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Asymptotic solvability of an imaginary cubic oscillator with spikes

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Abstract

For complex potentials $V(x) = -(\mathrm{i}x)^3 - \beta^2(\mathrm{i}x)^{-2} - 2\beta\delta(\mathrm{i}x)^{1/2}$ which are $\mathcal{PT}$ symmetric, we show that in $\beta \gg 1$ strong coupling regime the low-lying bound states almost coincide with harmonic oscillators whenever the spectrum remains real (this means, at all $\delta < \delta_{\mathrm{critical}}(\beta) \approx 1$).

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1. Introduction

Radial Schrödinger equations

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_{(\mathrm{eff})}(r)\right]\psi(r) = E\psi(r) \qquad V_{(\mathrm{eff})}(r) = \frac{\ell(\ell+1)}{r^2} + V(r) \tag{1}$$

characterized by the *large* angular momenta ℓ appear in molecular or nuclear physics [1]. The strongly repulsive phenomenological core G/r^2 of $V(r)$ with $G \gg 1$ is often added directly to the centrifugal term in three dimensions, $\ell(\ell+1) = \tilde{\ell}(\tilde{\ell}+1) + G$, $\tilde{\ell} = 0, 1, \ldots$, and in the latter context, even the effective dimensions $D \neq 3$ in $\tilde{\ell} = m + (D-3)/2$, $m = 0, 1, \ldots$, may become extremely large [2].

Similar situations have inspired the development of a few efficient $\ell \gg 1$ approximation techniques applicable to many particular Hermitian models (cf [3] and references therein). Thorough tests of their reliability are amply available [4]. Similar studies are missing in the non-Hermitian context, and our present purpose is to fill this gap.

For the sake of definiteness, let us recollect the popular anharmonic oscillator

$$V_{\mathrm{eff}}(r) = \frac{\ell(\ell+1)}{r^2} + \omega^2 r^2 + g r^N \tag{2}$$

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which has been studied in many papers at large ℓ. The encouraging results of these studies (cf [5] and references therein) show that the effective potential possesses a deep minimum at certain *real* coordinate $r_0 > 0$. Near this value, the effective potential is very well approximated by the *exactly solvable* harmonic oscillator. Thus, choosing $\omega = 0$ and $N = 4$ for definiteness we have

$$V_{\rm eff}(r) = V_{\rm eff}(r_0) + \tfrac{1}{2}V''_{\rm eff}(r_0)(r - r_0)^2 + \mathcal{O}(r - r_0)^3 \qquad r_0 = \sqrt[6]{\frac{\ell(\ell+1)}{2g}}$$

where the higher-order contributions prove small.

The latter Hermitian example is a key guide to our present study. We shall just ask what happens when the potential and/or coordinates cease to be real in a way proposed, e.g., by Bender and Boettcher [6]. The deepest physical motivation of the similar generalizations may probably be found in the field theory where the *non-Hermitian* oscillators emerge in the most natural manner (cf concluding remarks in [7] or recent considerations in [8]).

One of the first explicit studies of a non-Hermitian model (2) has been offered by Caliceti *et al* [9] who revealed the amazing reality of energies in the manifestly complex potential V with cubic anharmonicity $N = 3$ and with a purely imaginary coupling g in one dimension (i.e. still at the real coordinates r and with the parity $\ell = -1, 0$). For a long time, this result has been treated as a mere isolated curiosity in the literature, in spite of the well-known existence of its fully natural analytic continuation to the whole domain of analyticity of the potential, i.e. into the cut complex plane of coordinates r. The details concerning the purpose of such a complexification have been summarized, e.g., in [10].

A quartic, $N = 4$, parallel of the cubic model emerged a few years later in connection with the puzzling coincidence (up to a sign) between energy corrections in two different perturbative models [11]. An explanation has been given by Buslaev and Grecchi [12] who discovered that the connection was mediated by an auxiliary non-Hermitian potential (2) with $N = 4$, negative g and the most suitable complex choice of the coordinate $r = x - {\rm i}\varepsilon$ where $x \in (-\infty, \infty)$. Its purely real and discrete spectrum was proved to be bounded below.

Both the above non-Hermitian anharmonic oscillator examples share the commutativity of their Hamiltonian with the product of operations $\mathcal{P}x\mathcal{P} = -x$ and $\mathcal{T}{\rm i}\mathcal{T} = -{\rm i}$ interpreted as parity and time reversal, respectively,

$$H = \mathcal{P}\mathcal{T}H\,\mathcal{P}\mathcal{T} \equiv H^{\ddagger}. \tag{3}$$

The relevance of such a type of anti-linear symmetry was appreciated only after Bender and Boettcher [6] reanalysed the $\mathcal{PT}$ symmetric potentials (2) with complex couplings $g \sim {\rm i}^N$. Putting $\omega = 0$ for simplicity, they found that the numerical and WKB analysis supports the hypothesis that the spectrum remains discrete, bounded below and purely real at *any* real exponent $N \geqslant 2$. This inspired further intensive research and, within the resulting conjecture of the so-called $\mathcal{PT}$ symmetric quantum mechanics [13], the validity of equation (3) has been interpreted as a certain analogue or a weaker form of Hermiticity [12–14].

