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Quantum quadratic-attractive plus quartic-repulsive potential in a box†

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Abstract. The solution of the Schrödinger equation for the two-well oscillator in a symmetric box is formulated exactly, and high-accuracy numerical results are obtained for the lowest states. Perturbative solutions for boxes whose walls are (i) fairly close to each other, (ii) in the vicinity of the inflection points of the potential, (iii) at the position of the minima of the potential, and (iv) very far from each other are also obtained and compared with the exact ones.

1. Introduction

Some time ago Banerjee and Bhatnagar (1978) investigated the two-well oscillator

$$V(x)=-\tfrac{1}{2}kx^2+\tfrac{1}{2}\lambda x^4 \tag{1}$$

by a non-perturbative method and in the WKB approximation. They also argued why the problem does not admit of a straightforward perturbative solution. Recently, Killingbeck (1981) has considered the same problem. In contrast, we show in the present paper that the modified problem of the two-well oscillator in a symmetric box, with the potential of equation (1) inside the box ($|x|<R$) and an infinite potential outside the box ($|x|>R$), admits of an exact solution as well as perturbative solutions.

We use the reduced Hamiltonian

$$H(k=1,\lambda)=\tfrac{1}{2}(p^2-x^2+\lambda x^4) \tag{2}$$

and impose the boundary condition on the wavefunctions

$$\psi(|x|=R)=0 \tag{3a}$$

at the position of the walls. Furthermore, since the Hamiltonian is even under reflection, $H(x)=H(-x)$, its eigenfunctions have a well defined parity. We can restrict the problem to the interval $0\leqslant x\leqslant R$, by introducing the corresponding boundary condition at the origin,

$$\left.\frac{d\psi^{(+)}}{dx}\right|_{x=0}=0 \tag{3b}$$

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and

$$\psi^{(-)}(x=0)=0, \tag{3c}$$

for the even and odd wavefunctions, respectively.

An exact solution of the eigenvalue problem can be formulated by using the expansions of the wavefunctions,

$$\psi_m^{(+)}(x)=\sum_{n=0}^{\infty} c_{mn}^{(+)}\phi_n^{(+)}(x), \tag{4a}$$

$$\psi_m^{(-)}(x)=\sum_{n=0}^{\infty} c_{mn}^{(-)}\phi_n^{(-)}(x), \tag{4b}$$

in terms of the complete orthonormal bases of eigenfunctions of the free particle in the box,

$$|n+)=\phi_n^{(+)}(x)=R^{-1/2}\cos[(2n+1)\pi x/2R], \tag{5a}$$

$$|n-)=\phi_n^{(-)}(x)=R^{-1/2}\sin(n\pi x/R), \tag{5b}$$

which obviously satisfy the boundary conditions of equations ($3a$), and ($3b$) and ($3c$), respectively. Then the expansion coefficients $c_{mn}^{(\pm)}$ and the eigenvalues $\varepsilon_m^{(\pm)}$ are obtained from the diagonalisation of the corresponding matrices of the Hamiltonian, $(n'\pm|H|n\pm)$, which are explicitly constructed in § 2. In principle, the sums in equations ($4a$) and ($4b$) involve an infinite number of terms, but in practice we can use a finite number of them and test the convergence and accuracy of the numerical results.

In § 3, we develop perturbative solutions for boxes whose walls are (i) fairly close to each other, $R<1$, taking the free particle in the box as the unperturbed system, (ii) in the vicinity of the points of inflection of the potential, $R\approx(6\lambda)^{-1/2}$, taking the linear potential as the unperturbed system, (iii) at the position of the minimum of the potential, $R=(2\lambda)^{-1/2}$, taking the half-oscillator potential as the unperturbed system, and (iv) very far from each other, $R\gg\lambda^{-1/2}$, taking the harmonic oscillator potential as the unperturbed system.

Our numerical results are presented in § 4. The exact results illustrate how the degeneracy of the lowest states, by pairs, sets in as the separation of the walls is increased, especially for very small values of λ. Comparison of the perturbative and exact solutions allows us to ascertain the validity of the former.

