The energy levels for a symmetric and nonsymmetric double-well potential in a two-dimensional system using the Hill determinant approach

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Energy levels of the Schrödinger equation for a double-well potential $V(x, y; Z_x^2, Z_y^2, \lambda) = -Z_x^2 x^2 - Z_y^2 y^2 + \lambda [a_{xx} x^4 + 2a_{xy} x^2 y^2 + a_{yy} y^4]$ in a two-dimensional system are calculated using the Hill determinant approach for several eigenstates and over a wide range of values of the perturbation parameters (λ, Z_x^2, Z_y^2) . Some of the results calculated by the Hill determinant approach are compared with those results produced by the inner product technique.

1. Introduction

The Schrödinger equation for the one-dimensional double-well potential

$$V(x;Z^2) = -Z^2 x^2 + x^4 \tag{1}$$

has been the subject of numerous investigations with high calculational accuracy cannot be doubted, and the corresponding literature is abundant [1-7]. These studies have been carried out from both analytical and numerical points of view often in the study of systems for which the potential has been modeled as a doubleminimum well, e.g. the ammonia molecule or a hydrogen-bonded solid. Unfortunately most of these investigations have not been extended to multidimensional systems.

In this paper we present extensive numerical calculations which use the Hill determinant technique (in an iterative form) to calculate the energy levels of the Schrödinger equation for a double well potential for a wide range of values of the perturbation parameters Z_x^2 , Z_y^2 , λ and for several eigenstates.

In this work, the general form of the Schrödinger equation for the double-well potential $V(x, y; Z_x^2, Z_v^2, \lambda)$ in a two-dimensional system is taken in the form

$$\left[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(x, y; Z_x^2, Z_y^2, \lambda)\right] \Psi_{n_x, n_y}(x, y) = E_{n_x, n_y} \Psi_{n_x, n_y}(x, y), \qquad (2)$$

where $V(x, y; Z_x^2, Z_y^2, \lambda)$ is given as

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$$V(x, y; Z_x^2, Z_y^2, \lambda) = -Z_x^2 x^2 - Z_y^2 y^2 + \lambda \left[a_{xx} x^4 + 2a_{xy} x^2 y^2 + a_{yy} y^4 \right].$$
(3)

The eigenvalue spectrum of the Schrödinger equation (2) with $V(x, y; Z_x^2, Z_y^2, \lambda)$ has the feature that the lower eigenvalues for states E_{00}, E_{11} , and $(E_{01} = E_{10})$ are closely bunched together if the values of Z_x^2 and Z_y^2 are sufficiently large at small values of λ . As Z_x^2 and Z_y^2 increase, the magnitude of the splitting between these levels decreases i.e. $|E_{11} - E_{00}| \approx 0$ or $|E_{01} - E_{00}| \approx 0$. These energy levels are shown in figs. 1 and 2.

The depth of the double well is controlled by the parameters Z_x^2 , Z_y^2 at constant value of the perturbation parameters $(\lambda, a_{xx}, a_{xy}, a_{yy})$ (see fig. 3). The Hill determinant approach works well for small and medium values of Z_x^2 , Z_y^2 at small values of λ ; as Z_x^2 and Z_y^2 increase the depth of the well increases and for deep wells the degree of convergence decreases.

Our work illustrate the high flexibility of the Hill determinant approach; this gives it an advantage over the inner product technique, which can only work for small values of Z_x^2 and Z_y^2 , at which the potential minima are shallow [8].

Since many of our results for this problem are not available in the literature it was found useful to check them using another method of calculation such as the inner product technique. The agreement in the results calculated by two different methods suggests accuracy yielded by our calculations is good (see table 4).

For purposes of clarity, this paper is divided into three sections. Section two is concerned with the Hill determinant approach and its use to calculate the energy eigenvalues for double well potential, and section three contains a discussion of the results.



Fig. 1. Graph of three energy levels for different values of Z^2 for the case $a_{xx} = a_{yy} = 1$, $a_{xy} = 0$; at $Z_x^2 = Z_y^2 = Z^2$ and $\lambda = 1$.



Fig. 2. Graph of three energy levels for different values of Z^2 for the case $a_{xx} = a_{yy} = a_{xy} = 1$; at $Z_x^2 = Z_y^2 = Z^2$ and $\lambda = 1$.

