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Solvable simulation of a double-well problem in \mathcal{PT} -symmetric quantum mechanics

Miloslav Znojil

Department of Theoretical Physics, Institute of Nuclear Physics, Academy of Sciences,
250 68 Řež, Czech Republic

E-mail: znojil@ujf.cas.cz

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Abstract

Within the framework of \mathcal{PT} -symmetric quantum mechanics of bound states (which works with parity-pseudo-Hermitian Hamiltonians $H = \mathcal{P}H^\dagger\mathcal{P}$ and real spectra) we mimic some effects of the double-well structure of potentials by a pair of δ functions with mutually complex conjugate strengths. The model is solvable by the standard matching technique and exhibits several interesting features. We observe an amazingly robust absence of any \mathcal{PT} -symmetry breaking. A quasi-degeneracy which occurs in the high-energy domain is interpreted as a manifestation of certain ‘quantum beats’.

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1. Introduction

In current textbooks, many phenomena (e.g., vibrational spectra) and methods (e.g., perturbation expansions) of quantum mechanics are best illustrated by the one-dimensional Schrödinger equation for bound states in a real and symmetric well $V(x) = V^*(x) = V(-x)$,

$$\left[-\frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x). \quad (1)$$

In such a setting, the transition of the so-called \mathcal{PT} -symmetric quantum mechanics (say, in its form proposed by Bender and Boettcher [1]) may most easily be illustrated by an inclusion of an asymmetric and purely imaginary additional potential in the same equation,

$$V(x) = V_S(x) + iV_A(x) \quad V_S(x) = V_S^*(x) = V_S(-x) \quad V_A(x) = V_A^*(x) = -V_A(-x). \quad (2)$$

Exactly solvable examples abound [2, 3]. As their most elementary and transparent example we may recollect the harmonic oscillator in D dimensions [4] with

$$V(x) = \frac{\ell(\ell+1)}{(x-ic)^2} + B(x-ic)^2 \quad c > 0. \quad (3)$$

Here, the centrifugal barrier is regularized and proportional to $\ell = (D - 3)/2 + m$ in the m th partial wave.

The studies of models (2) also often involve much more complicated potentials, which are not exactly solvable. An encouragement is provided by their more immediate applicability as well as by the efficiency of many semiclassical [5], perturbative [6] and/or purely numerical techniques [7]. In the pioneering paper, Caliceti *et al* [8] paid attention to the very unusual imaginary cubic \mathcal{PT} -symmetric anharmonicity. Within sophisticated perturbation theory, she (together with her co-authors) succeeded in showing that in spite of the non-Hermiticity of the Hamiltonian, the spectrum of energies may remain real.

Buslaev and Grecchi [9] returned to the more standard, quartic \mathcal{PT} -symmetric anharmonic oscillator

$$V(x) = \frac{\ell(\ell + 1)}{(x - ic)^2} + B(x - ic)^2 + D(x - ic)^4 \quad c > 0 \quad (4)$$

with a similar motivation stemming from field theory [10]. They were the first who demonstrated that the bound-state energies of a non-Hermitian, \mathcal{PT} -symmetric model (4) may coincide with the spectrum of a certain *Hermitian* double-well problem. Their sophisticated and explicit, Fourier-type equivalence transformation between the Hermitian and non-Hermitian partners may be now better understood in the language of Mostafazadeh [11].

Let us note that the presence of the centrifugal term in equation (4) played an important technical role in [9], while a similar term has been absent in all the original studies of the imaginary cubic forces [5, 8]. Curiously enough, only a reintroduction of this term in the generalized model

$$V(x) = \frac{\ell(\ell + 1)}{(x - ic)^2} + B(x - ic)^2 + iC(x - ic)^3 \quad c > 0 \quad (5)$$

seems to have opened the way towards the rigorous proof of the reality of the spectrum of the imaginary cubic oscillators [12]. In the light of this proof, the special regular case of equation (5) with vanishing $\ell(\ell + 1) = 0$ is not exceptional at all. *In contrast*, the inclusion of a strong repulsion $\ell(\ell + 1) \gg 1$ in equation (5) seems instructive and productive in having paved the way towards the recent clarification of the applicability of the current $1/\ell$ technique in the \mathcal{PT} -symmetric context in [13]. Thus, we shall assume that ℓ is large in all the potentials of type (3), (4) or (5). At this point, we get quite close to the subject of our present paper since the implementation of the $1/\ell$ technique proved *entirely different* in the Hermitian and \mathcal{PT} -symmetric models, and we intend to re-analyse the latter case via certain simplified models.