2. Formulation of the exact solution

It is straightforward to construct the matrices of the Hamiltonian equation (2) in the bases of equations ($5a$) and ($5b$), respectively,

$$\begin{aligned}(n'+|H|n+)={}&\{(2n+1)^2\pi^2/8R^2-[\tfrac{1}{6}-(2n+1)^{-2}\pi^{-2}]R^2\\&+\tfrac{1}{2}[\tfrac{1}{5}-4(2n+1)^{-2}\pi^{-2}+24(2n+1)^{-4}\pi^{-4}]\lambda R^4\}\delta_{n'n}\\&+[\![[(n+n'+1)^{-2}-(n-n')^{-2}](-1)^{n-n'}\pi^{-2}R^2\\&-\{[(n+n'+1)^{-2}-(n-n')^{-2}]4\pi^{-2}\\&-[(n+n'+1)^{-4}-(n-n')^{-4}]24\pi^{-4}\}\tfrac{1}{2}(-1)^{n-n'}\lambda R^4]\!](1-\delta_{n'n}),\end{aligned} \tag{6a}$$

$$
\begin{aligned}
(n'-|H|n-) = \{ & n^2\pi^2/2R^2 - [\tfrac{1}{6}-(2n)^{-2}\pi^{-2}]R^2 \\
& + \tfrac{1}{2}[\tfrac{1}{5}-4(2n)^{-2}\pi^{-2}+24(2n)^{-4}\pi^{-4}]\lambda R^4\}\delta_{n'n} \\
& + [\![[(n+n')^{-2}-(n-n')^{-2}](-1)^{n-n'}\pi^{-2}R^2 \\
& - \{[(n+n')^{-2}-(n-n')^{-2}]4\pi^{-2} - [(n+n')^{-4}-(n-n')^{-4}]24\pi^{-4}\} \\
& \times \tfrac{1}{2}(-1)^{n-n'}\lambda R^4]\!](1-\delta_{n'n}).
\end{aligned} \qquad (6b)
$$

In these equations, it is easy to recognise the diagonal and non-diagonal contributions of the kinetic energy, quadratic and quartic terms in the Hamiltonian.

In the matrix representation, the solution of the eigenvalue problem is reduced to the solution of the secular equations

$$
\det |H^{(\pm)}_{n'n} - \varepsilon^{(\pm)}\delta_{n'n}| = 0. \qquad (7)
$$

However, as already mentioned in § 1, the matrices are of infinite dimension and in practice we work with submatrices of finite dimensions, testing the convergence and accuracy of the numerical results as the dimensions are increased.

3. Perturbative solutions

The two-well potential, equation (1), has zeros at $x=0$, $\pm(k/\lambda)^{1/2}$, minima at $x=\pm(k/2\lambda)^{1/2}$, and inflection points at $x=\pm(k/6\lambda)^{1/2}$. Next, we develop perturbative solutions for boxes whose walls are located in the vicinity of such points. We pay special attention to the interesting situation of very small values of λ.

3.1. *Very small boxes, $R<1$*

We take the free particle in the box, i.e. the kinetic energy term in equation (2) and its eigenfunctions of equations (5*a*) or (5*b*), as the unperturbed system, so that the potential itself, equation (1), is the perturbation. The matrix elements of equations (6*a*) and (6*b*) can be used directly to obtain the explicit forms of the Rayleigh–Schrödinger perturbation expansion

$$
\begin{aligned}
\varepsilon^s_N = {} & N^2\pi^2/8R^2 - (\tfrac{1}{6}-N^{-2}\pi^{-2})R^2 + \tfrac{1}{2}(\tfrac{1}{5}-4N^{-2}\pi^{-2}+24N^{-4}\pi^{-4})\lambda R^4 \\
& - 2S_1\pi^{-6}R^6 + 16\lambda S_2\pi^{-6}R^8 + [16(\tfrac{1}{6}-N^{-2}\pi^{-2})\pi^{-8}S_{10} \\
& - 8\pi^{-10}S_4 - 8\pi^{-8}S_5 - 32\lambda^2\pi^{-6}S_3]R^{10} \\
& + 8[4(2S_6+S_7)\pi^{-2} + 8S_8 + S_9 - (\tfrac{1}{5}-4N^{-2}\pi^{-2}+24N^{-4}\pi^{-4})S_{10} \\
& - 16(\tfrac{1}{6}-N^{-2}\pi^{-2})S_{11}]\lambda\pi^{-8}R^{12}
\end{aligned} \qquad (8)
$$

where

$$
N = \begin{cases} 2n+1 & \text{for even-parity states,} \quad n=0,1,2,\ldots, \\ 2n & \text{for odd-parity states,} \quad n=1,2,3,\ldots. \end{cases}
$$

The S_i ($i=1,\ldots,11$) are defined in the Appendix. In the expression (8) we have kept terms up to R^{12}.

