Inner product perturbation theory: Energy levels of double-well potentials for two-dimensional quantum systems by expanding the potential functions around their minima

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Energy eigenvalues of double-well potentials for two-dimensional systems are calculated by the approach of expanding the potential functions such as $V(x, y; Z^2, \lambda) = -Z^2[x^2 + y^2] + \lambda[x^4 + 2x^2y^2 + y^4]$ around their minima, using the inner product technique, for various values of perturbation parameters Z^2 and λ. Some of the results calculated by the inner product technique are compared with the results produced by other means.

1. Introduction

The double-well potential for one-dimensional quantum system has been the subject of intensive study in the last two decades. The literature on this topic, voluminous as it is, has recently been thoroughly referenced by several workers [1–9,11,14,19,20]. Unfortunately, comparable study have not been extended to multidimensional systems in spite of some progress that has been made to calculate their energy eigenvalues [12,15–18].

The numerical solution of the Schrödinger equation, by the approach of expanding some potentials around their minima in one-dimensional space is now customary. Different techniques are competing. For example, hypervirial perturbation theory [19], inner product perturbation theory [18], and so on. In contrast to the potential functions in multidimensional space, which have not been treated by the same approach by any worker in the past.

In this work, the general form of Schrödinger equation for the double-well potential in two-dimensional system can be written as

$$\left[-\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial y^2} + V(x, y; Z^2, \lambda) \right] \Psi(x, y) = E\Psi(x, y). \tag{1}$$

In the present paper, the inner product technique is applied to a double-well potential in two-dimensions,

$$V\left(x, y; Z^2, \lambda\right) = -Z^2\left[x^2 + y^2\right] + \lambda\left[x^4 + 2x^2y^2 + y^4\right]. \tag{2}$$

The depth of the double-well is controlled by the parameters Z^2 and λ. If the potential barrier between the two wells were of infinite height, the two wells would be totally "disconnected" and the energy spectrum would consist of same set of energy eigenvalues in each well. Thus, each energy eigenvalue of the system would be doubly degenerate.

Physically, when the potential well is very deep (for large Z^2/λ values) the classical turning points for the lowest bound states are very close to the minimum of each well; therefore the particle, even quantum mechanically, can in the main see only the region of the potential near the minima. The lower levels for this potential have therefore very nearly degenerate eigenvalues.

The eigenvalue spectrum of the Schrödinger equation (2) with $V(x, y; Z^2, \lambda)$ has the feature that the lower eigenvalues are closely bunched in one group if the values of the Z^2/λ are sufficiently large. As Z^2/λ increases, the magnitude of the splitting between these levels decreases, i.e.,

$$|E_{11} - E_{00}| \approx |E_{11} - E_{10}| = \Delta E \cong 0. \tag{3}$$

The splitting ΔE will be small at the bottom of the well and will increase as the levels approach the top of the barrier. When ΔE has its minimum value, the nearly degenerate eigenfunctions have equal weight in each potential well.

The paper is organized as follows. Section 2 is concerned with the inner product technique and its use to calculate the energy eigenvalues for the double-well potentials in two dimensions for several eigenstates. Section 3 contains a discussion of the numerical results.

2. The double-well potential in two-dimensions $V(X, Y; Z^2, \lambda)$ and the recurrence relation

The inner product technique is perturbative technique used to treated the perturbed oscillator in one, two and three dimensions with even parity. In this work, we modify and extend the inner product technique to treat a potential functions with mixed parity.

The idea of expanding the double-well potential function $V(x, Z^2, \lambda)$ around its minimum using a Taylor series has been used by Witwit and Killingbeck [19] and applied to the double-well potential in a one-dimensional system to calculate the energy eigenvalues. We have since established that the idea can be extended quite easily to apply to a double-well in multidimensional quantum systems.

Most of the ideas of a potential function in one dimension may be easily generalized to the potential function of two or more variables but the labour is greatly increased. If the potential function V has more than one independent variable, say

$V = V(x, y)$, the Taylor expansions of $V(x - x_m, y - y_m)$ around $x = x_m$ and $y = y_m$ can be written as

