Imaginary cubic oscillator
and its square-well approximations
in $x$– and $p$–representation

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Abstract
Schrödinger equation with imaginary $\mathcal{PT}$ symmetric potential $V(x) = i x^3$ is studied using the numerical discretization methods in both the coordinate and momentum representations. In the former case our results confirm that the model generates an infinite number of bound states with real energies. In the latter case the differential equation is of the third order and a square-well, solvable approximation of kinetic energy is recommended and discussed. One finds that in the strong-coupling limit, the exact $\mathcal{PT}$ symmetric solutions converge to their Hermitian predecessors.

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1 Introduction

An interest in 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

\[ H_{BZ} = p^2 + i x^3 \]

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 possible methodical relevance in relativistic quantum field theory \[3\]. They emphasized that the apparent reality of the spectrum of energies \(E_{BZ}\) is quite puzzling.

The conjecture of a full compatibility of similar Hamiltonians with the postulates of quantum mechanics \[4\] opened many new and interesting questions. The current Hermiticity of Hamiltonians was replaced by a weaker condition of their commutativity with a product \(PT\) of the spatial parity \(P\) and of the complex conjugation \(T\). The latter factor is to be understood as a one-dimensional version of the operator of time reversal.

The 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 the energies has been confirmed by the WKB and perturbative studies \[7,8\] and by the quasi-exact and exact models \[9\] where the admissible unavoided level crossings \[10\] prove sometimes followed by the spontaneous breakdown of \(PT\) symmetry \[11\].

In such a context we propose here an extremely elementary approach to similar models replacing interactions which admit just a numerical treatment (typically, \(V(x) = ix^3\)) by their exactly solvable square-well analogues.

2 Models in coordinate representation

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

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

In this spirit one can also replace the antisymmetric and imaginary homework potential \(V_{BZ}(x) = ix^3\) by its elementary square-well analogue

\[ V^{(ISQW)}(x) = \begin{cases} 
-i T^2, & x \in (-\infty, -\pi), \\
0, & x \in (-\pi, \pi), \\
+i T^2, & x \in (\pi, \infty).
\end{cases} \]
Schrödinger equation which appears in such a setting,

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

(2)

will be complemented 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 [12]

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

(4)

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

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

(5)

we shall guarantee the full compatibility of such a convention with the symmetry requirements (4) by the choice of the purely imaginary constant \(B = iG/k\) in wave functions (5).

3 Matching conditions at \(x = \pi\)

Let us split \(\sigma = p + iq\) in its real and imaginary part with a fixed sign, \(p, q \geq 0\). This gives \(p^2 + k^2 = q^2\) and \(2pq = T^2\). These rules 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)

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 matching of logarithmic derivatives at \(x = \pi\),

\[
G = -i k \tan(k + \Omega)\pi. \tag{7}
\]

The 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,

\[
\tan \left[ \frac{\pi T \sin \alpha^{(+)} \sqrt{2 \cos \alpha^{(+)}}}{\sqrt{2 \cos \alpha^{(+)}}} \right] = \tan \left[ \frac{\pi \alpha^{(+)} - \pi}{2} \right], \tag{9}
\]

\[
\tan \left[ \frac{\pi T \sin \alpha^{(-)} \sqrt{2 \cos \alpha^{(-)}}}{\sqrt{2 \cos \alpha^{(-)}}} \right] = \tan \left[ -\frac{\alpha^{(-)} - \pi}{2} \right]. \tag{10}
\]

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

## 4 Energies

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, \(\tan[(\pi - \alpha^{(+)})/2] \in (1, \infty)\) and \(\tan[\alpha^{(-)}/2] \in (0, 1)\). A priori this indicates that our roots \(k = k(\alpha_n^{(\pm)})\) will all lie within well determined intervals,

\[
k_n^{(+)} \in \left( n + \frac{1}{4}, n + \frac{1}{2} \right), \quad n = 0, 1, \ldots,
\]

\[
k_m^{(−)} \in \left( m + \frac{3}{4}, m + 1 \right) \quad m = 0, 1, \ldots.
\]

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,

\[
k_n^{(+)} = n + \frac{1}{2} - \frac{\omega_n^{(+)}}{4}, \quad k_n^{(−)} = m + 1 - \frac{\omega_m^{(−)}}{4}, \quad \omega_n^{(\pm)} = \frac{2\alpha_n^{(\pm)}}{\pi} \in (0, 1).
\]

After an elementary change of 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

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

In a graphical interpretation this equation represents 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 \(N = 0, 1, \ldots\).
Figure 1: Graphical solution of eq. (11) \((y = \omega_N/2, \ T = 1)\).

