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COMMENT

Comment on a recent paper by Mezincescu

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Abstract

It has been conjectured that for $\epsilon \geqslant 0$ the entire spectrum of the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian $H_N = p^2 + x^2(\mathrm{i}x)^\epsilon$, where $N = 2 + \epsilon$, is real. Strong evidence for this conjecture for the special case $N = 3$ was provided in a recent paper by Mezincescu (Mezincescu G A 2000 *J. Phys. A: Math. Gen.* **33** 4911) in which the spectral zeta function $Z_3(1)$ for the Hamiltonian $H_3 = p^2 + \mathrm{i}x^3$ was calculated exactly. Here, the calculation of Mezincescu is generalized from the special case $N = 3$ to the region of all $N \geqslant 2$ ($\epsilon \geqslant 0$) and the exact spectral zeta function $Z_N(1)$ for H_N is obtained. Using $Z_N(1)$ it is shown that to extremely high precision (about three parts in 10^{18}) the spectrum of H_N for other values of N such as $N = 4$ is entirely real.

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1. Introduction

There is strong numerical evidence that the class of non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians defined by

$$H_N = p^2 + x^2(\mathrm{i}x)^\epsilon \qquad (N = 2 + \epsilon, \epsilon \geqslant 0) \tag{1.1}$$

possesses a spectrum that is entirely discrete, real, and positive [1, 2]. It is believed that the reality and positivity of the spectrum is a consequence of $\mathcal{PT}$ symmetry. Hamiltonians such as those in (1.1) are interesting because the Schrödinger eigenvalue problem associated with H_N may be regarded as a deformation of a Sturm–Liouville problem into the complex plane.

In a recent paper [3], Mezincescu calculated the spectral zeta function $Z_3(1)$, the sum of the inverses of the energy eigenvalues of the Hamiltonian H_3 in (1.1) for the case $N = 3$:

$$Z_3(1) = \sum_{n=0}^{\infty} \frac{1}{E_n} = \frac{\Gamma^2\left(\frac{1}{5}\right)}{5^{6/5}\Gamma^2\left(\frac{3}{5}\right)}\left(3 - 2\cos\frac{\pi}{5}\right). \tag{1.2}$$

Using the numerical values of the first few eigenvalues and the WKB formula for the high eigenvalues [1], Mezincescu concluded that to about an accuracy of two parts in 10^6 there are no other eigenvalues in the spectrum other than the real ones found by Bender *et al*.

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In this Comment we point out that the method used by Mezincescu immediately generalizes to *all* Hamiltonians H_N in the class in (1.1). The result for all $N > 2$ is given by the following elegant and compact formula:

$$Z_N(1) = \frac{4\sin^2\left(\frac{\pi}{N+2}\right)\Gamma\left(\frac{1}{N+2}\right)\Gamma\left(\frac{2}{N+2}\right)\Gamma\left(\frac{N-2}{N+2}\right)}{(N+2)^{\frac{2N}{N+2}}\Gamma\left(\frac{N-1}{N+2}\right)\Gamma\left(\frac{N}{N+2}\right)}. \tag{1.3}$$

This equation reduces to that in (1.2) for the special case $N = 3$. Note that $Z_N(1)$ is singular at $N = 2$ ($\epsilon = 0$) because for the harmonic oscillator the energy eigenvalues E_n grow linearly with n.

We have obtained an even more general formula for the two-parameter class of Hamiltonians [2]

$$H_{2K,\epsilon} = p^2 + x^{2K}(\mathrm{i}x)^\epsilon \qquad (K = 1, 2, 3, \ldots, \epsilon \geqslant 0). \tag{1.4}$$

In terms of the variable $N = 2K + \epsilon$ we have

$$Z_{2K,\epsilon}(1) = \left[1 + \frac{\cos\left(\frac{3\epsilon\pi}{2N+4}\right)\sin\left(\frac{\pi}{N+2}\right)}{\cos\left(\frac{\epsilon\pi}{2N+4}\right)\sin\left(\frac{3\pi}{N+2}\right)}\right]\frac{\Gamma\left(\frac{1}{N+2}\right)\Gamma\left(\frac{2}{N+2}\right)\Gamma\left(\frac{N-2}{N+2}\right)}{(N+2)^{\frac{2N}{N+2}}\Gamma\left(\frac{N-1}{N+2}\right)\Gamma\left(\frac{N}{N+2}\right)}. \tag{1.5}$$

This formula reduces to that in (1.3) when $K = 1$.