2. The recurrence relation for the double-well potential $V(x, y; Z_x^2, Z_y^2, \lambda)$ using the Hill determinant approach

The traditional literature on Hill determinants deals with one-dimensional problems; the extension to two or three dimensions necessarily involves the use of a product basis set, leading to large matrix or determinantal problems, which are conveniently handled by a relaxation method.

In this section we use the Hill determinant approach to calculate the energy levels of quantum-mechanical systems whose potential functions have symmetric and nonsymmetric behaviour. An extended analysis of numerical calculations is carried out for a double-well potential in a two dimensional system, and illustrate the applicability of the Hill determinant approach for handling potentials in a multidimensional system.

To find the recurrence relations which allow us to calculate the eigenvalues for the Schrödinger equation (2), we introduce the wavefunction in the form:

$$\Psi_{n_x,n_y}(x,y) = \exp{-\frac{\alpha}{2} \left[x^2 + y^2\right] \sum_{M,N} H(M,N) \left(x^M y^N\right)}.$$
(4)

The next step is to substitute $\Psi_{n_x,n_y}(x, y)$ in the Schrödinger equation (2). After some algebra, we obtain the recurrence relation

$$[2\alpha(M+N+1) - E]H(M,N) = W(M,N), \qquad (5)$$

where



Fig. 3. The double well potential in two-dimensional system given by eq. (3). (a) $Z_x^2 = 10$; $Z_y^2 = 10^3$ at $\lambda = 1$. (b) $Z_x^2 = Z_y^2 = 100$ at $\lambda = 1$. (c) $Z_x^2 = Z_y^2 = 100$ at $\lambda = 10^6$.

$$W(M,N) = (M+2)(M+1)H(M+2,N) + (N+2)(N+1)H(M,N+2) + (\alpha^2 + Z_x^2)H(M-2,N) + (\alpha^2 + Z_y^2)H(M,N-2) - \lambda[a_{xx}H(M-4,N) + 2a_{xy}H(M-2,N-2) + a_{yy}H(M,N-4)].$$
(6)

The recurrence relation (5) is used as follows. First the state numbers n_x and n_y (0, 1, 2...) are chosen, specifying which particular state is being treated. Initial values of $(M_0 = n_x \text{ and } N_0 = n_y)$ are taken to start the calculations, and the initial coefficient $H(M_0, N_0)$ is set equal to one.

In matrix-theoretic terms, the calculation is using a Gauss-Seidel (R = 1) or successive-over-relaxation $(R \neq 1)$ approach to calculate the low eigenvalues of a large matrix. Increasing M and N corresponds to increasing the number of basis states ie the dimension of the matrix. In the present approach the relevant matrix elements are very simple, as seen from eq. (5), and the iterative solution method, although often only useful for low eigenvalues, avoids explicit storage and manipulation of large matrices. In the iterations, all the H(M, N) with $(M, N) \neq (M_0, N_0)$ are adjusted according to the assignment

$$H(M,N) = W(M,N)[2\alpha(M+N+1) - E]^{-1}$$
(7)

for some fixed α and some trial E value. In order to speed the convergence of the energy, we must choose an appropriate initial value of α . The energy is found from the relation (7) for the special case $M = M_0$, $N = N_0$, when the coefficient on the left-hand side becomes $H(M_0, N_0) = 1$. After this adjustment process a revised E estimate is calculated using the assignment statements

$$E_e = 2\alpha (M_0 + N_0 + 1) - W(M_0, N_0), \qquad (8)$$

$$E = RE_e + (1 - R)E.$$
⁽⁹⁾

The relaxation parameter R can be changed in value to help in stabilizing the convergence to a desired eigenvalue. R replaces E by a new value intermediate between the old E and the computed E_e ; an R value between 0 and 1 often produces convergence in cases where the direct replacement of E by E_e (the case R = 1) would give divergence.