2. Double wells

All three \mathcal{PT} -symmetric potentials (3)–(5) offer a very good testing ground for the comparison of the Hermitian and \mathcal{PT} -symmetric calculations. Firstly, they may serve as an elementary illustration of the $1/\ell$ technique in the Hermitian case because their Hermitian versions emerge simply in the limit $c \rightarrow 0$. Secondly, one immediately notes that such a step is not *mathematically* trivial since their centrifugal barriers become strongly singular. Fortunately, this does not play any role at all because simultaneously, we have to ‘shrink’ the full real axis of the coordinates to the mere positive ‘radial’ half-axis [4]. A fully rigorous discussion of this point is available in [9] and enables us to reinterpret our differential Schrödinger equation (1) with the *real and constrained* coordinates $x = x_{\text{Hermitian}} = x_{(c=0)} > 0$ as the standard central bound-state problem on the half-axis. In such a context, the perturbative $1/\ell$

recipe (as reviewed, e.g., in paper [14] and/or in many other references which are quoted therein) is virtually trivial. One simply imagines that the potential $V(x)$ possesses an absolute minimum at some real and positive coordinate $R > 0$ (for example, in equation (3) we get the *unique* minimum at $R = [\ell(\ell + 1)/B]^{1/4}$, etc). In the vicinity of this minimum, the shape of the potential $V(x)$ may be approximated by an appropriate harmonic oscillator well, $V(R + \xi) \approx \text{const} + \omega^2 \xi^2 + \mathcal{O}(1/R)$. At this point one discovers that the quality of the latter ‘zero-order’ approximation *increases quickly* with the growth of ℓ . Moreover, the expansion of the binding energies and wavefunctions in the powers of $1/R$ remains feasible and exhibits very good convergence properties in practice [14].

After a return to the non-Hermitian equation (1) with $x \in (-\infty, \infty)$, an application of the same idea requires a much more careful analysis. As long as all our sample potentials $V(x)$ remain smooth, analytic and confining for *all* the shift parameters $c \neq 0$, our wavefunctions $\psi(x)$ stay analytic and *normalizable* all over the lower half-plane of the complex plane of x [1]. At the same time, the manifest non-Hermiticity of our sample Hamiltonians at $c > 0$ leads to the necessity of a reinterpretation of their eigenstates. In the spirit of our remarks [15, 16] (cf also the later reviews [11, 17]), one must replace the concepts of Hermiticity by pseudo-Hermiticity while the unitarity becomes weakened to pseudo-unitarity. As a consequence, the probabilistic interpretation of \mathcal{PT} -symmetric quantum mechanics acquires the forms which find their immediate guidance in the relativistic quantum mechanics, with one of the most popular examples provided by the Feshbach–Villars pseudo-Hermitian reformulation of the Klein–Gordon equation [18].

The net consequence of all these introductory remarks is that within the framework of our above exemplification of the \mathcal{PT} -symmetric quantum mechanics we are *free* to work with *any complex* coordinate R of the minimum of $V(x)$. As long as we assume that $\ell(\ell + 1) \gg 1$ is large, we discover that there exist *many* minima R generating, in principle, *many* alternative large- ℓ expansions. For example, equation (3) with $c > 0$ gives the minimum of $V(x)$ whenever $x^4 = R^4 = \ell(\ell + 1)/B$. Even in this trivial example (where we know all the final solutions in advance!), we have no clear criterion for the choice not only between the above-mentioned real $R = R_{(+)} = \varrho$ (with the large $\varrho = |[\ell(\ell + 1)/B]^{1/4}| \gg 1$) and its negative partner $R_{(-)} = -\varrho$, but also between the two new purely complex extremes at $R = R_{(\text{lower})} = -i\theta$ and $R = R_{(\text{upper})} = R_{(\text{lower})}^* = +i\theta$ (with the same real parameter $\theta = \varrho \gg 1$). Moreover, the transition to the potentials (4) and (5) (both with $B = 0$ for simplicity) gives the respective rules $R^6 = \ell(\ell + 1)/(2D)$ and $iR^5 = 2\ell(\ell + 1)/(3C)$ so that, generically, one has to deal with several pairs of the *complex* minima such that

$$V(R + \xi) \approx \Omega^2 \xi^2 \quad R = R_{(\pm)} = \pm\varrho - i\theta \quad \Omega^2 = \Omega_{(\pm)}^2 = \omega^2 \pm i\eta \quad (6)$$

where we only know that $|R| \gg 1$. In such a setting, we may choose the shift of the axis in such a way that $c \equiv \theta$, *without* causing any change in the spectrum of course.

A fully exhaustive discussion of the particular cubic example (5) may be found in [13]. For the simpler quartic oscillator (4), the same large- ℓ construction would lead to vanishing and non-vanishing θ at the positive and negative couplings $D > 0$ (occurring, e.g., in [19]) and $D < 0$ (chosen, e.g., in [9, 20]), respectively. Thus, in contrast to the Hermitian case where the real position of the absolute minimum of $V(x)$ is unique in the majority of cases of practical interest, the regularization mediated by the shifts $c \neq 0$ leads, in accordance with the pattern (6), to the most frequent occurrence of two symmetric minima in $V(x)$ at once. Now we may conclude our introductory considerations by a declaration that *any* \mathcal{PT} -symmetric double well (6) with the *complex* (and complex conjugate) strengths $\Omega_{(\pm)}^2$ has not been found solvable in our preceding paper [13], and that this offered the main motivation for our forthcoming considerations, therefore.

