

Comment on “Comparison of quantal and classical behavior of PT-symmetric systems at avoided crossings”

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Abstract

After a thorough numerical analysis of the quantized Barbanis' system (= two harmonic oscillators coupled by $V_{int} = \sqrt{g} x y^2$), A. Nananyakkara [Phys. Lett. A 334 (2005) 144] conjectured that there exist no true level crossings (= degeneracies), for the first 150 energy levels at least. Here we report an opposite observation. A systematic improvement of the precision of the calculations forces us to conclude that in the system in question one finds no avoided crossings at all. Our twin explanation of the discrepancy is based on the false convergence of the variational method and on an unexpected (and unaccounted) degeneracy of the unperturbed energies in *loc. cit.*

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1 Introduction

The coupling-dependence of the energies is one of the most interesting and important characteristics of any quantized system. In a numerical experiment paying attention to the complex version of the so called Barbanis' potential

$$V^{(B)}(x) = \frac{1}{2}(\omega_x^2 x^2 + \omega_y^2 y^2) + \sqrt{g} x y^2, \quad (1)$$

Asiri Nanayakkara [1] conjectured recently that at certain sufficiently high excitations $n \geq n_0$, the sudden emergence of the irregularities characterized by the very large second differences $\Delta_n = E_n(f + \delta) - 2E_n(f) + E_n(f - \delta)$ (cf. Fig. 3, *loc. cit.*) might be interpreted as a clear manifestation of an onset of a quantum analogue of the classical chaos even in the manifestly non-Hermitian regime with the negative g .

He attributed all these anomalously large differences Δ_n to the occurrence of the avoided level crossings and concluded that there appears to be a more or less complete analogy between the Hermitian and non-Hermitian systems. He supported such a conjecture by the (harmonic-oscillator) large-basis variational calculations (cf. Fig. 4, *loc. cit.*).

In an independent numerical test he tried to re-confirm his observations by the (non-degenerate) high-order perturbation calculations (cf. Fig. 5, *loc. cit.*). Unfortunately, this test only proved successful for the low-lying part of the spectrum. Thus, he finally formulated his conclusion that certain predictions of his perturbation calculation “need not be the same” (as the exact results) “when applying non-degenerate perturbation theory to irregular states”.

A slightly puzzling form of the later conclusion inspired us to return to the model (1) and to re-analyze a few separate technicalities supporting the ambitious conjectures of ref. [1].

The presentation of our results starts in Sec. 2 where only the purely imaginary interaction potential in eq. (1) is considered. We re-analyze there the Nanayakkara's assertion that “no level crossings were observed for first 150 eigenstates”. Our numerical results lead us to an opposite conjecture, *viz.*, that all the energy levels do degenerate and cross exactly.

The most straightforward and immediate foundation of our alternative conjecture lies in our more consequent and systematic control of the numerical errors. It reveals that the size of the apparent observation of the avoided

Figure 1: Energy crossings for the perturbed circular (left) and elliptic (right) models (1).

level crossing depends and changes in fact with the rounding errors (cf. Sec. 2 for more details).

In Sec. 3 we turn attention to the positive parameters $g > 0$ which lead to the non-separable interaction term $V_{int} = \sqrt{g} x y^2$ with the real strength \sqrt{g} . Rigorously we prove that the quantum Hamiltonians associated with the real version of the potential (1) are ill defined. From the physical point of view this is an important observation, invalidating all the $g > 0$ results of ref. [1].

In the last part of our comment we return to the Nanayakkara’s perturbative analysis of the model (1) where, at a “random” choice of the asymmetric, elliptic unperturbed well with $\omega_x = 0.7$ and $\omega_y = 1.3$ he assumed a non-degeneracy of the unperturbed spectrum. This particular point in fact attracted us to the problem since the very explicit Fig. 5b of *loc. cit.* clearly shows that the unperturbed levels in question *appear* to be “almost degenerate”.

In Sec. 4 our hypothesis of their full degeneracy will be confirmed. Our exhaustive analysis of the degeneracy problem remains straightforward and implies that the Nanayakkara’s non-degenerate Rayleigh-Schrödinger perturbation expansions happen to be, quite unfortunately, entirely inapplicable in his particular numerical illustration. As a consequence, also all the related puzzling discrepancies between his perturbative and variational results (as discussed in the summary of his work) become clarified in an elementary manner.