For the case of symmetric double-well potential, we use a parity index P_{xy} (for interchange symmetry $x \leftrightarrow y$) in order to cut down the amount of computation required. If $P_{xy} = 1$, then the relation (for the interchange $x \leftrightarrow y$).

$$H(M,N) = H(N,M) \tag{10}$$

holds; for the case of odd parity $P_{xy} = -1$, the relation becomes

$$H(M,N) = -H(N,M).$$
⁽¹¹⁾

As suggested by the referees, if we take the wavefunction (4) in the alternative form

$$\Psi_{n_x,n_y}(x,y) = \exp \left[-\frac{1}{2} \left[\alpha_x x^2 + \alpha_y y^2\right] \sum_{M,N} H(M,N) \left(x^M y^N\right) \right]$$
(12)

and substitute the wavefunction (10) in the Schrödinger equation (2), we obtain the following recurrence relation

$$\left[\left(2\alpha_{x}M+2\alpha_{y}N+\alpha_{x}+\alpha_{y}\right)-E\right]H(M,N)=W_{xy}(M,N)\,,\tag{13}$$

where

$$W_{xy}(M,N) = (M+2)(M+1)H(M+2,N) + (N+2)(N+1)H(M,N+2) + (\alpha_x^2 + Z_x^2)H(M-2,N) + (\alpha_y^2 + Z_y^2)H(M,N-2) - \lambda[a_{xx}H(M-4,N) + 2a_{xy}H(M-2,N-2) + a_{yy}H(M,N-4)].$$
(14)

The above relation (13) has been used to calculate some energy levels for different values of the parameters λ , Z_x^2 , Z_y^2 . In our computations, we have not observed any fundamental difference in behaviour between the relations (5) and (14) as we vary the adjustable parameters α , α_x^2 , α_y^2 to achieve the best convergence. Aitken's transformation was found to be effective to increase the accuracy of our results and to accelerate the rate of convergence of our calculations; if E_n , E_{n+1} , E_{n+2} are three successive partial sums of a series whose convergence is approximately geometric, then an improved estimate is

$$E_n = E_n - \frac{[\Delta E_n]^2}{\Delta^2 E_n} = E_n - \frac{[E_{n+1} - E_n]^2}{[E_{n+2} - 2E_{n+1} + E_n]}.$$
(15)

3. Results and discussion

The Hill determinant approach has been applied in this paper for the Schrödinger equation equation with a double-well potential in a two-dimensional system. Eigenvalues for different values of Z_x^2 , Z_y^2 , λ and state numbers n_x , n_y are listed in table 1. Note that the degeneracy between the states (0, 1) and (1, 0) is intrinsic to the Hamiltonian and it cannot be broken by the perturbation used here when the potential has exchange symmetry. As a general remark, we note the degree of accuracy (ie the number of digits) in the eigenvalues that we have able to obtain by our approach appears to diminish slowly with the increase in the values Z_x^2 , Z_y^2 at low values of the λ . Also the accuracy is usually greater for larger values of λ than for smaller values of λ , at the same values of Z_x^2 , Z_y^2 .

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Table 1

Eigenvalues of a double-well potential $V(x, y; Z_x^2, Z_y^2, \lambda)$ in a two-dimensional system for several eigenstates (n_x, n_y) .

