

## Converging bounds for the eigenvalues of multiminima potentials in two-dimensional space

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1996 J. Phys. A: Math. Gen. 29 6967

(<http://iopscience.iop.org/0305-4470/29/21/027>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.68

The article was downloaded on 02/06/2010 at 03:03

Please note that [terms and conditions apply](#).

# Converging bounds for the eigenvalues of multim minima potentials in two-dimensional space

H Taşeli and R Eid

Department of Mathematics, Middle East Technical University, 06531 Ankara, Turkey

Received 29 May 1996

**Abstract.** The eigenvalue problem in  $L_2(\mathbb{R}^2)$  of Schrödinger operators with a polynomial perturbation has been replaced by one corresponding to the system confined in a box  $\Omega$  with impenetrable walls. It is shown that the Dirichlet and the von Neumann problems in  $L_2(\Omega)$  generate upper and lower bounds, respectively, to the eigenvalues of the unbounded system. To illustrate the method, rapidly converging two-sided bounds for the energy levels of two- and three-well oscillators are presented, using simple trigonometric basis functions.

## 1. Introduction

The two-dimensional perturbed oscillator Hamiltonian in the dimensionless form

$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + x^2 + y^2 + \varepsilon Q(x, y) \quad (1.1)$$

has received attention, especially from the viewpoint of perturbation theory due to its applications in quantum field theory and molecular spectroscopy. Regarding  $\varepsilon$  as a perturbation parameter, it has been well known, since the late 1960s, that the resulting perturbation series are divergent for all  $\varepsilon > 0$  [1, 2]. The quartic oscillator,

$$Q(x, y) = a_{20}x^4 + 2a_{11}x^2y^2 + a_{02}y^4 \quad (1.2)$$

is the most studied system of this kind, where the  $a_{ij}$  are the coupling constants. Several methods of finding estimates of the eigensolutions of (1.2) have been introduced, including large order and inner product perturbation theories [3–6], renormalized perturbation and power series [6, 7], and modified perturbative and moment methods [8–10]. The inner product technique was also applied to potentials other than the quartic oscillators [11, 12].

Almost all these approaches start with the use of the classical harmonic oscillator solution and deal with renormalized convergence parameter and/or resummation methods such as Padé approximants to obtain satisfactory results, owing to the divergent nature of the perturbation problem being considered. In any case, however, an obvious accuracy loss is noticeable for strong anharmonic couplings. This can easily be attributed to the fact that a harmonic-like reference function does not represent properly the asymptotic behaviour of the true wavefunction.

In a recent article [13] by the same authors, it was shown numerically that the Dirichlet boundary value problem,

$$\left[ -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(x, y) \right] \Psi = E\Psi \quad \Psi \in L_2(\Omega) \quad (1.3)$$

where the wavefunction  $\Psi$  vanishes over the boundaries of a sufficiently large finite rectangular region  $\Omega$ , can be effectively used in calculating the spectrum of the usual Schrödinger equation defined in  $\mathbb{R}^2$  with the quartic and the sextic perturbations. Such a truncation of the unbounded domain of the problem was justified analytically in [14]. However, having no error estimates at hand may raise a question about the accuracy of the numerical results, especially in the case of multiwell oscillators with nearly degenerate minima.

In this paper, we deduce in section 2 that the eigenvalues of the Dirichlet and the von Neumann problems are upper and lower bounds, respectively, for the eigenvalues of the relevant unbounded system. Section 3 presents complete orthonormal basis sets in terms of circular functions satisfying the boundary conditions of Dirichlet and von Neumann types to be utilized in the Rayleigh–Ritz variational method. In section 4, we attack the more challenging problem of multiwell potentials in two dimensions, reporting rapidly converging exact bounds to the eigenvalues for a wide range of the coupling constants. The last section is devoted to the discussion of the numerical results and the concluding remarks.

## 2. Dirichlet and von Neumann problems

Let us consider the enclosed Schrödinger equation

$$\mathcal{L}\Psi(x, y) = 0 \quad \mathcal{L} = -\nabla^2 + V(x, y) - E \quad (x, y) \in \Omega \quad (2.1)$$

where  $\Omega$  has been specified to be a square region such that

$$\Omega = \{(x, y) : x \in (-\ell, \ell) \text{ and } y \in (-\ell, \ell)\}. \quad (2.2)$$

For a nice analysis, we assume that  $V(x, y)$  is a well (multiwell) potential having both reflection and interchange symmetries. The end conditions imposed on the wavefunction  $\Psi(x, y)$  are

$$A\Psi_x(\mp\ell, y) + B\Psi(\mp\ell, y) = 0 \quad (2.3)$$

for all  $y$ , and

$$A\Psi_y(x, \mp\ell) + B\Psi(x, \mp\ell) = 0 \quad (2.4)$$

for all  $x$ , where the subscripts denote partial derivatives. The constants  $A$  and  $B$  are either zero or unity so that a Dirichlet or a von Neumann boundary value problem is under discussion according to whether  $A$  or  $B$  are equal to zero. If we regard the eigenfunctions and the eigenvalues of (2.1) as functions of the boundary parameter  $\ell$ ,

$$\Psi = \Psi(x, y; \ell) \quad E = E(\ell) \quad (2.5)$$

then the eigensolutions of the unbounded Schrödinger equation corresponding to (2.1) may formally be obtained through the limit operations

$$\Psi_{(\infty)}(x, y) = \lim_{\ell \rightarrow \infty} \Psi(x, y; \ell) \quad E_{(\infty)} = \lim_{\ell \rightarrow \infty} E(\ell). \quad (2.6)$$

In what follows, equation (2.1) can be differentiated with respect to  $\ell$  to give a result

$$\Psi \frac{dE}{d\ell} = \mathcal{L}\Psi_\ell \quad (2.7)$$

from which, on multiplying by  $\Psi$  and integrating over  $\Omega$ , it follows immediately that

$$\frac{dE}{d\ell} = \langle \mathcal{L}\Psi_\ell, \Psi \rangle \quad (2.8)$$

where we have assumed that the wavefunction is normalized so that  $\langle \Psi, \Psi \rangle = 1$ . If  $\mathcal{L}^*$  stands for the formal adjoint of the differential operator  $\mathcal{L}$ , (2.8) can then be written in the form

$$\frac{dE}{d\ell} = \text{boundary terms} + \langle \Psi_\ell, \mathcal{L}^* \Psi \rangle. \quad (2.9)$$

Note that the last inner product vanishes from (2.1) since  $\mathcal{L}$  is formally self-adjoint, i.e.  $\mathcal{L}^* = \mathcal{L}$ . Thus we have

$$\frac{dE}{d\ell} = \int_{-\ell}^{\ell} (\Psi_x \Psi_\ell - \Psi \Psi_{x\ell})|_{x=-\ell}^{\ell} dy + \int_{-\ell}^{\ell} (\Psi_y \Psi_\ell - \Psi \Psi_{y\ell})|_{y=-\ell}^{\ell} dx. \quad (2.10)$$

The use of the total differential of  $\Psi(x, y; \ell)$ ,

$$d\Psi = \Psi_x dx + \Psi_y dy + \Psi_\ell d\ell \quad (2.11)$$

allows the expression of (2.10) in a more informative form. In fact, if  $x = x(\ell)$  then  $dx = (dx/d\ell) d\ell$  and hence

$$d\Psi = \left( \Psi_\ell + \frac{dx}{d\ell} \Psi_x \right) d\ell + \Psi_y dy \quad (2.12)$$

showing that  $\Psi_\ell = \Psi_\ell + (dx/d\ell)\Psi_x$ , where on the left-hand side  $\Psi_\ell$  is to be regarded as the partial derivative of the function  $\Psi\{x(\ell), y; \ell\}$  of  $\ell$  and  $y$  only. Likewise for  $y = y(\ell)$  we infer that

$$d\Psi = \Psi_x dx + \left( \Psi_\ell + \frac{dy}{d\ell} \Psi_y \right) d\ell \quad (2.13)$$

so that

$$\Psi_\ell = \Psi_\ell \mp \Psi_x \quad \text{and} \quad \Psi_\ell = \Psi_\ell \mp \Psi_y \quad (2.14)$$

when  $x = \mp \ell$  and  $y = \mp \ell$ , respectively. By means of these operational relations, differentiating the boundary conditions in (2.3) and (2.4) with respect to  $\ell$  now yields the equations

$$A[\Psi_{x\ell}(\mp \ell, y) \mp \Psi_{xx}(\mp \ell, y)] + B[\Psi_\ell(\mp \ell, y) \mp \Psi_x(\mp \ell, y)] = 0 \quad (2.15)$$

and

$$A[\Psi_{y\ell}(x, \mp \ell) \mp \Psi_{yy}(x, \mp \ell)] + B[\Psi_\ell(x, \mp \ell) \mp \Psi_y(x, \mp \ell)] = 0. \quad (2.16)$$