3.2. Boxes whose walls are in the vicinity of the inflection points, $R \approx (6\lambda)^{-1/2}$

In this case, we work in the interval $-R \leqslant x \leqslant 0$, and make the change of variable $y = x + R$. Then the Hamiltonian becomes

$$H = -\tfrac{1}{2}\,\mathrm{d}^2/\mathrm{d}y^2 - \tfrac{1}{2}(y-R)^2 + \tfrac{1}{2}\lambda(y-R)^4$$
$$= -\alpha(\lambda, R) - \tfrac{1}{2}\,\mathrm{d}^2/\mathrm{d}y^2 + \tfrac{1}{2}\beta^3(\lambda, R)y - \tfrac{1}{2}\gamma(\lambda, R)y^2 - 2\lambda R y^3 + \tfrac{1}{2}\lambda y^4, \qquad (9a)$$

where

$$\alpha(\lambda, R) = \tfrac{1}{2}(R^2 - \lambda R^4), \qquad (9b)$$

$$\beta^3(\lambda, R) = 2R - 4\lambda R^3, \qquad (9c)$$

$$\gamma(\lambda, R) = 1 - 6\lambda R^2. \qquad (9d)$$

For fixed values of λ and R, the term in α is fixed and gives the value of the potential at the position of the walls. The next two terms in equation ($9a$) correspond to the Hamiltonian for a linear potential, which we take as the unperturbed system. Then the perturbation includes the quadratic, cubic and quartic terms.

For small values of λ, the boxes under consideration are rather large, and the degeneracy of the lowest pairs of even–odd states already appears. Thus, we will refer to both members of the pair simultaneously. Also, the interval of y can be taken as infinite since its values go from 0 to $R \gg 1$. Then the eigenfunctions of the unperturbed system are the regular Airy functions $\mathrm{Ai}(\beta y - 2\varepsilon^{(0)}/\beta^2)$ (Abramowitz and Stegun 1971), subject to the boundary condition of vanishing at the wall, i.e. for $y = 0$ which determines the unperturbed eigenvalues,

$$\varepsilon_n^{(0)} = -\tfrac{1}{2}\beta^2 a_n, \qquad (10a)$$

in terms of the zeros of such functions. Let us recall that those zeros are negative, so that the eigenvalues are positive. Notice that in practice these Airy functions also satisfy both boundary conditions at the centre of the box, equations ($3b$) and ($3c$), for $y = R \to \infty$.

The coefficient γ of the quadratic term is very close to zero, while the coefficients of the cubic and quartic terms are also very small, being of order $\lambda^{1/2}$ and λ, respectively. Therefore, we limit our calculation to first order in the perturbation, for which we need the expectation values of the second, third and fourth powers of y with the Airy functions. We take these directly from (Castilho Alcarás and Leal Ferreira 1975)

$$\langle y^2\rangle_n = 8(a_n/\beta)^2/15, \qquad (10b)$$

$$\langle y^3\rangle_n = (\tfrac{16}{35} + \tfrac{3}{7}|a_n|^{-3})(|a_n|/\beta)^3, \qquad (10c)$$

$$\langle y^4\rangle_n = (\tfrac{128}{315} + \tfrac{80}{63}|a_n|^{-3})(a_n/\beta)^4. \qquad (10d)$$

Then we obtain the perturbative solutions

$$\varepsilon'_n = -\alpha + \tfrac{1}{2}\beta^2|a_n| - \tfrac{4}{15}\gamma(a_n/\beta)^2 - \tfrac{2}{7}\lambda R(\tfrac{16}{5} + 3|a_n|^{-3})(|a_n|/\beta)^3 + \tfrac{8}{63}\lambda(\tfrac{8}{5} + 5|a_n|^{-3})(a_n/\beta)^4, \qquad (11)$$

to be compared with the lowest states $\varepsilon_{n-1}^{(+)} \approx \varepsilon_n^{(-)}$ for $n = 1, 2, \ldots$ and $R \approx (6\lambda)^{-1/2}$.