λ	Z_x^2	Z_y^2	$a_{xx} = a_{yy} = 1, a_{xy} = 0$					
			(0,0)	(0, 1)	(1,0)	(1, 1)		
1	0.0	0.1	2.0841715337663	4.7692941552708	4.8234824730835	7.5086050945881		
1	0.0	0.5	1.9303796088558	4.3941414203712	4.6696905481730	7.1334523596884		
1	1	0	1.7180150956649	4.4573260349821	3.8948982926035	6.6352092319207		
1	0.5	0.1	1.8938269616537	4.5789495831583	4.3575887731691	7.0427113946737		
1	1	1.5	1.0743592007601	2.9541245141742	3.2512423976987	5.1310077111129		
1	1.5	2.5	.22409791811492	1.4931409266214	2.1038632315920	3.3729062400356		
0.5	4	3	-7.662038794	-7.4942886374	-7.642606595	-7.4748559359		
1	4.5	5.5	-6.981636412	-6.8978480243	-6.8978480243	-6.6152131325		
1	10	12	-51.821526428	-51.821426077	-51.8212396100	-51.821396247		
1	10	10	-41.267153405	-41.267123587	-41.267123587	-41.267093768		
1	15	15	-101.6827745684	-101.6827745684	-101.6827745684	-101.6827745684		
100	15	20	6.8662171904777	17.164418433274	17.785495511134	28.083696753929		
250	25	30	10.286268250845	24.567605781305	25.021048900435	39.625322847091		
500	75	50	10.460542081481	28.688520566212	26.848500343116	45.076478827847		
10 ³	100	150	10.743592007601	29.541245141743	32.512423976987	51.310077111129		
104	250	150	38.651724088558	93.859780423166	91.263170299536	146.47122663415		
10 ⁵	500	400	91.269496459576	213.73023322005	212.54700375903	335.00774051950		
106	500	500	208.43480554835	479.66223652101	479.66223652102	750.88966749370		
106	500	600	208.06893892985	478.75425715647	479.29636990253	749.98168812734		
$\overline{\lambda}$	Z_x^2	Z_y^2	$a_{xx} = a_{yy} = a_{xy} = 1$					
			(0,0)	(0, 1)	(1,0)	(1, 1)		
1	0.0	0.1	2.3119803260619	5.3092354547368	5.3659738933654	8.8513398937019		
1 1	0.0 0.0	0.1 0.0	2.3119803260619 2.3448290727443	5.3092354547368 5.3942271641723	5.3659738933654 5.3944271641723	8.8513398937019 8.9280821998500		
1 1 5	0.0 0.0 0.0	0.1 0.0 0.0	2.3119803260619 2.3448290727443 4.0096013134609	5.3092354547368 5.3942271641723 9.2239987016447	5.3659738933654 5.3944271641723 9.2239987016447	8.8513398937019 8.9280821998500 15.266805811696		
1 1 5 5	0.0 0.0 0.0 1.5	0.1 0.0 0.0 2.5	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740		
1 1 5 5 10	0.0 0.0 0.0 1.5 5	0.1 0.0 0.0 2.5 10	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112		
1 1 5 5 10 1	0.0 0.0 0.0 1.5 5 4.5	0.1 0.0 0.0 2.5 10 5.5	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 -3.450758028297	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694		
1 1 5 5 10 1 1.5	0.0 0.0 0.0 1.5 5 4.5 5	0.1 0.0 2.5 10 5.5 7.5	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226 -4.416766701613	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 3.450758028297 4.196728942146	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165 -1.830547414181	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694 -1.0407661371727		
1 1 5 5 10 1 1.5 1	0.0 0.0 1.5 5 4.5 5 6	0.1 0.0 2.5 10 5.5 7.5 8	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226 -4.416766701613 -10.8152168029	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 -3.450758028297 -4.196728942146 -10.8043513558	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165 -1.830547414181 -8.239822679133	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694 -1.0407661371727 -8.1332227637539		
1 1 5 5 10 1 1.5 1 1	0.0 0.0 1.5 5 4.5 5 6 10	0.1 0.0 2.5 10 5.5 7.5 8 10	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226 -4.416766701613 -10.8152168029 -20.69255783668	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 -3.450758028297 -4.196728942146 -10.8043513558 -20.4574196849	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165 -1.830547414181 -8.239822679133 -20.4574196849	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694 -1.0407661371727 -8.1332227637539 -19.764280025300		
1 1 5 5 10 1 1.5 1 1 1	0.0 0.0 1.5 5 4.5 5 6 10 15	0.1 0.0 2.5 10 5.5 7.5 8 10 15	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226 -4.416766701613 -10.8152168029 -20.69255783668 -50.8775172003	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 -3.450758028297 -4.196728942146 -10.8043513558 -20.4574196849 -50.733091622	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165 -1.830547414181 -8.239822679133 -20.4574196849 -50.733091622	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694 -1.0407661371727 -8.1332227637539 -19.764280025300 -50.3012984043		
1 1 5 5 10 1 1.5 1 1 1 1	0.0 0.0 1.5 5 4.5 5 6 10 15 20	0.1 0.0 2.5 10 5.5 7.5 8 10 15 20	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226 -4.416766701613 -10.8152168029 -20.69255783668 -50.8775172003 -93.7526635	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 3.450758028297 -4.196728942146 10.8043513558 -20.4574196849 50.733091622 93.647517	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165 -1.830547414181 -8.239822679133 -20.4574196849 -50.733091622 -93.647517	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694 -1.0407661371727 -8.1332227637539 -19.764280025300 -50.3012984043 -93.33247428		
1 5 5 10 1 1.5 1 1 1 7.5	0.0 0.0 1.5 5 4.5 5 6 10 15 20 4.5	0.1 0.0 2.5 10 5.5 7.5 8 10 15 20 5.5	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226 -4.416766701613 -10.8152168029 -20.69255783668 -50.8775172003 -93.7526635 2.7282030231309	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 3.450758028297 4.196728942146 -10.8043513558 -20.4574196849 -50.733091622 93.647517 7.2758911537284	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165 -1.830547414181 -8.239822679133 -20.4574196849 -50.733091622 -93.647517 7.6130141154314	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694 -1.0407661371727 -8.1332227637539 -19.764280025300 -50.3012984043 -93.33247428 13.322867448641		
1 5 5 10 1 1.5 1 1 1 7.5 100	0.0 0.0 1.5 5 4.5 5 6 10 15 20 4.5 25	0.1 0.0 2.5 10 5.5 7.5 8 10 15 20 5.5 30	2.3119803260619 2.3448290727443 4.0096013134609 3.2007409755799 2.3621424429482 -3.783427828226 -4.416766701613 -10.8152168029 -20.69255783668 -50.8775172003 -93.7526635 2.7282030231309 6.5789824847560	5.3092354547368 5.3942271641723 9.2239987016447 7.6704702674755 6.4158733970732 -3.450758028297 -4.196728942146 -10.8043513558 -20.4574196849 -50.733091622 -93.647517 7.2758911537284 17.474999520183	5.3659738933654 5.3944271641723 9.2239987016447 8.0271612515257 8.0140448541912 -2.284993651165 -1.830547414181 -8.239822679133 -20.4574196849 -50.733091622 -93.647517 7.6130141154314 18.183174517204	8.8513398937019 8.9280821998500 15.266805811696 13.418326231740 13.401706386112 -1.2602872067694 -1.0407661371727 -8.1332227637539 -19.764280025300 -50.3012984043 -93.33247428 13.322867448641 31.822958099766		
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$\overline{\lambda}$	Z_x^2	Z_y^2	$a_{xx} = 0.5, a_{yy} = 0.75, a_{xy} = 0.6$					
			(0, 0)	(0, 1)	(1,0)	(1, 1)		
1	0.0	0.5	1.8010121367096	4.2516467433369	4.2622966646949	7.1363578422002		
1	1.5	2.5	-0.011279310633	1.2561396074382	1.5974724778474	3.4619147639219		
2	4.5	5	-2.098288791127	-0.605352402503	-1.291658247144	1.0470708477221		
5	8	4	-1.000482656637	3.2323080807639	-0.156981253998	4.9593759170571		
10	5	7.5	1.6857304334994	5.6211037556562	5.5603027478250	10.650808702939		
100	25	30	3.9465741811223	13.168907709666	11.889693704429	23.578973289838		
10 ³	100	120	10.318423329712	31.256016563324	28.461311611779	54.520815541659		
104	250	300	32.472510107721	84.153336581936	77.853234823537	139.42771472640		
10 ⁵	400	300	86.490662484974	210.70869414175	194.15031210123	337.81372446629		
10 ⁶	500	600	194.95862716579	466.33288082779	435.50923225175	747.77465947203		

