Solvable analogue of $V(x) = ix^3$

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Abstract

We prove that the purely imaginary square well generates an infinite number of bound states with real energies. In the strong-coupling limit, our exact $\mathcal{PT}$ symmetric solutions coincide, utterly unexpectedly, with their textbook, well known Hermitian predecessors.

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1 Introduction

An interest in the imaginary cubic anharmonic oscillators dates back to their perturbation analysis by Caliceti et al [1]. The simplified homework example with the mere two-term non-Hermitian Hamiltonian

$$H_{BZ} = p^2 + ix^3$$

has been proposed by D. Bessis and J. Zinn-Justin who had in mind its possible applicability in the context of statistical physics [2]. The example has been revitalized by C. Bender et al due to its further possible methodical relevance in the relativistic quantum field theory [3].

The apparent reality of the spectrum of energies $E_{BZ}$ proved quite puzzling and inspired a conjecture of the existence of the whole “modified quantum mechanics” paying attention to similar Hamiltonians [4]. This conjecture opened many new and interesting questions when it replaced the current Hermiticity of Hamiltonians by a weaker condition of their commutativity with a product $\mathcal{PT}$ of the spatial parity $\mathcal{P}$ and the complex conjugation $\mathcal{T}$ where the latter factor is to be understood as a one-dimensional version of the operator of time reversal.

The recent discussion between C. Bender and A. Mezincescu [5] pointed out that one of the key problems of the new studies lies in the ambiguity of the spectrum which depends quite crucially on our choice of the boundary conditions which can be, in general, complexified [6]. The fragile character of the reality of energies has been confirmed by the WKB and perturbative studies [7] and by the quasi-exact and exact models [8] where the admissible unavoided level crossings [9] prove sometimes followed by the spontaneous breakdown of the $\mathcal{PT}$ symmetry [10].

In such a context we intend to propose an extremely elementary $\mathcal{PT}$ symmetric model which would replace the BZ interaction $ix^3$ (which admits just a numerical treatment) by its exactly solvable square-well analogue.
2 Model

In a search for analogies between the solvable and unsolvable models in one dimension, all the possible forms of a confining well are often being approximated by the ordinary real and symmetric square well

\[ V^{(SQW)}(x) = \begin{cases} 
S^2, & x \in (-\infty, -\pi) \cup (\pi, \infty), \\
0, & x \in (-\pi, \pi).
\end{cases} \] (1)

In this spirit we intend to replace here the above-mentioned antisymmetric and imaginary homework potential \( V_{BZ}(x) = ix^3 \) by its elementary square-well analogue

\[ V^{(ISQW)}(x) = \begin{cases} 
-iT^2, & x \in (-\infty, -\pi), \\
0, & x \in (-\pi, \pi), \\
+iT^2, & x \in (\pi, \infty).
\end{cases} \]

Schrödinger equation which appears in such a setting,

\[ \left[ -\frac{\hbar}{2m} \frac{d}{dx^2} + V^{(ISQW)}(x) \right] \psi(x) = E\psi(x) \] (2)

will be complemented here by the standard \( L^2(\mathbb{R}) \) boundary conditions

\[ \psi(\pm\infty) = 0. \] (3)

The well known \( \mathcal{PT} \) symmetric normalization convention will be employed, with a free real parameter \( G \) in the unbroken \( \mathcal{PT} \)-symmetry requirements [11]

\[ \psi(0) = 1, \quad \partial_x \psi(0) = iG. \] (4)

Putting \( \hbar = 2m = 1 \) and using the ansatz

\[ \psi(x) = \begin{cases} 
\cos k x + B \sin k x, & x \in (0, \pi), \quad k^2 = E, \\
(L + iN) \exp(-\sigma x), & x \in (\pi, \infty), \quad \sigma^2 = iT^2 - k^2,
\end{cases} \] (5)

we guarantee its full compatibility with the symmetry requirements (4) by the choice of the purely imaginary constant \( B = iG/k \) in the wave functions (5).
3 Matching conditions at $x = \pi$

We may split $\sigma = p + i q$ in its real and imaginary part with $p, q \geq 0$. This gives the rules $p^2 + k^2 = q^2$ and $2pq = T^2$ as a consequence. They are easily re-parameterized in terms of a single variable $\alpha$,

$$p = q \cos \alpha, \quad k = q \sin \alpha, \quad q = \frac{T}{\sqrt{2 \cos \alpha}}, \quad \alpha \in (0, \pi/2).$$

(6)

