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Research Article

Two Simple Models Derived from a Quantum-Mechanical Particle on an Elliptical Path

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We analyze two simple models derived from a quantum-mechanical particle on an elliptical path. The first Hamiltonian operator is non-Hermitian but isomorphic to an Hermitian operator. It appears to exhibit the same two-fold degeneracy as the particle on a circular path. More precisely, $E_n = n^2 E_1, n = 1, 2, \ldots$ (in addition to an exact eigenvalue $E_0 = 0$). The second Hamiltonian operator is Hermitian and does not exhibit such degeneracy. In this case the nth excited energy level splits at the nth order of perturbation theory. Both models can be described in terms of the same point-group symmetry.

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1. Introduction

Most textbooks on quantum mechanics and quantum chemistry[1] resort to exactly-solvable models in order to illustrate some of the features of quantum-mechanical systems. Among the simplest models one finds the particle in a box, the harmonic oscillator and the planar rigid rotator. The latter model is one of the few cases of one degree of freedom that exhibits degeneracy. It is mathematically similar to a single particle moving along a circular path. An interesting deformation of this model is the case of a particle moving along an elliptical path. The purpose of this paper is a straightforward analysis of the latter model.

In section 2 we derive the Hamiltonian operator for the first model and discuss the possible scalar product for the states as well as other useful features. In section 3 we derive an analytical expression for the spectrum from first-order perturbation theory. In section 4 we obtain accurate eigenvalues by means

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of the Rayleigh-Ritz method (RRM)[1] that yields increasingly accurate upper bounds[2][3]. From the secular determinant we derive perturbation corrections of greater order. In section 5 we introduce an alternative model, but in this case with an Hermitian Hamiltonian, and carry out similar calculations. Finally, in section 6 we summarize the main results of the paper and draw conclusions.

2. The model

We consider a particle of mass m that moves freely on an elliptical path. The Hamiltonian operator is

$$H=-\frac{\hbar^2}{2m}\nabla^2, \tag{1}$$

where ∇^2 is the Laplacian in two dimensions. The motion of the particle is restricted to a closed path given by all points (x,y) that satisfy

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}=1, \tag{2}$$

where a and b are positive real numbers (the ellipse semi-axes). If we write

$$x=a\cos\phi, y=b\sin\phi, \tag{3}$$

which satisfy equation (2), we obtain

$$\begin{aligned}\nabla^2 &= \frac{1}{\sqrt{a^2+(b^2-a^2)\cos^2\phi}}\frac{d}{d\phi}\frac{1}{\sqrt{a^2+(b^2-a^2)\cos^2\phi}}\frac{d}{d\phi}=\frac{1}{a^2}\tilde{\nabla}^2,\\ \tilde{\nabla}^2 &= \frac{1}{\sqrt{1+\xi\cos^2\phi}}\frac{d}{d\phi}\frac{1}{\sqrt{1+\xi\cos^2\phi}}\frac{d}{d\phi}, \xi=\frac{b^2-a^2}{a^2},\end{aligned} \tag{4}$$

where $-1<\xi<\infty$. The point $\xi=-1$ is expected to be a singularity because it leads to $b=0$.

We can define a dimensionless Hamiltonian operator as[4]

$$\tilde{H}=\frac{2ma^2}{\hbar^2}H=-\tilde{\nabla}^2, \tag{5}$$

and from now on we will focus on the dimensionless eigenvalue equation

$$\begin{aligned}H\psi_n(\phi)=E_n\psi_n(\phi), \psi_n(\phi+2\pi)=\psi_n(\phi),\\ H=-\frac{1}{\sqrt{g}}\frac{d}{d\phi}\frac{1}{\sqrt{g}}\frac{d}{d\phi}, g=1+\xi\cos^2\phi.\end{aligned} \tag{6}$$

The Hamiltonian operator (6) is Hermitian with respect to the scalar product

$$\langle u|v\rangle=\int_0^{2\pi}u^*(\phi)v(\phi)\sqrt{g}d\phi, \tag{7}$$

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where $\sqrt{g}$ is the Jacobian of the transformation. However, this scalar product exhibits two difficulties. The first one is that the only variable parameter ξ of the dimensionless model appears in it. The second drawback is that it makes the calculation of matrix elements more complicated. For these reasons, in what follows we choose

$$\langle u|v\rangle = \int_0^{2\pi} u^*(\phi)v(\phi)d\phi, \tag{8}$$

which facilitates the numerical calculation based on Fourier basis sets (although it changes the nature of the model). As a result, the Hamiltonian operator H is not Hermitian because

$$H^\dagger = -\frac{d}{d\phi}\frac{1}{\sqrt{g}}\frac{d}{d\phi}\frac{1}{\sqrt{g}}. \tag{9}$$