Table 1 (continued)

In table 1 the values of the energy are calculated for several eigenstates over a wide range of Z_x^2 , Z_y^2 , λ and for different values of (a_{xx}, a_{xy}, a_{yy}) , for several eigenstates such as E_{00} , E_{11} , E_{01} and E_{10} . Emphasis is placed on the larger values of Z_x^2 , Z_y^2 , because the eigenvalues for different states E_{00} , E_{10} , E_{01} , E_{11} , have almost degenerate eigenvalues. As Z_x^2 , Z_y^2 increase (at low values of λ), the magnitude of the splitting between these levels decreases, i.e. $|E_{11} - E_{00}| \approx |E_{10} - E_{00}| = \Delta E \cong 0$, as illustrated by our results in table 1.

When the potential $V(x, y; Z_x^2, Z_y^2, \lambda)$ is separable is $a_{xy} = 0$, the total energy E_{n_x,n_y} of a state is the sum of two components $E_{ts} = E_x + E_y$, but when $a_{xy} \neq 0$ the potential is nonseparable and the total energy of a state is the sum of three components $E_{tnos} = E_x + E_y + E_{xy}$. When the system is separable, it is clear that the splitting ΔE vanishes for smaller values of Z_x^2 , Z_y^2 , in contrast to the case for the nonseparable system, in which the splitting vanishes for larger values of Z_x^2 , Z_y^2 .