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 behavior of the wave functions near the origin [remember that \(B = iG/k\) in eq. (5)]. For its analysis let us introduce an auxiliary linear function of \(\omega\) and \(N\),

\[
\sqrt{R}(\omega_N, N) = \frac{2N + 2 - \omega_N}{4T} \in \left(\frac{N + 1/2}{2T}, \frac{N + 1}{2T}\right).
\]

Our secular eq. (11) can be then read 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 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 small square-well heights \(T\) 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

\[
\frac{\pi}{2} \eta_N = \arcsin \frac{1}{R + \sqrt{R^2 + 1}} \approx \frac{1}{2R} - \frac{5}{48R^3} + \ldots
\]
represents 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 a priori expectations, the value of $p = p_N = \text{Re}\sigma \approx q/2R$ lies very close to zero. 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 $\psi(x) \approx \exp(-ikx)$ 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. (1) with $S \to \infty$). The complex-rotation transition from the Hermitian well $V^{(\text{SQW})}(x)$ of eq. (1) (with $S \gg 1$) to its present non-Hermitian $\mathcal{PT}$ symmetric alternative $V^{(\text{ISQW})}(x)$ of eq. (2) (with $T \gg 1$) proves amazingly smooth.

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

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

In the interior domain of $x \in (-\pi, \pi)$ the wave functions with superscripts $\text{(+)}$ and $\text{(-)}$ become dominated by their spatially even and odd components $\cos kx$ and $\sin kx$, respectively. The superscript mimics (or at least keeps the trace of) the quantum number of the slightly broken spatial parity $\mathcal{P}$.

We can summarize that our present $\mathcal{PT}$ symmetric model is quite robust. Independently of the coupling $T$ the spectrum is unbounded from above and remains constrained by 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” $\mathcal{PT}$ symmetric Hamiltonian $H_{BZ}$ appears closer than expected.

7 Transition to the momentum representation

Let us turn our attention to one-dimensional harmonic oscillator $H^{(\text{HO})} = p^2 + x^2$ which is exactly solvable and which appears in virtually any textbook on quantum
mechanics. In \(\mathcal{PT}\) symmetric quantum mechanics a similar guiding role can be and has been attributed to the non-Hermitian cubic Hamiltonian \(H^{(CO)} = p^2 + ix^3\) of Bender et al \[4\]. We have seen that a straightforward numerical and semi-classical analysis of the related Schrödinger equation

\[
H^{(CO)} \psi_n = E_n^{(CO)} \psi_n, \quad n = 0, 1, \ldots
\]

(15)
supports a highly plausible conjecture that the spectrum of energies is real, discrete and bounded below. The conjectured absence of its imaginary components is indicated by the Hilbert-Schmidt analysis \[5\] and by the perturbation calculations in both the weak-coupling regime \[13\] or in its strong-coupling, purely numerically generated re-arrangement \[12\].

Certainly, the problem deserves a change of the traditional perspective. Let us, therefore, move now to its momentum representation. This would give the momentum as a mere number, \(p \in (-\infty, \infty)\) while the coordinate \(x\) becomes represented by the differential operator \(\hat{x} = i \partial_x\). Equation (15) then acquires a new form containing the purely real differential Schrödinger operator \(H^{(CO)} - E\) of third order,

\[
\left[ \frac{d^3}{dp^3} + p^2 \right] \psi(p) = E \psi(p), \quad \psi(p) \in \mathcal{L}_2(\mathbb{R}).
\]

This gives an unusual formulation of our bound-state problem where the quadratic \(p\)–dependence of the kinetic term \(T(p) = p^2\) does not seem to make the equation any easier to solve. For this reason we shall drastically simplify the kinetic term and deduce some consequences.