$$V(x - x_m, y - y_m) = V(x_m, y_m) + (x - x_m)\frac{\partial V}{\partial x} + (y - y_m)\frac{\partial V}{\partial y}$$
$$+ \frac{1}{2!}\left[(x - x_m)^2\frac{\partial^2 V}{\partial x^2} + 2(x - x_m)(y - y_m)\frac{\partial^2 V}{\partial x \partial y}\right.$$
$$\left. + (y - y_m)^2\frac{\partial^2 V}{\partial y^2}\right]$$
$$+ \frac{1}{3!}\left[(x - x_m)^3\frac{\partial^3 V}{\partial x^3} + 3(x - x_m)^2(y - y_m)\frac{\partial^3 V}{\partial x^2 \partial y}\right.$$
$$\left. + 3(x - x_m)(y - y_m)^2\frac{\partial^3 V}{\partial x \partial y^2} + (y - y_m)^3\frac{\partial^3 V}{\partial y^3}\right]$$
$$+ \frac{1}{4!}\left[(x - x_m)^4\frac{\partial^4 V}{\partial x^4} + 4(x - x_m)^3(y - y_m)\frac{\partial^4 V}{\partial x^3 \partial y}\right.$$
$$+ 4(x - x_m)^2(y - y_m)^2\frac{\partial^4 V}{\partial x^2 \partial y^2}$$
$$\left. + (x - x_m)(y - y_m)^3\frac{\partial^4 V}{\partial x \partial y^3} + (y - y_m)^4\frac{\partial^4 V}{\partial y^4}\right] \qquad (4)$$

with all derivatives evaluated at the point (x_m, y_m). For example, at $(Z^2 = 1, \lambda = 4)$ and $(Z^2 = 16, \lambda = 4)$, and replacing $x = x - x_m$, $y = y - y_m$, the equation (4) takes the following two forms, respectively:

$$V(x, y; Z^2 = 1, \lambda = 4) = -\frac{1}{16} + [x^2 + y^2] + 4[x^3 + y^3] + 4[x^4 + y^4]$$
$$+ [x + 2x^2][2y + 4y^2], \qquad (5)$$

$$V(x, y; Z^2 = 3, \lambda = 12) = -\frac{3}{16} + 3[x^2 + y^2] + 12[x^3 + y^3] + 12[x^4 + y^4]$$
$$+ [x + 2x^2][6y + 12y^2]. \qquad (6)$$

The general form for the expansion of the potential $V(x, y; Z^2, \lambda)$ when $Z^2 = \lambda$ can be expressed as

$$V(x, y; Z^2, \lambda) = -\frac{Z^2}{4} + Z^2[x^2 + 2x^3 + x^4 + y^2 + 2y^3 + y^4] + 2Z^2[x + x^2][y + y^2]. \quad (7)$$

The energy perturbation series is expected to be divergent, so we start by introducing a renormalized parameter β, and write the potential in equation (4) $V(x, y; Z^2, \lambda)$ in a renormalized form,

$$V_\beta^r(x, y; Z^2, \lambda) = [\mu_x^2 - \underline{\lambda}\beta]x^2 + [\mu_y^2 - \underline{\lambda}\beta]y^2 + C(x^3)x^3 + C(y^3)y^3$$

$$+ C(x^4)x^4 + C(y^4)y^4 + C(xy)xy + C(xy^2)xy^2$$
$$+ C(x^2y)x^2y + C(x^2y^2)x^2y^2 + V(x_m, y_m). \qquad (8)$$

The double-well potential given by equation (8) in two dimensions is in general non-separable in Cartesian coordinates, showing symmetrical behaviour, and due to this behaviour a great deal of computation is not required to arrive at our results:

$$\mu_x^2 = C(x^2) + \underline{\lambda}\beta, \qquad \mu_y^2 = C(y^2) + \underline{\lambda}\beta, \quad \underline{\lambda} = 1, \qquad (9)$$

where $C(x^N y^M)$ $(N, M = 0, 1, \ldots, 4)$ are the coefficients of the expanded potential.

The double-well potential has minimum at ($x = x_m$ and $y = y_m$), the probability of finding the particle is locally maximal at $x = x_m$ and $y = y_m$. Its low energy levels should involve wave functions which present the maximal probability density at a position close to the minimum of the two-well potential. In this case we expand $V(x, y; Z^2, \lambda)$ around the minimum.

The central idea of this work is to expand the potential $V(x, y; Z^2, \lambda)$ in a Taylor series about its minimum value, and solve the resulting approximate problem by inner product theory. The expanded potential $V_\beta^\tau(x, y; Z^2, \lambda)$ of equation (8) is of mixed parity type. It is clear from equation (8), that we can regard the first two terms as unperturbed terms and the other terms as the perturbation.

To find the recurrence relations which allow us to calculate the eigenvalues for the Schrödinger equation (1) we use the reference function

$$\Phi(x, y) = (x^I y^J) \exp\left[-\frac{1}{2}(\mu_x x^2 + \mu_y y^2)\right], \qquad (10)$$

where I and J are non-negative integers. The methods of calculation used by the author start from the equation