3. The model

We shall try to simulate the effects of the general double attraction in the following schematic square-well-like model:

$$V(x) = (-\omega^2 - i\eta)\delta(x+a) + (-\omega^2 + i\eta)\delta(x-a) \quad x \in (-1, 1) \quad (7)$$

where, in the spirit of [3], the forces are reduced to the mere \mathcal{PT} -symmetric pair of the delta functions at a distance measured by the variable $a \in (0, 1)$. This means that we plan to solve equation (1) with the boundary conditions

$$\psi(\pm 1) = 0 \quad \frac{d}{dx}\psi(\pm a + 0) - \frac{d}{dx}\psi(\pm a - 0) = (-\omega^2 \pm i\eta)\psi(\pm a) \quad (8)$$

by the standard matching technique as described in textbooks [21]. Under the usual \mathcal{PT} -symmetric normalization convention [16]

$$\psi(x) = \psi_S(x) + i\psi_A(x) \quad \psi_S(x) = \psi_S^*(x) = \psi_S(-x) \quad \psi_A(x) = \psi_A^*(x) = -\psi_A(-x) \quad (9)$$

this enables us to denote $E = \kappa^2$ in the obvious ansatz for the wavefunctions on the three sub-intervals of the whole domain in question,

$$\psi(x) = \begin{cases} \psi_L(x) = (\alpha - i\beta) \sin \kappa(x+1) & x \in (-1, -a) \\ \psi_C(x) = \gamma \cos \kappa x + i\delta \sin \kappa x & x \in (-a, a) \\ \psi_R(x) = (\alpha + i\beta) \sin \kappa(-x+1) & x \in (a, 1) \end{cases} \quad (10)$$

Moreover, as long as we have

$$\psi'(x) = \begin{cases} \psi'_L(x) = \kappa(\alpha - i\beta) \cos \kappa(x+1) & x \in (-1, -a) \\ \psi'_C(x) = -\kappa\gamma \sin \kappa x + i\kappa\delta \cos \kappa x & x \in (-a, a) \\ \psi'_R(x) = -\kappa(\alpha + i\beta) \cos \kappa(-x+1) & x \in (a, 1) \end{cases} \quad (11)$$

the appropriate insertions in equation (8) lead to the four-by-four matrix set of equations

$$\begin{pmatrix} \sin \kappa(1-a) & 0 & -\cos \kappa a & 0 \\ 0 & \sin \kappa(1-a) & 0 & -\sin \kappa a \\ -\mu(\omega) & \nu(\eta) & \sin \kappa a & 0 \\ \nu(\eta) & \mu(\omega) & 0 & \cos \kappa a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = 0. \quad (12)$$

Here, $\mu(\omega) = \cos \kappa(1-a) - \omega^2 \kappa^{-1} \sin \kappa(1-a)$ and $\nu(\eta) = \eta \kappa^{-1} \sin \kappa(1-a)$ are mere abbreviations.

We may conclude that the matching conditions may be satisfied if and only if the secular determinant $F(\kappa)$ vanishes in equation (12). This condition has the following form:

$$F(\kappa) = (2\kappa) + \frac{\omega^2}{\kappa} [\cos(2\kappa) - \cos(2\kappa a)] + \frac{\omega^4 + \eta^2}{\kappa^2} \sin(2\kappa a) \sin^2[2\kappa(1-a)] = 0. \quad (13)$$

Its main merit is its compact form, not quite expected in the light of the previous complicated matching formula (12). By its structure it resembles the textbook solution of the simple square well so that, in this sense, it is a mere implicit representation of the spectrum itself. In fact, one might even believe that an explicit construction of this spectrum might be possible (say, in the form of an infinite power series in some of the parameters) but due to the utterly elementary character of equation (13), one might still deduce the majority of the relevant features of the spectrum from this implicit definition. In order to demonstrate this expectation in detail, the