In this language the standard matching at the point of discontinuity is immediate,

$$\cos k\pi + B \sin k\pi = (L + i N) \exp(-\sigma \pi),$$

$$- \sin k\pi + B \cos k\pi = - \frac{\sigma}{k} (L + i N) \exp(-\sigma \pi).$$

After we abbreviate $\sigma/k = - \tan \Omega \pi$, we get an elementary complex condition of the matching of logarithmic derivatives at $x = \pi$,

$$G = -i k \tan(k + \Omega)\pi.$$  (7)

Its real part defines our first unknown parameter, $G = G(\alpha)$. Due to our normalization conventions, the imaginary part of the right-hand-side expression must vanish, $\text{Re}[\tan(k + \Omega)\pi] = 0$. An elementary re-arrangement of such an equation acquires the form of an elementary quadratic algebraic equation for $X = \tan k\pi$. Its two explicit solutions read

$$X_1 = \frac{p + q}{k}, \quad X_2 = \frac{p - q}{k}$$

(8)

or, after all the insertions,

$$\tan \left[ \frac{\pi T \sin \alpha^{(+)} }{\sqrt{2 \cos \alpha^{(+)} }} \right] = \tan \left[ \frac{\pi - \alpha^{(+)} }{2} \right],$$

$$\tan \left[ \frac{\pi T \sin \alpha^{(-)} }{\sqrt{2 \cos \alpha^{(-)} }} \right] = \tan \left[ - \frac{\alpha^{(-)} }{2} \right].$$

(9) (10)

These equations specify, in implicit manner, the two respective infinite series of the appropriately bounded real roots $\alpha = \alpha_n^{(\pm)} \in (0, \pi/2)$. 

3
4 Energies

Even before any numerical considerations we immediately see that for \( \alpha \in (0, \pi/2) \) the left-hand-side arguments \([\ldots]\) in eqs. (9) and (10) run from zero to infinity. Their tangens functions oscillate infinitely many times from minus infinity to plus infinity. Within the same interval, the limited variation of the argument \( \alpha \) makes both the eligible right-hand side functions monotonic, very smooth and bounded, \( \tan[(\pi - \alpha^{(\pm)})/2] \in (1, \infty) \) and \( \tan[\alpha^{(-)/2}] \in (0, 1) \). *A priori* this indicates that our roots \( k = k(\alpha^{(\pm)}) \) will all lie within the fairly well determined intervals,

\[
\begin{align*}
  k^{(+)}_n &\in \left(n + \frac{1}{4}, n + \frac{1}{2}\right), \quad n = 0, 1, \ldots, \\
  k^{(-)}_m &\in \left(m + \frac{3}{4}, m + 1\right) \quad m = 0, 1, \ldots.
\end{align*}
\]

After such an approximate localization of the roots, an unexpected additional merit of our parametrization (6) manifests itself in an unambiguous removal of the tangens operators from both eqs. (9) and (10). This gives the following two relations,

\[
\begin{align*}
  k^{(+)}_n &= n + \frac{1}{2} - \frac{\omega^{(+)}}{4}, \quad k^{(-)}_m = m + 1 - \frac{\omega^{(-)}}{4}, \quad \omega^{(\pm)}_n = \frac{2\alpha_n^{(\pm)}}{\pi} \in (0, 1).
\end{align*}
\]

After an elementary change of the notation with \( \omega^{(+)}_n = \omega_{2n} \) and \( \omega^{(-)}_n = \omega_{2n+1} \), we may finally combine the latter two rules in the single secular equation

\[
\sin\left(\frac{\pi}{2} \omega_N\right) = \frac{2N + 2 - \omega_N}{4T} \cdot \sqrt{2 \cos\left(\frac{\pi}{2} \omega_N\right)} \quad N = 0, 1, \ldots, \quad (11)
\]

In a graphical interpretation this equation represents again an intersection of a tangens-like curve with the infinite family of parallel lines. This is illustrated in Figure 1. The equation generates, therefore, an infinite number of the real roots \( \omega_N \in (0, 1) \) at all the non-negative integers \( N = 0, 1, \ldots \).
5 Wave functions in the weak coupling regime

Equation (7) in combination with eqs. (9) and (10) determines the real parameter
\[ G = G(\pm) = -\frac{k^2}{q \pm p} \]  
(12)

responsible for the behaviour of the wave functions near the origin [remember that \( B = iG/k \) in eq. (3)]. For its deeper analysis let us first introduce an auxiliary linear function of \( \omega \) and \( N \),
\[ \sqrt{R(\omega_N, N)} = \frac{2N + 2 - \omega_N}{4T} \in \left( \frac{N + 1/2}{2T}, \frac{N + 1}{2T} \right) \]
and re-interpret our secular eq. (11) as an algebraic quadratic equation with the unique positive solution,
\[ \cos \left( \frac{\pi}{2} \omega_N \right) = \frac{1}{R(\omega_N, N) + \sqrt{R^2(\omega_N, N) + 1}} . \]  
(13)

This is an amended implicit definition of the sequence \( \omega_N \). As long as the right hand side expression is very smooth and never exceeds one, the latter formula re-verifies that the root \( \omega_N \) is always real and bounded as required.