$$EW(I, J) = \langle \Psi | H | \Phi \rangle, \qquad (11)$$
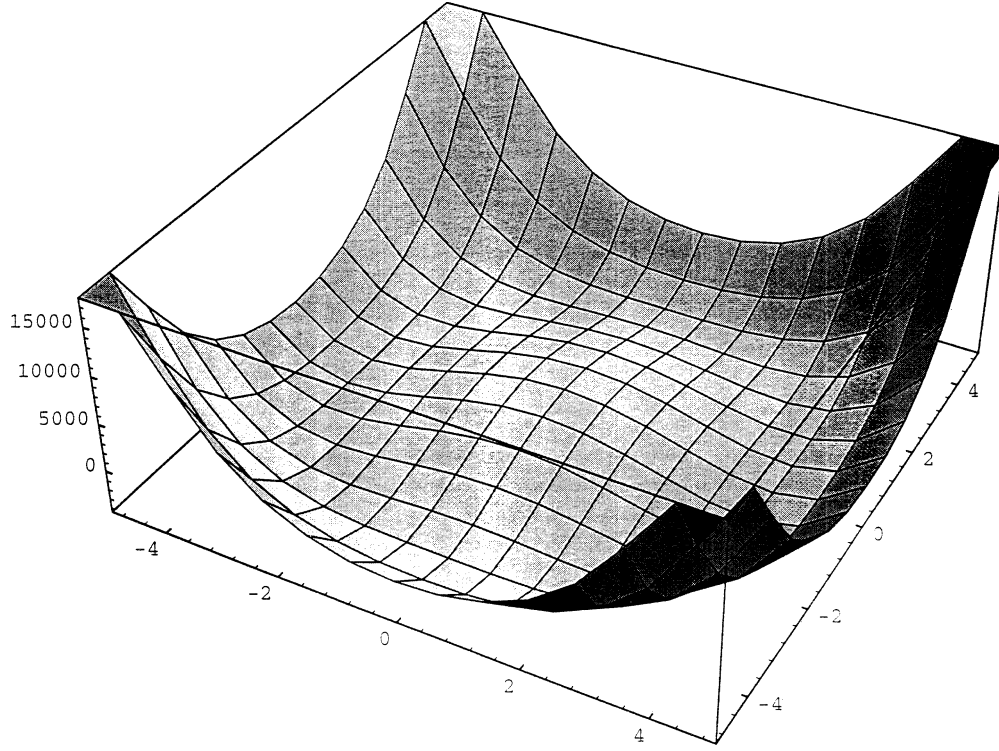
obtained by taking the inner product of the Schrödinger equation (1) with the reference function (10). The $W(I, J)$, sometimes called moments, are defined by

$$W(I, J) = \langle \Phi | \psi \rangle. \qquad (12)$$

Then substituting the perturbation expansions

$$W(I, J) = \sum_M W(I, J, M)\underline{\lambda}^M, \qquad (13)$$

$$E = \sum_N E(N)\underline{\lambda}^N \qquad (14)$$

Figure 1. Double-well potential $V(x, y; Z^2 = 625, \lambda = 25)$.

into the $W(I, J)$ recurrence relation given by equation (11) leads to a recurrence relations for the coefficients. For the renormalized potential $V_\beta^r(x, y; Z^2, \lambda)$ given by equation (8) the relation can be written as

$$
\sum_{N=0}^{M=60} E(N) W(I, J, M - N)
$$

$$
\begin{aligned}
&= C(x^3) W(I + 3, J, M - 1) + C(y^3) W(I, J + 3, M - 1) \\
&\quad + C(x^4) W(I + 4, J, M - 1) + C(y^4) W(I, J + 4, M - 1) \\
&\quad + C(xy) W(I + 1, J + 1, M - 1) - C(xy^2) W(I + 1, J + 2, M - 1) \\
&\quad + C(x^2 y) W(I + 2, J + 1, M - 1) + C(x^2 y^2) W(I + 2, J + 2, M - 1) \\
&\quad - \beta \big[S(I + 1, J, M - 1) + S(I, J + 1, M - 1) \big] \\
&\quad + \big[\mu_x(2I + 1) + \mu_y(2J + 1) \big] W(I, J, M) \\
&\quad - I(I - 1) W(I - 2, J, M) - J(J - 1) W(I, J - 2, M).
\end{aligned}
\tag{15}
$$