2. Comparison with numerical and analytic data

We have examined (1.3) for several values of N. We present two cases below:

Case 1. Large-ϵ limit of the $x^2(\mathrm{i}x)^\epsilon$ potential. The large-ϵ limit of a $x^2(\mathrm{i}x)^\epsilon$ potential is exactly solvable in terms of Bessel functions [4]. For large $N = 2+\epsilon$ the asymptotic behaviour of the nth energy level is given by

$$E_n \sim \tfrac{1}{16}(2n+1)^2 N^2 \qquad (N \to \infty). \tag{2.1}$$

Thus, if we calculate the spectral zeta function $Z_\infty(1)$, we obtain

$$\begin{aligned} Z_\infty(1) &\sim \frac{16}{N^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2} && (N \to \infty) \\ &\sim \frac{16}{N^2}\frac{\pi^2}{8} && (N \to \infty) \\ &\sim \frac{2\pi^2}{N^2} && (N \to \infty). \end{aligned} \tag{2.2}$$

We can verify this result by examining the large-N behaviour of $Z_N(1)$ in (1.3). The result is precisely that in (2.2).

Case 2. The $-x^4$ potential ($N = 4$). From (1.3), the exact value of $Z_N(1)$ at $N = 4$ is

$$Z_4^{\text{exact}}(1) = 1.526\,605\,869\,546\,945\,566\,99. \tag{2.3}$$

We can test this result using the numerically calculated energy levels of the Hamiltonian $H_4 = p^2 - x^4$, the first 11 of which are $E_0^{\text{numerical}} = 1.477\,149\,753\,577\,995$, $E_1^{\text{numerical}} = 6.003\,386\,083\,308\,277$, $E_2^{\text{numerical}} = 11.802\,433\,595\,134\,78$, $E_3^{\text{numerical}} = 18.458\,818\,704\,077\,12$, $E_4^{\text{numerical}} = 25.791\,792\,378\,517\,22$, $E_5^{\text{numerical}} = 33.694\,279\,876\,607\,79$,

$E_6^{\text{numerical}} = 42.093\,807\,710\,826\,17$, $E_7^{\text{numerical}} = 50.937\,404\,324\,545\,14$, $E_8^{\text{numerical}} = 60.184\,331\,266\,082\,70$, $E_9^{\text{numerical}} = 69.802\,096\,674\,912\,04$, $E_{10}^{\text{numerical}} = 79.764\,065\,824\,381\,80$. The remaining energy levels are taken from the second-order WKB calculation [5]

$$E_n^{\text{WKB}} \sim \left[\frac{\sqrt{18\pi}\,\Gamma\left(\frac{3}{4}\right)\left(n+\frac{1}{2}\right)}{\Gamma\left(\frac{1}{4}\right)}\right]^{4/3}\left[1+\frac{1}{18\pi\left(n+\frac{1}{2}\right)^2}\right] \qquad (n\to\infty). \tag{2.4}$$

Thus,

$$\frac{1}{E_n^{\text{WKB}}} \sim \left[\frac{\Gamma\left(\frac{1}{4}\right)}{\sqrt{18\pi}\,\Gamma\left(\frac{3}{4}\right)}\right]^{4/3}\left[\frac{1}{\left(n+\frac{1}{2}\right)^{4/3}}-\frac{1}{18\pi\left(n+\frac{1}{2}\right)^{10/3}}\right] \qquad (n\to\infty) \tag{2.5}$$

and

$$\sum_{n=0}^{\infty}\frac{1}{E_n^{\text{WKB}}} = \left[\frac{\Gamma\left(\frac{1}{4}\right)}{\sqrt{18\pi}\,\Gamma\left(\frac{3}{4}\right)}\right]^{4/3}\left[\left(2^{4/3}-1\right)\zeta\left(\frac{4}{3}\right)-\frac{2^{10/3}-1}{18\pi}\zeta\left(\frac{10}{3}\right)\right]$$
$$= 1.524\,768\,398\,149. \tag{2.6}$$