3.3. *Boxes whose walls are at the position of the minima, $R=(2\lambda)^{-1/2}$*

This time we make the change of variable $z=x-(2\lambda)^{-1/2}$, and the Hamiltonian becomes

$$H=-\tfrac{1}{2}(\mathrm{d}^2/\mathrm{d}z^2)-\tfrac{1}{2}[z+(2\lambda)^{-1/2}]^2+\tfrac{1}{2}\lambda[z+(2\lambda)^{-1/2}]^4$$
$$=-1/8\lambda-\tfrac{1}{2}(\mathrm{d}^2/\mathrm{d}z^2)+z^2+(2\lambda)^{1/2}z^3+\tfrac{1}{2}\lambda z^4. \qquad (12)$$

Again, the first term is constant and corresponds to the value of the potential at its minima. The next two terms correspond to a harmonic oscillator of frequency $\sqrt{2}$, which here and in § 3.4 we take as the unperturbed system. Then the perturbation consists of the anharmonic cubic and quartic terms. Notice that the linear term drops out because the origin has been shifted to the position of the minimum of the potential. Also, for small values of λ the boxes under consideration are even larger than those in § 3.2, so that the degeneracy of the lowest pairs of even–odd states is established, and the interval of the variable extends from $z=-(2\lambda)^{-1/2}\to-\infty$ to $z=0$.

The boundary condition, equation (3*a*), when the walls are at the position of the minima corresponds to $\psi(z=0)=0$, which means that we have to choose the odd functions of the harmonic oscillator as the unperturbed wavefunctions. Both boundary conditions at the centre of the box, equations (3*b*) and (3*c*), are also satisfied in practice by such functions because their gaussian exponential factors tend to vanish at $z=-(2\lambda)^{-1/2}\to-\infty$. Furthermore, the matrix elements of the perturbation can be directly calculated.

Since the coefficients of the cubic and quartic terms in equation (12) are of order $\lambda^{1/2}$ and λ, respectively, we have to be consistent in the inclusion of the terms in the perturbation series. Thus, in order to include all the terms of order λ, we take the quartic terms in first order of perturbation theory but the cubic term up to second order. This can be appreciated in the successive terms of the following expression for the lowest states:

$$\varepsilon^m=-1/8\lambda+3\sqrt{2}/2-4(2\lambda/\pi)^{1/2}2^{-3/4}+15\lambda/16-1.958\,486\,406\lambda$$
$$=-1/8\lambda+2.121\,320\,344-1.897\,699\,993\sqrt{\lambda}-1.020\,986\,406\lambda, \qquad (13)$$

to be compared with $\varepsilon_0^{(+)}\approx\varepsilon_1^{(-)}$ for $R=(2\lambda)^{-1/2}$.

3.4. *Very large boxes, $R\gg\lambda^{-1/2}$*

In this case, the Hamiltonian in the form of equation (12), with the variable in the interval from $z=-(2\lambda)^{-1/2}\to-\infty$ to $z=R\to\infty$, allows us to choose the complete harmonic oscillator as the unperturbed system. Again, the corresponding wavefunctions in practice satisfy the boundary conditions equations (3*a*), (3*b*) and (3*c*), because of their gaussian exponential factors. In addition, since these wavefunctions and also the cubic and quartic terms in the perturbation have well defined parities, the corresponding selection rules automatically eliminate some terms in the perturbation series. For instance, in the energy of the lowest states including all the terms of order λ^2,

$$\varepsilon^l=-1/8\lambda+\tfrac{1}{2}\sqrt{2}+3\lambda/16-11\lambda/16-21\lambda^2/2^7\sqrt{2}+171\lambda^2/2^6\sqrt{2}-465\lambda^2/2^7\sqrt{2}$$
$$=-1/8\lambda+\sqrt{1/2}-\tfrac{1}{2}\lambda+(9/8\sqrt{2})\lambda^2, \qquad (14)$$

the cubic term does not contribute in first or third order by itself, but it does lower the energy in second and fourth order, while the quartic term makes a positive contribution

Table 1. Exact (variational) eigenvalues of the lowest states of the two-well oscillator in symmetric boxes of different sizes.