As a result, in the case of the problem (2.1) with the prescribed Dirichlet conditions,  $A = 0$  and  $B = 1$ , substituting (2.15) and (2.16) into (2.10) leads to

$$\frac{dE}{d\ell} = - \int_{-\ell}^{\ell} [\Psi_x^2(\ell, y) + \Psi_x^2(-\ell, y)] dy - \int_{-\ell}^{\ell} [\Psi_y^2(x, \ell) + \Psi_y^2(x, -\ell)] dx \quad (2.17)$$

which may be written in the form

$$\frac{dE}{d\ell} = -4 \int_{-\ell}^{\ell} \Psi_u^2(\ell, u) du \quad (2.18)$$

whenever the wavefunction possesses reflection and interchange symmetries. In any case, however,  $dE/d\ell$  is negative implying that the eigenvalues of the Dirichlet problem,  $E_{(u)}$  say, decreases monotonically to its limit  $E_{(\infty)}$  as  $\ell$  increases.

On the other hand, if the problem being considered obeys the boundary conditions of the von Neumann type, i.e.  $A = 1$  and  $B = 0$ , we then find in a similar fashion that

$$\begin{aligned} \frac{dE}{d\ell} &= \int_{-\ell}^{\ell} [\Psi(\ell, y)\Psi_{xx}(\ell, y) + \Psi(-\ell, y)\Psi_{xx}(-\ell, y)] dy \\ &\quad + \int_{-\ell}^{\ell} [\Psi(x, \ell)\Psi_{yy}(x, \ell) + \Psi(x, -\ell)\Psi_{yy}(x, -\ell)] dx. \end{aligned} \quad (2.19)$$

Taking advantage of the symmetry prescriptions we obtain

$$\frac{dE}{d\ell} = 2 \int_{-\ell}^{\ell} \{\Psi(x, y)\nabla^2\Psi(x, y)\}|_{y=\ell} dx = 2 \int_{-\ell}^{\ell} \{\Psi(x, y)\nabla^2\Psi(x, y)\}|_{x=\ell} dy \quad (2.20)$$

which reduces to

$$\frac{dE}{d\ell} = 2 \int_{-\ell}^{\ell} \{[V(x, y) - E]\Psi^2(x, y)\}|_{y=\ell} dx = 2 \int_{-\ell}^{\ell} \{[V(x, y) - E]\Psi^2(x, y)\}|_{x=\ell} dy \quad (2.21)$$

from (2.1). Clearly  $dE/d\ell$  is positive provided that  $\ell$  is beyond the classical turning points. Therefore, the eigenvalues of the von Neumann problem,  $E_{(l)}$  say, approaches  $E_{(\infty)}$  from below as  $\ell$  increases.

As a consequence, the Dirichlet and von Neumann problems generate error bounds to the eigenvalues  $E_{(\infty)}$  required, in the sense that

$$E_{(l)} \leq E_{(\infty)} \leq E_{(u)}. \quad (2.22)$$

All that is left now is the establishment of an efficient algorithm to solve the Schrödinger equation (2.1) accompanying with both Dirichlet and von Neumann conditions, in estimating rigorous upper and lower bound eigenvalues, respectively.

### 3. Trigonometric basis sets

The Schrödinger equation for a free particle

$$-\nabla^2\Psi = \lambda\Psi \quad \Psi \in L_2(\Omega) \quad (3.1)$$

is considered to construct a complete orthonormal basis for the space  $L_2(\Omega)$ . Our approach is guided by recent successful variational studies of anharmonic oscillators in one and two dimensions [15–17, 13]. It is an easy matter to show that Laplace's operator in (3.1) has the normalized sequence of eigenfunctions, for  $m, n = 0, 1, \dots$ ,

$$\phi_{mn}(x, y) = \frac{1}{\ell} \cos\left[\left(m + \frac{1}{2}\right)\frac{\pi}{\ell}x\right] \cos\left[\left(n + \frac{1}{2}\right)\frac{\pi}{\ell}y\right] \quad (3.2a)$$

$$\phi_{mn}(x, y) = \frac{1}{\ell} \cos\left[\left(m + \frac{1}{2}\right)\frac{\pi}{\ell}x\right] \sin\left[\left(n + 1\right)\frac{\pi}{\ell}y\right] \quad (3.2b)$$

$$\phi_{mn}(x, y) = \frac{1}{\ell} \sin\left[\left(m + 1\right)\frac{\pi}{\ell}x\right] \cos\left[\left(n + \frac{1}{2}\right)\frac{\pi}{\ell}y\right] \quad (3.2c)$$

$$\phi_{mn}(x, y) = \frac{1}{\ell} \sin\left[\left(m + 1\right)\frac{\pi}{\ell}x\right] \sin\left[\left(n + 1\right)\frac{\pi}{\ell}y\right] \quad (3.2d)$$

and

$$\varphi_{mn}(x, y) = \frac{1}{\ell} \gamma_{mn} \cos\left(m\frac{\pi}{\ell}x\right) \cos\left(n\frac{\pi}{\ell}y\right) \quad (3.3a)$$

$$\varphi_{mn}(x, y) = \frac{\sqrt{2}}{\ell} \gamma_{m,0} \cos\left(m \frac{\pi}{\ell} x\right) \sin\left[\left(n + \frac{1}{2}\right) \frac{\pi}{\ell} y\right] \tag{3.3b}$$

$$\varphi_{mn}(x, y) = \frac{\sqrt{2}}{\ell} \gamma_{n,0} \sin\left[\left(m + \frac{1}{2}\right) \frac{\pi}{\ell} x\right] \cos\left(n \frac{\pi}{\ell} y\right) \tag{3.3c}$$

$$\varphi_{mn}(x, y) = \frac{1}{\ell} \sin\left[\left(m + \frac{1}{2}\right) \frac{\pi}{\ell} x\right] \sin\left[\left(n + \frac{1}{2}\right) \frac{\pi}{\ell} y\right] \tag{3.3d}$$

satisfying Dirichlet and von Neumann conditions, respectively, where

$$\gamma_{mn} = (1 + \delta_{m,0} + \delta_{n,0} + \delta_{m,0}\delta_{n,0})^{-1/2} \tag{3.4}$$

in which  $\delta_{ij}$  is the Kronecker delta. Henceforth, the basis sets in (3.2) and (3.3) are referred to as  $\textcircled{1}_u, \textcircled{2}_u, \textcircled{3}_u, \textcircled{4}_u$  and  $\textcircled{1}_l, \textcircled{2}_l, \textcircled{3}_l, \textcircled{4}_l$ , respectively.

The symmetric structure of the problem suggests the decomposition of the spectrum into four subsets. Actually, the sets  $\textcircled{1}_u, \textcircled{1}_l$  and  $\textcircled{4}_u, \textcircled{4}_l$  can be used to determine energy levels with the same parity, i.e. both even or both odd. On the other hand, we may deal with the eigenvalues having different parity, one even and one odd, by means of the sets  $\textcircled{2}_u, \textcircled{3}_u$  and  $\textcircled{2}_l, \textcircled{3}_l$ . Hence we can propose as our trial functions

$$\Psi_{(u)}(x, y) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} h_{mn} \phi_{mn}(x, y) \tag{3.5}$$

and

$$\Psi_{(l)}(x, y) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} f_{mn} \varphi_{mn}(x, y) \tag{3.6}$$

in calculating upper and lower bounds to  $E_{(\infty)}, E_{(u)}$  and  $E_{(l)}$ , of the perturbed Schrödinger equation, respectively, where the  $h_{mn}$  and  $f_{mn}$  are the linear combination coefficients. The potential function is chosen as a general polynomial of degree  $2M$  of the form

$$V(x, y) = \sum_{i=1}^M v_{2i} \sum_{j=0}^i a_{i-j,j} \binom{i}{j} x^{2(i-j)} y^{2j} \quad M = 1, 2, \dots \tag{3.7}$$

with the coupling constants  $v_{2i}$  and  $a_{i-j,j}$ . It is obvious that  $V(x, y)$  has the reflection symmetries

$$V(x, y) = V(-x, y) = V(x, -y) = V(-x, -y) \tag{3.8}$$

as well as an interchange symmetry,

$$V(x, y) = V(y, x) \tag{3.9}$$

when  $a_{i-j,j} = a_{j,i-j}$ .