In what follows, we constrain our attention to the $N = 3$ anharmonicity and pick up a one-parametric $\mathcal{PT}$ symmetric generalization of equation (2) in sections 2 and 2.1. In section 2.2 we then recollect a few basic formal ingredients and, in particular, explain the relation between the $\mathcal{PT}$ symmetry and boundary conditions. A way in which the smallness of $1/\ell$ may play a crucial role is outlined in section 3. In section 4 we describe our main results concerning the closed asymptotic representation of the energies in the two separate (namely, weak- and strong-coupling) regimes of the non-Hermitian cubic-plus-square-root models. A few numerical tests and illustrations confirm our assertions in section 5 and are complemented by a non-numerical discussion in section 6. A short summary is given in section 7.

2. The problem

2.1. Characteristic example: cubic oscillator with spikes

The short history of the $\mathcal{PT}$ symmetric quantum mechanics climaxed with the recent work by Dorey, Dunning and Tateo (DDT, [15]) who succeeded in proving rigorously that the generalized cubic model with $\omega = 0$, namely

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2} - \alpha\sqrt{\mathrm{i}r} + \mathrm{i}r^3\right]\psi(r) = E\psi(r) \qquad r = x - \mathrm{i}\varepsilon \quad x \in (-\infty, \infty) \tag{4}$$

possesses a real and discrete spectrum whenever the angular momentum ℓ is sufficiently large:

$$\ell > \max\left[\tfrac{1}{4}(2\alpha - 7), -\tfrac{1}{2}\right]. \tag{5}$$

The reality of the spectrum under a suitable constraint is a characteristic feature of many pseudo-Hermitian models [16]. Within this class, the $\mathcal{PT}$ symmetric DDT oscillator (4) is distinguished by the presence of two spikes near the origin. Moreover, the preliminary tests performed on a simplified model in [15] indicate that the reality of the spectrum becomes spontaneously broken. At some $\ell_{\mathrm{minimal}}(\alpha)$, only slightly below the bound (5), at least two energy levels have to merge and form a complex conjugate pair. In the other words, we may tolerate the non-Hermiticity of the Hamiltonian $H^{(\mathrm{DDT})}$ as *acceptably weak* in the semi-infinite interval of the angular momenta $\ell \in (\ell_{\mathrm{minimal}}, \infty)$ where ℓ_{minimal} grows with α for $\alpha > 5/2$.

The interference between the two spikes becomes particularly interesting in the strong-coupling domain of $\alpha \gg 1$. In this interval, the square-root dynamics may be understood as weakly non-Hermitian (in the sense of generating the real spectrum) if and only if the kinematical centrifugal repulsion also remains strong, $\ell = \mathcal{O}(\alpha)$. The latter observation has attracted our attention since the non-Hermiticity may in general worsen the feasibility of the construction of the solutions while, as we have already noted, many of the difficulties with the construction of the bound states may in principle be avoided due to the presence of the small parameter $1/\ell$.

2.2. Complex boundary conditions

The ℓ-dependence in the Schrödinger equations remains the same for the real and complex potentials. The latter case is exemplified by our equation (4) and illustrated in figure 1 where, for simplicity, the smooth term $\mathrm{i}r^3$ is completely omitted. The real part of the effective potential is displayed there for the complex shift $\varepsilon = 0.8$ and angular momentum $\ell = 13/4 \approx \ell_{\mathrm{minimal}}(\alpha)$ at the medium $\alpha = 10$. The figure shows how the square-root force $-\alpha\sqrt{\mathrm{i}r(x)}$ dominates at the large coordinates while the centrifugal spike prevails near the origin. Both these spikes would become more pronounced closer to the real axis and vice versa.

With the wavefunctions unconstrained by boundary conditions, we may construct two independent solutions $\psi_{1,2}(r)$ of our imaginary cubic Schrödinger differential equation (4) which are analytic functions of r and/or x. In a way described in more detail in [10], we may cut the complex plane of $r = r(x)$ from the origin upwards. This means that we parametrize

$$r = \xi\,\mathrm{e}^{\mathrm{i}\varphi} \qquad \xi \in (0, \infty) \qquad \varphi \in (-3\pi/2, \pi/2).$$