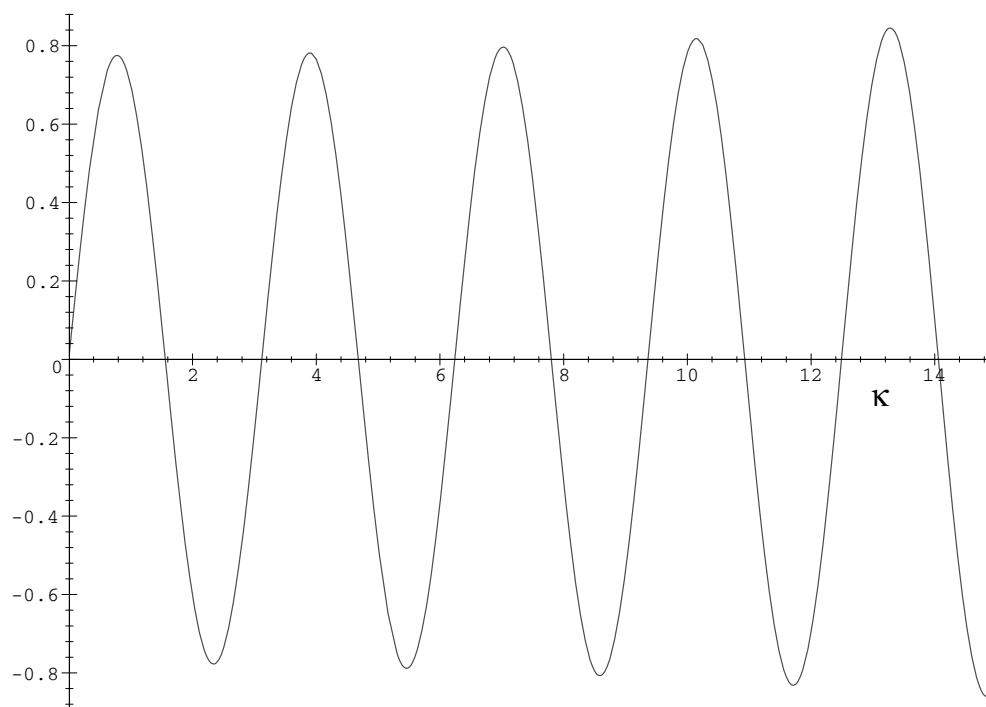


Figure 1. The sinus-like left-hand side curve $F(\kappa)$ of equation (13) in the weakly perturbed square-well regime, i.e., at a ‘large’ distance $a = 0.95$ of the ‘shallow’ wells with a weak strength $\omega = 1.5$ and with a (virtually irrelevant) asymmetry measure $\eta = 20$.

roots of equation (13) will be studied here via the graphs of the function $F(\kappa)$. In this sense, we shall determine and display the various qualitative features of the spectrum of the energies $E_n = \kappa_n^2$ in a series of pictures, via their presentation in the form of the sequences of the nodal zeros κ_n of the function $F(\kappa)$.

4. Discussion

The results of our study are sampled in figures 1–7 for the different sets of couplings. In all these cases we observed, first of all, that the influence of the changes of η is not too relevant so that we have fixed, in all our pictures, $\eta = 20$ for the sake of definiteness.

In figure 1 we simulated the system of two weakly attractive wells which lie far from each other. We see that the choice of $a = 0.95$ and $\omega = 3/2$ still leads to the mere very weak perturbation of the very well-known spectrum of the $\omega = 0$ energies in a square well. The function $F(\kappa)$ oscillates very regularly and its overall amplitude, although not quite constant, exhibits just a small slow variation and remains almost independent of our choice of the interval of κ (the figure takes $\kappa = \sqrt{E} \in (0, 15)$).

In figure 2 we see that for the same distance of the wells, the growth of their attractive strength up to $\omega = 15\,000$ leads to significant growth of the average magnitude of the amplitude of $F(\kappa)$ and to the emergence of an ‘envelope’ (i.e., an auxiliary curve $F_{av}(\kappa)$ which connects the maxima or minima) with much slower oscillations. In addition we discover an overall asymptotic decrease of $F_{av}(\kappa)$ and certain less apparent periodic structure when we try to connect some of the ‘subdominant’ local maxima/minima of $F(\kappa)$.

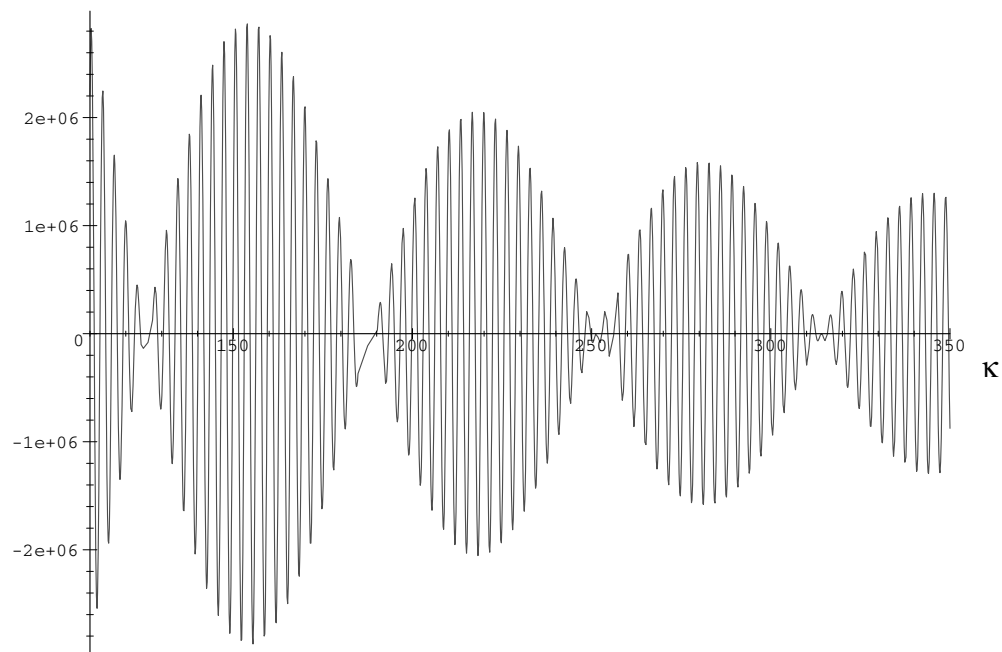


Figure 2. Graphical determination of the high-lying energies $E = \kappa^2$ (at nodes of $F(\kappa)$) for a very strong attraction at $\omega = 15 \times 10^3$ (the other parameters are the same as in figure 1).