We then obtain our numerical approximation to $Z_4(1)$ by calculating

$$Z_4^{\text{numerical}}(1) = \sum_{n=0}^{10}\frac{1}{E_n^{\text{numerical}}}+\sum_{n=0}^{\infty}\frac{1}{E_n^{\text{WKB}}}-\sum_{n=0}^{10}\frac{1}{E_n^{\text{WKB}}}$$
$$= 1.526\,605\,869\,911. \tag{2.7}$$

The difference between $Z_4^{\text{numerical}}(1)$ in (2.7) and $Z_4^{\text{exact}}(1)$ in (2.3) is 3.64×10^{-10}. Thus, the relative error is $2.38\times10^{-8}\%$. This extremely small number provides what we believe is convincing evidence supporting the conjecture that the entire spectrum of H_4 is real and that there are no complex eigenvalues.

We can extend this calculation beyond second order. Using fourth-order WKB the relative error decreases to $1.6\times10^{-10}\%$; in sixth-order WKB the relative error further decreases to $1.0\times10^{-12}\%$; in eighth-order WKB the relative error is $9.8\times10^{-15}\%$; in tenth-order WKB the relative error decreases to $2.6\times10^{-16}\%$. Thus, it would be astonishing indeed if there were any complex eigenvalues.

3. Final remarks

It is interesting to compare the spectral zeta function (1.3) for the Hamiltonian H_N in (1.1) with the spectral zeta function for the conventional Hermitian quantum mechanical Hamiltonian [6]

$$H_N = p^2 + |x|^N. \tag{3.1}$$

Using the same methods that give (1.3) (see [7]), we obtain for the Hamiltonian H_N in (3.1) the exact result

$$Z_N(1) = \frac{4\sin\left(\frac{\pi}{N+2}\right)\cos^2\left(\frac{\pi}{N+2}\right)\Gamma\left(\frac{1}{N+2}\right)\Gamma\left(\frac{2}{N+2}\right)\Gamma\left(\frac{N-2}{N+2}\right)}{\sin\left(\frac{3\pi}{N+2}\right)(N+2)^{\frac{2N}{N+2}}\Gamma\left(\frac{N-1}{N+2}\right)\Gamma\left(\frac{N}{N+2}\right)}. \tag{3.2}$$

It is easy to check this result. For example, if we let $N\to\infty$, the potential $|x|^N$ becomes a square well, whose energy levels are $E_n = \frac{1}{4}n^2\pi^2$. The exact spectral zeta function for this potential is $Z_\infty(1) = \frac{2}{3}$.

What is most remarkable is the striking similarity between the spectral zeta functions (1.3) and (3.2) for the non-Hermitian and Hermitian Hamiltonians in (1.1) and (3.1). Indeed, the only structural difference is in the trigonometric functions.

Furthermore, the results of this paper suggest that the eigenfunctions $\psi_n(x)$ of the complex Hamiltonian H_N are complete. To explain this assertion, we review the calculational technique that gives the spectral zeta function. The Green function $G(x, y)$ has the representation

$$G(x, y) = \sum_{n=0}^{\infty} \frac{\psi_n(x)\psi_n(y)}{E_n}. \tag{3.3}$$

This Green function satisfies the differential equation

$$HG(x, y) = \delta(x - y) \tag{3.4}$$

where

$$\delta(x - y) = \sum_{n=0}^{\infty} \psi_n(x)\psi_n(y) \tag{3.5}$$

is the usual statement of completeness. The correctness of our calculation of the spectral zeta function in terms of $G(x, x)$,

$$Z_N(1) = \sum_{n=0}^{\infty} \frac{1}{E_n} = \int \mathrm{d}x\, G(x, x) \tag{3.6}$$

implicitly relies on the assumption of completeness. In an earlier paper [8] a numerical study of the zeros of the eigenfunctions was presented to argue that the eigenfunctions are complete. The current paper strengthens this assertion enormously.

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