The unperturbed energy can be expressed as

$$
E(0) = \mu_x(2n_x + 1) + \mu_y(2n_y + 1) + V(x_m, y_m)
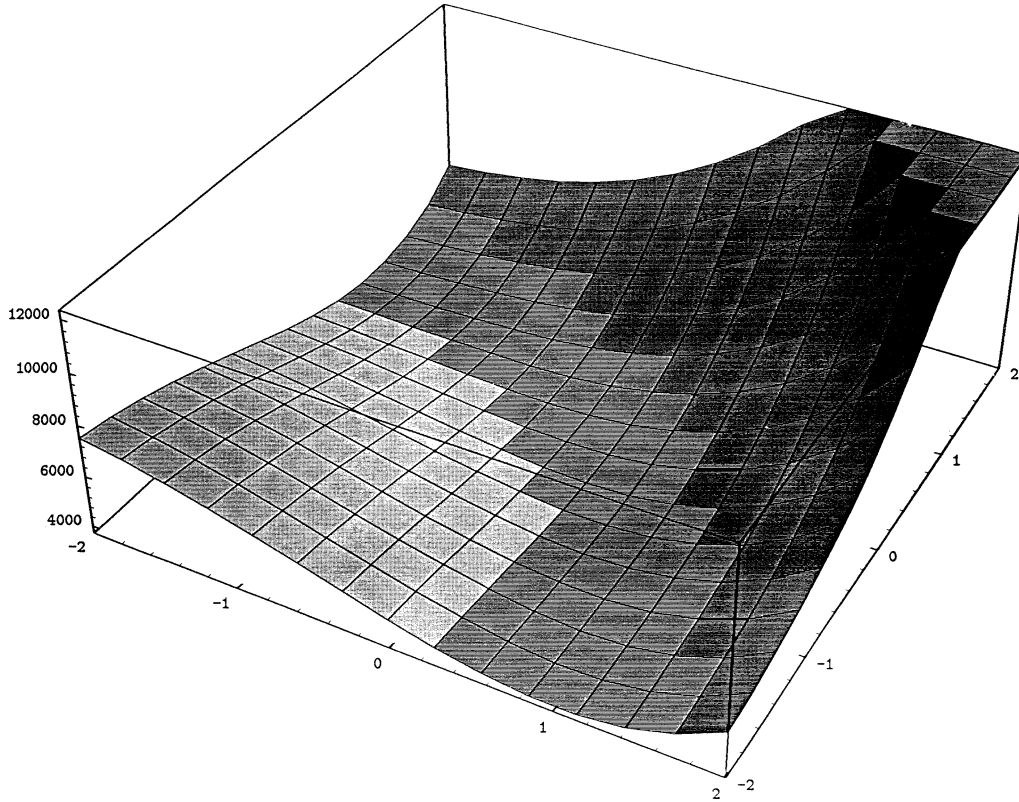\tag{16}
$$

Figure 2. The expanded double-well potential $V(x, y; Z^2 = 625, \lambda = 25)$ around their minima $x_m = y_m = 2.5$.

and the initial coefficient to start our calculations is given as

$$W(n_x, n_y, 0) = 1, \quad n_x, n_y = 0, 1. \tag{17}$$

The indices are scanned in the order I, J, M as explained in [13] and the relation (15) is used to work out $W(I, J, M)$ in terms of lower-order elements that are already known. $E(N)$ is found from the relation (15) for the special case $I = n_x$, $J = n_y$, and the sum on the left-hand side becomes $E(N)$, because of the intermediate normalization convention $W(n_x, n_y, 0) = 1$ that we impose on the algorithm.

Up to 60 coefficient of the perturbation series for the double potential for three energy levels were computed according to

$$E_{n_x, n_y}(\underline{\lambda}) = \sum_{N=0}^{60} E(N) \underline{\lambda}^N. \tag{18}$$

We should point out that Aitken's transformation has been used in order to increase the accuracy of our results and to accelerate the rate of convergence of our calculations.

The power series method [13] can be used to compute the energy eigenvalues for the Schrödinger equation when potential (2) has a circular symmetry in two dimensions, i.e., $x = r \sin\theta$, $y = r \cos\theta$, $r^2 = x^2 + y^2$.

The general form for the Schrödinger equation in two dimensions can be written as

$$\left[-\frac{d^2}{dr^2} + \left(m^2 - \frac{1}{4} \right) r^{-2} + V\left(r; Z^2, \lambda\right) \right] \Psi(r) = E\Psi(r), \tag{19}$$

where m is the magnetic quantum number. The potential $V(r; Z^2, \lambda)$ can be expressed as

$$V\left(r; Z^2, \lambda\right) = -Z^2 r^2 + \lambda r^4. \tag{20}$$

The energy levels are then most appropriately characterized by the quantum numbers (n_r, l) rather than (n_x, n_y). The energies of the unperturbed levels are

$$E(0) = (4n_r + 2m + 2), \tag{21}$$

$$2n_r + m \equiv n_x + n_y, \tag{22}$$

where n_r is called the radial quantum number and l the angular momentum.

3. Results and discussion

The inner product technique has been applied in this paper for a double-well potentials on two-dimensional systems. In this paper we expand the potential functions around their minima at x_m and y_m in order to estimate the eigenvalues around their minima x_m, y_m. Eigenvalues for different values of Z^2, λ and state numbers n_x, n_y are listed in tables 1–3.

In table 1, we list the energy eigenvalues for a double potential in two-dimensional system $V(x, y; Z^2, \lambda)$ for the case $Z^2 = \lambda$, for the ground state E_{00} and the first two excited state E_{10} and E_{11}, over a wide range of $1/6 \leqslant Z^2 = \lambda \leqslant 5 \times 10^3$.