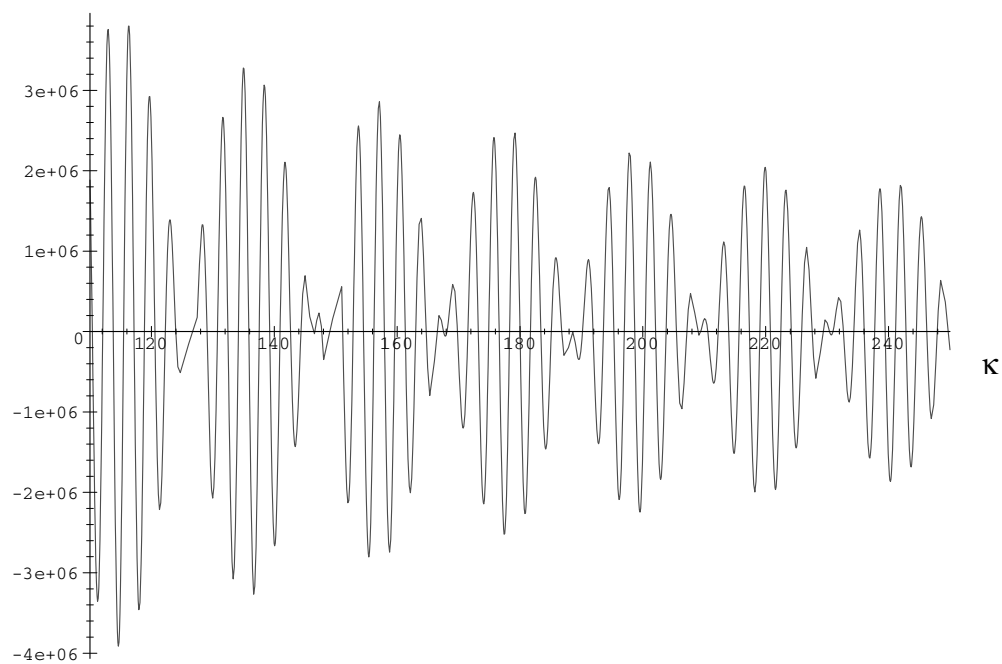


Figure 3. A shortening of the 'beats' of figure 2 after the shortening of the distance between wells to $a = 0.85$.

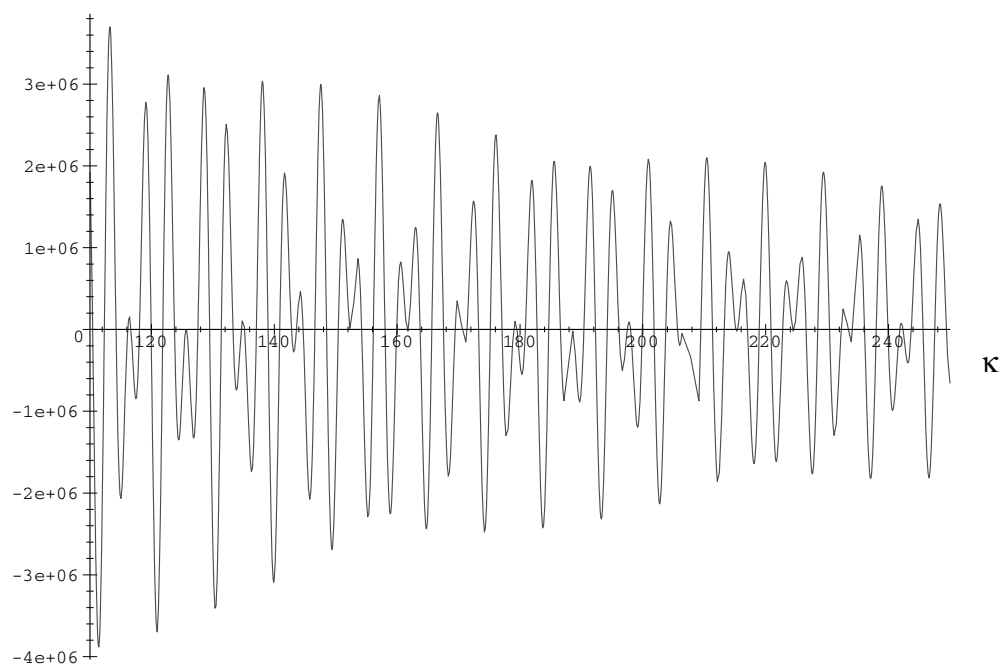


Figure 4. The emergence of overlaps between multiple 'beats' at a still shorter distance $a = 0.65$.