Substituting (3.5) into (2.1) now yields the secular equations

$$\sum_{k=0}^{\infty} \sum_{l=0}^{\infty} [H_{klmn} - E_{(u)} \delta_{km} \delta_{ln}] h_{kl} = 0 \quad m, n = 0, 1, \dots \tag{3.10}$$

where

$$H_{klmn} = \int_{-\ell}^{\ell} \int_{-\ell}^{\ell} [-\nabla^2 \phi_{kl}(x, y) + V(x, y) \phi_{kl}(x, y)] \phi_{mn}(x, y) dx dy \tag{3.11}$$

from which it follows that

$$\begin{aligned} H_{klmn} = & \sum_{i=1}^M v_{2i} \left(\frac{\ell}{\pi}\right)^{2i} \sum_{j=0}^i a_{i-j,j} \binom{i}{j} [R_{k-m}^{(i-j)} + s_1 R_{k+m+1+p_1}^{(i-j)}] [R_{l-n}^{(j)} + s_2 R_{l+n+1+p_2}^{(j)}] \\ & + \frac{\pi^2}{4\ell^2} [(2k+1+p_1)^2 + (2l+1+p_2)^2] \delta_{km} \delta_{ln}. \end{aligned} \tag{3.12}$$

In this definition of  $H_{klmn}$  we have introduced four integer parameters  $s_1, s_2, p_1$  and  $p_2$  to include all four bases in (3.2) such that

$$s_1 = s_2 = 1 \quad p_1 = p_2 = 0 \quad (3.13a)$$

$$s_1 = 1 \quad s_2 = -1 \quad p_1 = 0 \quad p_2 = 1 \quad (3.13b)$$

$$s_1 = -1 \quad s_2 = 1 \quad p_1 = 1 \quad p_2 = 0 \quad (3.13c)$$

and

$$s_1 = s_2 = -1 \quad p_1 = p_2 = 1 \quad (3.13d)$$

for the sets ①<sub>u</sub>, ②<sub>u</sub>, ③<sub>u</sub> and ④<sub>u</sub>, respectively. Furthermore, the  $R_k^{(j)}$  denote the simple integrals of the type

$$R_k^{(j)} = \frac{1}{\pi} \int_0^\pi \xi^{2j} \cos k\xi \, d\xi \quad (3.14)$$

which may be evaluated both recursively and explicitly. The recursive relation,

$$k^2 R_k^{(j)} = 2j(-1)^k \pi^{2j-2} - 2j(2j-1)R_k^{(j-1)} \quad j = 1, 2, \dots, M \quad (3.15)$$

with the initial condition that  $R_k^{(0)} = 0$ , is preferable from a computational point of view [16].

Starting from the solution  $\Psi_{(l)}(x, y)$  in (3.6), the variational formulation of the von Neumann problem may be worked out by the same way. The result is again the reduction of the Schrödinger equation to the system of algebraic equations

$$\sum_{k=0}^{\infty} \sum_{l=0}^{\infty} [F_{klmn} - E_{(l)} \delta_{km} \delta_{ln}] f_{kl} = 0 \quad m, n = 0, 1, \dots \quad (3.16)$$

where

$$F_{klmn} = \sigma \sum_{i=1}^M v_{2i} \left(\frac{\ell}{\pi}\right)^{2i} \sum_{j=0}^i a_{i-j,j} \binom{i}{j} [R_{k-m}^{(i-j)} + s_1 R_{k+m+p_1}^{(i-j)}] [R_{l-n}^{(j)} + s_2 R_{l+n+p_2}^{(j)}] + \frac{\pi^2}{4\ell^2} [(2k+p_1)^2 + (2l+p_2)^2] \delta_{km} \delta_{ln} \quad (3.17)$$

with  $s_1, s_2, p_1, p_2$  being the same as those defined by (3.13), for the von Neumann basis sets in (3.3) as well. Besides,  $\sigma$  is an additional adjustable parameter which should be taken as

$$\sigma = \gamma_{kl} \gamma_{mn} \quad \sigma = 2\gamma_{k,0} \gamma_{m,0} \quad \sigma = 2\gamma_{l,0} \gamma_{n,0} \quad \text{and} \quad \sigma = 1 \quad (3.18)$$

for ①<sub>l</sub>, ②<sub>l</sub>, ③<sub>l</sub> and ④<sub>l</sub>, respectively.

For numerical purposes, we naturally truncate the wavefunctions by writing

$$\Psi_{(u)}(x, y) = \sum_{m=0}^{N_u-1} \sum_{n=0}^{N_u-1} h_{mn} \phi_{mn}(x, y) \quad \Psi_{(l)}(x, y) = \sum_{m=0}^{N_l-1} \sum_{n=0}^{N_l-1} f_{mn} \varphi_{mn}(x, y) \quad (3.19)$$

where  $N$  ( $N_u$  or  $N_l$ ) is the number of basis elements considered in the expansions. Now equations (3.10) and (3.16) describe finite algebraic systems of order  $N^2$ . As long as  $N$  is finite it may be interesting to point out that recoding the entries defined by  $H_{klmn}$  and  $F_{klmn}$ , these systems are expressible in the form of standard matrix eigenvalue problems [13]. To this end, the integer transformation  $T, T: \mathbb{N}_0^4 \rightarrow \mathbb{N}^2$  defined by

$$T = \{(i, j) \in \mathbb{N}^2 : i = mN + n + 1 \text{ and } j = kN + l + 1 \forall (k, l, m, n) \in \mathbb{N}_0^4\} \quad (3.20)$$

reduces  $H_{klmn}$  ( $F_{klmn}$ ) and  $\delta_{km}\delta_{ln}$  to a matrix  $[A_{ij}]$  and the identity matrix  $[\delta_{ij}]$  of orders  $N^2$ , respectively, where  $\mathbb{N} = \{1, 2, \dots\}$  is a subset of the set of natural numbers and  $\mathbb{N}_0 = \{0\} \cup \mathbb{N}$ . The  $[A_{ij}]$  turns out to be a symmetric matrix due to the block symmetry of  $H_{klmn}$  ( $F_{klmn}$ ), i.e.  $H_{klmn} = H_{mnlk}$  ( $F_{klmn} = F_{mnlk}$ ). Furthermore, the mapping  $S, S : \mathbb{N}_0^2 \rightarrow \mathbb{N}$

$$S = \{j \in \mathbb{N} : j = kN + l + 1 \ \forall (k, l) \in \mathbb{N}_0^2\} \tag{3.21}$$

transforms  $h_{kl}$  ( $f_{kl}$ ) with  $k, l = 0, 1, \dots, N - 1$  into  $g_j$  with  $j = 1, 2, \dots, N^2$ . Hence we may represent (3.10) and (3.16) in the form

$$\sum_{j=1}^{N^2} (A_{ij} - E\delta_{ij})g_j = 0 \quad i = 1, 2, \dots, N^2 \tag{3.22}$$

whose diagonalization employing available routines [18] results in the truncated upper and lower bound eigenvalues.

#### 4. Two- and three-well oscillators

The particular example which we first consider in this paper is that of the Schrödinger equation with a quartic anharmonicity where  $M = 2$  in (3.7). In spite of the possibility of treating this potential in its full generality, we have exploited the interchange symmetry of the coordinates, that is,  $a_{10} = a_{01}$  and  $a_{20} = a_{02}$ , to minimize the number of coupling constants. Thus we take the potential

$$V(x, y; a, v_2, v_4) = v_2(x^2 + y^2) + v_4(x^4 + 2ax^2y^2 + y^4) \tag{4.1}$$

where  $v_4 > 0$  and  $a \geq -1$  to have a positive quartic perturbation, and hence a well potential. If  $v_2$  is negative then  $V(x, y; a, v_2, v_4)$  describes a double-well potential (figure 1). In such a situation, however, the parameter  $a$  should not be equal to  $-1$  since the resulting potential then tends to  $-\infty$  along the straight line  $y = |x|$ .

