]).

Let us now return to the Hamiltonian H in (1). The Schrödinger equation associated with H is

$$-\psi''(x) + (x^4 + \mathrm{i}Ax)\psi(x) = E\psi(x). \tag{6}$$

[8] The transition at $N = 2$ can be seen at the classical level. When $N \geqslant 2$ the classical trajectories $x(t)$ are periodic closed orbits in the complex-x plane. However, when $1 < N < 2$, the classical motion is no longer periodic; the trajectories $x(t)$ spiral outward to infinity (see [5]). For the case of the Hamiltonian H in (1), where there are only a finite number of complex eigenvalues for all A, one observes no transition at the classical level at $|A| = 3.169$. Indeed, the classical trajectories continue to be closed periodic orbits for all values of A.

Table 1. Values of A at which the energies of figure 1 become degenerate, approximations $A_{\rm WKB}$ from equations(13), percentage error, and scaled parameters $a = AE^{-3/4}$. The values of a extrapolate to $a_{\rm crit} = 1.1838363072914\cdots$.

A	$A_{\rm WKB}$	$\dfrac{A - A_{\rm WKB}}{A_{\rm WKB}}$	a
3.169	3.097	2.32%	1.3330
7.625	7.596	0.38%	1.2355
12.110	12.097	0.11%	1.2150
16.609	16.597	0.07%	1.2063
21.109	21.098	0.05%	1.2001

It is relatively straightforward to show that some eigenvalues E must become degenerate for sufficiently large values of $|A|$. The argument is similar to one due to Simon [11]. Treating $g = \mathrm{i}A$ as a perturbation parameter, we argue that $E(g)$ is a *Herglotz* function of g. (A Herglotz function is one whose imaginary part has the same sign as the imaginary part of its argument; the function is real when its argument is real.) The Herglotz property of $E(g)$ is verified by multiplying (6) by $\psi^*(x)$, integrating with respect to x, and taking the imaginary part of the resulting equation. Next, we apply the theorem that if a function is both entire and Herglotz, then it is linear. It is easy to verify by calculating to second order in perturbation theory that $E(g)$ is not a linear function of g so we conclude that $E(g)$ has singularities, and these are the square-root singularities (degeneracies) that are shown in figure 1 and that occur for pure imaginary values of g[9].

Letting $x = E^{1/4}t$ gives the scaled version of (6):

$$-\varepsilon^2\psi''(t) + (t^4 + \mathrm{i}at)\psi(t) = \psi(t) \tag{7}$$

where $a = AE^{-3/4}$ and $\varepsilon = E^{-3/4}$. The parameter ε is small for large energies E. In table 1 we display the scaled values of the degeneracy points.

We can use conventional WKB techniques like those used to derive (4) to calculate the large eigenvalues E of (6). However, these techniques are not powerful enough to predict the degeneracies shown in figure 1. Instead, we use complex WKB methods [3], which take into account reflections off *all* turning points and not just the principal turning points.

The complex WKB method incorporates the subdominant exponentials that can appear and disappear across Stokes lines issuing from turning points in the complex-x plane. In the present case there are four turning points $x_i(E, A)$ (illustrated in figure 2 for $E = A = 1$), defined by

$$E - x_i^4 - \mathrm{i}Ax_i = 0. \tag{8}$$

The turning points x_1 and x_2 lie just below the real axis, and are the continuations for $A > 0$ of the two real turning points generating the simplest WKB approximation for the pure quartic oscillator; x_3 and x_4, which lie on the imaginary axis, are the complex turning points that are responsible for the degeneracies. The Stokes lines from x_i (see figure 2) are defined by

$$\mathrm{Re}\, w(x_i, x; E, A) = 0 \tag{9}$$

where

$$w(x_i, x; E, A) = \int_{x_i}^{x} \mathrm{d}t\, \sqrt{E - t^4 - \mathrm{i}At}. \tag{10}$$

[9] This argument fails for the Hamiltonian $p^2 + x^2 + \mathrm{i}Ax$. Indeed, for this shifted quadratic potential the eigenvalues $E_n = 2n + 1 + \frac{1}{4}A^2$ are entire functions of A for all n. For this special case, the integral $\int \mathrm{d}x\, x\psi^*(x)\psi(x)$ vanishes.