In the domain of the large and almost constant \( R \gg 1 \) (i.e., for the small square-well height \( T \) or at the higher excitations), our new secular equation (13) gives a better picture of our bound-state parameters \( \omega_N = 1 - \eta_N \) which all lie very close to one. The estimate
\[ \frac{\pi}{2} \eta_N = \arcsin \frac{1}{R + \sqrt{R^2 + 1}} \approx \frac{1}{2R} - \frac{5}{48 R^3} + \ldots \]
represents also a quickly convergent iterative algorithm for the efficient numerical evaluation of the roots \( \omega_N \). One can conclude that in a way compatible with our \textit{a priori} expectations, the value of \( p = p_N = \text{Re} \sigma \approx q/2R \) is very close to zero and, as a consequence, the asymptotic decrease of our wave functions remains slow. We have \( q = q_N = \text{Im} \sigma \approx k \) so that, asymptotically, our wave functions very much resemble free waves \( \exp(-ikx) \). In the light of eq. (12) we have also \( \psi(x) \approx \exp(-ikx) \) near the origin.
6 Wave functions in the strong coupling regime

For the models with a very small $R$ (i.e., for the low-lying excitations in a deep well with $T \gg 1$) we get an alternative estimate

$$\frac{\pi}{4} \omega_N = \arcsin \sqrt{\frac{1}{2} \left[ R - \left( \sqrt{1 + R^2} - 1 \right) \right]} \approx \frac{1}{2} R - \frac{1}{4} R^2 + \ldots \ll \frac{\pi}{4}.$$  

In the limit $R \to 0$ the present spectrum of energies moves towards (and precisely coincides with) the well known levels of the infinitely deep Hermitian square well of the same width $I = (-\pi, \pi)$ (cf. eq. (11) with $S \to \infty$). In this sense, the “complex-rotation” transition from the Hermitian well $V^{(SQW)}(x)$ of eq. (11) (with $S \gg 1$) to its present non-Hermitian $PT$ symmetric alternative $V^{(ISQW)}(x)$ of eq. (12) (with $T \gg 1$) proves amazingly smooth.

The wave functions exhibit the similar tendency. In the outer region, they are proportional to $\exp(-px)$ and decay very quickly since $p = \mathcal{O}(R^{-1/2})$. The parameter $G^{(\pm)}$ becomes strongly superscript-dependent,

$$G^{(+)}/q + p = \mathcal{O}(R^{3/2}), \quad G^{(-)} = -(q + p) = \mathcal{O}(R^{-1/2}).$$

This means that in the interior domain of $x \in (-\pi, \pi)$, the wave functions with the superscript $(+)$ and $(−)$ become dominated by their spatially even and odd components $\cos kx$ and $\sin kx$, respectively. In this sense, the superscript mimics (or at least keeps the trace of) the quantum number of the slightly broken spatial parity $P$.

We can summarize that our present $PT$ symmetric model is, unexpectedly, quite robust. Almost irrespectively of the coupling $T$, the spectrum is unbounded from above and remains constrained by the inequalities

$$\frac{(N + 1/2)^2}{4} \leq E_N \leq \frac{(N + 1)^2}{4}. \quad (14)$$

The analogy between our exactly solvable square-well model and the standard or “paradigmatic” $PT$ symmetric Hamiltonian $H_{BZ}$ appears to be closer than expected.
7 Outlook

The exact solvability of our present purely imaginary square well model throws a new light on some properties of the $\mathcal{PT}$ symmetric wave functions which are hardly accessible by approximative techniques. In the nearest future, one can expect that the further detailed study of the $\mathcal{PT}$ symmetric square wells will give new answers to the recent puzzles as formulated in ref. [12] and concerning the irregular behaviour of the nodal zeros in the complex plane. Our present example indicates that a surprising alternative to the Sturm Liouville oscillation theorem could, perhaps, emerge in connection with the study of zeros of the separate real and imaginary parts of the $\mathcal{PT}$ symmetric wave functions.

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Figure captions

Figure 1. Graphical solution of eq. (11) ($y = \omega_N/2$, $T = 1$)
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Figure 1