A linear transformation shows that the eigenvalues of the Schrödinger equation with (4.1) have the scaling relationship,

$$E(a, v_2, v_4) = v_4^{1/3} E(a, Z^2, 1) \quad Z^2 = -v_2 v_4^{-2/3} \tag{4.2}$$

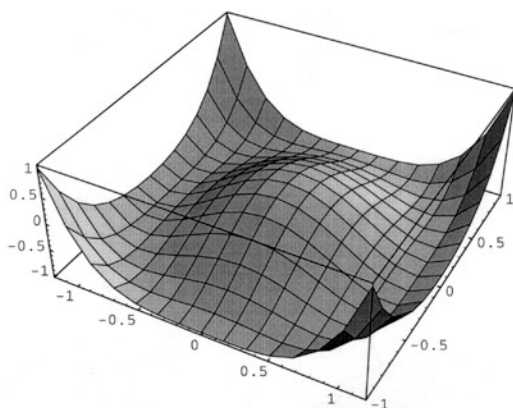


Figure 1. A two-well oscillator in two dimensions.



where  $a > -1$  and  $Z^2 > 0$ . Therefore, the two-well oscillators may be best characterized by a potential of the form

$$V(x, y; a, Z^2) = -Z^2(x^2 + y^2) + x^4 + 2ax^2y^2 + y^4 \quad (4.3)$$

containing two effective parameters  $a$  and  $Z^2$ , so that  $E = E(a, Z^2)$ . Note also that both  $a$  and  $Z^2$  should remain finite. Indeed, if  $a \rightarrow \infty$  then we encounter the infinite-field limit Hamiltonian with  $V(x, y) = 2x^2y^2$ , which is no longer a double-well potential, while if  $Z^2 \rightarrow \infty$  then the resulting equation with  $V(x, y) = -x^2 - y^2$  does not define a physical problem.

Furthermore, if we introduce new variables  $\xi$  and  $\eta$  such that

$$\xi = (\frac{1}{2}v)^{1/2}(x + y) \quad \eta = (\frac{1}{2}v)^{1/2}(x - y) \quad (4.4)$$

the Schrödinger equation is unaltered in form:

$$\left[ -\frac{\partial^2}{\partial \xi^2} - \frac{\partial^2}{\partial \eta^2} - \frac{Z^2}{v^2}(\xi^2 + \eta^2) + \xi^4 + 2\alpha\xi^2\eta^2 + \eta^4 - E \right] \Psi(\xi, \eta) = 0 \quad (4.5)$$

where

$$v = [(1 + a)/2]^{1/3} \quad \alpha = (3 - a)/(1 + a) \quad (4.6)$$

indicating clearly that the range of  $a \geq 1$  is taken into the interval  $(-1, 1]$  of the parameter  $\alpha$ , which plays in (4.5) the same role with  $a$ . The connection between the eigenvalues of the original and the transformed Schrödinger equations,

$$E(a, Z^2) = vE(\alpha, Z^2/v^2) \quad (4.7)$$

now implies the investigation of the problem only for the values of  $a \in (-1, 1]$ , without any loss of generality. For instance,

$$E(3, 4^{1/3}Z^2) = 2^{1/3}E(0, Z^2) \quad E(15, 4Z^2) = 2E(-\frac{3}{4}, Z^2) \quad (4.8)$$

so that we present the numerical results at  $a = -\frac{1}{2}, 0, \frac{1}{2}$  and 1 covering the interval of  $a$  of the main interest, for a variety of  $Z^2$  values ranging from 0.001 up to 20 in tables 2–6.

As a second example, we handle the sextic oscillators in (3.7) with  $M = 3$ . This potential is equivalent to

$$V(x, y) = v_2(x^2 + y^2) + v_4(x^4 + 2ax^2y^2 + y^4) + v_6(x^6 + 3bx^4y^2 + 3bx^2y^4 + y^6) \quad (4.9)$$

when  $V(x, y) = V(y, x)$ , namely,  $a_{10} = a_{01}$ ,  $a_{20} = a_{02}$ ,  $a_{21} = a_{12}$  and  $a_{30} = a_{03}$ . Obviously, we have a well potential if  $v_6 > 0$  and  $b \geq -\frac{1}{3}$ . It may be shown, in analogy with the sextic oscillators in one dimension [16], that the same potential with a non-negative harmonic and a strictly negative quartic couplings, i.e.  $v_2 \geq 0$  and  $v_4 < 0$  with  $a > -1$ , possesses three minima provided that  $v_4^2 > 3v_2v_6$  (figure 2). In this case, the resulting three-well potential is bounded below if  $b > -\frac{1}{3}$ .

Instead of (4.9) we may consider the rescaled potential of the form

$$V(x, y; a, b, c_2, c_4) = c_2(x^2 + y^2) - c_4(x^4 + 2ax^2y^2 + y^4) + x^6 + 3bx^4y^2 + 3bx^2y^4 + y^6 \quad (4.10)$$

for which

$$a > -1 \quad b > -\frac{1}{3} \quad c_2, c_4 > 0 \quad c_4^2 > 3c_2 \quad (4.11)$$

such that

$$E(a, b, v_2, v_4, v_6) = v_6^{1/4}E(a, b, c_2, c_4) \quad (4.12)$$

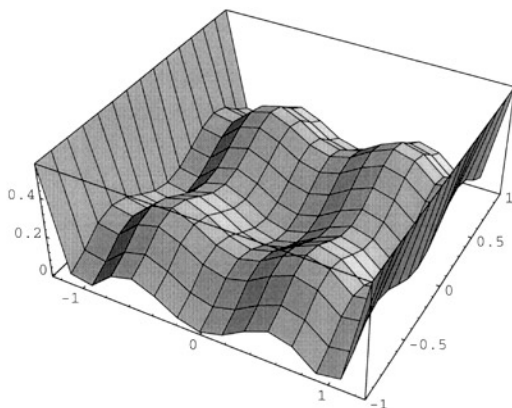


Figure 2. A three-well oscillator in two dimensions.

where

$$c_2 = v_2 v_6^{-1/2} \quad c_4 = -v_4 v_6^{-3/4}. \tag{4.13}$$

Now making use of the substitutions in (4.4) with  $\mu$  replaced by  $v$ , we deduce that the Hamiltonian  $\mathcal{H}$ ,

$$\mathcal{H}(x, y; a, b, c_2, c_4) = -\nabla^2 + V(x, y; a, b, c_2, c_4) \tag{4.14}$$

admits the similarity properties

$$\mathcal{H}(x, y; a, b, c_2, c_4) = \mu \mathcal{H}(x, y; \alpha, \beta, c_2/\mu^2, c_4 v^3/\mu^3) \tag{4.15}$$

and

$$E(a, b, c_2, c_4) = \mu E(\alpha, \beta, c_2/\mu^2, c_4 v^3/\mu^3) \tag{4.16}$$

where  $v$  and  $\alpha$  are the same parameters in (4.6) and

$$\mu = [(1 + 3b)/4]^{1/4} \quad \beta = (5 - b)/(1 + 3b). \tag{4.17}$$

It is important to notice that  $\beta$  ranges from  $-\frac{1}{3}$  to 1 when  $b \geq 1$ . Hence we suffer no loss of generality by setting  $b \in (-\frac{1}{3}, 1]$  as well as  $a \in (-1, 1]$  to cope with the problem of

Table 1. Convergence rates of lower and upper bound eigenvalues as a function of  $\ell$ , for  $E_{00}$  of the two-well potential  $V(x, y; a, Z^2)$  where  $a = \frac{1}{2}$  and  $Z^2 = 1$ .

$\ell$	$E_{00}$	$N$
2.25	1.486/499	6
2.75	1.493 278/315	9
3.00	1.493 297 105/822	10
3.25	1.493 297 475/482	11
3.50	1.493 297 478 496/524	12
3.75	1.493 297 478 510 209/257	15
4.00	1.493 297 478 510 233 435/468	18
4.25	1.493 297 478 510 233 451 925/934	20
4.40	1.493 297 478 510 233 451 929 801/834	22
4.50	1.493 297 478 510 233 451 929 817 302/979	25
4.60	1.493 297 478 510 233 451 929 817 638/651	28
4.70	1.493 297 478 510 233 451 929 817 644 312/52 2	30

**Table 2.** Lower and upper bounds to the eigenvalues of the two-well potentials  $V(x, y; a, Z^2)$  at  $Z^2 = 0.001$  as a function of  $a$ .