λ \ R		0.1	0.5	1.0	2.0	4.0	8.0	15.0
0.01	$\varepsilon_0^{(+)}$	123.369 401 6	4.918 469 4	1.167 968 1	0.007 536 348 8	−3.214 392 44	−11.568 330 8	−11.797 975 7
	$\varepsilon_1^{(-)}$	493.478 806 7	19.703 901 7	4.793 484 5	0.642 611 427 0	−3.214 363 36	−11.568 330 8	−11.797 975 7
	$\varepsilon_2^{(+)}$	1110.328 941 1	44.374 418 8	10.948 811 0	2.180 821 111 6	−0.966 319 19	−9.781 727	−10.414 903
	$\varepsilon_3^{(-)}$	1973.919 277 0	78.916 809 0	19.579 907 8	4.318 148 131	−0.939 142 67	−9.781 727	−10.414 903
	$\varepsilon_4^{(+)}$	3084.249 749 3	123.329 461 1	30.680 946 9	7.082 911 143	0.167 268 02	−7.987 470	−9.064 956
	$\varepsilon_5^{(-)}$	4441.320 342 1	177.611 976 8	44.250 410 3	10.469 083 86	0.710 174 98	−7.987 470	−9.064 956
0.20	$\varepsilon_0^{(+)}$	123.369 402 0	4.918 713 9	1.171 979 3	0.097 617 547 92	−0.154 122 690	−0.154 124 483	−0.154 124 825
	$\varepsilon_1^{(-)}$	493.478 807 8	19.704 579 5	4.804 453 5	0.842 803 682 44	0.142 771 618	0.142 765 101	0.142 765 09
	$\varepsilon_2^{(+)}$	1110.328 942 6	44.375 357 1	10.963 838 1	2.416 597 187 36	1.010 215 375	1.010 188 899	1.010 188 9
	$\varepsilon_3^{(-)}$	1973.919 278 6	78.917 851 7	19.596 570 3	4.578 256 746 11	1.949 245 007	1.949 137 37	1.949 137 4
	$\varepsilon_4^{(+)}$	3084.249 751 0	123.330 554 6	30.698 417 7	7.356 954 871 49	3.058 959 419	3.058 567 34	3.058 57
	$\varepsilon_5^{(-)}$	4441.320 343 9	177.613 098 4	44.268 335 3	10.751 515 516 54	4.289 961 687	4.288 658 66	4.288 66
1.00	$\varepsilon_0^{(+)}$	123.369 403 61	4.919 743 045	1.188 743 519	0.343 424 175 3	0.328 826 502	0.328 826 501	0.328 826 6
	$\varepsilon_1^{(-)}$	493.478 812 39	19.707 433 577	4.850 433 229	1.492 371 909 4	1.417 268 100	1.417 268 099	1.417 269
	$\varepsilon_2^{(+)}$	1110.328 948 93	44.379 307 622	11.027 016 336	3.332 364 017	3.081 950 626	3.081 950 62	3.081 96
	$\varepsilon_3^{(-)}$	1973.919 285 6	78.922 242 156	19.666 726 856	5.661 517 480	5.019 323 058	5.019 323 05	5.019 4
	$\varepsilon_4^{(+)}$	3084.249 758 4	123.335 158 718	30.772 007 695	8.529 861 78	7.186 203 249	7.186 203 24	7.186
	$\varepsilon_5^{(-)}$	4441.320 351 4	177.617 821 38	44.343 843 546	11.970 416 04	9.542 859 34	9.542 857 33	9.543

in first order and a negative one in second order. In addition, both the cubic and quartic terms combine the products of two matrix elements of the former with one of the latter to make a positive contribution in third order. The energies in equation (14) are to be compared with $\varepsilon_0^{(+)} \approx \varepsilon_1^{(-)}$ for $R \gg \lambda^{-1/2}$.