However, it follows from

$$g^{1/4}Hg^{-1/4} = g^{-1/4}H^\dagger g^{1/4} = \mathcal{H} = -g^{-1/4}\frac{d}{d\phi}g^{-1/2}\frac{d}{d\phi}g^{-1/4}, \tag{10}$$

that both H and $H^\dagger$ are isomorphic to the Hermitian operator $\mathcal{H}$ and, therefore, share the same real spectrum. If $H\psi = E\psi$ and $H^\dagger\varphi = E\varphi$ then one can easily prove that the Hellmann-Feynman theorem (HFT)[5][6] in this case reads

$$\frac{dE}{d\xi} = \frac{\left\langle\varphi\left|\frac{dH}{d\xi}\right|\psi\right\rangle}{\langle\varphi|\psi\rangle}. \tag{11}$$

The HFT is valid even for degenerate states as discussed elsewhere for Hermitian operators[7].

The Hamiltonian operator H is invariant under the operations $\phi \to -\phi$ and $\phi \to \phi + \pi$; therefore, we expect that $\psi(-\phi) = \pm\psi(\phi)$ and $\psi(\phi + \pi) = \pm\psi(\phi)$. For this reason we can separate the states into four clases given by $(+,+)$, $(+,-)$, $(-,+)$ and $(-,-)$ from which we conclude that the problem can be described by means of the symmetry point groups D_2 or C_{2v}, both with one-dimensional irreducible representations[8]. It is clear that the functions into the classes $(+,+)$ and $(-,+)$ are periodic of period π. The relation between present notation and the one in standard books on group theory[8] is given in the following table

$$\begin{array}{ccc} D_2 & C_{2v} & \Pr esent \\ A & A_1 & (+,+) \\ B_1 & A_2 & (-,+) \\ B_2 & B_1 & (+,-) \\ B_3 & B_2 & (-,-) \end{array}. \tag{12}$$

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3. Perturbation theory

When $\xi = 0$ the dimensionless Hamiltonian operator becomes $H_0 = -\frac{d^2}{d\phi^2}$ so that

$$H_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}, E_n^{(0)} = n^2, \psi_n^{(0)}(\phi) = \frac{1}{\sqrt{2\pi}}e^{in\phi}, n = 0, \pm 1, \pm 2, \ldots \tag{13}$$

By means of perturbation theory (PT) we can obtain approximate solutions in terms of power series

$$E_n = \sum_{j=0}^{\infty} E_n^{(j)}\xi^j, \psi_n = \sum_{j=0}^{\infty} \psi_n^{(j)}\xi^j. \tag{14}$$

Note that we have an exact solution given by $E_0 = E_0^{(0)} = 0$ and $\psi_0(\phi) = \psi_0^{(0)}(\phi)$ for all ξ that will not be relevant for present discussion.

The perturbation correction of first order can be derived by means the non-Hermitian operator

$$H_1 = \left.\frac{dH}{d\xi}\right|_{\xi=0} = \cos^2\phi\frac{d^2}{d\phi^2} - \sin(\phi)\cos(\phi)\frac{d}{d\phi}. \tag{15}$$

Since

$$\left\langle\psi_{-n}^{(0)}\middle|H_1\middle|\psi_n^{(0)}\right\rangle = \left\langle\psi_n^{(0)}\middle|H_1\middle|\psi_{-n}^{(0)}\right\rangle = 0, \left\langle\psi_n^{(0)}\middle|H_1\middle|\psi_n^{(0)}\right\rangle = \left\langle\psi_{-n}^{(0)}\middle|H_1\middle|\psi_{-n}^{(0)}\right\rangle = -\frac{n^2}{2}, \tag{16}$$

we conclude that

$$E_n = n^2\left(1 - \frac{\xi}{2}\right) + \mathbf{O}\left(\xi^2\right). \tag{17}$$

We obtain exactly the same result using $H_1^\dagger$ as expected from the argument given in the preceding section. Besides, the HFT at $\xi = 0$

$$\left.\frac{dE}{d\xi}\right|_{\xi=0} = -\frac{n^2}{2}, \tag{18}$$

predicts that all the eigenvalues have a negative slope at origin.