In figs. 1 and 2 we plot some of our results from table 1, for the double well potential in a two dimensional system for the symmetric case $(Z_x^2 = Z_y^2 \equiv Z^2)$ at $\lambda = 1$ for the three energy levels E_{00} , E_{10} , E_{11} for different values of Z^2 . It can be seen that the energy levels are degenerate for higher values of Z^2 .

It is important to point out that the an adjustable parameter α has played an important role in the convergence process in our calculations. The best α values in this calculation have been obtained by numerical search, and our calculations reveal the importance of finding these best values. The general consideration which governs our choice is that, as Z_x^2 , Z_y^2 , λ increase the value of α increases. This is illustrated by the data in table 2, the convergence of our results is influenced by the value of the adjustable parameter α for the the energy levels E_{00} , E_{10} and E_{11} . Also the accuracy possible is usually greater for the symmetric ($Z_x^2 = Z_y^2$) case than for the nonsymmetric case ($Z_x^2 \neq Z_y^2$). However, from a practical view point handling the symmetric case is preferable; the computation is more quickly performed than that for the nonsymmetric case, and requires less memory. Next we consider the use Table 2

Convergence for some eigenvalues for (n_x, n_y) for the double-well potential for the case $a_{xx} = a_{yy} = a_{xy} = 1$ with various values of the adjustable parameter α .

λ	Z_x^2	Z_y^2	(0,0)	α	(1,0)	α	(1,1)	α
1	2.5	1.5		1.5		0		1.5
				2	2.44	2.5		2.5
			0.745377488	3.5	2.442820952	3.6	5.5209345	3.5
			0.745377488284	4.5	2.4428209523016	4.8	5.209345985547	4.5
			0.7453774882843	5.7	2.4428209523016	6	5.5209345985547	5.5
1000	80	100		20		20		20
			17.1295	30	43.8738	30	74.93	30
			17.129556790947	40	43.873825041950	40	74.939654090303	40
			17.129556790947	50	43.873825041950	50	74.939654090303	50
10 ⁶	550	500		250		250		250
			231.0489	300	533.349	300	884.77	300
			231.048917720	370	533.3497757	360	884.773513	350
			231.04891772053	410	533.34977574434	410	884.77351306400	408

of two adjustable parameter α_x , α_y . Our results for three energy levels E_{00} , E_{10} and E_{11} , along with the values of Z_x^2 , Z_y^2 , λ , α_x and α_y are shown in table 3. We wish to draw attention to the fact that the Hill determinant approach works equally well for ($\alpha_x = \alpha_y$) and ($\alpha_x \neq \alpha_y$) as adjustable parameters. We used two values of α_x and α_y to verify the convergence of the Hill determinant for this calculation. The calculated energy eigenvalues for case $Z_x^2 < Z_y^2$ at low values of λ converge faster if we used $\alpha_x < \alpha_y$ instead of using ($\alpha_x = \alpha_y$). The two examples show that are ($\lambda = 1, Z_x^2 = 0, Z_y^2 = 7.5$) and ($\lambda = 1, Z_x^2 = 0.5, Z_y^2 = 5$).

As suggested by the referees, comparison with the results of the inner product technique has been made in table 4, for various values of λ and Z^2 (for three energies levels $E_{1,1}^+$, $E_{0,2}^+$ and $E_{2,0}^-$, for two special cases, i.e. $a_{xx} = a_{yy} = a_{xy} = 1$ and $a_{xx} = a_{yy} = 1$, $a_{xy} = 3$. The results for the case $a_{xx} = a_{yy} = a_{xy} = 1$ illustrate the presence of a special circular symmetry. The energy levels characterized by labels (11, +; 20, -), and (11, +; 02, +) have crossings when $a_{xx} = a_{xy} = a_{yy} = 1$, $a_{xx} = a_{yy} = 1$, $a_{xy} = 3$, respectively, for all values of λ and Z^2 .

The crossing is removed when the $a_{yy} \neq 1$ and $a_{xy} \neq 3$ and the energy level then splits into two levels, as shown by our results in table 4. From the listed results in table 3, we observed that the accuracy produced by Hill determinant approach in general, is better than that produced by inner product technique.

Higher accuracies can be achieved at the expense of greater computation times. The higher values of parameters Z_x^2 , Z_y^2 and lower values of λ require greater computation times.