Using such a polar representation of $r(x)$ we may assign a unique meaning to the square root expression $\sqrt{\mathrm{i}r(x)}$. In accordance with figure 1 the real part of this long-range spike is oriented upwards, $\mathrm{Re}\,\sqrt{\mathrm{i}r} \geqslant 0$. This convention makes our potential uniquely defined. Its complex and ε-dependent effective form reads

$$V_{(\mathrm{eff})}[r(x)] = \frac{\ell(\ell+1)}{r^2(x)} - \alpha\sqrt{\mathrm{i}r(x)} + \mathrm{i}r^3(x) \qquad r(x) + \mathrm{i}\varepsilon = x \in (-\infty, \infty). \tag{6}$$

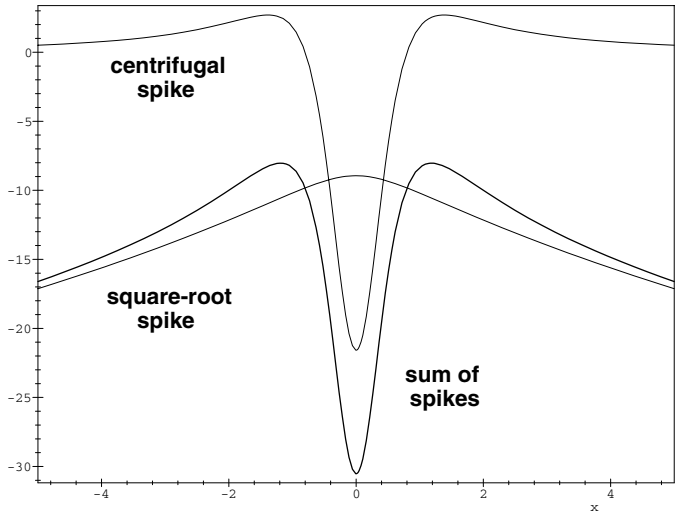

Figure 1. Real parts of the spikes in equation (4) at $\varepsilon = 0.8$.

Due to the analyticity of this function in the cut complex plane, we may freely deform the integration path. The spectrum $E^{(\mathrm{DDT})}$ remains unchanged for all the constant shifts $\varepsilon > 0$ so that one may work with Buslaev and Grecchi's [12] asymptotic boundary conditions $\psi(-\mathrm{i}\varepsilon \pm \infty) = 0$. Bender and Boettcher [6] emphasized that a further generalization of these boundary conditions may be admitted and reads

$$\begin{aligned} &\psi(\xi \mathrm{e}^{\mathrm{i}\varphi_+}) = \psi(\xi \mathrm{e}^{\mathrm{i}\varphi_-}) = 0 \qquad && \xi \to +\infty \\ &\varphi_+ \in (-3\pi/10, +\pi/10) && \varphi_- \in (-11\pi/10, -7\pi/10). \end{aligned} \tag{7}$$

All of these boundary conditions are mutually equivalent and form an elementary analytic continuation of their standard special case $\psi(\pm\infty) = 0$ in the wedge-shaped vicinity (7) of both the ends of the real axis. This is illustrated in figure 2 where the asymptotic wedge permitted for the cubic oscillator is marked by symbol CO. Its boundary also avoids the upwards-running cut which starts at $r = 0$.

In the context of textbook quantum mechanics, the removal of the origin $r = 0$ from our considerations has two immediate consequences. First, in the spirit of [12] (where more details may be found) we may always return to the current Hermitian radial-equation case (in more dimensions, with $r \in (0, \infty)$) by a suitable limiting transition ($\varepsilon \to 0$ in our above notation). In this sense, one need not change the mathematical results but discards merely 'a half' of the available solutions as 'manifestly unphysical' due to the divergence of their norm in this limit. Thus, for example, one simply crosses out all the quasi-even states in the solvable example of [17].

Second, there exists an alternative physical context where the presence of the spikes of the form $\ell(\ell + 1)/r^2$ is a dynamical assumption [18]. Then, the Hermitian quantum system usually remains to be defined on the whole real axis, $r \in (-\infty, \infty)$. All the solutions retain their physical meaning even after the limiting transition $\varepsilon \to 0$ which merely represents a regularization recipe. Such a regularization is also needed within the so-called supersymmetric quantum mechanics [19].

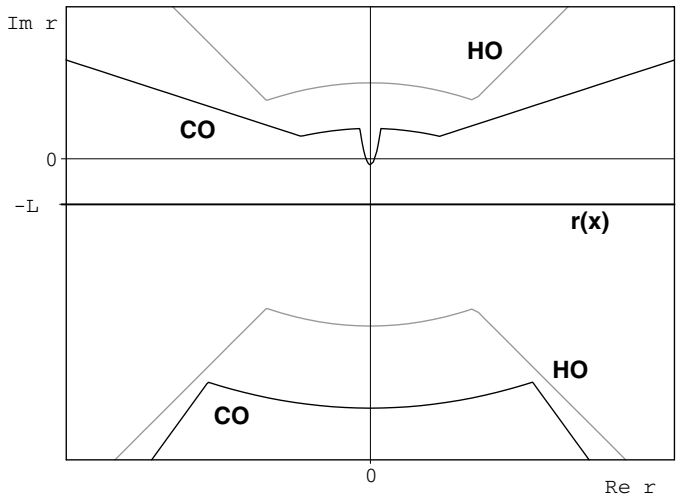

Figure 2. Optimal path $r(x)$ and asymptotic wedges: boundary CO for the cubic oscillator (4) and boundary HO for its harmonic-oscillator approximant (15).