Since the eigenvalues are expected to be singular when $\xi = -1$ it appears convenient to try the improved perturbation approximation

$$E_n \approx \left\langle\psi_n^{(0)}\middle|H\middle|\psi_n^{(0)}\right\rangle = \frac{n^2}{\sqrt{1+\xi}}, \tag{19}$$

that yields the correct linear term and is singular at $\xi = -1$.

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4. Rayleigh-Ritz method

The RRM[1] is a well known variational procedure that provides increasingly accurate upper bounds[2][3]. In order to apply this approach we need a suitable basis set.

The standard Fourier basis set is suitable for the application of the RRM. However, we found it easier to calculate the necessary matrix elements, by means of our old-fashioned computer-algebra software, with the alternative basis sets

$$\begin{aligned} (+,+) &: \left\{\cos^{2n}\phi, n=0,1,\ldots\right\}, \\ (+,-) &: \left\{\cos^{2n+1}\phi, n=0,1,\ldots\right\}, \\ (-,+) &: \left\{\sin\phi\cos^{2n+1}\phi, n=0,1,\ldots\right\}, \\ (-,-) &: \left\{\sin\phi\cos^{2n}\phi, n=0,1,\ldots\right\}. \end{aligned} \tag{20}$$

We followed a brute-force procedure consisting of obtaining the roots of the secular determinant $|\mathbf{H}-W\mathbf{S}|$ where the elements of the $N\times N$ matrices $\mathbf{H}$ and $\mathbf{S}$ are given by[1][7]

$$H_{ij}=\langle\varphi_i|H|\varphi_j\rangle, S_{ij}=\langle\varphi_i|\varphi_j\rangle, i,j=0,1,\ldots,N-1. \tag{21}$$

N	$n=0$	$n=2$	$n=4$	$n=6$
5	0	2.705129367	10.82054064	24.39391541
6	0	2.705129365	10.82051747	24.34655624
7	0	2.705129365	10.82051746	24.34616541
8	0	2.705129365	10.82051746	24.34616429
9	0	2.705129365	10.82051746	24.34616429
10	0	2.705129365	10.82051746	24.34616429

Table 1. $(+,+)$ RRM eigenvalues of model (6) for $\xi=1$

N	$n=1$	$n=3$	$n=5$	$n=7$
5	0.6762823414	6.086541072	16.9071682	33.23425983
6	0.6762823414	6.086541072	16.90705871	33.13897689
7	0.6762823414	6.086541072	16.90705853	33.13783974
8	0.6762823414	6.086541072	16.90705853	33.13783474
9	0.6762823414	6.086541072	16.90705853	33.13783472
10	0.6762823414	6.086541072	16.90705853	33.13783472

Table 2. $(+,-)$ RRM eigenvalues of model (6) for $\xi=1$

N	$n=1$	$n=3$	$n=5$	$n=7$
5	0.6762823414	6.086541072	16.9071682	33.23425983
6	0.6762823414	6.086541072	16.90705871	33.13897689
7	0.6762823414	6.086541072	16.90705853	33.13783974
8	0.6762823414	6.086541072	16.90705853	33.13783474
9	0.6762823414	6.086541072	16.90705853	33.13783472
10	0.6762823414,	6.086541072,	16.90705853,	33.13783472

Table 3. $(-,-)$ RRM eigenvalues of model (6) for $\xi=1$

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N	$n=2$	$n=4$	$n=6$	$n=8$
5	2.705129365	10.82051747	24.34655624	43.45817399
6	2.705129365	10.82051746	24.34616541	43.28492974
7	2.705129365	10.82051746	24.34616429	43.28208765
8	2.705129365	10.82051746	24.34616429	43.2820699
9	2.705129365	10.82051746	24.34616429	43.28206985
10	2.705129365	10.82051746,	24.34616429,	43.28206985

Table 4. $(-,+)$ RRM eigenvalues of model (6) for $\xi=1$

Tables 1, 2, 3 and 4 show the rate of convergence of the RRM eigenvalues for $\xi=1$ in terms of the dimension N of the secular determinant[1][7]. If we order the eigenvalues E_n in such a way that $E_{n+1}>E_n$, we appreciate that the states with $n>0$ are two-fold degenerate within the accuracy of present calculation (10 digits). The two states that share the eigenvalue E_{2n} have symmetries $(+,+)$ and $(-,+)$, while those that share E_{2n+1} have symmetries $(+,-)$ and $(-,-)$. Besides, the RRM eigenvalues of those four tables suggest that

$$E_n=n^2E_1, n=1,2,\ldots. \tag{22}$$

Figure 1 shows the RRM eigenvalues and the PT ones given by equations (17) and (19) with $n=1,2,3,4$ for $-0.5\leq\xi\leq 0.5$. We appreciate that the accuracy of PT decreases with n and that equation (19) provides a noticeably improvement over (17).