## 8 Piecewise constant approximate kinetic energy

In a way proposed by Prüfer \[14\] many wave functions can be visualized as certain deformations of solutions which correspond to a locally constant potential, \(\psi(x) \approx c_1 \sin[\varrho(x)] + c_2 \cos[\varrho(x)]\). In the standard quantum mechanics such a trick found immediate applications in numerical computations \[15\] while it still admits an easy interpretation via some traditional Sturm Liouvillean oscillation theorems \[16, 17\]. Using this idea as a methodical guide let us now replace the kinetic energy operator \(T(p) = p^2\) by the most elementary square well of a finite depth \(Z > 0\),

\[
T(p) = \begin{cases} 
Z, & p \in (-\infty, -1), \\
0, & p \in (-1, 1), \\
Z, & p \in (1, \infty).
\end{cases}
\]

In the bounded range of energies \(E < Z\) this splits our toy model in the two separate differential equations,

\[
\left[ \frac{d^3}{dp^3} - 8 \alpha^3 \right] \psi(p) = 0, \quad p \in (-1, 1),
\]
\[
\left[ \frac{d^3}{dp^3} + 8 \beta^3 \right] \psi(p) = 0, \quad p \in (-\infty, -1) \cup (1, \infty).
\]

The two auxiliary parameters \( \alpha = \alpha(E) > 0 \) and \( \beta = \beta(E) > 0 \) are defined in such a way that \( Z = E + 8 \beta^3 > E = 8 \alpha^3 \). They appear in the three independent (exponential) solutions of our equation. Their general superpositions are complex but they may be given the real, trigonometric form. Near the origin we have

\[
\psi_0(p) = d e^{2\alpha p} + f e^{-\alpha p} \cos(\tilde{\alpha} p + \theta), \quad p \in (-1, 1), \quad \tilde{\alpha} = \sqrt{3} \alpha
\]

where the symbols \( d, f \) and \( \theta \) stand for the three undetermined constant parameters.

In the right and left asymptotic regions we obtain the similar formulae. After we omit their exponentially growing and normalization-violating unphysical components we get the one-parametric family

\[
\psi_+(p) = g e^{-2\beta p}, \quad p \in (1, \infty).
\]

The two-parametric left-barrier counterpart of this formula reads

\[
\psi_-(p) = c e^{\beta p} \cos(\tilde{\beta} p + \eta), \quad p \in (-\infty, -1), \quad \tilde{\beta} = \sqrt{3} \beta.
\]

At the right discontinuity \( p = 1 \) we have to guarantee the continuity of \( \psi(p) \), \( \partial_p \psi(p) \) and \( \partial_p^2 \psi(p) \). This is equivalent to the three matching conditions

\[
\begin{align*}
d e^{2\alpha} + f e^{-\alpha} \cos(\tilde{\alpha} + \theta) &= g e^{-2\beta}, \\
2\alpha d e^{2\alpha} - \alpha f e^{-\alpha} [\cos(\tilde{\alpha} + \theta) + \sqrt{3} \sin(\tilde{\alpha} + \theta)] &= -2\beta g e^{-2\beta}, \\
4\alpha^2 d e^{2\alpha} - 2\alpha^2 f e^{-\alpha} [\cos(\tilde{\alpha} + \theta) - \sqrt{3} \sin(\tilde{\alpha} + \theta)] &= 4\beta^2 g e^{-2\beta}.
\end{align*}
\]

(16)

The weighted sum of these equations re-scales and interrelates the unknown coefficients \( d \) and \( g \) in terms of a new energy parameter \( t = t(E) = \beta(E)/\alpha(E) > 0 \) or rather \( R = R(E) = (1 - t + t^2)^{-1/2} > 0 \),

\[
d e^{2\alpha} \equiv D(E) = \frac{3}{G(E)} R(E), \quad G(E) \equiv g e^{-2\beta}.
\]

After we eliminate \( G \) from the last two equations which are linear in \( d \) and \( f \) we obtain the elementary formula which defines the shift \( \theta = \theta(E) \),

\[
\tan(\tilde{\alpha} + \theta) = \frac{\sqrt{3}}{2/t - 1}.
\]

The trigonometric factors become fixed up to their common sign \( \varepsilon = \pm 1 \),

\[
\cos(\tilde{\alpha} + \theta) = \varepsilon [1 - t(E)/2] R(E), \quad \sin(\tilde{\alpha} + \theta) = \frac{\sqrt{3}}{2} \varepsilon t(E) R(E).
\]

The same sign enters our last decoupled definition

\[
f e^{-\alpha} \equiv F(E) = \frac{2[t(E) + 1] G(E)}{3 \varepsilon R(E)}.
\]
Up to an overall normalization (say, \( g = 1 \)) in our wave functions matched at \( p = 1 \), all the free parameters become specified as functions of the energy.

