

Application of the inner product technique to double-well potentials in three-dimensional quantum systems by expanding the potential functions around their minima

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Energy eigenvalues of double-well potentials for three-dimensional systems are calculated by means of an expansion of the potential function $V(x, y, z; Z^2, \lambda, a_{IJ}) = -Z^2[x^2 + y^2 + z^2] + \lambda\{x^4 + y^4 + z^4 + 2a_{IJ}[x^2y^2 + x^2z^2 + y^2z^2]\}$ around its minimum, using the inner product technique, for various values of perturbation parameters Z^2 , λ and a_{IJ} . Some of the results calculated by this technique are compared with results obtained by other methods.

1. Introduction

There are a large number of physical and chemical systems whose properties can be studied (modelled) assuming that the potential function responsible for such properties is well represented by means of a function with two valleys and a barrier between them.

Some of the problems to which the double-well potential model has been applied are the interpretation of the infrared spectra of the NH_3 molecule, infrared and Raman spectra of hydrogen-bonded systems, inversion characteristics of isomers, structural phase transitions, formation of noble-gas monolayers on a graphite substrate, macroscopic quantum coherence in superconducting Josephson devices, and so on [1,5]. In the theory of these problems, the most important characteristics are related to the separation between the two lowest-lying energy levels as it defines the tunnelling rate through the double-well barrier.

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 [11], inner product perturbation theory [9] and so on, in contrast to the potential functions in multi-dimensional space, which have not been treated by the same approach by any worker in the past.

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 [11], and

by Witwit [10], and applied to the double-well potential in one- and two-dimensional systems, respectively. We have since established that the idea can be extended to apply to a double well in three-dimensional quantum systems.

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

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

There now exist a number of techniques that provide very good approximations of eigenvalues of Hamiltonians, especially in one dimension. Among these techniques, the so-called inner product technique has provided high precision results for various important quantum systems [3,4,6].

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

$$V(x, y, z; Z^2, \lambda, a_{IJ}) = -Z^2[x^2 + y^2 + z^2] + \lambda\{x^4 + y^4 + z^4 + 2a_{IJ}[x^2y^2 + x^2z^2 + y^2z^2]\}. \quad (2)$$

The eigenvalue spectrum of the Schrödinger equation (1) with potential $V(x, y, z; Z^2, \lambda, a_{IJ})$ has the feature that the lower eigenvalues are closely bunched into a single group if the values of Z^2/λ are sufficiently large. As Z^2/λ increases, the magnitude of the splitting between these levels decreases, i.e.,

$$|E_{111} - E_{000}| \approx |E_{000} - E_{100}| \approx |E_{100} - E_{110}| = \Delta E \cong 0. \quad (3)$$

In the theory of double-wells, the most important characteristics are related to the separation between the two lowest-lying energy levels, which defines the tunneling rate through the double-well barrier.

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 almost degenerate eigenfunctions have equal weight in each potential well.

This paper is organized as follows: in section 2, we derive the formalism of the inner product technique for a double-well in three-dimensional space together with the method that has been used to handle our calculations. In section 3 we present results and discussion.

2. The double-well potential in three dimensions $V(x, y, z; Z^2, \lambda, a_{IJ})$ and the recurrence relation

The inner product technique has been applied to many three-dimensional problems. However, until now, it has not been applied to a double-well potential in multi-dimensional spaces which have been expanded around their minima.

The recent analysis by the work [10] of a double-well potential in two dimension compel us to investigate the relevance of the inner product technique to treat the