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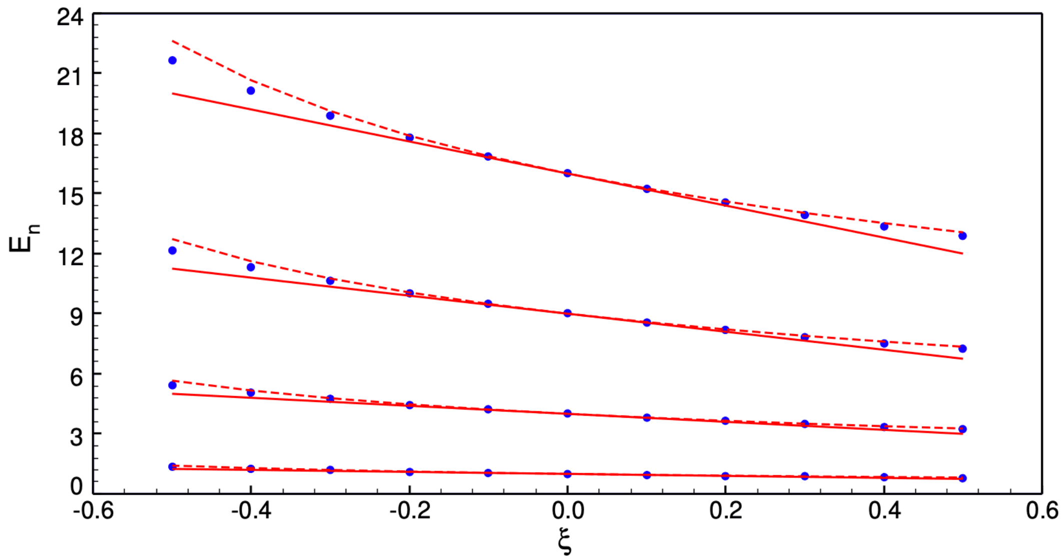

Figure 1. RPM (blue circles), PT (solid red line) and improved PT (dashed red line) eigenvalues with $n = 1, 2, 3, 4$ of model (6)

We can obtain perturbation corrections of greater order by means of a straightforward procedure. We substitute the perturbation series (14) and the Taylor expansion of $g^{-1/2}$ about $\xi = 0$ into the secular determinant and solve for the perturbation coefficients $E_n^{(j)}$. In this way we obtain

$$\begin{aligned} E_1 &= 1 - \frac{1}{2}\xi + \frac{9}{32}\xi^2 - \frac{11}{64}\xi^3 + \frac{917}{8192}\xi^4 + \mathcal{O}\left(\xi^5\right), \\ E_2 &= 4 - 2\xi + \frac{9}{8}\xi^2 - \frac{11}{16}\xi^3 + \frac{917}{2048}\xi^4 + \mathcal{O}\left(\xi^5\right), \\ E_3 &= 9 - \frac{9}{2}\xi + \frac{81}{32}\xi^2 - \frac{99}{64}\xi^3 + \frac{8253}{8192}\xi^4 + \mathcal{O}\left(\xi^5\right), \\ E_4 &= 16 - 8\xi + \frac{9}{2}\xi^2 - \frac{11}{4}\xi^3 + \frac{917}{512}\xi^4 + \mathcal{O}\left(\xi^5\right), \\ E_5 &= 25 - \frac{25}{2}\xi + \frac{225}{32}\xi^2 - \frac{275}{64}\xi^3 + \frac{22925}{8192}\xi^4 + \mathcal{O}\left(\xi^5\right), \\ E_6 &= 36 - 18\xi + \frac{81}{8}\xi^2 - \frac{99}{16}\xi^3 + \frac{8253}{2048}\xi^4 + \mathcal{O}\left(\xi^5\right), \end{aligned} \tag{23}$$

which clearly confirm the conjecture (22).