2 Unavoided level crossings at $g < 0$

Fig. 1 shows two examples of our numerical results for both circular ($\omega_x = \omega_y = 1$) and elliptic ($\omega_x = 0.7, \omega_y = 1.3$) cases. We employed the collocation spectral method [3], [4]. We checked the stability of our results and proceeded with very fine step in g . Comparing our Fig. 1 and the results presented on Fig. 4b and Fig. 5b in [1] we find the main difference in the way of the levels cross. Within the best precision we are able to control, the energy lines

Figure 2: Contour plots of real and imaginary parts of the 72nd and 73rd wave functions of (1) for $\omega_x = 0.7, \omega_y = 1.3$, and $g = -0.002$.

intersect in all instances we investigated. This is, however, at variance with the conclusions of [1].

In order to support our conclusions we visualized the corresponding wave functions. Fig. 2 may help to understand the situation. It is related to the Fig. 1b (*i.e.* $\omega_x = 0.7, \omega_y = 1.3$). The levels that cross there still preserve the patterns determined by the wave functions of the unperturbed elliptic oscillator. We discuss levels Nr. 72 and 73, whose numbers are $(0, 8)$ and $(15, 0)$, respectively. Both of them show a substantially one-dimensional dominance. As the g approaches the critical value $g_c = -0.0025297676$ the shape of the wave functions changes smoothly keeping the character of pattern unchanged (*e.g.* the nodal curves are slightly deformed but no new structure appears). Passing through g_c brings no substantial change, however, the order of these two levels is *swapped*. It strongly supports our conjecture based on numerical “evidence” that the crossings are genuine, *i.e.* that the levels are degenerated.

A more detailed study of the crossings is left to a separate paper.

3 The physical inconsistency of quantization at $g > 0$

Let us turn attention to the quantum Barbanis model with the apparently “physical” real couplings $h = \sqrt{g}$. The differential map

$$f \longrightarrow Tf = -\frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}\right) + \frac{1}{2}(\omega_x^2 x^2 + \omega_y^2 y^2)f + h x y^2 f \quad (2)$$

acting on Schwartz space $\mathcal{S}(\mathbb{R}^2)$ defines a self-adjoint operator which maps \mathcal{S} into \mathcal{S} [2]. For positive $h > 0$ it is an unbounded operator with spectrum not bounded below. In order to see this we chose a test function from \mathcal{S} ,

$$\psi_0(x, y) := \sqrt{\frac{2}{\pi}} e^{-x^2 - y^2}$$

and complement it by the family of the shifted test functions

$$\psi_n(x, y) := \psi_0(x - n, y - n),$$

where $n \in \mathbb{Z}$. Clearly $\|\psi_n\| = \|\psi_0\| = 1$.

Now, let us suppose that the norm of the operator (2), *i.e.*, the value $T := \sup(\|Tf\|; \|f\| = 1)$ is finite. It is straightforward to find $\|T\psi_n\|$ by direct evaluation. The result is a square root of a polynomial of the sixth degree

$$\|T\psi_n\| = \sqrt{P_6(n)}, \dots, P_6(n) = h^2 n^6 + h(\omega_x^2 + \omega_y^2)n^5 + \dots$$

As long as we can always chose $n > 0$ sufficiently large to make $\|T\psi_n\| > T$, the operator (2) cannot be bounded.

In order to assess the spectrum from below we evaluate $(\psi_n, T\psi_n)$ choosing $n < 0$. We arrive at another polynomial

$$(\psi_n, T\psi_n) = Q_3(n) = hn^3 + \frac{1}{2}(\omega_x^2 + \omega_y^2)n^2 + \dots$$

We see that the spectrum cannot be bounded below, because the leading term is negative so that we can always get a value lower than any bound.