3. The method

As we have seen, the non-Hermiticity is most easily introduced in a Schrödinger equation by a downward complex shift of the coordinate. The typical consequences of this complexification may be illustrated via the simplest example (2) with the vanishing $g = 0$ and scaled-out $\omega = 1$. This offers us a suitable guide towards the $1/\ell$ approximations in their non-Hermitian generalizations.

Although the $\mathcal{PT}$ symmetric $g = 0$ oscillator is exactly solvable and its spectrum is real, it still exhibits certain unusual features [17]. The energies remain non-equidistant and have to be numbered by the integer $n = 0, 1, \ldots$ and by the superscript $(\pm)$,

$$E_n^{(\pm)} = 4n + 2 \pm (2\ell + 1). \tag{8}$$

Once we abbreviate $[\ell(\ell+1)]^{1/4} = A = A(\ell) > 0$ and assume that this quantity is large, we arrive at the Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{A^4}{r^2} + r^2\right]\psi(r) = E\psi(r). \tag{9}$$

We may infer that the absolute minimum of $V_{(\mathrm{eff})}(r) = A^4/r^2 + r^2$ lies at the purely imaginary point $r = R_0 = -\mathrm{i}A$. In the domain of our interest concerning the large values of $A \gg 1$, it may be rewritten in a perturbative form using the new, shifted variable $t = r - R_0$,

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}t^2} - 2A^2 + 4t^2 + \mathcal{O}\left(\frac{t^3}{A}\right)\right]\psi(t + R_0) = E\psi(t + R_0). \tag{10}$$

Obviously, the textbook perturbation solution of this problem is straightforward [20] and shows that the contribution of the corrections is asymptotically small. We get the following harmonic-oscillator leading-order energy estimate for the low-lying part of the spectrum:

$$E = -2A^2 + 2(2n+1) + \mathcal{O}\left(\frac{n^2}{A^2}\right) \qquad n = 0, 1, \ldots. \tag{11}$$

It is worth emphasizing that our *non-Hermitian* equation degenerates to its *Hermitian* harmonic-oscillator approximation which does not contain any centrifugal barrier.

Table 1. Energy levels of the solvable model (9) with $\ell = 5$.

Exact solution	Numerical solution	Large-ℓ approximation	Difference
−9	−9.000 00	−8.954	0.046
−5	−5.000 00	−4.954	0.046
−1	−1.000 00	−1.954	0.046
3	3.000 00	3.046	0.046
7	7.000 00	7.046	0.046
11	11.000 00	11.046	0.046
13	13.000 00	—	—
15	15.000 00	15.046	0.046
17	17.000 00	—	—
19	19.000 00	19.046	0.046

The numerical reliability of equation (11) is documented in the third column of table 1. In the light of the table, the harmonic-oscillator approximation reproduces the low-lying part of the toy spectrum $E_n^{(-)}$ with reasonable quality even at very small $A = \sqrt[4]{30} \approx 2.34$.

Of course, the second, quasi-odd series $E_n^{(+)} = 2\ell + 4n^{(+)} + 3$ of energies is not reproduced here at all. The reason is given by the error term in equation (11). As soon as we moved in the domain of the extremely large $\ell \to \infty$, the value of the lowest quasi-even excitation energy $E_0^{(+)} = 2\ell + 3$ is already comparable with our error estimate. The high-lying energy $E_0^{(+)}$ cannot be reproduced within the framework of our harmonic-oscillator fit.

4. Energies $E^{(\mathrm{DDT})}$ at the large ℓ

The main merit of the freedom in the choice of the shift $\varepsilon > 0$ in our non-Hermitian Schrödinger equation as well as in the related boundary conditions is that we may let the axis $r(x)$ pass through a minimum of the *complex* interaction term. A full analogy with the Hermitian case is achieved in this manner. The systematic search for all the possible *complex* extremes of the effective potentials is easy and may be based on the elementary mathematical rule

$$\partial_r V_{(\mathrm{eff})}(r)|_{r=R} = 0. \tag{12}$$

In the vicinity of the extreme, we may approximate the unsolvable potentials by their reduction to the solvable harmonic-oscillator wells.

