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.

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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 simple 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 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 of the Rayleigh-Ritz method (RRM)[1] that yields increasingly accurate upper bounds[2][3]. In section 5 we

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introduce an alternative model 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 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

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

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 of the model ξ appears in it. The second drawback is that

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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. An immediate consequence of the latter property is the straightforward validity of the Hellmann-Feynman theorem (HFT)[5][6]

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

This expression is valid even for degenerate states as discussed elsewhere[7].

3. Perturbation theory

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

$$H_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}, E_n^{(0)} = n^2, \psi_n^{(0)}(\phi) = \frac{1}{\sqrt{2\pi}}e^{in\phi}, n = 0, \pm1, \pm2, \ldots. \tag{12}$$

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

$$E_n = \sum_{j=0}^{\infty} E_n^{(j)}\xi^j, \psi_n = \sum_{j=0}^{\infty}\psi_n^{(j)}\xi^j. \tag{13}$$

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 we will omit from now on.

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

$$H_1 = \left.\frac{dH}{d\xi}\right|_{\xi=0} = \cos^2\phi\frac{d^2}{d\phi^2} - \sin(\phi)\cos(\phi)\frac{d}{d\phi}. \tag{14}$$

Since

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$$\left\langle\psi_{-n}^{(0)}\middle|H_1\middle|\psi_n^{(0)}\right\rangle=\left\langle\psi_n^{(0)}\middle|H_1\middle|\psi_{-n}^{(0)}\right\rangle=0,\left\langle\psi_n^{(0)}\middle|H_1\middle|\psi_n^{(0)}\right\rangle=\left\langle\psi_{-n}^{(0)}\middle|H_1\middle|\psi_{-n}^{(0)}\right\rangle=-\frac{n^2}{2}, \tag{15}$$

we conclude that

$$E_n=n^2\left(1-\frac{\xi}{2}\right)+\mathbf{O}\left(\xi^2\right). \tag{16}$$

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

$$\left.\frac{dE}{d\xi}\right|_{\xi=0}=-\frac{n^2}{2}, \tag{17}$$

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

$$E_n\approx\left\langle\psi_n^{(0)}\middle|H\middle|\psi_n^{(0)}\right\rangle=\frac{n^2}{\sqrt{1+\xi}}, \tag{18}$$

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

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.

Since the dimensionless Hamiltonian operator H in equation (6) is invariant under the transformation given by $\phi\rightarrow-\phi$ it is more convenient to resort to basis sets of even ($\varphi_{en}(\phi)$) and odd ($\varphi_{on}(\phi)$) functions; for example:

$$\begin{aligned}\{\varphi_{en}(\phi),n=0,1,\ldots\}&=\left\{\frac{1}{\sqrt{2\pi}},\frac{1}{\pi}\cos\left(n\phi\right),n=1,2,\ldots\right\},\\ \{\varphi_{on}(\phi),n=1,2,\ldots\}&=\left\{\frac{1}{\pi}\sin\left(n\phi\right),n=1,2,\ldots\right\}.\end{aligned} \tag{19}$$

However, our old-fashioned computer-algebra software found it easier to calculate the desired matrix elements by means of the non-orthogonal basis sets

$$\{\varphi_{en}(\phi)=\cos^n\left(\phi\right),n=0,1,\ldots\},\{\varphi_{on}(\phi)=\sin\left(\phi\right)\cos^n\phi,n=0,1,\ldots\}. \tag{20}$$

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]

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

For example, for $N = 3$ and even basis functions we have the non-symmetric matrix

$$\mathbf{H} = \begin{pmatrix} 0 & 0 & \frac{2\pi(2\sqrt{\xi+1}-\xi-2)}{\xi\sqrt{\xi+1}} \\ 0 & \frac{\pi}{\sqrt{\xi+1}} & 0 \\ 0 & 0 & \frac{2\pi(\sqrt{\xi+1}-1)}{\xi\sqrt{\xi+1}} \end{pmatrix}. \tag{22}$$

Note that the matrix elements ehibit the singularity discussed above.