At the second, \( p = -1 \) discontinuity we have to satisfy three matching conditions as well. In terms of abbreviations

\[
L_1 = de^{-2\alpha} + f e^\alpha \cos(-\tilde{\alpha} + \theta),
L_2 = 2\alpha de^{-2\alpha} - \alpha f e^\alpha [\cos(-\tilde{\alpha} + \theta) + \sqrt{3} \sin(-\tilde{\alpha} + \theta)],
L_3 = 4\alpha^2 de^{-2\alpha} - 2\alpha^2 f e^\alpha [\cos(-\tilde{\alpha} + \theta) - \sqrt{3} \sin(-\tilde{\alpha} + \theta)]
\]

they read

\[
L_1(\alpha, d, f, \theta) = ce^{-\beta} \cos(-\tilde{\beta} + \eta),
L_2(\alpha, d, f, \theta) = \beta ce^{-\beta}[\cos(-\tilde{\beta} + \eta) - \sqrt{3} \sin(-\tilde{\beta} + \eta)],
L_3(\alpha, d, f, \theta) = -2\beta^2 ce^{-\beta}[\cos(-\tilde{\beta} + \eta) + \sqrt{3} \sin(-\tilde{\beta} + \eta)].
\]

They determine the values of \( c = c(E) \) and \( \eta = \eta(E) \). Their properly weighted sum gives

\[
\sqrt{3} F(E) \sin(-\tilde{\alpha} + \theta) + (2t - 1) F(E) \cos(-\tilde{\alpha} + \theta) + 2 \frac{1 - t + t^2}{t + 1} D(E) e^{-6\alpha} = 0.
\]

After its slight re-arrangement we arrive at the amazingly transparent relation

\[
(1 - 4t + t^2) \cos(2\sqrt{3}\alpha) + \sqrt{3}(1 - t^2) \sin(2\sqrt{3}\alpha) = \left( \frac{1 - t + t^2}{1 + t} e^{-3\alpha} \right)^2. \quad (17)
\]

It should be read as an implicit definition of physical energies \( E \).

Figure 1.

Figure 2: Graphical solution of equation (17) at \( Z = 1/1000 \).
9 The $Z$–dependence of the spectrum

It is quite instructive to search for the physical energies numerically. Starting from the very-shallow-well extreme in eq. (17) we find the two clearly distinguished energy roots. The qualitative features of the graph of secular determinant remain unchanged in a broad interval of the inverse strengths $1/Z$. Its shape is sampled in Figure 2 at $Z = 10^{-3}$. We have tested that even the approximate height $\approx -5$ of its left plateau stays virtually unchanged between $Z = 10^{-5}$ and $Z = 10^{-3}$. Within the same interval of the shallowest wells the left zero grows from the value 0.00280 till 0.0241. Beyond the broad, downwards-oriented peak one finds the second, right zero moving from the value 0.01047 (found very close to the instantaneous threshold 0.01077) up the value 0.1056 (not very far from its threshold 0.1077, either) within the same interval of $1/Z$.

![Figure 2](image)

Figure 2: Figure 3: Local maximum giving the new doublet of roots at $Z = 5.3005$.

A new feature emerges around $Z = 10^{-1}$ (with the left zero at 0.0445 and with the right zero 0.222 still quite close to the threshold 0.232) and $Z = 1$ (with the left zero at 0.072 and with the right zero 0.446, not that close already to the threshold 1/2) in the left half of the picture. The plateau develops a local, safely negative maximum.

In the subsequent domain of $Z > 1$ we have to switch our attention back to the right half of our graph. Immediately before the coupling reaches the integer value of $Z = 5$, the end of the curve returns to the negative half-plane near the maximal (i.e., threshold) energy. This means that there emerges the third energy level there. The total number of bound states grows to $N = 3$ (cf. the leftmost items in our Table 1).
Table 1.

Number of levels $N$ and its changes $\Delta$ with growing $Z$.

| $N$ | 2  | 3  | 5  | 3  | 4  | 5  | 7  | 8  | 6  | 7  | 9  | 10 |
|-----|----|----|----|----|----|----|----|----|----|----|----|----|
| $\Delta$ | 1  | 2  | $-2$ | 1  | 1  | 2  | 1  | $-2$ | 1  | 2  | 1  | 1  |

Beyond $Z = 5$, our attention has to return quickly to the left half of the picture where the very slow growth of the local maximum creates a new quality at last. The top of the local bump touches and crosses the horizontal axis at $Z \approx 5.3003$ and $E \approx 0.6244$. At $Z = 5.3005$ a new doublet of energies is formed in a way illustrated in Figure 3. The number of levels jumps to $N = 5$.