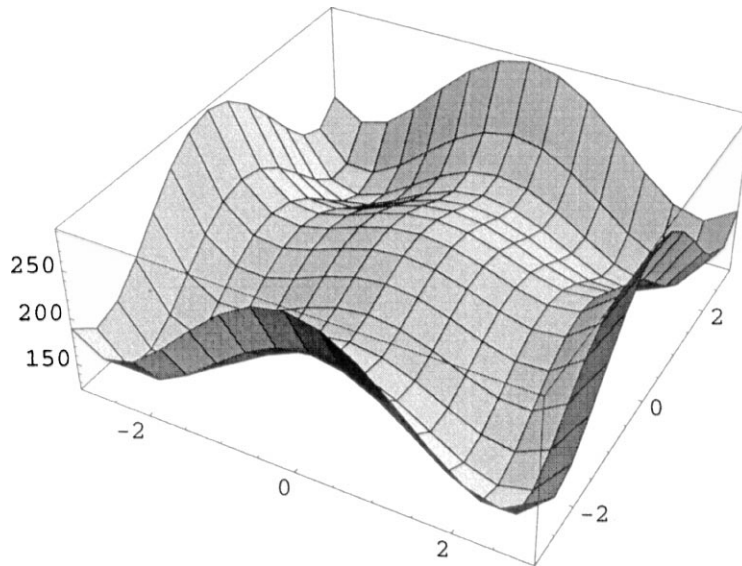


Figure 1. Double-well potential $V(x, y, z = 4; Z^2 = 2, \lambda = 3, \beta = -1/3)$.

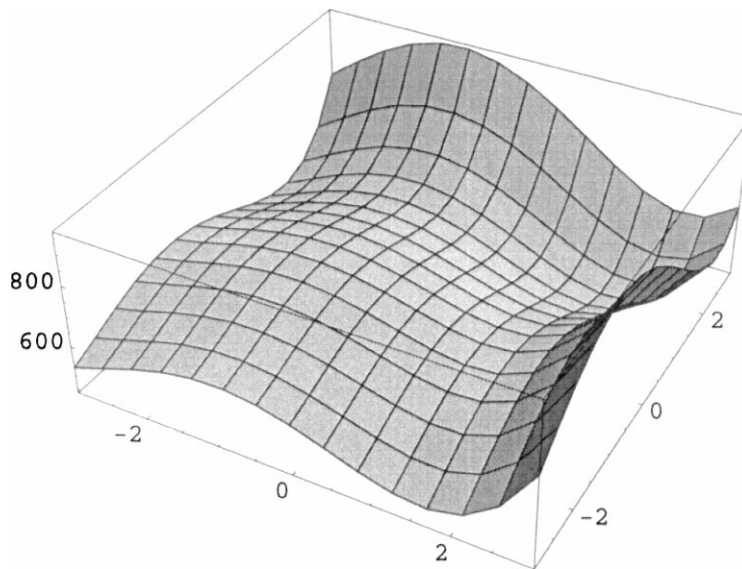


Figure 2. The expanded double-well potential $V(x, y, z = 4; Z^2 = 2, \lambda = 3, \beta = -1/3)$ around their minima $x_m = y_m = z_m = 1$.

expansion a double-well potentials in three-dimensional spaces. This problem is of interest because it is related to several interesting physical and chemical problems [1,5].

Most of the ideas of a potential function in two dimensions may be easily generalized to the potential function of three variables but the labour is greatly increased.

To calculate the energy eigenvalue for a double-well potential in three dimensions, we expand $V(x, y, z; Z^2, \lambda, a_{IJ})$ around its minimum at x_m, y_m and z_m .

We may write the Taylor expansion of $V(x, y, z; Z^2, \lambda, a_{IJ})$ around $x = x_m, y = y_m$ and $z = z_m$ in the symbolic form

$$V(x_I, \dots; Z^2, \lambda, a_{IJ}) = \sum_{n=0}^4 \frac{1}{n!} \left[\sum_{I=1}^3 (x_I - x_{Im}) \frac{\partial}{\partial x_I} \right]^n V(x_I, \dots; Z^2, \lambda, a_{IJ}) \Big|_{x_I=x_{Im}}. \quad (4)$$

Here, and subsequently, all the indices run over 1,2,3, so that the coordinate x_I runs over x, y and z , and all derivatives are evaluated at the point (x_m, y_m, z_m) . For example, at $(Z^2 = 12/243, \lambda = 2/243, a_{IJ} = 1)$ and $(Z^2 = 1/3, \lambda = 1/2, a_{IJ} = -1/3)$, replacing $x = x - x_m, y = y - y_m, z = z - z_m$, equation (4) takes the following two forms, respectively:

$$\begin{aligned} & V\left(x, y, z; Z^2 = \frac{12}{243}, \lambda = \frac{2}{243}, a_{IJ} = 1\right) \\ &= -\frac{2}{27} + \frac{8}{243} [x^2 + y^2 + z^2] + \frac{8}{243} [x^3 + y^3 + z^3] + \frac{2}{243} [x^4 + y^4 + z^4] \\ &+ [2x + x^2] \left[\frac{8}{243} y + \frac{4}{243} y^2 \right] + [2x + x^2] \left[\frac{8}{243} z + \frac{4}{243} z^2 \right] \\ &+ [2y + y^2] \left[\frac{8}{243} z + \frac{4}{243} z^2 \right], \end{aligned} \quad (5)$$