We performed special external checking calculations for the case $Z_x^2 = Z_y^2$

Table 3

Convergence for some eigenvalues for (n_x, n_y) of the double-well potential for the case $a_{xx} = a_{yy} = a_{xy} = 1$ for several sets of parameters λ , Z_x^2 and Z_y^2 for various values of the adjustable parameters α_x and α_y . The empty spaces mean the eigenvalues cannot be obtained with values of α_x and α_y .

λ	Z_x^2	Z_y^2	(0, 0)	(1,0)	(1, 1)	α _x	α_y
1	0	7.5	-7.6652 -7.66524734 -7.6652473452608 -7.6652473452608	-2.3365 -2.33657101 -2.3365710173287 -2.3365710173287	-2.30908 -2.309079665 -2.3090796649906 -2.3090796649906	5 5 8 10	5 10 10 10
1	0.5	5	1.46915460 1.4691546031127 1.4691546031127	2.353113116 2.3531131167167 2.3531131167167	3.028200588 30.28005882115 3.0282005882115	2 5 5 10	5 5 10 10
2	2.5	3.5	1.100258 1.100258 1.100258397 1.1002583974694 1.1002583974694	4.048106 4.048106 4.0481063006 4.0481063006864 4.0481063006864	7.24385 7.24385 7.243850857 7.2438508578048 7.2438508578048	2.5 4 4.5 5.5 6	3.5 4 4.5 5.5 6.5 6
10	1	10	3. 3.004305 3.0043046029903 3.0043046029908	9.7 9.670838 9.6078384845395 9.6708384845395	14.8 14.857282 14.857282473671 14.857282473671	4 5 8 12 18	10 12 15 18 18
10	5	10	2.3621424429482 2.3621424429482 2.3621424429482	8.0140448541912 8.0140448541912 8.0140448541912	13.40 13.401706386112 13.401706386112 13.401706386112	5 10 10 15	10 12 15 15
10	15	20	-3.1559 -3.1558978137322 -3.1558978137322 -3.15589781373	0.67917 0.6791738707284 0.6791738707284 0.6791738707	3.9 3.922304 3.9223038374693 3.9223038374693 3.9223038375	4 5 8 10 15 20	8 10 12 15 17 20
10 ³	50	100	18.2066 18.206646679 18.20664667940 18.206664667940	46.59674 46.5967459122 46.596745912223 46.596745912223	77.3559 77.3559681236 77.355968123686 77.355968123686	20 30 40 50 60	30 40 50 60 60

Table 4

Comparison of some eigenvalues of the double-well potential $V(x, y; Z^2, \lambda)$ which have been calculated by the Hill determinant approach with those calculated by the Inner product technique. The empty space means the eigenvalue cannot be obtained by the inner product technique for these values of parameters λ and Z^2 .

$a_{xx} = a_{yy} = 1$						
		$a_{xy} = 1, E_{1,1}^+ = E_{2,0}^-$	$a_{xy} = 3, E_{1,1}^+ = E_{0,2}^+$			
λ	Z^2	Hill determinant	Inner product	Hill determinant	Inner product	
1	4	1.3684785185289	1.36848	4.826751073372	4.82675107	
2	2.5	7.9813272546529	7.981327254	10.850900243477	10.8509002434	
2.5	7.5	1.6267273035404	1.6267	6.382873519709	6.382873519	
10	25	-4.769515583332	-4.76	4.910470558482	4.91047	
20	50	-17.7762342		-1.844421514	-1.8444	
500	100	50.102533167839	50.102533167	68.215542621441	68.2155426214	
10 ³	150	64.675606957923	64.6756069579	87.183652998410	87.18365299841	
104	200	177.89453442368	177.89453442368	219.12726110436	219.15726110436	
10 ⁵	300	404.47451462012	404.4745146201	489.74302312367	489.7430231237	
106	500	885.15703420306	885.157034203	1066.5698268491	1066.569826849	

 $= Z^2$; $a_{xx} = a_{yy} = 1$, $a_{xy} = 0$. For this special case the potential (3) reduces to two identical independent double-well potential

$$V(x, y; Z^2) = -Z^2[x^2 + y^2] + \lambda[x^4 + y^4].$$
(16)

We have checked the energies obtained by the present technique against results obtained by other methods [1-7].

In conclusion, we have demonstrated how the Hill determinant approach can be applied to a double-well potential in two dimensional space. This approach has been shown to be very effective and simpler than other methods.

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