4.1. Weak-coupling domain, $\alpha \ll \ell$

As long as the value of ℓ is assumed to be very large in our particular DDT example, it makes sense to abbreviate $2\ell(\ell+1)/3 = L^5$ and replace ℓ by the alternative large parameter $L = L(\ell) \gg 1$. The range of α is then limited by condition (5) so that we may rescale $\alpha = \sqrt{6L^5}\delta$ with $0 \leqslant \delta \lesssim 1$. This simplifies our Schrödinger equation (4),

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + L^5 W(y)\right]\psi(r) = L^2 E\psi(r) \qquad r = Ly. \tag{13}$$

The exact form of the rescaled effective potential

$$W(y) = \frac{3}{2y^2} - \delta\sqrt{6\mathrm{i}y} + \mathrm{i}y^3$$

is L-independent. This simplifies the implicit definition of the minimum/minima of $V_{(\mathrm{eff})}(r)$ which rescales with $r = Ly$ to the elementary formula

$$\partial_y W(y)|_{y=Y} = 0. \tag{14}$$

In writing the solutions of this equation, we shall distinguish between the two separate intervals of α. In the weak-coupling regime with negligible $|\alpha| \ll \ell$ (i.e. vanishing $\delta \approx 0$), equation (14) is trivial ($Y^5 = -\mathrm{i}$) and implies that the extremes of $V_{(\mathrm{eff})}(r)$ are located at the five complex points numbered by $k = 0, 1, 2, 3, 4$,

$$r = R_k = \left|\left[\tfrac{2}{3}\ell(\ell+1)\right]^{1/5}\right| Y_k \qquad Y_k = -\mathrm{i}\exp\{\mathrm{i}(-8+4k)\pi/10\} \quad \delta = 0.$$

After the overall change of scale of $r = Ly$ with $L = \mathcal{O}(\ell^{2/5}) \gg 1$ we get our effective potential $W(y) = V_{(\mathrm{eff})}(Ly)/L^3$ rewritten in the form of the Taylor series,

$$W(y) = \frac{3/2}{y^2} + \mathrm{i}y^3 = \frac{5}{2Y_k^2} + \frac{15}{2Y_k^4}(y - Y_k)^2 + \mathcal{O}\big[(y - Y_k)^3\big]. \tag{15}$$

As long as $\mathrm{Re}\, Y_k^4$ is negative if and only if $k = 0$ or $k = 4$ while $\mathrm{Im}\, Y_k^4$ is non-zero unless $k = 2$, the *unique absolute minimum* of the effective potential $W(y)$ exists and lies at the point $y = Y_2 = -\mathrm{i}$. This implies that in the first two orders in our auxiliary small parameter $1/\ell^{\mathrm{const}} \ll 1$ we get the low-lying spectrum

$$E_n^{(\mathrm{DDT})} \approx -\frac{5L^3}{2} + \sqrt{\frac{15L}{2}}(2n+1) \qquad n = 0, 1, \ldots. \tag{16}$$

We see that the choice of the integration path $r(x)$ with $\varepsilon = L = \mathrm{i}R_2$ enables us to replace our differential Schrödinger equation (4) by its harmonic-oscillator approximation. The asymptotic compatibility of the related boundary conditions is illustrated in figure 2.

4.2. Strong-coupling regime, $\alpha = \mathcal{O}(\ell)$

The strength α of the long-range spike is constrained by rule (5). This means that the $\mathcal{PT}$ symmetry breaks down at the couplings $\delta_{\mathrm{critical}} \approx 1$ in a way described in [15]. The choice of $\delta \in (0, \delta_{\mathrm{critical}})$ remains compatible with the reality of the spectrum and characterizes the strongly spiked regime where both our free parameters are comparably large, $\alpha = \mathcal{O}(\ell)$.

For the small non-vanishing $\delta \approx 0$ we may expect that the positions Y_k of the five weak-coupling extremes of $W(y)$ become only slightly shifted. In the vicinity of the absolute minimum with $k = 2$ we abbreviate $r = -\mathrm{i}Lq$ and write

$$W(y) = 3/(2y^2) + \mathrm{i}y^3 - \delta\sqrt{6\mathrm{i}y} = -\frac{3}{2q^2} - \delta\sqrt{6q} - q^3.$$

Equation (14) remains quadratic in the fifth power of the rescaling factor in $R = -\mathrm{i}LQ$,

$$1 - \left(2 + \frac{\delta^2}{6}\right) Q^5 + Q^{10} = 0.$$

We abbreviate $Q^5 = Z$ and arrive at the two eligible roots. Both of them are real and share the obligatory weak-coupling limit $Z_\pm = 1$. When δ grows from 0 to 1, they split and move to their respective strong-coupling extremes,

$$[Z_\pm = 1]_{\delta=0} \longrightarrow \left[Z_+ = \tfrac{3}{2}, Z_- = \tfrac{2}{3}\right]_{\delta=1}.$$