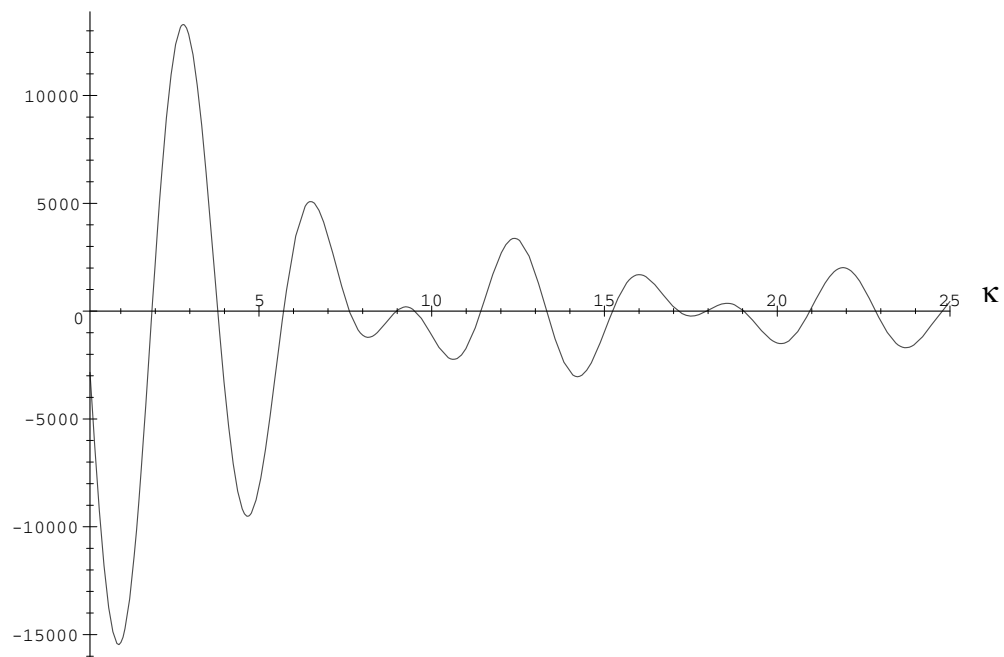


Figure 5. A return to the lowest energy levels in figure 4 and to the weaker attraction with $\omega = 150$.

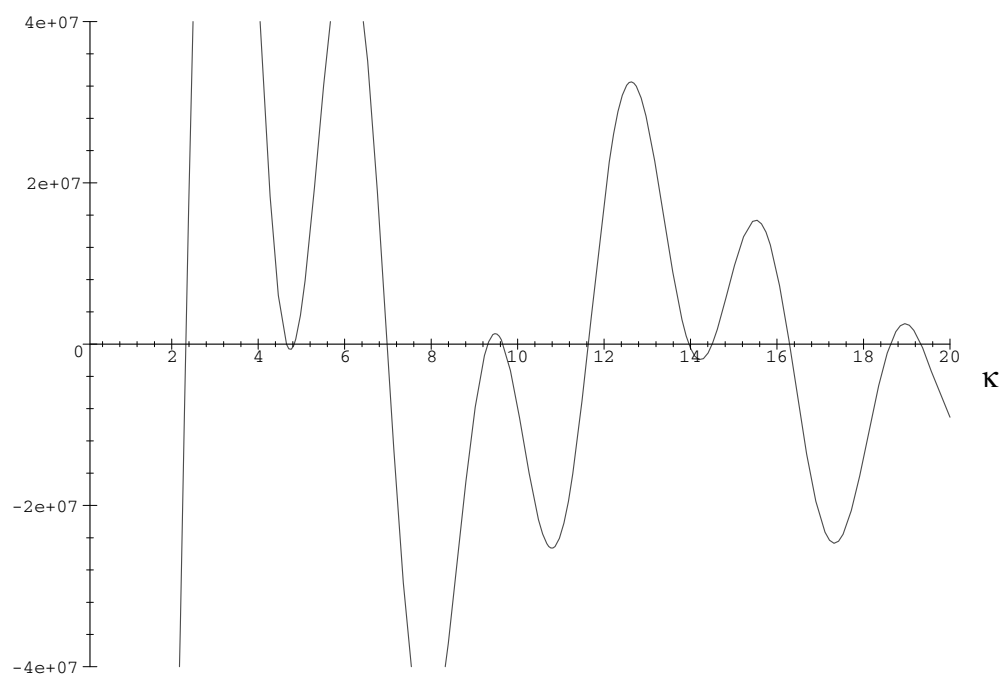


Figure 6. The quasi-degeneracy of levels for the 'deep' wells with $\omega = 15 \times 10^3$ at a comparatively small distance $a = 0.35$.