4. Numerical results and discussion

In this section, we discuss illustrative samples of the numerical results obtained with the several approximations in each region in which the original problem was separated. Comparison with the exact (variational) results is also made through the tables.

In table 1, we present the exact results for the first six energy levels, for several values of R and λ. We have used different dimensions for the matrices (6) to be diagonalised, namely, for $R \leqslant 1$ and $\lambda = 0.01$, 0.20 we diagonalised matrices of dimensions up to 10; for $R > 1$, we diagonalised matrices of dimensions up to 35, for all values of λ considered; finally, for $R \leqslant 0.5$ and $\lambda = 1$, the greatest dimension was taken as 25. We used different dimensions in order to ensure convergence of the eigenvalues up to the number of decimals shown in the table. For $R = 15$ and $\lambda = 0.01$, 0.20, we have already obtained, up to the shown precision, the four exact energy levels of Banerjee and Bhatnagar (1978), which correspond to the asymptotic condition $R = \infty$.

Table 2. Comparison of perturbative eigenvalues for very small boxes with exact eigenvalues for the lowest states. The first two levels are the perturbative ε_+^s and ε_-^s as given by equations (8). The second pair of levels are the corresponding exact ones.

R \ λ	0.01		0.20		1.00	
0.1	123.369 4016	123.369 4016	123.369 4020	123.369 4020	123.369 4036	123.369 4036
	493.478 8067	493.478 8067	493.478 8078	493.478 8078	493.478 8124	493.478 8124
0.2	30.839 9002	30.839 9002	30.839 9065	30.839 9065	30.839 9328	30.839 9328
	123.364 4024	123.364 4024	123.364 4198	123.364 4198	123.364 4928	123.364 4928
0.3	13.701 9040	13.701 9040	13.701 9357	13.701 9357	13.702 0688	13.702 0688
	54.818 4195	54.818 4195	54.818 5073	54.818 5073	54.818 8769	54.818 8769
0.4	7.700 1760	7.700 1760	7.700 2760	7.700 2760	7.700 6972	7.700 6972
	30.819 9123	30.819 9123	30.820 1898	30.820 1898	30.821 3583	30.821 3583
0.5	4.918 4694	4.918 4694	4.918 7139	4.918 7139	4.919 7430	4.919 7430
	19.703 9017	19.703 9017	19.704 5795	19.704 5795	19.707 4336	19.707 4336
0.6	3.403 4207	3.403 4207	3.403 9285	3.403 9285	3.406 0661	3.406 0660
	13.656 9508	13.656 9508	13.658 3576	13.658 3576	13.664 2800	13.664 2800
0.7	2.485 7168	2.485 7168	2.486 6605	2.486 6605	2.490 6305	2.490 6305
	10.001 8418	10.001 8418	10.004 4517	10.004 4517	10.015 4351	10.015 4351
0.8	1.885 7652	1.885 7652	1.887 3826	1.887 3826	1.894 1795	1.894 1793
	7.620 2616	7.620 2616	7.624 7233	7.624 7233	7.643 4873	7.643 4872
0.9	1.469 9778	1.469 9778	1.472 5857	1.472 5856	1.483 5242	1.483 5230
	5.977 9464	5.977 9464	5.985 1143	5.985 1143	6.015 2237	6.015 2231
1.0	1.167 9680	1.167 9681	1.171 9795	1.171 9793	1.188 7486	1.188 7435
	4.793 4845	4.793 4845	4.804 4537	4.804 4535	4.850 4358	4.850 4332

Table 3. Comparison of perturbative eigenvalues for boxes whose walls are in the vicinity of inflection points of the potential with exact eigenvalues for lowest states. The central column for each λ corresponds to the inflection point of the potential; the other two correspond to neighbouring values.