In the light of our original equation (14) which may be rewritten in the form

$$1 - Z = \delta\sqrt{\frac{Z}{6}}$$

the larger root gives the wrong sign on the right-hand side and must be discarded for positive δ. The solution becomes unique and its value $Z = Z_- \leqslant 1$ decreases with the growing δ. Near its absolute minimum, our effective potential $W(y)$ depends on δ only via the function $Z = Z(\delta)$,

$$W(y) = \frac{1}{Z^{2/5}}\left(-\frac{15}{2} + 5Z\right) + \frac{15}{4Z^{4/5}}(1+Z)\left(y + \mathrm{i}Z^{1/5}\right)^2 + \cdots. \tag{17}$$

As long as $Z^{1/5}(1) \approx 0.922$, this is a fairly weak dependence. The formula leads to our final energy estimate

$$E_m^{(\mathrm{DDT})} = \frac{1}{Z^{2/5}}\left[\left(-\frac{15}{2} + 5Z\right)L^3 + \sqrt{\frac{15(1+Z)}{4}}L^{1/2}(2m+1) + \cdots\right] \tag{18}$$

with $m = 0, 1, \ldots$. Near $\delta = 0$ the deformation of the spectrum (16) is continuous and smooth.

5. Numerical tests

Let us support the idea of applicability of our formulae by their immediate comparison with exact results generated by a suitable 'brute-force' numerical method. All the necessary calculations will be performed with the help of the discrete variable representation (DVR) approach of Harris *et al* [21]. Since its use is rather new in the present context, let us start from its brief description.

In the simplest case, the DVR approach can be regarded as a variational method for finding bounded solutions of the Schrödinger equation. As a first step, we have to choose a suitable set of orthonormal functions $\{\phi_k(r)\}_{k=0}^N$ that should be real for a $\mathcal{PT}$ symmetric case. Then we evaluate matrix elements of the Hamiltonian:

$$H_{ij} = T_{ij} + V_{ij} \tag{19}$$

$$T_{ij} = -\int \phi_i(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi_j(x)\,\mathrm{d}x \tag{20}$$

$$V_{ij} = \int \phi_i(x)V(x)\phi_j(x)\,\mathrm{d}x. \tag{21}$$

The approximate bounded solutions and their energies are finally obtained as eigenvectors and eigenvalues of the Hamiltonian matrix H.

Since the basis set is usually formed by special functions (e.g. orthogonal polynomials), the former integrals (20) can be evaluated analytically. However, the evaluation of the latter ones (equation (21)) is tedious. Therefore in the DVR, the Hamiltonian matrix is expressed and approximated in another representation. We calculate matrix elements of the coordinate operator

$$X_{ij} = \int \phi_i(x)x\phi_j(x)\,\mathrm{d}x \tag{22}$$

which mostly can be done analytically. Then we transform the obtained matrix into its diagonal representation Λ:

$$X \to \Lambda = Q^{-1}XQ. \tag{23}$$

The Hamiltonian matrix is now approximated in the Λ-representation as

$$H(\Lambda) = T(\Lambda) + V(\Lambda) \tag{24}$$

$$T(\Lambda) = Q^{-1}TQ \tag{25}$$

$$V_{ij}(\Lambda) \approx \delta_{ij}V(\Lambda_{ii}). \tag{26}$$

The approximation basically arises from the fact that an eigenvector of the coordinate matrix X should correspond to a function that is localized around the appropriate eigenvalue Λ_{ii}. The level of the approximation is further discussed in [22].

The DVR can also be regarded as a method that allows us to construct wavefunctions in a set of discrete points, i.e. on a grid. For each set of basis functions we obtain a corresponding grid, and an appropriate approximation of the kinetic energy operator $T(\Lambda)$. The grid can be shifted in the complex plane or even scaled or rotated, provided that a corresponding scaling or rotation is also performed with the kinetic energy operator. The choice of basis functions affects only the spacing between successive points. For example, with $\phi_k(x) \sim \sin kx$, the grid is nearly equidistant while with the Hermite polynomials we obtain a grid that is symmetrical and denser in the middle.

In our calculations, we used Hermite polynomials as basis functions (see e.g. [23] for a precise definition of this DVR). The grid consisted of up to 1001 points from the interval $x \in \langle -17.5, 17.5\rangle$ with $\epsilon \in \langle 0.5, 5\rangle$. The Hamiltonian matrix was diagonalized with the help of the QR routine for general complex matrices from the EISPACK package [24][4]. The results were verified to be stable with respect to the changes of the grid.

As a case study, let us first contemplate the exactly solvable equation (2) at $g = 0$. The sample of the exact energies is given in the first column of table 1. Their purely numerical DVR reproduction appears in the second column and we see that the method is fully reliable.