5. Alternative model

The model discussed in section 2 can be written as $H = -AA$, where $A = g^{-1/2}\frac{d}{d\phi}$. We can derive an Hermitian variant by simply writing $H = -A^\dagger A$; that is to say

$$H=-\frac{d}{d\phi}g^{-1}\frac{d}{d\phi}, \quad (24)$$

that is Hermitian with the scalar product (8). Note that

$$H()-H()=-\frac{g'}{2g^{2}}\frac{d}{d\phi}. \quad (25)$$

We carry out the same RPM calculation as in the preceding model. Table 5 shows the lowest eigenvalues for each of the symmetries discussed above and $\xi=1$. We appreciate that the degeneracy is broken but the magnitude of the splitting decreases with n. It is worth mentioning that in this case we also have the exact solution $E_0=0, \psi_0(\phi)=\frac{1}{\sqrt{2\pi}}$.

$(+,+)$	$(-,+)$	$(+,-)$	$(-,-)$
0			
2.642467139	2.79431927	0.7959412608	0.5700037793
10.81697747	10.84750548	6.135514729	6.062735007
24.35498746	24.35945236	16.92430649	16.91237359
43.29263030	43.29320664	33.14957349	33.1479519

Table 5. Lowest eigenvalues of model (24) for $\xi=1$

In this case we can roughly resort to the improved perturbation expression (19). Figure 2 shows the lowest RPM eigenvalues in the interval $-0.5\leq\xi\leq 0.5$ and the perturbation expression just mentioned. The splitting between the states indicated by blue circles and red squares is almost indistinguishable because of the scale of the figure and, for this reason, the approximate perturbation expression (19) appears to provide reasonable results for those values of the parameter ξ.

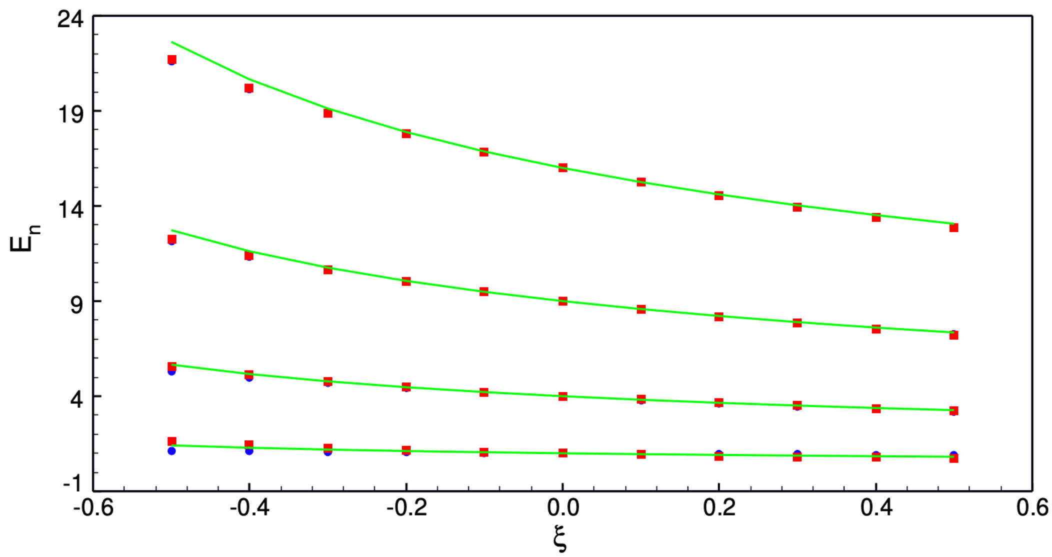

Figure 2. Lowest RPM eigenvalues (blue circles and red squares) and improved PT eigenvalues (solid green line) of model (24)

By means of the perturbation expansion based on the secular determinant already described above we obtain