λ		0.0025			0.01			0.20	
R	7.50	8.16	8.50	3.50	4.08	4.50	0.80	0.91	1.00
$\varepsilon_0^{(+)}$	−18.533 47	−22.058 30	−23.866 17	−2.052 08	−3.418 81	−4.492 13	1.887 38	1.428 55	1.171 98
$\varepsilon_1^{(-)}$	−18.533 47	−22.058 30	−23.866 17	−2.050 88	−3.418 80	−4.492 13	7.624 72	5.811 65	4.804 45
ε_1^{i}	−18.532 29	−22.058 07	−23.866 15	−2.029 85	−3.413 12	−4.491 35	0.244 92	0.266 89	0.272 92
$\varepsilon_2^{(+)}$	−14.450 52	−17.853 03	−19.619 5	−0.251 70	−1.119 69	−2.000 14	17.255 96	13.205 51	10.963 84
$\varepsilon_3^{(-)}$	−14.450 52	−17.853 03	−19.619 5	−0.017 07	−1.102 68	−1.999 03	30.747 13	23.565 71	19.596 57
ε_2^{i}	−14.441 29	−17.850 26	−19.618 6	0.082 86	−1.032 49	−1.974 14	1.992 40	1.617 03	1.450 82
$\varepsilon_4^{(+)}$	−11.239 49	−14.501 10	−16.213 8	0.905 72	0.077 51	−0.400 02	48.094 93	36.888 35	30.698 42
$\varepsilon_5^{(-)}$	−11.239 49	−14.501 10	−16.213 8	1.916 88	0.540 38	−0.265 64	69.298 55	53.172 48	44.268 34
ε_3^{i}	−11.207 98	−14.489 28	−16.208 4	1.474 86	0.637 56	−0.149 76	10.823 84	9.178 86	8.523 17

We can see from table 1 that for small λ, and R not too large, e.g. $R = 15$, we have already obtained the degeneracy by pairs of the even and odd lowest levels, as it should be. We also note that for small R the energy levels are quite independent of the λ considered, due to the dominance, in this case, of the quadratic term of the Hamiltonian.

In table 2, we show in the first column, for each λ, the first two energy levels for several R as obtained from the perturbative expansion given by equation (8). These values should be compared with the corresponding exact ones shown in the second column. We observe the monotonic increase of the energy as the size of the box diminishes, due to the dominance of the kinetic energy term. We call attention to the fact that the perturbative and exact values almost coincide for relatively small values of R and λ.

In table 3, we show the lowest perturbative eigenvalues of the potential having the cut-off at its inflection points, as obtained from expression (11), for comparison with the eigenvalues associated with the two exact parity states. As an illustration of the behaviour of the levels, we also show them for two neighbouring boxes. We see that for very small values of λ (which correspond to relatively large values of the box) this 'perturbation' method gives very good results, especially for the first two levels. For $\lambda = 0.20$, which corresponds to a small box, the results are bad and in this case the perturbative expansion (8) has proved better, as shown in table 2.

Table 4. Comparison of perturbative eigenvalues for boxes whose walls are at the minima of the potential with exact eigenvalues for lowest states.

λ	R_m	ε_0^m	$\varepsilon_0^{(+)}$	$\varepsilon_1^{(-)}$
0.0025	14.1	−47.976 117 12	−47.976 323 76	−47.976 323 76
0.01	7.1	−10.578 659 52	−10.580 532 79	−10.580 532 79
0.02	5.0	−4.417 474 691	−4.423 476 899	−4.423 476 718
0.03	4.1	−2.404 667 196	−2.417 160 572	−2.416 959 822
0.04	3.5	−1.424 059 111	−1.448 297 740	−1.442 983 384
0.05	3.2	−0.854 067 5953	−0.904 323 755	−0.872 290 6617
0.07	2.7	−0.237 947 2151	−0.383 352 0439	−0.205 742 1169
0.10	2.2	0.169 116 2735	−0.077 916 5382	0.391 453 0158
0.15	1.8	0.399 863 0023	0.173 102 6141	1.095 080 5124
0.20	1.6	0.443 445 8252	0.350 304 6718	1.687 958 2983

In table 4, we show the lowest perturbative eigenvalue associated with the boxes passing through the minimum of the potential as obtained from expression (13), for comparison with the two lowest eigenvalues associated with the two exact parity states. As the difference between the perturbative and exact levels is proportional to $\lambda^{3/2}$, we see that the levels tend to coincide as λ becomes smaller and smaller.