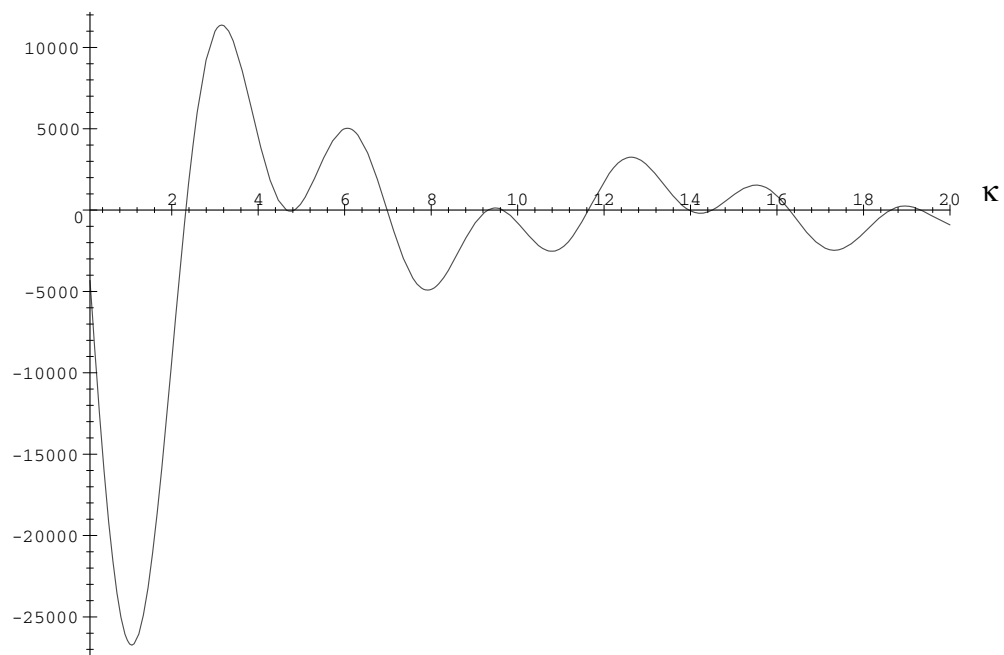


Figure 7. Same as figure 6, with a 'wobbling-type' irregularity in the energy nodes for 'shallow' wells with $\omega = 150$.

Figures 3 and 4 show the effect of the movement of the two wells towards each other. Even a not too significant shortening of their distance (to $a = 0.85$ and $a = 0.65$, respectively) shows that the period of the envelopes becomes shorter and, in the latter case, one can see a clear competition between several parallel envelopes which start to overlap each other.

In order to reveal the latter pattern clearly, we omitted the low-lying levels. This enabled us to see that the interplay between different periods remains fairly regular. Step by step, it introduces a much more complicated pattern to the energy spectrum, anyhow. The separate levels behave in a more and more chaotic manner, especially when we return to the low-lying part of the spectrum in a way illustrated in figure 5 where we kept $a = 0.65$ and weakened $\omega = 150$.

The remarkable feature of all this pattern is that our numerical experiments never revealed a merger of the two levels followed, presumably, by their disappearance in the complex plane. In the other models, such a phenomenon may exist and is usually interpreted as the so-called spontaneous \mathcal{PT} -symmetry breaking [22]. Here, figure 6 with the fairly small distance $a = 0.35$ (and with the original very strong $\omega = 15 \times 10^3$) illustrates the situation where one gets very close to such a possibility and where several pairs of the real energies appear to be almost degenerate.

In figure 7 where $\omega = 150$, we finally demonstrate that the ‘chaotic’ character of the eigenvalues in our schematic and exactly solvable \mathcal{PT} -symmetric point-interaction double wells may be weakened and partially removed by a return to their weaker strengths. We see in the picture that the characteristic pairwise ‘irregular’ quasi-degeneracies persist. This type of irregularity has a slightly different source in an ultimate slowdown of the oscillations of the envelopes, the ‘wobbles’ of which become comparable to the nodal distances.

We may summarize that the double-well-like structure of our complex, non-Hermitian example complies with some of our intuitive expectations. Thus, the ‘robust’ reality of the spectrum or an emergence of the quasi-degeneracy has been reconfirmed. At the same time, a few other observations (say, of the multiple and/or superimposed ‘beats’ in the curve $F(\kappa)$) wait for a deeper understanding and/or a generic explanation in the future.