The energy eigenvalues for a double potential in a two-dimensional system $V(x, y; Z^2, \lambda)$ and their energy eigenvalues are quoted in tables 2 and 3 for the ground state E_{00} and the first two excited states E_{00} and E_{11}, for different values of Z^2 and λ lying between $0.25 \leqslant \lambda \leqslant 10^4$ and $0.25 \leqslant Z^2 \leqslant 625$. In the same tables, we listed the values of the minimum points x_m and y_m, and also we listed the values of these potentials $V(x_m, y_m)$ corresponding to these points, we also present the coefficients (A, B, C, D, E, F) of the expanding potential in table 3, which can be expressed as

$$V\left(x, y; Z^2, \lambda\right) = -V(x_m, y_m) + A\left[x^2 + y^2\right] + B\left[x^3 + y^3\right] + C\left[x^4 + y^4\right] + Dxy$$
$$+ E\left[x^2 y + xy^2\right] + Fx^2 y^2. \tag{23}$$

The general forms of the potentials (23) enable other workers in the future to study this problem in order to understand the typical features of their energy spectra.

Table 1

Eigenvalues of a double-well potential $V(x, y; Z^2, \lambda)$ for several sets of perturbation parameters for three eigenstates E_{00}, E_{10} and E_{11}. First line – power series method; <u>second line</u> – inner product technique.

Z^2	E_{00}	$E_{10} = E_{01}$	E_{11}
1/6	1.0843151777768309192	2.61649090835940491	4.439089607962285029
	<u>1.084315</u>	<u>2.61649</u>	<u>4.43908</u>
1	1.6374879527236908208	4.19968538748636154	7.328144388065296548
	<u>1.63748</u>	<u>4.19968</u>	<u>7.32814</u>
2	1.8044830442464193546	4.86881781300593481	8.676133945433321839
	<u>1.8044</u>	<u>4.8688</u>	<u>8.67613</u>
3	1.8488321914370639803	5.22422325263170673	9.474465483207472146
	<u>1.8488</u>	<u>5.2242</u>	<u>9.4744</u>
4	1.8385590283544875739	5.43724394566261425	10.020506633563638597
	<u>1.8385</u>	<u>5.4372</u>	<u>10.0205</u>
5	1.7968689041605638879	5.56732946175554058	10.418323520678918695
	<u>1.796</u>	<u>5.567</u>	<u>10.418</u>
6	1.7346246501862441306	5.64268198028411299	10.717618348733334183
	<u>1.734</u>	<u>5.642</u>	<u>10.717</u>
7	1.6578208954336511232	5.67904295688764262	10.946294283550039271
	<u>1.657</u>	<u>5.679</u>	<u>10.946</u>
8	1.5701260000887291455	5.68614299833470901	11.121689047527532774
	<u>1.570</u>	<u>5.686</u>	<u>11.122</u>
9	1.4739514548646148314	5.67043750462078796	11.255359002152461509
	<u>1.474</u>	<u>5.670</u>	<u>11.255</u>
10	1.3709684666267474547	5.63643781301499726	11.355415550499845011
	<u>1.371</u>	<u>5.636</u>	<u>11.355</u>
15	0.7871869197830882583	5.28296005117310908	11.516108578101458477
	<u>0.787</u>	<u>5.283</u>	<u>11.516</u>
20	0.1326082762362237966	4.74587424739272832	11.333999585344506495
25	−0.5646018123013606328	4.10489140261927649	10.956328072930601301
30	−1.2917235797372086225	3.39667660362108241	10.451760973533783270
35	−2.0418946945009686787	2.64116844530880466	9.858066497432172239
40	−2.8109577662735971057	1.85041586313421799	9.198286922415046065
45	−3.5961728350773893302	1.03225453866347263	8.487527481546965620
50	−4.3956121483598687690	0.19206498384905919	7.736229151400722751
60	−6.0317660261179082664	−1.53998339323537888	6.140159922629425277
70	−7.7112576514331486264	−3.32509459910430469	4.450515567992847895
80	−9.4285608314216875014	−5.15087752945364766	2.691667923680334379
90	−11.1795481987876144131	−7.00928422595450137	0.879427807681633035
100	−12.9609269649048695144	−8.89476918524743711	−0.975373241579171062
150	−22.2395988119109852032	−18.61734851058081198	−10.675569055062844518
200	−31.9843137660799431163	−28.67964434783808212	−20.809796825585514889
250	−42.0559962998298213887	−31.202833229778826495	−38.97510605095315706
300	−52.3678827136362476641	−41.775103082675892486	−49.44730794073281388
400	−73.5037724106590025923	−63.298132190341071527	−70.78987207245184340
500	−95.1183975652991801459	−85.183093550308476614	−92.52792314464256671
600	−117.0687809193023407232	−107.332160745065192644	−114.55905718073712544
700	−139.2708620634581284772	−129.686598805852351331	−136.81794904111663296
800	−161.6706545176345775351	−152.207257408023620635	−159.26001993510215814