$$\begin{aligned} & V\left(x, y, z; Z^2 = \frac{1}{3}, \lambda = \frac{1}{2}, a_{IJ} = -\frac{1}{3}\right) \\ &= -\frac{1}{2} + 2[x^2 + y^2 + z^2] + 2[x^3 + y^3 + z^3] + \frac{1}{2}[x^4 + y^4 + z^4] \\ &- \left[\frac{2}{3}x + \frac{1}{3}x^2 \right] [2y + y^2] - \left[\frac{2}{3}x + \frac{1}{3}x^2 \right] [2z + z^2] \\ &- \left[\frac{2}{3}y + \frac{1}{3}y^2 \right] [2z + z^2]. \end{aligned} \quad (6)$$

The most efficient way to overcome the divergence problem for the perturbation series is to convert $V(x, y, z; Z^2, \lambda, a_{IJ})$ to renormalized form using a renormalization parameter β ,

$$\begin{aligned} V_\beta^r(x, y, z; Z^2, \lambda, a_{IJ}) &= [\mu_x^2 - \lambda\beta]x^2 + [\mu_y^2 - \lambda\beta]y^2 + [\mu_z^2 - \lambda\beta]z^2 + C(x^3)x^3 \\ &+ C(y^3)y^3 + C(z^3)z^3 + C(x^4)x^4 + C(y^4)y^4 + C(z^4)z^4 \\ &+ C(xy)xy + C(xz)xz + C(yz)yz + C(xy^2)xy^2 \\ &+ C(x^2y)x^2y + C(xz^2)xz^2 + C(x^2z)x^2z + C(zy^2)zy^2 \end{aligned}$$

$$\begin{aligned}
& + C(z^2y)z^2y + C(x^2y^2)x^2y^2 + C(x^2z^2)x^2z^2 \\
& + C(y^2z^2)y^2z^2 + V(x_m, y_m, z_m), \tag{7}
\end{aligned}$$

with

$$\mu_x^2 = C(x^2) + \underline{\lambda}\beta, \quad \mu_y^2 = C(y^2) + \underline{\lambda}\beta, \quad \mu_z^2 = C(z^2) + \underline{\lambda}\beta, \quad \underline{\lambda} = 1. \tag{8}$$

We find that the perturbation series associated with the renormalized potential (7) has much improved convergence properties with appropriate choice of renormalization parameter β . Here $C(x^M y^N z^L)$ ($M, N, L: 0, 1, \dots, 4$) are the coefficients of the expanded potential.

The double-well potentials given by equation (7) in three dimensions are in general non-separable in Cartesian coordinates, showing symmetrical behaviour, and this behaviour simplifies the computation.

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

$$\Phi(x, y, z) = (x^I y^J z^L) \exp\left[-\frac{1}{2}(\mu_x x^2 + \mu_y y^2 + \mu_z z^2)\right]. \tag{9}$$

The next step is to work out the quantity

$$EW(I, J, L) = \langle \Psi | H | \Phi \rangle \tag{10}$$

obtained by taking the inner product of the Schrödinger equation (1) with the reference function (9). Here $W(I, J, L)$ is defined by

$$W(I, J, L) = \langle \Phi | \psi \rangle, \tag{11}$$

and substituting the perturbation expansions

$$W(I, J, L) = \sum_M W(I, J, L, M) \underline{\lambda}^M, \tag{12}$$

$$E = \sum_N E(N) \underline{\lambda}^N \tag{13}$$

into the $W(I, J, L)$ recurrence relation given by equation (10) leads to a recurrence relation for the coefficients. For the renormalized potential (7), the relation can be written as

$$\begin{aligned}
& \sum_{N=0}^{M=50} E(N)W(I, J, L, M - N) \\
& = C(x^3)W(I + 3, J, L, M - 1) + C(y^3)W(I, J + 3, L, M - 1) \\
& \quad + C(z^3)W(I, J, L + 3, M - 1) + C(x^4)W(I + 4, J, L, M - 1) \\
& \quad + C(y^4)W(I, J + 4, L, M - 1) + C(z^4)W(I, J, L + 4, M - 1) \\
& \quad + C(xy)W(I + 1, J + 1, L, M - 1) + C(xz)W(I + 1, J, L + 1, M - 1)
\end{aligned}$$