A few remarks may be added. Firstly, at any not too large real and, say, positive value of the Barbanis' parameter h in eq. (1) the shape of the potential $V(x, y)$ is easily visualized as a mere deformation of the circular (at $\omega_x = \omega_y$) or elliptic (at $\omega_x \neq \omega_y$) unperturbed (*i.e.*, $h = 0$) harmonic-oscillator well in the $x - y$ plane. For the generic $h > 0$, this deformation remains inessential at all the sufficiently negative coordinates $x < 0$. In contrast, in the half-plane of $x > 0$ the confining character of the $h = 0$ well proves discontinuously changed at an arbitrarily small non-zero $h > 0$. Indeed, once we introduce a real scaling parameter $\varrho = 1/h^{1/5}$ and re-scale the coordinates in the real Barbanis Hamiltonian $H^{(RB)}$ we get

$$H^{(RB)} = \frac{1}{\varrho^2} \hat{H}, \quad \hat{H} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \hat{\omega}_x^2 x^2 + \hat{\omega}_y^2 y^2 - xy^2 \quad (3)$$

where $\hat{\omega}_x = \omega_x \varrho^2$ and $\hat{\omega}_y = \omega_y \varrho^2$. We may see that in the re-scaled model the potential remains safely confining, in the y -direction, at any negative $z = x - \omega_y^2 < 0$. On the boundary of this half-plane our potential remains constant along the $z = 0$ line. Finally, at all the positive $z = x - \omega_y^2 > 0$

it acquires, in the y -direction, a clearly deconfining shape of downwards-oriented parabolas.

All our observations invalidate the applicability of both the standard perturbation recipes and/or of the variational techniques using functions centered around the origin. In the light of this argument, all the related numerical results of ref. [1] (cf., e.g., both the right halves of the graphs in Fig. 5, *loc. cit.*) are just artifacts. One should note that their apparent convergence is no paradox as it remains fully understood as compatible with both the divergent asymptotic-series character of the perturbation series as well as with the false convergence of the corresponding alternative variational energy estimates.

One should add that a suitable, phenomenologically motivated “regularization” of our Hamiltonian, say, by a spatial cut-off seems necessary. Unfortunately, a possible mathematical foundation as well as physical meaning of such a regularization remain unclear. All its tentative choices look equally artificial and leave the spectrum *very strongly* dependent on the form of the cut-off.

4 Perturbation theory for Barbanis’ Hamiltonians

In the domain of small couplings $g \approx 0$ the first few orders of perturbation theory are often credited as offering a comparably reliable guide to the coupling-dependence of the low-lying approximate eigenvalues. In this context the author of ref. [1] chooses an apparently standard procedure. In detail,

(a) he assumes that the spectrum of the model (1) with a “random” choice of $\omega_x = 7/10$ and $\omega_y = 13/10$ is non-degenerate for the quadruplet of the “randomly” chosen sample of levels Nr. 71, 72, 73 and 74;

(b) he constructs the non-degenerate Rayleigh-Schrödinger perturbation series and picks up its 15th-order truncation as a “sufficiently high order” candidate for for his empirical “sufficiently exact” and plausible closed energy formula;

(c) he employs, in parallel, a variational basis of as many as 2500 lowest harmonic-oscillator states. Such a basis gives the energies which, numerically, appear to converge up to four or five decimal places and seem to confirm the

perturbation results in the regime of the very small couplings.

Unfortunately, in spite of all the appearances, all these precautions proved insufficient. Indeed, in the “unperturbed” limit of the vanishing couplings, the quadruplet of the energy levels studied in ref. [1] happens to be composed of the two doubly degenerate doublets.

Our latter statement explains a number of “puzzles” encountered in [1]. It is also very easy to prove. Indeed, in the unperturbed $g = 0$ harmonic-oscillator system of ref. [1] with $\omega_x/\omega_y = 7/13$ and with the energies

$$E_{n,N} \sim 7n + 13N, \quad n, N = 0, 1, \dots \quad (4)$$

we may order the energy levels in accord with Table 1. No degeneracy is encountered within its limits so that the items $E_{0,N} = 13N$ represent the K -th energy levels with $K = N(N + 1)$, followed by the next N values of $E_{2j,N-j} = 13N + j$ and $j = 1, 2, \dots, N$. Then one has to jump to the L -th energy level $E_{1,N} = 13N + 7$ [with $L = (N + 1)^2$] followed by the N -plet $E_{2j+1,N-j} = 13N + 7 + j$ and $j = 1, 2, \dots, N$.