N	$n=1$	$n=2$	$n=3$	$n=4$
5	0.6762816118	2.705333163	6.3947862	11.43680246
6	0.6762824936	2.705333163	6.08832183	11.43680246
7	0.6762824936	2.705129814	6.08832183	10.82772904
8	0.6762823438	2.705129814	6.086544511	10.82772904
9	0.6762823438	2.705129367	6.086544511	10.82054064
10	0.6762823414	2.705129367	6.086541072	10.82054064
11	0.6762823414	2.705129365	6.086541072	10.82051747
12	0.6762823414	2.705129365	6.086541072	10.82051747
13	0.6762823414	2.705129365	6.086541072	10.82051746
14	0.6762823414	2.705129365	6.086541072	10.82051746
15	0.6762823414	2.705129365	6.086541072	10.82051746

Table 1. Even RRM eigenvalues E_n of (6) for $\xi = 1$

N	$n=1$	$n=2$	$n=3$	$n=4$
5	0.6762824936	2.705333163	6.08832183	11.43680246
6	0.6762824936	2.705129814	6.08832183	10.82772904
7	0.6762823438	2.705129814	6.086544511	10.82772904
8	0.6762823438	2.705129367	6.086544511	10.82054064
9	0.6762823414	2.705129367	6.086541072	10.82054064
10	0.6762823414	2.705129365	6.086541072	10.82051747
11	0.6762823414	2.705129365	6.086541072	10.82051747
12	0.6762823414	2.705129365	6.086541072	10.82051746
13	0.6762823414	2.705129365	6.086541072	10.82051746
14	0.6762823414	2.705129365	6.086541072	10.82051746
15	0.6762823414	2.705129365	6.086541072	10.82051746

Table 2. Odd RRM eigenvalues E_n of (6) for $\xi = 1$

Tables 1 and 2 show the rate of convergence of the RRM eigenvalues for $\xi = 1$ in terms of the dimension N of the secular determinant[1][7]. We appreciate that the even and odd states remain degenerate within the accuracy of present calculation (10 digits). Besides, the RRM eigenvalues of both tables suggest that

$$E_n = n^2 E_1, n = 1, 2, \ldots. \tag{23}$$

Figure 1 shows the RRM eigenvalues and the PT ones given by equations (16) and (18) 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 (18) provides a noticeably improvement.

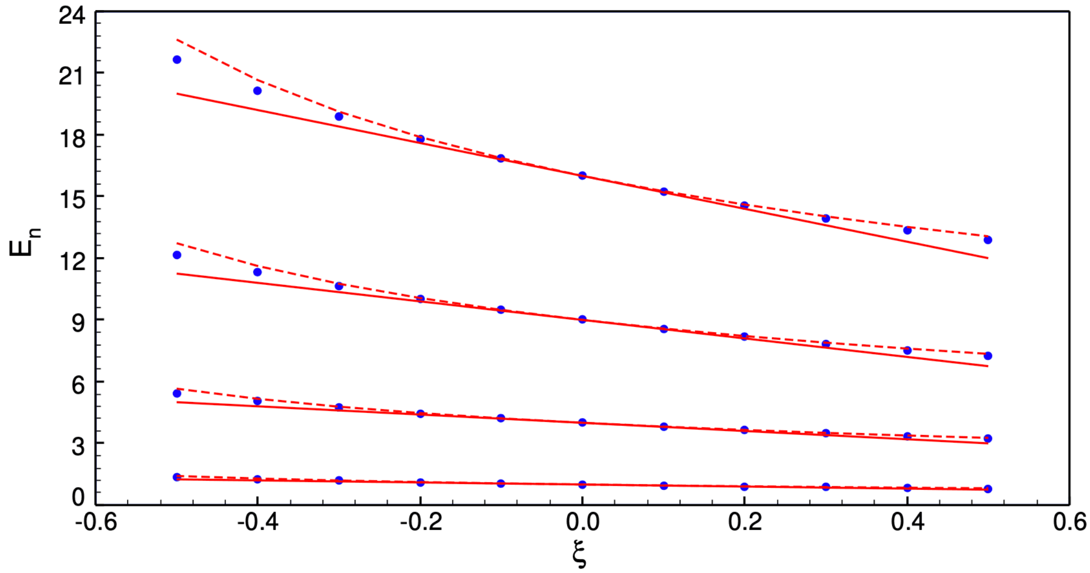

Figure 1. RPM (blue circles), PT (solid red line) and improved PT (dashed red line) eigenvalues with $n = 1, 2, 3, 4$ for (6)