$$\begin{aligned}
& + C(yz)W(I, J + 1, L + 1, M - 1) + C(xy^2)W(I + 1, J + 2, L, M - 1) \\
& + C(x^2y)W(I + 2, J + 1, L, M - 1) + C(xz^2)W(I + 1, J, L + 2, M - 1) \\
& + C(x^2z)W(I + 2, J, L + 1, M - 1) + C(zy^2)W(I, J + 2, L + 1, M - 1) \\
& + C(z^2y)W(I, J + 1, L + 2, M - 1) + C(x^2y^2)W(I + 2, J + 2, L, M - 1) \\
& + C(x^2z^2)W(I + 2, J, L + 2, M - 1) + C(y^2z^2)W(I, J + 2, L + 2, M - 1) \\
& - \beta[W(I + 1, J, L, M - 1) + W(I, J + 1, L, M - 1) \\
& \quad + W(I, J, L + 1, M - 1)] \\
& + [\mu_x(2I + 1) + \mu_y(2J + 1) + \mu_z(2L + 1)]W(I, J, L, M) \\
& - I[I - 1]W(I - 2, J, L, M) - J[J - 1]W(I, J - 2, L, M) \\
& - L[L - 1]W(I, J, L - 2, M). \tag{14}
\end{aligned}$$

We exploited the interchange symmetry between the coordinates x - y - z , if the eigenstates have even-symmetry such as $\Psi_{111}(x, y, z)$ and $\psi_{000}(x, y, z)$:

$$\begin{aligned}
W(I, J, L, M) &= W(J, I, L, M) = W(I, L, J, M) = W(J, L, I, M) \\
&= W(L, J, I, M) = W(L, I, J, M). \tag{15}
\end{aligned}$$

The unperturbed energy can be expressed as

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

and the initial condition imposed on the $W(I, J, L, M)$ is given as

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

The state-labelling indices n_x, n_y, n_z are used in equations (14)–(17) to select the particular state being treated, as explained in previous work [7].

The indices are scanned in the order I, J, L, M , as explained in [7], and relation (14) is used to work out $W(I, J, L, M)$ in term of lower-order elements which are already known. $E(N)$ is found from relation (14) for the special case $I = n_x, J = n_y, L = n_z$, and the sum on the left-hand side becomes $E(N)$ because of the intermediate normalization convention $W(n_x, n_y, n_z, 0) = 1$ which we impose on the algorithm.

Up to 50 coefficients of the perturbation series for the double-well potential for four energy levels were computed according to

$$E_{n_x, n_y, n_z} = \sum_{N=0}^{50} E(N)\lambda^N. \tag{18}$$

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.

Recently, we have seen the development of non-perturbative techniques to compute energy eigenvalues. Such techniques are necessary, since the perturbative techniques provide insufficient information about accuracy and give convergence difficulties. In the present work, we have used the power series method [8] to compute energy eigenvalues for the Schrödinger equation when the potential (2) has spherical symmetry in three dimensions, i.e., $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, $z = r \cos \theta$, $r^2 = x^2 + y^2 + z^2$.

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

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

The potential $V(r; Z^2, \lambda)$ can be expressed as

$$V(r; Z^2, \lambda) = -Z^2 r^2 + \lambda r^4. \quad (20)$$

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

$$E(0) = (4n_r + 2l + 3), \quad (21)$$

$$2n_r + l \equiv n_x + n_y + n_z, \quad (22)$$

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

3. Results and discussion

The inner product technique has been applied in this paper for double-well potentials in three-dimensional systems. We have expanded the potential functions around their minima at x_m , y_m and z_m in order to estimate eigenvalues. Eigenvalues for different values of Z^2 , λ and state numbers n_x, n_y, n_z are listed in tables 1 and 2.

The energy eigenvalues for the three-dimensional system $V(x, y, z; Z^2, \lambda, a_{IJ} = 1)$ are calculated, and their energy eigenvalues are quoted in table 1 for four eigenstates E_{000} , E_{100} , E_{110} and E_{111} over a wide range of parameters $12/243 \leq Z^2 \leq 324$ and $2/243 \leq \lambda \leq 216$.