Table 1
(Continued.)

| Z^2	E_{00}	$E_{10} = E_{01}$	E_{11}
900	-184.2311264703076048874	-174.866253309587203003	-181.85334567362862524
1000	-206.9255783668468765096	-197.642800253003109450	-204.57419684955686821
1500	-321.8416563257501696780	-312.827923845633274415	-319.57176725859997975
2000	-438.3504152100121300244	-429.489717801849096314	-436.12424871321182629
5000	$-1151.5572330234744599157$	-1143.03791006312355479	-1149.42396264921099512
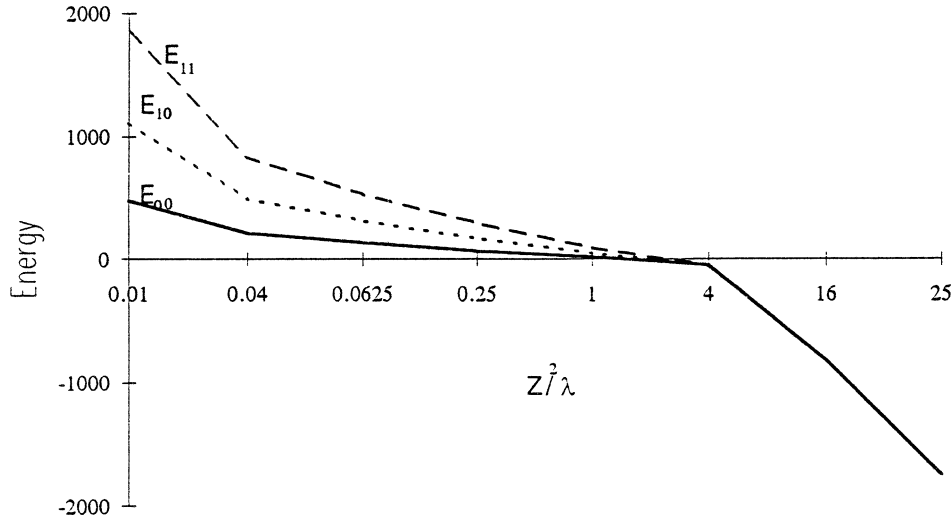
Figure 3. Graph of three energy levels E_{n_x, n_y} for the double-well potential $V(x, y; Z^2, \lambda)$. For small values of Z^2/λ, the positive energies are small, then it is necessary to multiply these energies by a factor of 10, in order to obtain a clear figure.

It is clear from our results in tables 2 and 3, that when Z^2/λ is large, the potential minimum occurs at large values of x and y, so that the wave function centered at x_m and y_m does not penetrate too much into left-hand well; obviously, this is not the case for small Z^2/λ.

In tables 2 and 3 emphasis is specially placed on the larger values of the depth Z^2 because for the three states E_{00}, E_{10} and E_{11} have almost degenerate eigenvalues. As Z^2/λ increases, the magnitude of the splitting between these levels decreases, i.e., $|E_{10} - E_{00}| \approx |E_{11} - E_{00}| = \Delta E \approx 0$, as is clear from the results listed in tables 2 and 3 and figure 3, and this confirmed the results conjectured by the previous works [17,18].

In tables 1–3 we compare the results obtained by the inner product technique with those obtained by power series method. The agreement between the two methods is in general good, but at large values of Z^2, the inner product technique faces difficulties in producing the eigenvalues, due to the convergence problem, while the power series is able to give high accuracy, and the accuracy seems insensitive to higher values of Z^2.

Table 2
Eigenvalues of a double-well potential $V(x, y; Z^2, \lambda)$ for several sets of perturbation parameters for two
eigenstates E_{00} and E_{10}. First line – power series method; <u>second line</u> – inner product technique.