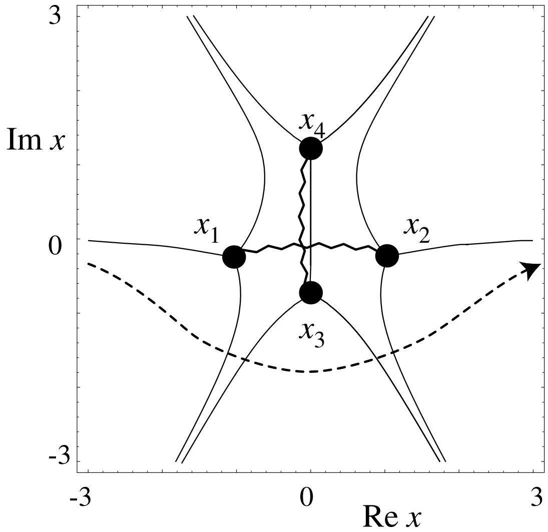

Figure 2. Complex-coordinate plane structure of Hamiltonian (1) for $E = 1$ and $A = 1$ as required for complex-WKB quantization. The four dots represent the turning points x_i, which obey the equation $1 - x^4 - ix = 0$. The solid curves represent the Stokes lines where subdominant exponentials appear. The dashed line is the connection path. The zigzag lines are branch cuts.

Beginning with a solution of (6) that decays exponentially towards $x = -\infty$, we continue along the path shown in figure 2 (with branch cuts avoiding the path, as indicated), incorporating the exponentials that appear as each Stokes line is crossed (with coefficient $-\mathrm{i}$ times that of the dominant exponential), and referring each exponent to the appropriate turning point. When the positive real-x axis is reached, we require the solution that decays towards $x = \infty$, so the coefficient of the growing exponential must be 0. This leads to the quantization condition

$$\exp[-\mathrm{i}w(x_1, x_2)] = 2\cos[w(x_3, x_2)]\cos[w(x_1, x_3)]. \tag{11}$$

(We temporarily suppress the dependence on E and A.) From the $\mathcal{PT}$ invariance of (1) and incorporating the effect of the branch cut between x_2 and x_3, we have

$$w(x_1, x_3) = -w(x_3, x_2)^* \equiv U + \mathrm{i}V \qquad \text{so that} \quad w(x_1, x_2) = 2\mathrm{i}V. \tag{12}$$

Thus (12) becomes, after a little simplification,

$$\cos(2U) = -\tfrac{1}{2}\exp(-2V). \tag{13}$$

This is the final form of the complex WKB quantization condition. Since U and V are functions of E and A, the solutions of (13) are eigenvalue curves in the (E, A) plane shown in figure 1. It is clear that all features of the exact energies, including the degeneracies (see table 1), are reproduced accurately, even for the low-lying states. For small A, V is positive, and $\exp(-2V)$ gives an exponentially small correction to the conventional WKB eigenvalues given by $\cos(2U) = 0$. (These eigenvalues arise from the turning points x_1 and x_2 because $2U$ is the action integral $w(x_1, x_2)$ when there is no branch cut joining x_2 and x_3.) When A increases, V becomes negative, and $\exp(-2V)$ is a positive exponential whose value can exceed 2. When this happens (13) has no solutions for which U or E is real. In effect, the disappearance of real eigenvalues (i.e. the occurrence of degeneracies) is a phenomenon where complex turning points dominate, rather than giving the familiar small corrections.

There is no simple exact formula for the parameter values A_{WKB} corresponding to the degeneracies given by (13). If U is regarded as energy and V as the parameter, then degeneracies occur at $V = -\frac{1}{2}\log 2 = -0.3466\cdots$. For high energies the degeneracies lie asymptotically on the curve $V(E, A) = 0$. To evaluate the integral (cf. (10) and (12)) we convert to scaled variables, expand the contour to enclose the branch point joining the turning points, expand the integral in powers of a, and integrate term by term. This gives

$$(2\pi)^{3/2}a + \sum_{n=0}^{\infty}(-1)^n a^{4n}\left[\frac{\Gamma\left(n+\frac{1}{4}\right)\Gamma\left(3n-\frac{3}{4}\right)}{(4n)!} - a^2\frac{\Gamma\left(n+\frac{3}{4}\right)\Gamma\left(3n+\frac{3}{4}\right)}{(4n+2)!}\right] = 0 \tag{14}$$

whose numerical solution is $a_{\mathrm{crit}} = 1.1838363072914\cdots$. This exact theoretical result agrees perfectly with the extrapolation from the numerically-determined eigenvalues.

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