In table 1 we compare the results obtained by the inner product technique with those obtained by the power series method. The power series method has been used for calculations outside the limits applicable to the inner product technique, particularly in respect to the values of the perturbation parameters. Generally speaking, the agreement between the two methods is good for small values of Z^2/λ .

In table 1 special emphasis is placed on larger values of Z^2/λ because the eigenvalues for four states E_{000} , E_{100} , E_{110} and E_{111} have almost degenerate eigenvalues. As Z^2/λ increases, the magnitude of the splitting between these four levels decreases,

Table 1

Eigenvalues of a double-well potential $V(x, y, z; Z^2, \lambda, a_{IJ} = 1)$ for the energy levels E_{000} , E_{100} , E_{110} , and E_{111} for a wide range values of the perturbation parameters. First line, power series method; second line, inner product technique. The empty spaces mean the corresponding eigenvalue cannot be calculated by the inner product technique.

Z^2	λ	E_{000}	E_{100}	E_{110}	E_{111}
16	216	20.322609863728 <u>20.322609</u>	39.014150696064 <u>39.014151</u>	60.41043570868 <u>60.41043</u>	83.985318455011 <u>83.98531</u>
10	60	12.470024829465 <u>12.470025</u>	24.307265751810 <u>24.307265</u>	37.95821990747 <u>37.958219</u>	53.061005938968 <u>53.061006</u>
6	25	9.171531010780 <u>9.17153</u>	17.949077316639 <u>17.94907</u>	28.09008136641 <u>28.09008</u>	39.320879559790 <u>39.32088</u>
6	16	7.285635127842 <u>7.28563</u>	14.577983739378 <u>14.57798</u>	23.08333091397 <u>23.08333</u>	32.551095537939 <u>32.55109</u>
1	6	6.398425455901 <u>6.398425</u>	12.171858607268 <u>12.17185</u>	18.74931960640 <u>18.74931</u>	25.977120661447 <u>25.97712</u>
18	27	5.139083693303 <u>5.139</u>	12.402570420632 <u>12.402</u>	21.31630782024 <u>21.316</u>	31.498816888040 <u>31.498</u>
20	30	5.050692919398 <u>5.0506</u>	12.474257546591 <u>12.4742</u>	21.62174221250 <u>21.6217</u>	32.091981392944 <u>32.0919</u>
6	9	5.038160840443 <u>5.0381</u>	10.647115651839 <u>10.6471</u>	17.31623749103 <u>17.3162</u>	24.815302617464 <u>24.8153</u>
100	216	4.179191764797 <u>4.1791</u>	16.634843631727 <u>16.6348</u>	32.69224911694 <u>32.6922</u>	51.464599661101 <u>51.4646</u>
2	3	4.145431521192 <u>4.1454</u>	8.308627615548 <u>8.3086</u>	13.16759355087 <u>13.1676</u>	18.578319450365 <u>18.5783</u>
3	2	2.325557748262 <u>2.3255</u>	5.438278030046 <u>5.4383</u>	9.23487789170 <u>9.2348</u>	13.558923495330 <u>13.5589</u>
6	4	1.957410772028 <u>1.9574</u>	5.530494926531 <u>5.5304</u>	10.01651452433 <u>10.0165</u>	15.197225262604 <u>15.1972</u>
24	25	1.916115995497 <u>1.916</u>	7.948839272506 <u>7.949</u>	15.74209136704 <u>15.742</u>	24.861565944107 <u>24.862</u>
9	6	1.397947262839 <u>1.3979</u>	5.211598776534 <u>5.2115</u>	10.11019089545 <u>10.1101</u>	15.827532595592 <u>15.8275</u>
12/81	2/81	0.586518557664 <u>0.58651</u>	1.324595495895 <u>1.32459</u>	2.21798113158 <u>2.21798</u>	3.231647695564 <u>3.23164</u>
12/243	2/243	0.527392569589 <u>0.52739</u>	1.087679254541 <u>1.08767</u>	1.74857916234 <u>1.74858</u>	2.488663141605 <u>2.48863</u>
12/27	12/27	0.440952665505 <u>0.44095</u>	1.360430005490 <u>1.36043</u>	2.52519815191 <u>2.52519</u>	3.875969554735 <u>3.87597</u>
1	1/6	-0.043279108811 <u>-0.0432</u>	0.975420620736 <u>0.9754</u>	2.34119643141 <u>2.3412</u>	3.966117958673 <u>3.9661</u>
12/9	2/9	-0.372040095527 <u>-0.37204</u>	0.666183480943 <u>0.66618</u>	2.09645966127 <u>2.09645</u>	3.818386741956 <u>3.81838</u>
27	18	-2.947904835215 <u>-2.948</u>	1.235841227941 <u>1.236</u>	7.14851236159 <u>7.148</u>	14.345520784119 <u>14.345</u>
4	2/3	-3.319554593771 <u>-3.319</u>	-2.315820019352 <u>-2.315</u>	-0.71912023622 <u>-0.7191</u>	1.326438564585 <u>1.3264</u>