Obviously, the degeneracies occur whenever $7n + 13N = 7n' + 13N'$, *i.e.*, whenever $n - n' = 13k$ while $N' - N = 7k$ at some $k = 1, 2, \dots$. Thus, the first ones with $k = 1$ appear at $n' = 0$, $n = 13$, $N = 0$ and $N' = 7$ (giving $E_{13,0} = E_{0,7} = 91$ and the coincidence of the 55th and 56th levels) and at $n' = 1$, $n = 14$, $N = 0$ and $N' = 7$ (giving $E_{14,0} = E_{1,7} = 98$ and the coincidence of the 63rd and 64th levels).

It is easy to reveal the first deviations from the above-described ordering scheme at the 70th and 71st levels which form the degenerate doublet $E_{13,1} = E_{0,8} = 104$. The next pair of the 72nd and 73rd energy levels forms another degenerate doublet with $E_{15,0} = E_{2,7} = 105$. Along these lines it is straightforward to discover the other two degenerate energy doublets with $E_{14,1} = E_{1,8} = 111$ and $E_{16,0} = E_{3,7} = 112$, etc.

For our present purposes the pairwise degeneracy of the levels Nr. 70 - 73 is precisely what we see in Fig. 5b of ref. [1] (obtained by the variational diagonalization method and using a numbering shifted by one). In similar situations, the non-degenerate version of the textbook Rayleigh-Schrödinger perturbation theory cannot work. This is seen in the complementary Fig. 5a, *loc. cit.*, the disagreement of which with Fig. 5a as formulated in the concise summary of ref. [1] just reflects the inadequacy of its generation by the non-degenerate Rayleigh-Schrödinger recipe.

5 Summary

We believe that several Nanayakkara’s numerically supported conclusions of ref. [1] were premature. Here we are offering their following modified versions.

- All quantum Hamiltonians associated with the real Barbanis’ potential (1) are ill defined. There are either no bound states or, if they do exist, they are embedded in the continuum. Their apparent variational convergence as observed in ref. [1] is spurious. The latter observation makes the majority of conclusions concerning the classical and quantum correspondence of the system presented in [1] unsubstantiated.
- For the well-defined quasi-Hermitian quantum Hamiltonians related to the imaginary Barbanis potential (1), no avoided level crossings were found in our calculations. We tend to the view that in this model, *all* the crossings are the genuine points of degeneracy. Even in this dynamical setting, a really unfortunate and unexpected degeneracy of the unperturbed levels as chosen in ref. [1] leaves both the employed non-degenerate perturbation method and its results entirely inapplicable.

Thus, we may summarize that in the Hermitian-like dynamical regime with $g > 0$ the Nanayakkara’s variational energies *must* in fact diverge to $-\infty$. In the language of physics this means that the quantized system would collapse [or rather, in the light of (3), “explode” in two directions in the $x > 0$ half-plane] immediately after the parameter g becomes negative.

In the alternative PT-symmetric, quasi-Hermitian and well-quantized regime (i.e., at certain sufficiently small and negative $g < 0$ at least), we easily spotted the reason of the failure of the Nanayakkara’s perturbation results. Hence, their improvement might be achieved after a transition to the degenerate Rayleigh-Schrödinger formalism.

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Table 1: Values (and ordering) of the unperturbed energy levels (4)

n	0	1	2	3	4	5	...
0	0 (0th)	7 (1st)	14 (3rd)	21 (5th)	28 (8th)	35 (11th)	...
1	13 (2nd)	20 (4th)	27 (7th)	34 (10th)	41 (14th)	48 (18th)	...
2	26 (6th)	33 (9th)	40 (13th)	47 (17th)	54 (22nd)	61 (27th)	...
3	39 (12th)	46 (16th)	53 (21st)	60 (26th)	67 (32nd)	74 (38th)	...

Figure captions

Figure 1 Energy crossings for the perturbed circular (left) and elliptic (right) models (1).

Figure 2 Contour plots of real and imaginary parts of the 72nd and 73rd wave functions of (1) for $\omega_x = 0.7$, $\omega_y = 1.3$, and $g = -0.002$.

Table captions

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References

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