$a$	$\ell$	$N$	$n_x$	$n_y$	$E_{n_x n_y}$	Basis set
$-\frac{1}{2}$	6.5	28	0	0	1.972 650 264 858 277 7453/4	① $1/u$
	6.5	29	0(1)	1(0)	4.475 162 794 565 222 5114/5	② $1/u$ -③ $1/u$
	6.5	30	1	1	6.641 712 094 923 313 6219/20	④ $1/u$
	6.5	31	0	2	7.669 059 033 652 040 4080/1	① $1/u$
	6.5	31	2	0	8.264 204 890 146 653 4235/6	① $1/u$
	6.5	31	2(1)	1(2)	9.848 784 120 634 441 8300/1	② $1/u$ -③ $1/u$
	6.5	30	0(3)	3(0)	12.074 103 696 791 181 174/5	② $1/u$ , ③ $1/u$
	6.5	30	2	2	12.968 730 654 846 365 630/1	① $1/u$
	6.5	30	1	3	13.151 363 771 658 962 864/5	④ $1/u$
	6.5	30	3	1	14.367 147 265 069 970 491/2	④ $1/u$
0	4.05	18	0	0	2.120 000 066 639 870 7314/23	① $1/u$
	4.15	19	0(1)	1(0)	4.858 771 399 736 927 0351/3	② $1/u$ -③ $1/u$
	4.15	19	1	1	7.597 542 732 833 983 3384/8	④ $1/u$
	4.20	20	0(2)	2(0)	8.514 453 210 582 725 7098/103	① $1/u$ -① $1/u$
	4.15	19	2(1)	1(2)	11.253 224 543 679 782 012/5	② $1/u$ -③ $1/u$
	4.20	20	0(3)	3(0)	12.703 187 588 395 680 274/8	② $1/u$ -③ $1/u$
	4.15	19	2	2	14.908 906 354 525 580 686/90	① $1/u$
	4.20	20	1(3)	3(1)	15.441 958 921 492 736 577/81	④ $1/u$ -④ $1/u$
	4.25	21	0(4)	4(0)	17.319 984 396 115 486 195/201	① $1/u$ -① $1/u$
	4.20	20	2(3)	3(2)	19.097 640 732 338 535 252/6	② $1/u$ -③ $1/u$
$\frac{1}{2}$	4.05	18	0	0	2.240 227 653 554 100 8436/40	① $1/u$
	4.10	18	0(1)	1(0)	5.150 498 521 885 328 4660/6	② $1/u$ -③ $1/u$
	4.10	18	1	1	8.323 657 717 248 752 6819/23	④ $1/u$
	4.20	20	0	2	8.731 601 993 203 248 7822/5	① $1/u$
	4.20	20	2	0	9.086 732 688 254 732 3651/3	① $1/u$
	4.10	19	2(1)	1(2)	12.192 229 876 891 851 315/21	② $1/u$ -③ $1/u$
	4.20	20	0(3)	3(0)	13.249 726 188 740 431 482/4	② $1/u$ -③ $1/u$
	4.20	20	2	2	16.199 816 348 987 009 082/4	① $1/u$
	4.15	19	1	3	16.318 297 369 933 702 846/50	④ $1/u$
	4.15	19	3	1	17.045 270 094 677 392 744/50	④ $1/u$
1	4.05	18	0	0	2.344 177 545 585 648 9362/4	① $1/u$
	4.10	19	0(1)	1(0)	5.393 100 635 284 337 9891/6	② $1/u$ -③ $1/u$
	4.10	19	0(1)	2(1)	8.926 555 327 142 081 7154/6	① $1/u$ -④ $1/u$
	4.20	20	2	0	9.528 384 527 506 382 9889/91	① $1/u$
	4.15	19	0(1)	3(2)	12.841 251 032 037 540 350/2	② $1/u$ -③ $1/u$
	4.15	19	2(3)	1(0)	13.809 389 558 946 551 647/54	② $1/u$ -③ $1/u$
	4.20	20	0(1)	4(3)	17.075 470 989 981 863 046/50	① $1/u$ -④ $1/u$
	4.20	20	2(3)	2(1)	18.308 236 791 422 879 338/53	① $1/u$ -④ $1/u$
	4.20	20	4	0	18.733 224 174 598 178 029/41	① $1/u$
	4.20	20	0(1)	5(4)	21.587 532 648 351 539 612/21	② $1/u$ -③ $1/u$

triple-well potentials. However, our aim is not to overfill the content of the article with any more tabular material by making a systematic investigation over the specified intervals of the coupling constants  $a$ ,  $b$ ,  $c_2$  and  $c_4$ . As a matter of fact, we present only some specimen calculations in table 7 to verify the applicability of the method to the sextic oscillators with three minima as well.

**Table 3.** Lower and upper bounds to the eigenvalues of the two-well potentials  $V(x, y; a, Z^2)$  at  $Z^2 = 1$  as a function of  $a$ . The last column includes the results in [22], where available, for comparison.

$a$	$\ell$	$N$	$n_x$	$n_y$	$E_{n_x n_y}$	Basis set	$E_{n_x n_y}$ in [22]
$-\frac{1}{2}$	6.5	30	0	0	1.065 604 946 028 825 7199/200	① <sub>l/u</sub>	
	6.5	30	0(1)	1(0)	2.885 821 319 192 803 5836/7	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	6.5	30	1	1	4.317 978 336 716 244 2592/3	④ <sub>l/u</sub>	
	6.5	31	0	2	5.539 936 438 724 869 6728/9	① <sub>l/u</sub>	
	6.5	31	2	0	6.492 219 662 651 952 9503/4	① <sub>l/u</sub>	
	6.5	31	0(3)	3(0)	7.148 202 959 554 446 3274/5	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	6.5	31	2(1)	1(2)	9.788 050 299 308 083 9496/7	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	6.5	32	1	3	9.910 938 512 029 913 0317/8	④ <sub>l/u</sub>	
	6.5	32	2	2	9.976 698 667 287 598 7063/4	① <sub>l/u</sub>	
	6.5	30	3	1	11.519 392 676 279 759 111/2	④ <sub>l/u</sub>	
0	4.05	18	0	0	1.315 306 010 361 430 2458/64	① <sub>l/u</sub>	1.315 060 103 6144 <sup>a</sup>
	4.20	19	0(1)	1(0)	3.492 189 207 300 019 3374/80	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.25	20	1	1	5.669 072 404 238 608 4292/4	④ <sub>l/u</sub>	5.669 072 404 238 57
	4.25	20	0(2)	2(0)	6.821 554 262 143 783 3635/44	① <sub>l/u</sub> -① <sub>l/u</sub>	6.821 554 262 1437
	4.25	21	2(1)	1(2)	8.998 437 459 082 372 4551/60	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.25	20	0(3)	3(0)	10.696 299 125 892 291 163/70	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.25	20	2	2	12.327 802 513 926 136 481/3	① <sub>l/u</sub>	
	4.30	21	1(3)	3(1)	12.873 182 322 830 880 257/9	④ <sub>l/u</sub> -④ <sub>l/u</sub>	12.873 182 322 831
	4.30	21	0(4)	4(0)	15.030 059 509 858 584 074/83	① <sub>l/u</sub> -① <sub>l/u</sub>	
	4.25	20	2(3)	3(2)	16.202 547 377 674 644 280/8	② <sub>l/u</sub> -③ <sub>l/u</sub>	
$\frac{1}{2}$	4.15	19	0	0	1.493 297 478 510 233 4518/20	① <sub>l/u</sub>	
	4.20	20	0(1)	1(0)	3.889 906 849 661 130 6937/40	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.20	20	1	1	6.594 814 582 164 737 4561/3	④ <sub>l/u</sub>	
	4.25	21	0	2	7.092 266 626 999 638 0857/62	① <sub>l/u</sub>	
	4.25	21	2	0	7.560 230 963 215 618 7530/4	① <sub>l/u</sub>	
	4.20	20	2(1)	1(2)	10.126 150 099 578 332 525/7	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.25	21	0(3)	3(0)	11.385 769 262 460 847 676/80	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.25	21	2	2	13.797 868 585 986 881 784/8	① <sub>l/u</sub>	
	4.20	20	1	3	13.915 106 190 762 756 469/78	④ <sub>l/u</sub>	
	4.20	20	3	1	14.779 052 108 152 612 242/50	④ <sub>l/u</sub>	
1	4.10	18	0	0	1.637 487 952 723 690 8204/11	① <sub>l/u</sub>	1.637 487 952 7233
	4.20	19	0(1)	1(0)	4.199 685 387 486 361 5444/6	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.15	19	0(1)	2(1)	7.328 144 388 065 296 5481/4	① <sub>l/u</sub> -④ <sub>l/u</sub>	7.328 144 388 065 29
	4.25	21	2	0	8.087 207 576 543 170 4575/8	① <sub>l/u</sub>	8.087 207 576 536
	4.20	19	0(1)	3(2)	10.883 871 503 101 303 367/71	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.25	20	2(3)	1(0)	12.039 932 859 791 980 212/5	② <sub>l/u</sub> -③ <sub>l/u</sub>	
	4.20	19	0(1)	4(3)	14.789 805 972 176 726 431/4	① <sub>l/u</sub> -④ <sub>l/u</sub>	14.789 805 972 1767
	4.20	19	2(3)	2(1)	16.216 922 537 509 726 271/5	① <sub>l/u</sub> -④ <sub>l/u</sub>	16.216 922 54
	4.30	22	4	0	16.716 860 324 044 199 940/3	① <sub>l/u</sub>	
	4.30	21	0(1)	5(4)	18.996 019 587 096 235 714/6	② <sub>l/u</sub> -③ <sub>l/u</sub>	