![Figure 3](image3.png)

Figure 3: The local maximum not giving the doublet of roots at $Z = 35$.

A smooth deformation of the graph takes place when the value of $Z$ grows on. During this evolution we discover that our (originally broad), downward-oriented peak shrinks quite quickly and moves comparatively slowly to the right. It gets close to the rightmost and, to its bad luck, slightly more slowly moving zero number five. The magnified picture of the resulting “collision” is displayed here in Figure 4. At $Z = 35$ it shows that in the threshold region of the energies,

- the wavy motion of the threshold end of our graph still did not manage to reach the zero axis;
- the downwards-oriented peak has already left the positive part (and moved to the negative part) of the curve in question.

As a consequence, the number of levels drops, quite unexpectedly, down to 3 again (cf. Table 1).
In the vicinity of \( Z = 40 \) the new, rightmost energy root emerges at last. Up to \( Z = 100 \) and beyond, the number of levels stays equal to 4. Then it increases to 5, due to the emergence of the next threshold zero. Only after that, the slowly moving downward peak reaches the domain of the fourth zero. At almost exactly \( Z = 190 \) its left (and temporarily negative) local maximum reaches the zero value again (cf. Figure 5). At this moment the number of states jumps up by two to seven. The magnified graphical proof is offered by Figure 5 at \( Z = 200 \).

The latter Figure illustrates nicely the rapid shrinking of our peak with \( Z \). The numerical detection of its position becomes more and more difficult. Although this position plays a crucial role in the practical determination of the number of levels at
a given $Z$, we must be very careful in distinguishing the subgraph of Figure 6 (with three zeros) from a simple straight line with the single zero.

The pattern is deceitful and the standard software which searches for roots has to be used with due care. *Vice versa*, the above analysis enables us to take into account all the specific features of the $Z$–dependence of the graph in eq. (17). We get a regular pattern summarized in Table 1 and exhibiting a certain regularity of the $Z$–dependence of the number of levels $N = N(Z)$.

**10 Energies in the square-well approximation**

The main consequence of the presence of the above-mentioned narrow peak is an unusual irregularity observed in the emergence of the new levels in the deeper wells. We may conclude that this irregularity is not an artifact of the computation method. The energy formula (17) for our square-well toy model is exact and the seemingly unpredictable emergence of its roots just reflects the fact that our Schrödinger equation is of the third order. In particular, there exists no symmetry/antisymmetry with respect to the parity $p \to -p$ etc.

![Figure 6.](image)

**Figure 6.**

![Figure 7](image)

**Figure 7:** Numerical invisibility of the narrow peak and of the new threshold root at $Z = 1200$.

Methodical consequences of our analysis are a bit discouraging. Firstly, the very symbolic-manipulation derivation of our present formulae proved unexpectedly complicated even in comparison with the multiple standard square wells in textbooks. That’s why we did not move to any further piece-wise constant approximations of $T(p)$.

Secondly, even our use of the most elementary solvable example revealed quite clearly a very real danger of the possible loss of certain levels. For an illustration let us imagine that our numerical study would have been started in the deep-well domain, i.e., at the large $Z$. It is quite easy to generate the graphs of eq. (17) there.
In the standard and routine finite-precision computer arithmetics one discovers that the results are very smooth and look virtually the same, say, in the interval of $Z \in (1000, 1200)$.

Let us pick up, for definiteness, the larger sample $Z = 1200$. We get a picture (cf. our last Figure 7) which is regular and, deceptively, indicates that $N(1200) = 7$. Unfortunately, the correct answer (appearing at the right end of our Table 1) is $N(1200) = 10$. Its derivation requires the use of a significantly enhanced precision. Otherwise, whenever we use just the standard 14 digits and Figure 7, we would have missed as much as three (i.e., cca 30% of all) energy levels.

In the light of our preceding considerations, an easy explanation of the latter numerical paradox lies in the presence of the narrow peak. *A priori*, it is hardly predictable of course. It is necessary to spot it by brute force. One finds that at $Z = 1000$, this anomalous peak still lives safely below the sixth energy level. The related number of levels is reliably confirmed as equal to seven, indeed.

In between $Z = 1000$ and $Z = 1200$, it is necessary to work in an enhanced precision arithmetics. One finds that the upper, threshold end of the curve crosses the horizontal axis only slightly above $Z = 1100$. Due to the very steep slope of the curve in this region, this crossing is not visible even at $z = 1200$ in Figure 7.