Z^2	λ	x_m	y_m	$-V(x_m, y_m)$	E_{00}	$E_{10} = E_{01}$
1/4	1	1/4	1/4	1/64	2.1787811759361418227	5.10862071412588021162
					<u>2.178781</u>	<u>5.108621</u>
1	1/4	1	1	1	0.1651653292236315486	1.29666328921032645832
					<u>0.16516</u>	<u>1.29666</u>
1	4	1/4	1/4	1/16	3.2988377079349240454	7.83701536032146873650
					<u>3.298837</u>	<u>7.837015</u>
4	1	1	1	4	−1.6746781702247934097	−0.56212069832440285085
					<u>−1.674</u>	<u>−0.5621</u>
$4\sqrt{2}$	$\sqrt{2}$	1	1	$4\sqrt{2}$	−2.8174073854179428693	−1.77619140084241815847
					<u>−2.817</u>	<u>−1.776</u>
$\sqrt{2}$	$4\sqrt{2}$	1/4	1/4	$1/(8\sqrt{2})$	3.6425216866654988021	8.69439952226333190438
					<u>3.64252</u>	<u>8.694399</u>
$\sqrt{3}$	$\sqrt{3}/4$	1	1	$\sqrt{3}$	−0.2389804937470944807	0.93186626245449553365
					<u>−0.238</u>	<u>0.931</u>
$4\sqrt{3}$	$\sqrt{3}$	1	1	$4\sqrt{3}$	−3.73128645772	−2.74168983870226523053
					<u>−3.731</u>	<u>−2.7416</u>
$\sqrt{5}$	$\sqrt{5}$	1/2	1/2	$\sqrt{5}/4$	1.8220774473995417074	4.97114476287340423439
					<u>1.8221</u>	<u>4.9711</u>
$4\sqrt{5}$	$\sqrt{5}$	1	1	$4\sqrt{5}$	−5.2322437042274371274	−4.31339791060492395451
					<u>−5.232</u>	<u>−4.313</u>
$4\sqrt{7}$	$\sqrt{7}$	1	1	$4\sqrt{7}$	−6.4901059947471383543	−5.61858663113509389619
					<u>−6.490</u>	<u>−5.618</u>
$\sqrt{7}$	$4\sqrt{7}$	1/4	1/4	$\sqrt{7}/16$	4.3281447185753846384	10.44233030057788965314
					<u>4.3281</u>	<u>10.44233</u>
4	16	1/4	1/4	1/4	4.8211659516406174280	11.73852456988894350935
					<u>4.8211</u>	<u>11.73852</u>
2	8	1/4	1/4	1/8	4.0119688764113039501	9.62939034169658128114
					<u>4.0119</u>	<u>9.62939</u>
8	2	1	1	8	−4.5221383627768976017	−3.57193644204140065221
					<u>−4.522</u>	<u>−3.572</u>
8	32	1/4	1/4	1/2	5.6939636162457358656	14.15336720753876425017
					<u>5.6939</u>	<u>14.15336</u>
16	64	1/4	1/4	1	6.5499518108947632830	16.79874154994544617789
					<u>6.54995</u>	<u>16.79874</u>
16	256	1/8	1/8	1/4	13.1953508317396961818	31.34806144128587494601
					<u>13.19535</u>	<u>31.348061</u>
25	625	1/10	1/10	1/4	18.0916528697467783409	42.76185477063849179901
					<u>18.091652</u>	<u>42.761854</u>
100	400	1/4	1/4	25/4	6.8664669974978532132	22.61989308848137033303
					<u>6.8665</u>	<u>22.61989</u>
40	10^3	1/10	1/10	2/5	20.7595245052678659655	49.33297281720582128802
					<u>20.759524</u>	<u>49.332972</u>
10^2	10^4	1/20	1/20	1/4	47.4432730968702205018	110.92285334174981146371
					<u>47.44327</u>	<u>110.922853</u>

Table 2
(Continued.)

Z^2	λ	x_m	y_m	$-V(x_m, y_m)$	E_{00}	$E_{10} = E_{01}$
16	4	1	1	16	-10.8205188690327884519	-10.05581964986195411208
32	8	1	1	32	-24.4341897872129731821	-23.78943195017113664216
64	16	1	1	64	-53.0974630504781789002	-52.51101643160262214682
256	16	2	2	1024	-824.3485304128287185987	$-824.20124841655491853453$
625	25	5/2	5/2	15625/4	$-1751.8599778851174516594$	$-1751.71184466088061526692$

Table 3
The coefficients of the expanded potentials $V(x, y; Z^2, \lambda) \equiv -V_m + A[x^2 + y^2] + B[x^3 + y^3] + C[x^4 + y^4] + Dxy + E[xy^2 + x^2y] + Fx^2y^2$ and the energy for the second excited state E_{11}. First line – power series; <u>second line</u> – inner product.