In table 5, we show the perturbative energy levels for very large boxes as given by expression (14), for comparison with the exact values and with the asymptotic values given in Abramowitz and Stegun (1971). We have taken $R = 15$ for the biggest box representing an asymptotic condition. As the difference between the perturbative and exact values is proportional to λ^3, we see that the levels tend to coincide as λ decreases.

As a general final comment, we should stress that all the perturbative solutions discussed here cannot be valid for larger values of λ or for highly excited states. This is

Table 5. Comparison of perturbative eigenvalues for very large boxes with exact eigenvalues for lowest states. The last two columns show values from Banerjee and Bhatnagar (1978).

λ	ε_0^{l}	$\varepsilon_0^{(+)}$	$\varepsilon_1^{(-)}$	ε_0	ε_1
0.0025	−49.294 148 19	−49.294 148 19	−49.294 148 19	—	—
0.01	−11.797 972 77	−11.797 975 7	−11.797 975 7	−11.797 975 70	−11.797 975 70
0.02	−5.553 211 417	−5.553 236	−5.553 236 2	−5.553 236 208	−5.553 236 207
0.03	−3.475 275 831	−3.475 365	−3.475 363 7	−3.475 365 945	−3.475 363 775
0.04	−2.439 166 011	−2.439 438	−2.439 346	−2.439 438 882	−2.439 345 769
0.05	−1.819 881 957	−1.820 789	−1.819 933	−1.820 788 948	−1.819 933 201
0.07	−1.117 505 431	−1.124 08	−1.114 031	−1.124 027 249	−1.114 031 478
0.10	−0.600 848 1701	−0.632 75	−0.576 53	−0.632 746 4185	−0.576 529 5655
0.15	−0.219 125 1925	−0.302 08	−0.122 79	−0.302 083 7093	−0.122 789 8883
0.17	−0.136 177 1457	−0.231 71	−0.003 18	−0.231 711 5381	−0.003 181 5516
0.20	−0.049 713 024	−0.154 12	+0.142 77	−0.154 124 8290	+0.142 765 1020

mainly due to the fact that the eigenfunctions of the several unperturbed systems considered do not satisfy in practice the proper boundary condition at the centre of the potential. Had we taken the eigenfunctions which satisfy this condition, we would obtain perturbative solutions which are good also for larger values of λ. Clearly, we should distinguish between states of different parity which are no longer degenerate. We can use such eigenfunctions as trial ones for an alternative variational analysis of the problem. In fact, an obvious suggestion is to use the eigenfunctions associated with the double oscillator in both situations of free and boxed systems.

Appendix

We give below explicit expressions for the sums S_i, $i = 1, 2, \ldots, 11$, appearing in the expression (8).

$$S_1 = \sum_M{}' (N|x^2|M)^2/(M^2 - N^2)$$

$$S_2 = \sum_M{}' (N|x^2|M)(M|x^4|N)/(M^2 - N^2)$$

$$S_3 = \sum_M{}' (N|x^4|M)^2/(M^2 - N^2)$$

$$S_4 = \sum_{\substack{M,P \\ M \neq P}}{}' (N|x^2|P)(P|x^2|M)(M|x^2|N)/(M^2 - N^2)(P^2 - N^2)$$

$$S_5 = \sum_M{}' (N|x^2|M)^2(M|x^2|M)/(M^2 - N^2)^2$$

$$S_6 = \sum_{\substack{M,P \\ M \neq P}}{}' (N|x^2|P)(P|x^2|M)(M|x^4|N)/(P^2 - N^2)(M^2 - N^2)$$

$$S_7 = \sum_{\substack{M,P \\ M \neq P}}{}' (N|x^2|P)(P|x^4|M)(M|x^2|N)/(P^2 - N^2)(M^2 - N^2)$$

$$S_8 = \sum_M{}' (N|x^2|M)(M|x^2|M)(M|x^4|N)/(M^2-N^2)^2$$

$$S_9 = \sum_M{}' (N|x^2|M)^2(M|x^4|M)/(M^2-N^2)^2$$

$$S_{10} = \sum_M{}' (N|x^2|M)^2/(M^2-N^2)^2$$

$$S_{11} = \sum_M{}' (N|x^2|M)(M|x^4|N)/(M^2-N^2)^2.$$

References

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