<sup>a</sup> There is most likely a misprint in this result.

Additional features of the energy levels of the Schrödinger equation for the multiwell oscillators will be discussed in the next section in connection with the numerical results reported.

**Table 4.** Lower and upper bounds to the eigenvalues of the two-well potentials  $V(x, y; a, Z^2)$  at  $Z^2 = 4$  as a function of  $a$ . The last column includes the results in [22], where available, for comparison.

$a$	$\ell$	$N$	$n_x$	$n_y$	$E_{n_x n_y}$	Basis set	$E_{n_x n_y}$ in [22]
$-\frac{1}{2}$	6.7	34	0	0	-8.696 896 343 354 576 0322/1	① $l/u$	
	6.7	34	0(1)	1(0)	-8.687 605 254 296 730 7420/19	② $l/u$ -③ $l/u$	
	6.7	35	1	1	-8.678 964 253 853 924 3967/6	④ $l/u$	
	6.7	36	0	2	-4.344 908 198 649 155 1073/2	① $l/u$	
	6.7	36	2	0	-4.114 067 653 855 145 6673/2	② $l/u$ -③ $l/u$	
	6.7	36	0(3)	3(0)	-3.904 565 953 569 948 8326/5	④ $l/u$	
	6.7	35	1	3	-1.332 303 318 677 593 5398/7	① $l/u$	
	6.7	36	2	2	-1.141 362 819 873 516 6616/5	① $l/u$	
	6.7	35	2(1)	1(2)	-1.090 023 184 715 436 1874/3	② $l/u$ -③ $l/u$	
6.7	36	3	1	-0.493 867 971 066 834 744 64/3	④ $l/u$		
0	4.45	24	0	0	-3.420 700 900 265 278 0253/46	① $l/u$	
	4.45	24	0(1)	1(0)	-2.958 272 942 198 852 9378/68	② $l/u$ -③ $l/u$	
	4.50	24	1	1	-2.495 844 984 132 427 8498/6	④ $l/u$	
	4.55	25	0(2)	2(0)	0.231 086 740 514 392 674 40/9	① $l/u$ -① $l/u$	
	4.60	25	0(3)	3(0)	0.693 514 698 580 817 762 04/6	② $l/u$ -③ $l/u$	
	4.55	25	2(1)	1(2)	2.902 593 002 006 533 6593/7	② $l/u$ -③ $l/u$	
	4.55	24	1(3)	3(1)	3.365 020 960 072 958 7469/73	④ $l/u$ -④ $l/u$	
	4.55	25	2	2	3.882 874 381 294 063 3737/9	① $l/u$	
	4.60	25	0(4)	4(0)	6.411 091 504 557 949 0579/82	① $l/u$ -① $l/u$	
4.55	25	2(2)	3(2)	6.554 380 642 786 204 3586/90	② $l/u$ -③ $l/u$		
$\frac{1}{2}$	4.40	23	0	0	-2.254 621 872 622 836 7812/07	① $l/u$	
	4.40	23	0(1)	1(0)	-1.370 734 193 369 988 5994/85	② $l/u$ -③ $l/u$	
	4.45	24	1	1	-0.127 226 612 982 704 802 21/15	④ $l/u$	
	4.50	25	0	2	0.893 378 274 844 259 334 54/70	① $l/u$	
	4.50	25	2	0	2.286 561 466 627 129 6005/7	① $l/u$	
	4.45	24	0(3)	3(0)	2.594 513 668 023 481 5207/15	② $l/u$ -③ $l/u$	
	4.50	25	2(1)	1(2)	4.872 176 890 108 528 6594/601	② $l/u$ -③ $l/u$	
	4.50	25	1	3	5.348 081 810 319 435 8015/7	④ $l/u$	
	4.50	25	2	2	5.410 618 715 746 547 1132/9	① $l/u$	
4.20	20	3	1	6.899 781 311 349 868 1198/200	④ $l/u$		
1	4.40	22	0	0	-1.674 678 170 224 793 4099/6	① $l/u$	-1.6745
	4.45	23	0(1)	1(0)	-0.562 120 698 324 402 850 92/80	② $l/u$ -③ $l/u$	
	4.35	22	0(1)	2(1)	1.368 478 518 528 928 8262/7	① $l/u$ -④ $l/u$	1.368 4785
	4.45	23	2	0	3.263 535 028 598 281 4819/27	① $l/u$	3.2626
	4.50	24	0(1)	3(2)	3.861 362 246 146 439 8555/7	② $l/u$ -③ $l/u$	
	4.50	24	2(3)	1(0)	6.039 564 286 788 146 1248/54	② $l/u$ -③ $l/u$	
	4.45	23	0(1)	4(3)	6.793 563 400 243 966 6015/9	① $l/u$ -④ $l/u$	
	4.45	23	2(3)	2(1)	9.148 520 711 638 172 9892/7	① $l/u$ -④ $l/u$	9.148 53
	4.50	24	4	0	10.090 615 272 745 345 835/9	① $l/u$	
4.45	23	0(1)	5(4)	10.091 137 573 384 104 288/94	② $l/u$ -③ $l/u$		

**5. Results and discussion**

In this paper, we calculate the eigenvalues of multiwell oscillators with high accuracy providing rigorous lower and upper bounds. Quite extensive numerical data are given for the double-well potentials in order to understand the typical features of their energy spectra. In the tables  $\ell$  and  $N$  denote the boundary parameter and the truncation order of

**Table 5.** Lower and upper bounds to the eigenvalues of the two-well potentials  $V(x, y; a, Z^2)$  at  $Z^2 = 8$  as a function of  $a$ .