We can obtain perturbation corrections of greater order by means of a straightforward procedure. We substitute the perturbation series (13) 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

$$\begin{aligned} E_1 &= 1 - \frac{1}{2}\xi + \frac{9}{32}\xi^2 - \frac{11}{64}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_2 &= 4 - 2\xi + \frac{9}{8}\xi^2 - \frac{11}{16}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_3 &= 9 - \frac{9}{2}\xi + \frac{81}{32}\xi^2 - \frac{99}{64}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_4 &= 16 - 8\xi + \frac{9}{2}\xi^2 - \frac{11}{4}\xi^3 + \mathcal{O}\left(\xi^4\right), \end{aligned} \tag{24}$$

for both even and odd states. These results confirm the conjecture (23).

5. Alternative model

In this section we explore the model given by the dimensionless Hamiltonian operator

$$H = -\frac{d}{d\phi} g^{-1} \frac{d}{d\phi}, \tag{25}$$

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

$$H(6) - H(25) = -\frac{g'}{2g^2}\frac{d}{d\phi}. \tag{26}$$

We carry out the same RPM calculation as in the preceding model. In this case the matrices are symmetric; for example, for $N = 3$ and even states we have

$$\mathbf{H} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{2\pi(\sqrt{\xi+1}-1)}{\xi} & 0 \\ 0 & 0 & -\frac{4\pi(2\sqrt{\xi+1}-\xi-2)}{\xi^2} \end{pmatrix}. \tag{27}$$

It is worth mentioning that for greater values of N the matrix $\mathbf{H}$ is no longer diagonal. In this case the matrix elements also reflect the singularity at $\xi = -1$.

n	**even**	**odd**
1	0.7959412608	0.5700037793
2	2.642467139	2.79431927
3	6.135514729	6.062735007
4	10.81697747	10.84750548

Table 3. Eigenvalues for even and odd states of (25) for $\xi = 1$

Table 3 shows the lowest eigenvalues for even and odd states with $n = 1, 2, 3, 4$ for $\xi = 1$. We appreciate that the degeneracy is broken and that $|E_{en} - E_{on}|$ decreases with n. It is worth mentioning that in this case we also have the exact solution $E_0 = 0, \psi_0(\phi) = \frac{1}{\sqrt{2\pi}}$ that is not shown in the table.

In this case we can also resort to the same improved perturbation expression (18). Figure 2 shows the lowest RPM eigenvalues for even and odd states in the interval $-0.5 \leq \xi \leq 0.5$ and the perturbation expression just mentioned. The difference $|E_{en} - E_{on}|$ is almost indistinguishable because of the scale of the figure and we appreciate that the approximate perturbation expression (18) provides reasonable results for those values of the parameter ξ.

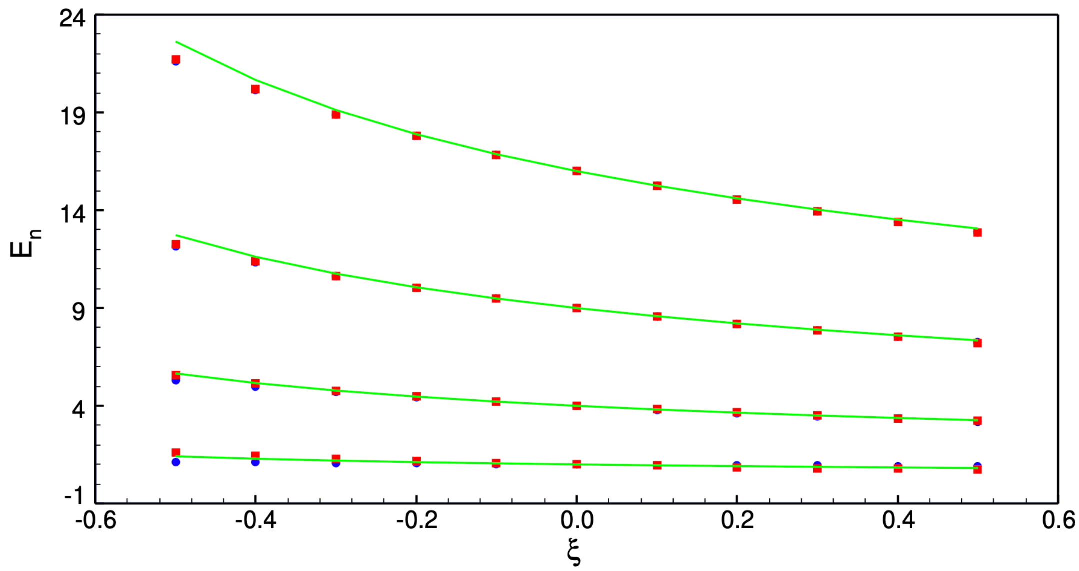

Figure 2. RPM even states (blue circles), RPM odd states (red squares) and improved PT eigenvalues (solid green line) with $n = 1, 2, 3, 4$ for (25)