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References

- [1] Bender C M and Boettcher S 1998 *Phys. Rev. Lett.* **24** 5243
- [2] Cannata F, Junker G and Trost J 1998 *Phys. Lett. A* **246** 219
- Znojil M 1999 *Phys. Lett. A* **264** 108
- Andrianov A A, Cannata F, Dedonder J P and Ioffe M V 1999 *Int. J. Mod. Phys. A* **14** 2675
- Bagchi B and Roychoudhury R 2000 *J. Phys. A: Math. Gen.* **33** L1
- Znojil M 2000 *J. Phys. A: Math. Gen.* **33** L61, 4561
- Bagchi B, Cannata F and Quesne C 2000 *Phys. Lett. A* **269** 79
- Lévai G and Znojil M 2000 *J. Phys. A: Math. Gen.* **33** 7165
- Ahmed Z 2001 *Phys. Lett. A* **286** 231
- Znojil M and Tater M 2001 *J. Phys. A: Math. Gen.* **34** 1793
- Tkachuk V M and Fityo T V 2001 *J. Phys. A: Math. Gen.* **34** 8673
- Klischovich S M and Plyushchay M S 2001 *Nucl. Phys. B* **616** 403
- Bagchi B, Mallik S and Quesne C 2002 *Int. J. Mod. Phys. A* **17** 51
- Lévai G, Cannata F and Ventura A 2002 *J. Phys. A: Math. Gen.* **35** 5041
- Bagchi B and Quesne C 2002 *Phys. Lett. A* **300** 18
- Sinha A and Roychoudhury R 2002 *Phys. Lett. A* **301** 163
- Jia C-S, Sun Y and Li Y 2002 *Phys. Lett. A* **305** 231

- [3] Znojil M 2001 *Phys. Lett. A* **285** 7
Albeverio S, Fei S M and Kurasov P 2002 *Lett. Math. Phys.* **59** 227
Nagasawa T, Sakamoto M and Takenaga K 2002 SUSY in QM with point interactions *Preprint* hep-th/0212192
- [4] Znojil M 1999 *Phys. Lett. A* **259** 220
- [5] Alvarez G 1995 *J. Phys. A: Math. Gen.* **27** 4589
Delabaere E and Pham F 1998 *Phys. Lett. A* **250** 25, 29
Bender C M, Boettcher S and Meisinger P N 1999 *J. Math. Phys.* **40** 2201
Delabaere E and Trinh D T 2000 *J. Phys. A: Math. Gen.* **33** 8771
Shin K C 2001 *J. Math. Phys.* **42** 2513
Nanayakkara A and Abayaratne C 2002 *Phys. Lett. A* **303** 243
- [6] Fernandez F, Guardiola R, Ros J and Znojil M 1999 *J. Phys. A: Math. Gen.* **32** 3105
Bender C M and Dunne G V 1999 *J. Math. Phys.* **40** 4616
- [7] Handy C R, Khan D, Wang Xiao-Xian and Tomczak C J 2001 *J. Phys. A: Math. Gen.* **34** 5593
Bernard C and Savage V M 2001 *Phys. Rev. D* **64** 085010
Bender C M and Weniger E J 2001 *J. Math. Phys.* **42** 2167
- [8] Caliceti E, Graffi S and Maioli M 1980 *Commun. Math. Phys.* **75** 51
- [9] Buslaev V and Grecchi V 1993 *J. Phys. A: Math. Gen.* **26** 5541
- [10] Seznec R and Zinn-Justin J 1979 *J. Math. Phys.* **20** 1398
Avron J and Seiler R 1981 *Phys. Rev. D* **23** 1316
- [11] Mostafazadeh A 2002 *J. Math. Phys.* **43** 205, 2814, 3944
- [12] Dorey P, Dunning C and Tateo R 2001 *J. Phys. A: Math. Gen.* **34** 5679, L391
- [13] Znojil M, Gemperle F and Mustafa O 2002 *J. Phys. A: Math. Gen.* **35** 5781
- [14] Bjerrum-Bohr N E J 2000 *J. Math. Phys.* **41** 2515
- [15] Znojil M 2001 Conservation of pseudo-norm in PT symmetric quantum mechanics *Preprint* math-ph/0104012
(*Suppl. ai Rendiconti del Circ. Matem. di Palermo* at press)
- [16] Bagchi B, Quesne C and Znojil M 2001 *Mod. Phys. Lett.* **16** 2047
- [17] Ramírez A and Mielnik B 2002 *Preprint* quant-ph/0211048 (*Rev. Fis. Mex.* at press)
- [18] Feshbach H and Villars F 1958 *Rev. Mod. Phys.* **30** 24
- [19] Znojil M 1999 *J. Phys. A: Math. Gen.* **32** 7419
Bender C M, Berry M, Meisinger P N, Savage V M and Simsek M 2001 *J. Phys. A: Math. Gen.* **34** L31
- [20] Bender C M and Boettcher S 1998 *J. Phys. A: Math. Gen.* **31** L273
Znojil M 2000 *J. Phys. A: Math. Gen.* **33** 4203
- [21] Fluegge S 1971 *Practical Quantum Mechanics I* (Berlin: Springer) p 39
- [22] Khare A and Mandal B P 2000 *Phys. Lett. A* **272** 53
Lévai G and Znojil M 2001 *Mod. Phys. Lett. A* **16** 1973
Ahmed Z 2001 *Phys. Lett. A* **282** 343
Znojil M and Lévai G 2001 *Mod. Phys. Lett. A* **16** 2273