Z^2	λ	x_m	y_m	$-V_m$	A	B	C	D	E	F	E_{11}
1/4	1	1/4	1/4	1/64	1/4	1	1	1/2	1	2	8.54203369483475573005 <u>8.542033</u>
1	1/4	1	1	1	1	1	1/4	2	1	1/2	2.87513314732153278819 <u>2.87513</u>
1	4	1/4	1/4	1/16	1	4	4	2	4	8	13.19306206246391090591 <u>13.193062</u>
4	1	1	1	4	4	4	1	8	4	2	1.36847851852892882643 <u>1.36847</u>
$4\sqrt{2}$	$\sqrt{2}$	1	1	$4\sqrt{2}$	$4\sqrt{2}$	$4\sqrt{2}$	$\sqrt{2}$	$8\sqrt{2}$	$4\sqrt{2}$	$2\sqrt{2}$	0.19646195361830885756 <u>0.19646</u>
$\sqrt{2}$	$4\sqrt{2}$	1/4	1/4	$1/8\sqrt{2}$	$\sqrt{2}$	$4\sqrt{2}$	$4\sqrt{2}$	$2\sqrt{2}$	$4\sqrt{2}$	$8\sqrt{2}$	14.67129708502542526061 <u>14.671297</u>
$\sqrt{3}$	$\sqrt{3}/4$	1	1	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}/4$	$2\sqrt{3}$	$\sqrt{3}$	$\sqrt{3}/2$	2.67386194727777643566 <u>2.67386</u>
$4\sqrt{3}$	$\sqrt{3}$	1	1	$4\sqrt{3}$	$4\sqrt{3}$	$4\sqrt{3}$	$\sqrt{3}$	$8\sqrt{3}$	$4\sqrt{3}$	$2\sqrt{3}$	-0.75681562553391021578 <u>-0.7568</u>
$\sqrt{5}$	$\sqrt{5}$	1/2	1/2	$\sqrt{5}/4$	$\sqrt{5}$	$2\sqrt{5}$	$\sqrt{5}$	$2\sqrt{5}$	$2\sqrt{5}$	$2\sqrt{5}$	8.89708405157769917376 <u>8.89708</u>
$4\sqrt{5}$	$\sqrt{5}$	1	1	$4\sqrt{5}$	$4\sqrt{5}$	$4\sqrt{5}$	$\sqrt{5}$	$8\sqrt{5}$	$4\sqrt{5}$	$2\sqrt{5}$	-2.32667388711564077242 <u>-2.3266</u>
$4\sqrt{7}$	$\sqrt{7}$	1	1	$4\sqrt{7}$	$4\sqrt{7}$	$4\sqrt{7}$	$\sqrt{7}$	$8\sqrt{7}$	$4\sqrt{7}$	$2\sqrt{7}$	$-3.63865699600365903 24$ <u>-3.638</u>
$\sqrt{7}$	$4\sqrt{7}$	1/4	1/4	$\sqrt{7}/16$	$\sqrt{7}$	$4\sqrt{7}$	$4\sqrt{7}$	$2\sqrt{7}$	$4\sqrt{7}$	$8\sqrt{7}$	17.71490107592092727 67 <u>17.714901</u>
4	16	1/4	1/4	1/4	4	16	16	8	16	32	20.00237600802916244995 <u>20.00237</u>
2	8	1/4	1/4	1/8	2	8	8	4	8	16	16.29400223524496885588 <u>16.294002</u>
8	2	1	1	8	8	8	2	16	8	4	-1.58417228650699250109 <u>-1.584</u>
8	32	1/4	1/4	1/2	8	32	32	16	32	64	24.35335078234699469491 <u>24.35335</u>

Table 3
(Continued.)

Z^2	λ	x_m	y_m	$-V_m$	A	B	C	D	E	F	E_{11}
16	64	1/4	1/4	1	16	64	64	32	64	128	29.31257755226118619289
											29.31257
16	256	1/8	1/8	1/4	16	128	256	32	128	512	52.77224824985564362062
											52.772248
25	625	1/10	1/10	1/4	25	250	625	50	250	1250	71.79964556193960785223
											71.799645
100	400	1/4	1/4	25/4	100	400	400	200	400	800	43.12239868785334026201
											43.12239
40	10^3	1/10	1/10	2/5	40	400	1000	80	400	2000	83.06120653309269041894
											83.061206
10^2	10^4	1/20	1/20	1/4	100	2000	10^4	200	2000	2×10^4	185.19350065722970401545
											185.1935006
16	4	1	1	16	16	16	4	32	16	8	-8.11578177921287062138
32	8	1	1	32	32	32	8	64	32	16	-21.95711140731594064126
64	16	1	1	64	64	64	16	128	64	32	-50.78120100250709703521
256	16	2	2	1024	256	128	16	512	128	32	$-823.75950939266511494548$
625	25	5/2	5/2	15625/4	625	250	25	1250	250	50	$-1751.26753124828917523964$

The quantity of great interest here is the splitting between energies levels

$$\Delta E_{10}^{11} = E_{11} - E_{10}, \qquad \Delta E_{00}^{10} = E_{10} - E_{00}, \tag{24}$$

that controls the tunnelling rate from one well to the other. It is generally believed to have an exponential character for deep wells [10]. It is clear from our results in tables 2 and 3, that for large values of Z^2/λ, the well is deep and wide and these state functions $\Psi_{00}(x, y)$, $\Psi_{10}(x, y)$ and $\Psi_{11}(x, y)$ are approximately peaked over the minima of the well. As Z^2/λ increases these minima move further and further out away from the origin.

We have plotted the variation of the first few energy levels in figure 3 as function of Z^2/λ to display the degeneracy of energy levels for our results in tables 2 and 3 for the double-well potential in two-dimensional systems for the energy levels E_{00}, E_{10} and E_{11} different values of Z^2/λ. We can observe in the figure 3 that the energy levels are degenerate for higher values of Z^2/λ.

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