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

$$\begin{aligned} E_{e1} &= 1 - \frac{1}{4}\xi + \frac{7}{128}\xi^2 - \frac{41}{4096}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_{o1} &= 1 - \frac{3}{4}\xi + \frac{71}{128}\xi^2 - \frac{1655}{4096}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_{e2} &= 4 - 2\xi + \frac{11}{12}\xi^2 - \frac{3}{8}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_{o2} &= 4 - 2\xi + \frac{17}{12}\xi^2 - \frac{9}{8}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_{e3} &= 9 - \frac{9}{2}\xi + \frac{657}{256}\xi^2 - \frac{5823}{4096}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_{o3} &= 9 - \frac{9}{2}\xi + \frac{657}{256}\xi^2 - \frac{7281}{4096}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_{e4} &= 16 - 8\xi + \frac{68}{15}\xi^2 - \frac{14}{5}\xi^3 + \mathcal{O}\left(\xi^4\right), \\ E_{o4} &= 16 - 8\xi + \frac{68}{15}\xi^2 - \frac{14}{5}\xi^3 + \mathcal{O}\left(\xi^4\right). \end{aligned} \tag{28}$$

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

Figure 3 shows accurate RPM results and the PT series for E_{e1} and E_{o1} in a scale that clearly reveals the splitting of the first energy level. We appreciate that the perturbation expansions are reasonably accurate in this range of values of ξ.

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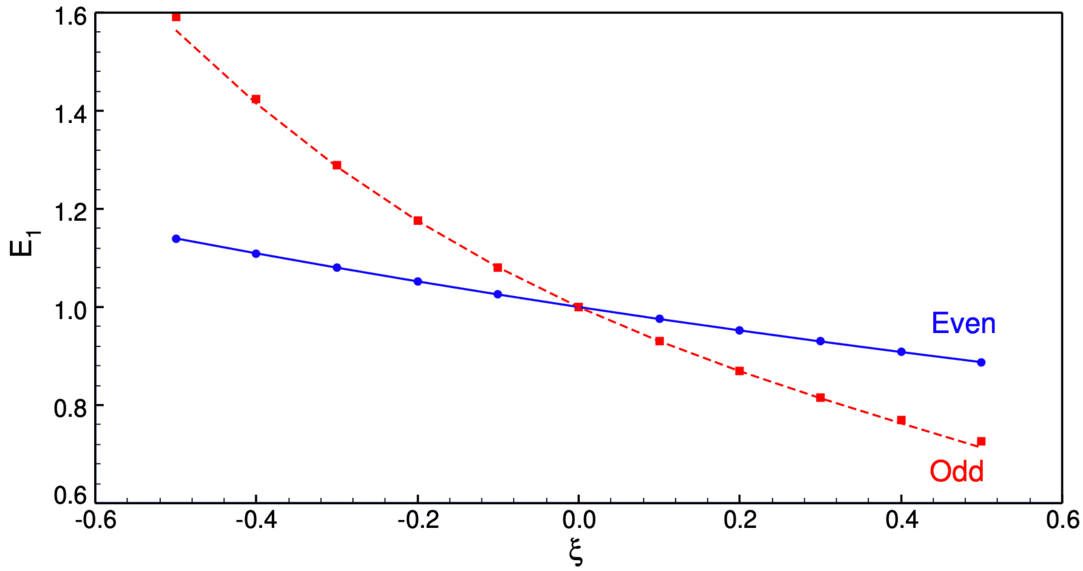

Figure 3. RPM even state (blue circles), RPM odd state (red squares) PT even state (solid blue line) and PT odd state (dashed red line) of (25) for $n = 1$

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 (23). In addition to it, there is an exact solution given by a constant eigenfunction and $E_0 = 0$.

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