Table 1
(Continued.)

Z^2	λ	E_{000}	E_{100}	E_{110}	E_{111}
16	6	-5.294355517505	-2.986259550300	0.55714395673	5.026185931482
		<u>-5.294</u>	<u>-2.986</u>	<u>0.557</u>	<u>5.026</u>
6	1	-5.706792517166	-4.753828775802	-3.14009821020	-1.011528832307
		<u>-5.707</u>	<u>-4.754</u>	<u>-3.140</u>	<u>-1.011</u>
12	2	-13.281256470256	-12.422667170734	-10.83271948386	-8.626809369541
25	6	-19.230129439376	-17.994590025001	-15.70553547383	-12.528671527420
54	25	-19.255152377144	-16.667764246440	-12.18557739039	-6.205123196976
36	6	-45.689583087436	-44.492772506211	-43.42968353770	-41.237584040939
216	100	-96.344549938019	-94.183896129206	-89.96479752739	-83.841630301644
108	18	-147.474240441548	-146.757190177266	-145.32923851634	-143.202120760436
324	54	-460.713361148955	-460.018916531067	-458.63174506173	-456.555237991687

Table 2

Eigenvalues of a double-well potential $V(x, y, z; Z^2, \lambda, a_{IJ})$ for the energy levels E_{000} , E_{100} , E_{110} and E_{111} . First line, Hill determinant approach; second line, inner product technique.

Z^2	λ	a_{ij}	E_{000}	E_{100}	E_{110}	E_{111}
1	1	-1/4	1.61201495328	3.456630036	5.091680638	6.5118037463
			<u>1.612</u>	<u>3.456</u>	<u>5.091</u>	<u>6.511</u>
1	4	-1/4	3.92504963643	7.516968915	10.813480513	13.7957014917
			<u>3.9250</u>	<u>7.516</u>	<u>10.813</u>	<u>13.7957</u>
3	1	1/4	-0.91563685322	0.441375057	1.972284285	3.6735907350
			<u>0.915</u>	<u>0.441</u>	<u>1.972</u>	<u>3.673</u>
2	6	1/4	4.92555576221	9.666420462	14.667807602	19.9129965248
			<u>4.9255</u>	<u>9.6664</u>	<u>14.6678</u>	<u>19.9129</u>
6/5	1	-1/5	1.38279308852	3.169417855	4.792321082	6.2485967403
			<u>1.382</u>	<u>3.169</u>	<u>4.792</u>	<u>6.248</u>
1	1	1/2	2.46833894498	5.052867093	7.914699484	11.0201191055
			<u>2.468</u>	<u>5.052</u>	<u>7.914</u>	<u>11.020</u>
4	1	1/2	-2.37986633699	-1.188402897	0.325865926	2.1526758814
			<u>2.379</u>	<u>-1.188</u>	<u>0.325</u>	<u>2.152</u>
2	3	-1/3	2.18516863370	4.645856146	6.653451744	8.2166399777
			<u>2.185</u>	<u>4.645</u>	<u>6.653</u>	<u>8.216</u>
1/3	1/2	-1/3	1.73311967226	3.359962807	4.763333493	5.9288653277
			<u>1.733</u>	<u>3.359</u>	<u>4.763</u>	<u>5.928</u>
1	3/10	1/3	0.42282607011	1.651835636	3.030258064	4.5473148364
			<u>0.422</u>	<u>1.651</u>	<u>3.030</u>	<u>4.547</u>

as is clear from our results listed in table 1. The quantity of great interest here is the splitting between energies levels

$$\Delta_{000}^{100}E = |E_{100} - E_{000}|, \quad \Delta_{100}^{110}E = |E_{110} - E_{100}|, \quad \Delta_{110}^{111}E = |E_{111} - E_{110}|, \quad (23)$$

which controls the tunneling rate from one well to the other. It is generally believed to have an exponential character for deep wells [2].