The last two columns of the table list the efficiency and practical values of our non-numerical estimate (11). We have to emphasize that even in the domain of not too large ℓ, the difference between the exact and approximate energies remains small, of the order of $\approx$0.5% for the ground state. The error term remains the same also for all the excited states but this should be understood as a mere peculiarity of our choice of the oversimplified illustrative example.

The genuine test of the present formulae (and of their merits as well as limitations of validity) only appears in table 2. The 'measure of smallness' $1/L$ lies there, roughly, in between 0.55 and 0.23. This choice makes the test quite stringent again. Its results are very encouraging. We witness, firstly, a quick improvement of the quality of the ground state, from $\sim$1% at $L \approx 2$ up to four-digit precision at $L \approx 4$. Secondly, the poor performance of our harmonic-oscillator approximation of excited states at $L \approx 2$ (giving an almost 100% error already for the second excited state) is in sharp contrast with the $L \approx 4$ results predicting a reasonably good two correct digits even for the 8th excited state.

In table 3 we extend the scope of our test beyond the weak-coupling regime with $|\alpha| \ll 2\ell$ and/or $\delta = 0$. The dependence of the energies on the non-vanishing values of the parameter $\alpha = 2\sqrt{\ell(\ell+1)}\delta \approx 20.98\,\delta$ is shown there to agree very well with our asymptotic prediction (18) even at the fairly small $L \approx 2.36$. We may note that the precision of our approximation appears to be almost α-independent in a broad range of α including also the domain of the negative values which were not discussed here in detail as safely protected against any possible spontaneous $\mathcal{PT}$ symmetry breaking [15].

6. Discussion

At the maximal $\delta \approx 1$, the estimate of the low-lying energies

$$E_m^{(\mathrm{DDT})} \approx \left(\tfrac{3}{2}\right)^{2/5}\left[-\tfrac{25}{6}L^3 + \tfrac{5}{2}\sqrt{L}(2m+1)\right] \qquad m = 0, 1, \ldots \quad \delta \approx 1 \tag{27}$$

[4] The Eigensystem Subroutines PACKage is available at the Internet address www.netlib.org/eispack. The subroutines represent public adaptations of the algorithms from [24].

Table 2. Energy levels of the generalized cubic model (4) with $\alpha = 0$ and increasing ℓ.

Parameters	Numerical solution	Large-ℓ approximation	Difference
$\ell = 5$	−11.521 91	−11.390	0.132
$L = 1.821$	−4.564 82	−4.000	0.565
	1.870 17	3.390	1.520
$\ell = 10$	−28.765 52	−28.686	0.079
$L = 2.361$	−20.598 67	−20.271	0.328
	−12.706 40	−11.855	0.851
	−5.116 63	−3.439	1.677
	2.140 32	4.976	2.836
$\ell = 20$	−68.726 46	−68.680	0.046
$L = 3.086$	−59.247 06	59.058	0.189
	−49.917 73	−49.435	0.482
	−40.745 89	−39.813	0.933
	−31.739 51	−30.191	1.549
	−22.907 12	−20.569	2.338
	−14.257 69	−10.947	3.311
	−5.800 54	−1.324	4.476
	2.454 91	8.298	5.843
$\ell = 50$	−211.135 55	−211.113	0.023
$L = 4.427$	−199.680 09	−199.589	0.091
	−188.294 59	−188.065	0.230
	−176.980 40	−176.541	0.440
	−165.738 89	−165.017	0.722
	−154.571 49	−153.493	1.079
	−143.479 67	−141.969	1.511
	−132.464 94	−130.444	2.020
	−121.528 86	−118.920	2.608

differs significantly from its weak-coupling counterpart (15). Moreover, in the light of the numerical experiments of [15] we may expect the end of the applicability of our straightforward harmonic-oscillator approximation. At the same time, the underlying shift of the minimum looks insignificant. We may conclude that the freedom in our choice of the shift ε may encounter its natural limitations near and beyond the value of $\delta = 1$.

The latter point may comparatively easily be discussed quantitatively. Returning to the rescaled form of our original Schrödinger equation (13) we may rewrite this complex differential equation in an equivalent form on real line,

$$\left\{-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + L^3\left[\frac{3}{2(x/L-\mathrm{i}\eta)^2} - \delta\sqrt{6\mathrm{i}(x/L-\mathrm{i}\eta)} + \mathrm{i}(x/L-\mathrm{i}\eta)^3\right]\right\}\phi(x) = E\phi(x).$$

Let us assume now that the shift $\eta = \varepsilon/L$ is not too small. This enables us to transform the effective potential in a series in the powers of L,

$$\left\{-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + L^3\left(-\frac{3}{2\eta^2} - \delta\eta^3 - \eta^3\right) + \mathrm{i}xL^2\left(\frac{3}{\eta^3} - \frac{\delta\eta^2}{2} - 3\eta^2\right) + x^2L\left(\frac{9}{2\eta^4} - \frac{\delta\eta}{8} + 3\eta\right) + R\right\}\phi(x) = E\phi(x). \tag{28}$$

The residual term can only generate $\mathcal{O}(1)$ corrections to the energies and may be omitted as irrelevant. As a consequence, we may once more shift the coordinate line, $x = z + \mathrm{i}\varrho$ and

Table 3. The lowest three energy levels of the generalized cubic model (4) with $\ell = 10$ and various α.