$a$	$\ell$	$N$	$n_x$	$n_y$	$E_{n_x n_y}$	Basis set
$-\frac{1}{2}$	6.9	39	0	0	-53.261 836 510 220 844 870/69	① $1/u$
	6.9	39	0(1)	1(0)	-53.261 836 509 446 004 842/1	② $1/u$ -③ $1/u$
	6.9	38	1	1	-53.261 836 508 711 166 588/7	④ $1/u$
	6.9	40	0	2	-45.689 525 312 106 483 616/5	① $1/u$
	7.0	40	0(3)	3(0)	-45.689 525 224 609 398 001/0	② $1/u$ -③ $1/u$
	6.9	39	1	3	-45.689 525 137 113 211 020/19	④ $1/u$
	7.0	40	2	0	-40.150 722 018 158 899 312/1	① $1/u$
	7.0	40	2(1)	1(2)	-40.150 721 759 730 984 713/2	② $1/u$ -③ $1/u$
	7.0	40	3	1	-40.150 721 501 300 901 320/19	④ $1/u$
	7.0	41	2	2	-38.354 036 147 542 773 744/3	① $1/u$
0	4.75	25	0	0	-24.272 661 441 386 951 221/17	① $1/u$
	4.75	25	0(1)	1(0)	-24.271 145 065 966 337 449/5	② $1/u$ -③ $1/u$
	4.75	25	1	1	-24.269 628 690 545 723 677/3	④ $1/u$
	4.80	26	0(2)	2(0)	-17.262 880 924 919 592 708/3	① $1/u$ -① $1/u$
	4.80	26	2(1)	1(2)	-17.261 364 549 498 978 936/1	② $1/u$ -③ $1/u$
	4.80	26	0(3)	3(0)	-17.147 244 032 195 922 974/69	② $1/u$ -③ $1/u$
	4.80	26	1(3)	3(1)	-17.145 727 656 775 309 202/197	④ $1/u$ -④ $1/u$
	4.85	27	0(4)	4(0)	-12.268 350 820 957 639 835/2	① $1/u$ -① $1/u$
	4.85	27	1(4)	4(1)	-12.266 834 445 537 026 063/0	② $1/u$ -③ $1/u$
	4.85	27	0(5)	5(0)	-10.716 668 140 570 039 193/86	② $1/u$ -③ $1/u$
$\frac{1}{2}$	4.65	23	0	0	-15.499 666 362 995 942 163/0	① $1/u$
	4.65	23	0(1)	1(0)	-15.394 859 895 531 839 812/09	② $1/u$ -③ $1/u$
	4.60	23	1	1	-15.274 247 089 243 241 363/55	④ $1/u$
	4.70	24	0	2	-12.483 951 958 383 685 683/78	① $1/u$
	4.70	24	0(3)	3(0)	-11.977 837 759 786 882 531/25	② $1/u$ -③ $1/u$
	4.70	24	1	3	-10.868 750 334 717 617 546/2	④ $1/u$
	4.70	24	2	0	-10.645 429 941 389 415 702/696	① $1/u$
	4.75	25	2(1)	1(2)	-9.233 034 904 664 678 8928/4	② $1/u$ -③ $1/u$
	4.70	24	3	1	-8.123 289 305 125 186 1552/0	④ $1/u$
	4.80	25	2	2	-7.447 329 538 506 703 3829/3	① $1/u$
1	4.70	24	0	0	-12.217 094 893 606 486 592/0	① $1/u$
	4.70	24	0(1)	1(0)	-11.894 715 975 085 568 322/0	② $1/u$ -③ $1/u$
	4.70	24	0(1)	2(1)	-10.978 555 703 657 970 323/19	① $1/u$ -④ $1/u$
	4.75	25	0(1)	3(2)	-9.548 167 682 237 708 0567/2	② $1/u$ -③ $1/u$
	4.80	25	0(1)	4(3)	-7.675 547 200 640 074 3391/89	① $1/u$ -④ $1/u$
	4.80	25	2(3)	1(0)	-5.416 824 334 005 841 5298/5	② $1/u$ -③ $1/u$
	4.80	25	2	0	-5.240 778 747 942 187 5797/3	① $1/u$
	4.80	25	0(1)	5(4)	-4.529 877 232 906 298 4043/36	② $1/u$ -③ $1/u$
	4.85	26	2(3)	2(1)	-3.019 285 192 831 561 2630/27	① $1/u$ -④ $1/u$
	4.80	25	0(1)	6(5)	-2.816 900 786 934 507 8248/1	① $1/u$ -④ $1/u$

the wavefunctions, respectively, for which the desired number of significant figures of an eigenvalue being considered with the quantum numbers  $n_x$  and  $n_y$  is reached. In presenting the limiting energies  $E_{(\infty)}$  in equation (2.6) the lower and upper bound evaluations, i.e. the eigenvalues of the von Neumann and Dirichlet problems, have been tabulated by means of a notation in which, for example, 1.493 278/315 means that  $1.493\ 278 < E_{(\infty)} < 1.493\ 315$ . Here, the lower bounds are truncated whereas the upper bounds are rounded up, if they are

**Table 6.** Lower and upper bounds to the eigenvalues of the two-well potentials  $V(x, y; a, Z^2)$  at  $Z^2 = 20$  as a function of  $a$ .

$a$	$\ell$	$N$	$n_x$	$n_y$	$E_{n_x n_y}$	Basis set
$-\frac{1}{2}$	7.3	49	0	0	-382.794 825 437 725 506 71/0	① $l/u$
	7.3	49	0(1)	1(0)	-382.794 825 437 725 506 71/0	② $l/u$ -③ $l/u$
	7.3	49	1	1	-382.794 825 437 725 506 71/0	④ $l/u$
	7.3	50	0	2	-370.306 396 584 749 528 19/8	① $l/u$
	7.3	49	0(3)	3(0)	-370.306 396 584 749 528 19/8	② $l/u$ -③ $l/u$
	7.3	49	1	3	-370.306 396 584 749 528 19/8	④ $l/u$
	7.3	50	2	0	-361.163 108 318 486 535 81/0	① $l/u$
	7.3	50	2(1)	1(2)	-361.163 108 318 486 535 81/0	② $l/u$ -③ $l/u$
	7.3	49	3	1	-361.163 108 318 486 535 81/0	④ $l/u$
	7.3	50	2	2	-357.896 882 466 392 549 09/8	① $l/u$
0	5.50	32	0	0	-187.452 741 835 721 117 13/1	① $l/u$
	5.50	31	0(1)	1(0)	-187.452 741 835 721 117 04/0	② $l/u$ -③ $l/u$
	5.50	31	1	1	-187.452 741 835 721 116 92/0	④ $l/u$
	5.55	33	0(2)	2(0)	-175.116 507 344 662 437 30/6	① $l/u$ -① $l/u$
	5.55	33	2(1)	1(2)	-175.116 507 344 662 437 25/19	② $l/u$ -③ $l/u$
	5.55	33	0(3)	3(0)	-175.116 507 344 662 387 69/3	② $l/u$ -③ $l/u$
	5.55	33	1(3)	3(1)	-175.116 507 344 662 387 58/2	④ $l/u$ -④ $l/u$
	5.60	34	0(4)	4(0)	-163.115 886 154 547 280 57/45	① $l/u$ -① $l/u$
	5.60	34	1(4)	4(1)	-163.115 886 154 547 280 47/34	② $l/u$ -③ $l/u$
	5.60	34	0(5)	5(0)	-163.115 886 154 536 762 17/04	② $l/u$ -③ $l/u$
$\frac{1}{2}$	5.35	29	0	0	-123.486 212 464 952 770 46/5	① $l/u$
	5.35	30	0(1)	1(0)	-123.486 212 342 145 509 24/3	② $l/u$ -③ $l/u$
	5.35	30	1	1	-123.486 212 219 338 227 89/8	④ $l/u$
	5.35	30	0	2	-116.535 029 936 968 695 19/8	① $l/u$
	5.35	30	0(3)	3(0)	-116.535 020 856 874 239 90/89	② $l/u$ -③ $l/u$
	5.35	30	1	3	-116.535 011 776 678 611 77/6	④ $l/u$
	5.35	30	2	0	-111.779 609 754 156 901 26/5	① $l/u$
	5.35	30	2(1)	1(2)	-111.779 530 816 018 060 83/2	② $l/u$ -③ $l/u$
	5.35	30	3	1	-111.779 451 875 843 545 64/3	④ $l/u$
	5.50	31	2	2	-109.271 256 591 795 413 09/8	① $l/u$
1	5.45	31	0	0	-93.752 663 561 353 941 555/46	① $l/u$
	5.45	31	0(1)	1(0)	-93.647 517 895 857 672 160/51	② $l/u$ -③ $l/u$
	5.50	32	0(1)	2(1)	-93.332 477 425 955 759 823/0	① $l/u$ -④ $l/u$
	5.50	32	0(1)	3(2)	-92.808 715 952 146 584 367/5	② $l/u$ -③ $l/u$
	5.50	32	0(1)	4(3)	-92.078 139 010 609 340 932/29	① $l/u$ -④ $l/u$
	5.50	32	2(3)	1(0)	-91.143 313 569 269 610 768/6	② $l/u$ -③ $l/u$
	5.50	32	2(3)	2(1)	-90.007 380 078 860 023 320/16	① $l/u$ -④ $l/u$
	5.50	32	0(1)	5(4)	-88.673 954 768 441 786 580/78	② $l/u$ -③ $l/u$
	5.50	32	0(1)	6(5)	-87.147 029 595 509 710 231/26	① $l/u$ -④ $l/u$
	5.50	32	2(3)	3(2)	-85.430 875 917 598 644 492/88	② $l/u$ -③ $l/u$

positive. An inverse procedure is adopted for negative eigenvalues. The energy levels are introduced in ascending order of magnitude indicating also their respective basis sets.