$$\begin{aligned}
E_1(-,-) &= 1-\frac{3}{4}\xi+\frac{71}{128}\xi^2-\frac{1655}{4096}\xi^3+\frac{113807}{393216}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_1(+,-) &= 1-\frac{1}{4}\xi+\frac{7}{128}\xi^2-\frac{41}{4096}\xi^3+\frac{527}{393216}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_2(+,+) &= 4-2\xi+\frac{11}{12}\xi^2-\frac{3}{8}\xi^3+\frac{1781}{13824}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_2(-,+) &= 4-2\xi+\frac{17}{12}\xi^2-\frac{9}{8}\xi^3+\frac{12533}{13824}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_3(-,-) &= 9-\frac{9}{2}\xi+\frac{657}{256}\xi^2-\frac{7281}{4096}\xi^3+\frac{7505613}{5242880}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_3(+,-) &= 9-\frac{9}{2}\xi+\frac{657}{256}\xi^2-\frac{5823}{4096}\xi^3+\frac{3773133}{5242880}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_4(+,+) &= 16-8\xi+\frac{68}{15}\xi^2-\frac{14}{5}\xi^3+\frac{5878}{3375}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_4(-,+) &= 16-8\xi+\frac{68}{15}\xi^2-\frac{14}{5}\xi^3+\frac{6628}{3375}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_5(-,-) &= 25-\frac{25}{2}\xi+\frac{5425}{768}\xi^2-\frac{2225}{512}\xi^3+\frac{566374475}{198180864}\xi^4+\mathcal{O}\left(\xi^5\right),\\
E_5(+,-) &= 25-\frac{25}{2}\xi+\frac{5425}{768}\xi^2-\frac{2225}{512}\xi^3+\frac{566374475}{198180864}\xi^4+\mathcal{O}\left(\xi^5\right).
\end{aligned} \tag{26}$$

These analytical expressions suggest that the splitting of the nth level takes place at perturbation order n.

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Figure 3 shows accurate RPM results and PT ones for $E_1(-,-)$ and $E_1(+,-)$ in a scale that clearly reveals the splitting of the energy level with $n=1$. We appreciate that the perturbation expansions are reasonably accurate in this range of values of ξ. The first-order perturbation expression (19) is not suitable for the description of these two levels with the required detail.

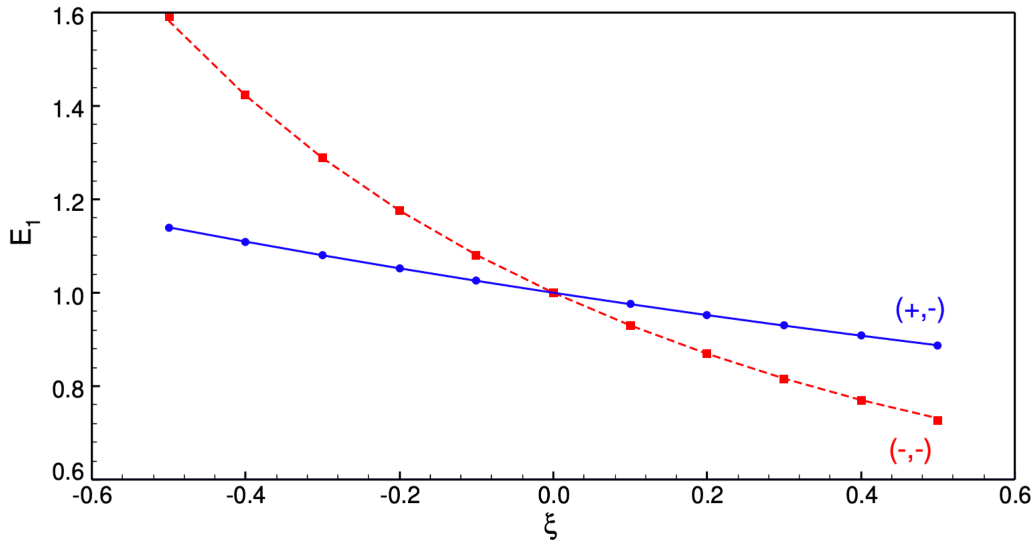

Figure 3. RPM eigenvalues (blue circles and red squares) and PT series (blue solid and red dashed lines) for the first and second excited states of model (24)

6. Conclusions

We have explored two Hamiltonian operators derived from the model of a quantum-mechanical particle on an elliptical path. The first one is non-Hermitian but it is isomorphic to an Hermitian operator. For this reason its eigenvalues are real. The most relevant feature of this quantum-mechanical model is that it appears to exhibit the same two-fold degeneracy as in the case $\xi=0$ (particle on a circular path). Both accurate numerical results and perturbation theory suggest that the eigenvalues follow the expression shown in equation (22). In addition to it, there is an exact solution given by a constant eigenfunction and $E_0=0$. We can separate the states of the system into four symmetry species which facilitates the calculation and the analysis of the problem.

The second example is an Hermitian modification of the previous Hamiltonian operator that exhibits the same type of symmetry. In this case the two-fold degeneracy at $\xi=0$ is broken when $\xi\neq 0$. Present low

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order perturbation expansions suggests that the splitting of the nth excited level takes place at the nth perturbation order.

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Declarations

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