We refer to some more general models for the double-well potential $V(x, y, z; Z^2, \lambda, a_{IJ} \neq 1)$ in three dimensions. When the parameter $a_{IJ} \neq 1$, the Schrödinger equation (1) is non-separable in spherical coordinates, and the potential $V(x, y, z; Z^2, \lambda, a_{IJ})$ does not have spherical symmetry. We used the Hill determinant approach and inner product technique to calculate the energy eigenvalues for different values of Z^2 , λ and a_{IJ} for four energy levels E_{000} , E_{100} , E_{110} and E_{111} . These two approaches work very well, and the results obtained are in good agreement with each other, though the Hill determinant approach gives better accuracy than the inner product technique, as is clear from our results listed in table 2. One main difference between the power series and the inner product technique and Hill determinant approach is that the power series method can only work for the special case $a_{IJ} = 1$, in which the Schrödinger equation is separable and reduces to a one-dimensional case. However, the inner product technique and Hill determinant approach deal with more general parameters such as $a_{IJ} = \pm 1/4, \pm 1/3, \dots$.

Next we draw attention to the fact that the total energy for each energy eigenvalue comes from two contributions: firstly, a negative contribution coming from $V(x_m, y_m, z_m)$ and, secondly, a positive contribution coming from the other component of the expanded potentials. For deep wells, the negative contribution from $V(x_m, y_m, z_m)$ is larger than the positive contribution, so that the total energy is negative, but for shallow wells, the contribution from $V(x_m, y_m, z_m)$ is smaller, and the total energy positive, as is very clear from our listed results.

We have plotted the variation of the first few energy levels in figure 3 as a function of Z^2/λ to display the degeneracy of energy levels for our results in table 1

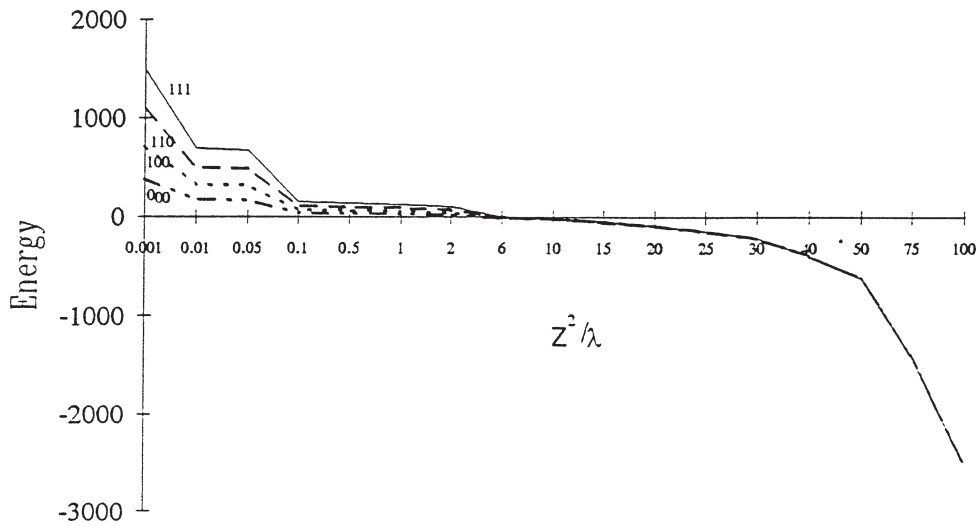


Figure 3. Graph of four energy levels E_{n_x, n_y, n_z} for the double-well potential $V(x, y, z; Z^2, \lambda, \beta = 1)$. For small values of Z^2/λ , the positive energies are small, and it is necessary to multiply these energies by a factor of 10, in order to obtain a clear figure.

for the double-well potential in three dimensions. Energy levels E_{000} , E_{100} , E_{110} and E_{111} are given for different values of Z^2/λ . We can observe in figure 3 that energy levels are degenerate for higher values of Z^2/λ .

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