One has to trace the narrow peak carefully. It overtakes the sixth energy level at $Z \approx 1190$ (and $E = 4.217$), in an arrangement resembling our Figure 5 above. Thus, one concludes, finally, that the new, almost degenerate pair of the energy levels emerges immediately beyond this point.

11 Wave functions and their zeros

A marginal merit of our use of the square-well-shaped $T(p)$ lies in the availability of the explicit wave functions. For the lack of space we have to omit illustrative pictures, mentioning just a few of their most characteristic features.

In the first step we notice that in the rightmost interval of $p$ the absence of any nodal zero in the wave function is in fact very similar to the usual Sturm Liouville behavior. Less expectedly, at the exact energy value one encounters an infinity of the nodal zeros in the leftmost subinterval of $p \in (-\infty, -1)$. In this domain we are fortunate in studying the exactly solvable case. The very presence of this infinite “left” set of nodal zeros is extremely sensitive to the numerical level of precision we use. Indeed, the errors are proportional to the unphysical $\psi^{(unphys.)}(p) \sim exp(-2\beta p)$ which is growing rapidly at $p \ll -1$.

After the smallest deviation of the energy $E$ from its absolutely precise bound-state value even the non-numerical and absolutely precise wave functions will be dominated by the growing asymptotics $\psi^{(unphys.)}(p) \sim exp(-2\beta p)$ near the left infinity. The change of sign of the asymptotics is a reliable source of information about the fact that the energy crossed its physical value. This observation survives in the shooting numerical algorithms [18] as well as in the rigorously proved versions of the method of Hill determinants [19]). In this context our present numerical experiments could be perceived as opening a number of new questions. Some of them emerge in
the purely numerical context of an appropriate generalization of the Prüfer-type algorithms. Especially in the vicinity of the correct physical energies they could lead to reliable and robust right-to-left shooting numerical recipes.

12 Outlook

In the $x$–representation of our problem our main emphasis has been put on the exact solvability of its replacement by the purely imaginary square well model. New light has been thrown on some properties of wave functions. One can expect that the further detailed study of the $\mathcal{PT}$ symmetric square wells will give new answers to the puzzles concerning the irregular behavior of the nodal zeros in the complex plane as formulated in ref. [20]. Our present study indicates that some complexified versions of the Sturm-Liouville oscillation theorems should be developed for the study of zeros of the separate real and imaginary parts of $\mathcal{PT}$ symmetric wave functions.

After the standard Fourier-transformation transition to the $p$–representation of our imaginary cubic oscillator the underlying eigenvalue problem can be seen from a different perspective. Its Hamiltonian is being replaced by a real differential expression. On a suitable Hilbert space this specifies the Hamiltonian operator with the numerical range (and, hence, spectrum) which is, obviously, real. This complements the extensive discussion of this topic in [5]. Among several immediate constructive consequences of the latter observation we underlined the consistency of the approximations imposed directly upon the kinetic term $T(p)$.

As long as the behavior of wave-function asymptotics at large $|p| \gg 1$ differs in the left and right infinity, several new qualitative aspects of the problem emerge and became clarified by our schematic piece-wise constant approximation of $T(p)$. At small $p \approx 0$ the emergence and motion of the nodal zeros can be interpreted in a graphical manner explaining some features of the $N(Z)$ dependence. In particular, the puzzling loss of its monotonicity seems confirmed by our solvable model.

The use of the momentum representation proved able to throw a new light on the counterintuitive bound states in $\mathcal{PT}$ symmetric quantum mechanics. The emergence/disappearance of our quasi-degenerate doublets should be emphasized as, perhaps, analogous to the unavowed level crossings in harmonic oscillators [10] and/or to the anomalous doubling of levels in the models of Natanzon type [21]. Similar irregularities in the spectra could be, perhaps, attributed to a peculiar combination of the analyticity and non-Hermiticity in $\mathcal{PT}$ symmetric systems.

In a brief summary of our numerical observations let us point out the regularity of the $Z$–dependence of the number $N(Z)$ of the bound states. This indicates that one should search for an improved application of Sturm-Liouville theory in complex domain [22]. The possibility of deduction of new oscillation-type theorems exists, first of all, in the middle interval of $p \in (-1, 1)$ where, for a continuously growing energy parameter $E$, a steady right-ward movement of the nodal zeros competes with the exponential terms which are varying slowly.
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