α	Numerical solution	Large-ℓ approximation	Difference
20	−58.621 90	−58.535	0.087
	−49.836 26	−49.533	0.303
	−41.290 14	−40.531	0.759
10	−43.852 23	−43.768	0.084
	−35.407 17	−35.083	0.324
	−27.230 03	−26.398	0.832
0	−28.765 52	−28.686	0.079
	−20.598 67	−20.271	0.328
	−12.706 40	−11.855	0.851
−10	−13.355 29	−13.282	0.073
	−5.407 17	−5.089	0.318
	2.276 17	3.104	0.828
−20	2.381 31	2.447	0.066
	10.164 62	10.463	0.298
	17.703 39	18.478	0.775

eliminate the redundant linear term in z via a suitable choice of ϱ. The new version of the potential reads

$$\frac{(36-\delta\eta^5+24\eta^5)L}{8\eta^4}z^2-\frac{(72+81\delta\eta^5+216\eta^5-3\delta^2\eta^{10}+34\delta\eta^{10}+12\eta^{10})L^3}{2\eta^2(36-\delta\eta^5+24\eta^5)}. \tag{29}$$

The derivation of the subsequent η-dependent energies will be skipped here as straightforward. Their role is less important in the present context but may be expected to grow in the perturbative context (of course, the explicit study of the higher-order perturbation corrections already lies beyond the scope of our present paper).

Formula (29) depends on a free parameter η and offers a more flexible harmonic-oscillator fit of the effective potential in equation (28). Its η-dependence may certainly prove useful in numerically oriented considerations, as it still gives the approximate energies up to a bounded $\mathcal{O}(R) = \mathcal{O}(1)$ error term. Non-numerically, formula (29) may be checked as reproducing *exactly* our previous equation (15) in the weak-coupling limit $\delta = 0$ with optimal $\eta = 1$.

A small decrease of $\eta = 1 - \lambda$ may be contemplated as a small perturbation. The deep, $\mathcal{O}(L^3)$ minimum of our η-dependent effective potential does not move in the first order at all. Only the shape becomes narrower pushing the $\mathcal{O}(\sqrt{L})$ component of the energies (16) upwards by the factor $1/\eta \approx 1 + \lambda$. This indicates a certain variational optimality of our previous leading-order results where the shift was in fact *not* arbitrary, $\eta = 1$.

7. Summary

In this paper, we paid attention to the complex and asymptotically cubic DDT oscillator (4). Within the so-called $\mathcal{PT}$ symmetric quantum mechanics, this oscillator represents one of the most characteristic examples of a non-Hermitian (or 'next to Hermitian') Hamiltonian with real spectrum. Although the model is not solvable in closed form, its appeal is enhanced by the presence of the variable coupling α and angular momentum ℓ.

We started from the observation that in the majority of the physical applications of the Schrödinger equation in D dimensions the relevant values of ℓ are usually small. In this context, the DDT model itself is exceptional. In the strongly spiked $\alpha \gg 1$ regime, it is formally consistent if and only if the angular momenta ℓ are very high. In this regime, the weak non-Hermiticity (supporting the real spectrum) *requires* the presence of a strong centrifugal repulsive core. We reinterpreted such a descriptive property of the model as its internal, formal feature. Its *mathematical* consistency is enhanced by the admissibility of the complex shifts and of a $\mathcal{PT}$ symmetric deformation of the axis of coordinates.

In this framework, our main purpose was to find a suitable technique which would give the approximate low-lying DDT spectrum non-numerically. This effort was inspired by the enormous success of the so-called $1/\ell$ expansions—techniques which proved extremely successful within the standard, Hermitian quantum mechanics. Our study revealed that the transition between the Hermitian and non-Hermitian models is entirely smooth. We discovered, in particular, that the angular momentum parameter $|\ell| \gg 1$ may serve as a guide to the introduction of the suitable harmonic-oscillator approximation of the low-lying (in our case, DDT) spectrum.

We may conclude that the feasibility of the harmonic-oscillator approximation (presumably, not only in our non-Hermitian model (4)) is encouraging. We may expect that in the future the more consequent and precise solution of the similar complex models will prove obtainable by perturbative techniques. The leading-order harmonic-oscillator construction will be followed by the systematically constructed series of corrections in a way which would parallel the $1/\ell$ expansions for the purely real potentials.

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