Table 1 illustrates how the method of this work can be applied to show the dependence of a specific energy level on the boundary parameter  $\ell$ . Clearly the lower and upper bound eigenvalues converge very rapidly to the limiting energy  $E_{(\infty)}$  as  $\ell$  increases, supporting numerically the theoretical findings of section 2.

**Table 7.** Lower and upper bounds to the eigenvalues of the three-well potential  $V(x, y; a, b, c_2, c_4)$  for which  $a = b = 0$ ,  $c_2 = 1$  and  $c_4 = 2$ .

$n_x$	$n_y$	$E_{n_x n_y}$	Basis set	$\ell$	$N$
0	0	1.714 654 094 198 951 8361/73	① <sub>l/u</sub>	3.20	24
0(1)	1(0)	4.024 199 895 443 115 5949/51	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.25	24
1	1	6.333 745 696 687 279 3531/5	④ <sub>l/u</sub>	3.25	24
0(2)	2(0)	7.686 165 214 700 426 6239/47	① <sub>l/u</sub> -① <sub>l/u</sub>	3.25	25
2(1)	1(2)	9.995 711 015 944 590 3821/30	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.25	26
0(3)	3(0)	12.579 407 545 521 240 012/7	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.25	26
2	2	13.657 676 335 201 901 411/3	① <sub>l/u</sub>	3.25	26
1(3)	3(1)	14.888 953 346 765 403 771/4	④ <sub>l/u</sub> -④ <sub>l/u</sub>	3.25	24
0(4)	4(0)	18.364 219 332 089 309 754/66	① <sub>l/u</sub> -① <sub>l/u</sub>	3.25	26
2(3)	3(2)	18.550 918 666 022 714 800/4	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.25	24
4(1)	1(4)	20.673 765 133 333 473 513/24	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.25	25
3	3	23.444 160 996 843 528 189/95	④ <sub>l/u</sub>	3.25	24
2(4)	4(2)	24.335 730 452 590 784 542/54	① <sub>l/u</sub> -① <sub>l/u</sub>	3.25	26
0(5)	5(0)	24.944 792 389 262 699 178/80	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.30	26
1(5)	5(1)	27.254 338 190 506 862 936/9	④ <sub>l/u</sub> -④ <sub>l/u</sub>	3.30	26
4(3)	3(4)	29.228 972 783 411 597 937/8	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.30	26
2(5)	5(2)	30.916 303 509 764 173 965/8	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.30	27
0(6)	6(0)	32.248 454 862 419 083 094/101	① <sub>l/u</sub> -① <sub>l/u</sub>	3.30	26
6(1)	1(6)	34.558 000 663 663 246 850/4	② <sub>l/u</sub> -③ <sub>l/u</sub>	3.30	27
4	4	35.013 784 569 979 667 673/95	① <sub>l/u</sub>	3.25	25

From tables 2–6 we may observe the behaviour of the low-lying state eigenvalues of the two-well oscillators as  $Z^2$  varies from 0.001 to 20. It should be mentioned that  $Z^2$  controls the depth of wells, and at  $Z^2 = 8$  the lower eigenvalues start to become nearly degenerate owing to the tunnelling through the potential barrier. This means that the two wells are sufficiently separated when  $Z^2 > 8$ , especially, for negative values of  $a$ . Such a situation appears evidently at  $Z^2 = 20$ , where the lower eigenvalues are closely bunched in quadruples. Note that the probability of tunnelling approaches zero for relatively small negative harmonic couplings, i.e.  $Z^2 \ll 8$ , for which the system behaves like a single-well oscillator. On the other hand,  $Z^2$  should not be much greater than 20 since the eigenvalue problem then tends to a non-physical one. Actually, we perceived the weak convergence property of the method for large enough values of  $Z^2$ .

In the problem under discussion, two special cases of the parameters  $a = b = 1$  and  $a = b = 0$  can be distinguished. In the former, the potential has a circular symmetry, and hence the spectrum may also be examined by the radial part of the Schrödinger equation,

$$\left(-\frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{l^2}{r^2} + v_2 r^2 + v_4 r^4 + v_6 r^6\right) \mathcal{R}(r) = E \mathcal{R}(r) \tag{5.1}$$

in another context. This is currently being investigated [19,20]. In the latter, the system reduces to two independent oscillators, for which

$$E_{n_x n_y} = E_{n_x} + E_{n_y} \tag{5.2}$$

where the  $E_{n_x}$  ( $E_{n_y}$ ) are the eigenvalues of the corresponding one-dimensional equation. So the results of this case may be checked by the accurate one-dimensional calculations in [16,21]. Furthermore, only for positive values of  $a$ , there are some two-dimensional results as well, which are quoted in tables 3 and 4 for comparison [22]. However, the inner product technique used in [22] seems to be insufficient in determining the aforementioned nearly degenerate eigenstates.



The energy level crossings may be analysed by the representation of the eigenvalues  $E_{n_x, n_y}$  as groups denoted by the integer number  $G$  such that  $G = n_x + n_y$ . It can be seen, from tables 2–6, that the eigenvalues in the groups  $2G + 1$ , which are treated by either the sets ②<sub>l/u</sub> or ③<sub>l/u</sub>, remain doubly degenerate throughout the interval of  $a$ ,  $a \in (-1, 1]$ . This is a consequence of the interchange symmetry of the coordinates  $x$  and  $y$ . Additional doubly degenerate levels occur at  $a = 0$  and  $a = 1$  due to the relation in (5.2) and the circular symmetry of the potential, respectively. However, these particular degenerate levels split into two levels when  $a$  is different from 0 and 1. In [7] and [13], certain ordering rules for the eigenvalues of anharmonic oscillators belonging to a specific group  $G$  were investigated. Unfortunately, in the case of multiwell potentials, we could not devise similar rules which are independent of  $Z^2$ . In fact, the eigenvalues in a group  $G$  cannot be ordered according to an identical rule for small and large  $Z^2$  regimes, with a fixed  $a$ .

The reported truncation orders  $N$  imply that the trigonometric basis sets in (3.2) and (3.3) have virtually the same convergence properties. It is clear that there is no uncertainty in the tabulated results since we have estimated two-sided exact eigenvalue bounds. Furthermore, as is shown from table 7 the method can be extended to three-well potentials without any loss of accuracy. However, a fairly detailed numerical analysis of the spectrum of such an oscillator is left to a future study.

## References

- [1] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
- [2] Bender C M and Wu T T 1973 *Phys. Rev. D* **7** 1620
- [3] Banks T, Bender C M and Wu T T 1973 *Phys. Rev. D* **8** 3346
- [4] Banks T and Bender C M 1973 *Phys. Rev. D* **8** 3366
- [5] Killingbeck J P and Jones M N 1986 *J. Phys. A: Math. Gen.* **19** 705
- [6] Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 4535
- [7] Hioe F T, MacMillen D and Montroll E W 1978 *Phys. Rep.* **43** 305
- [8] Ari N and Demiralp M 1985 *J. Math. Phys.* **26** 1179
- [9] Fernandez F M, Meson A M and Castro E A 1985 *Phys. Lett.* **112A** 107
- [10] Vrscay E R and Handy C R 1989 *J. Phys. A: Math. Gen.* **22** 823
- [11] Witwit M R M 1992 *J. Math. Phys.* **33** 4196
- [12] Witwit M R M and Killingbeck J P 1993 *J. Phys. A: Math. Gen.* **26** 3659
- [13] Taşeli H and Eid R 1996 *Int. J. Quantum Chem.* **59** 183
- [14] Nunez M A 1994 *Int. J. Quantum Chem.* **50** 113
- [15] Taşeli H 1992 *J. Comput. Phys.* **101** 252
- [16] Taşeli H 1993 *Int. J. Quantum Chem.* **46** 319
- [17] Taşeli H 1996 Accurate lower and upper bounds of the energy spectrum for the asymmetrical two-well potentials *Int. J. Quantum Chem.* in press
- [18] Press H W, Flannery B P, Teukolsky S A and Vetterling W T 1986 *Numerical Recipes* (Cambridge: Cambridge University Press) p 335
- [19] Taşeli H and Zafer A 1996 A Fourier–Bessel expansion for solving radial Schrödinger equation in two dimensions *Int. J. Quantum Chem.* in press
- [20] Taşeli H and Zafer A 1996 Bessel basis with applications:  $N$ -dimensional isotropic polynomial oscillators *Int. J. Quantum Chem.* submitted
- [21] Fernandez F M, Meson A M and Castro E A 1985 *J. Phys. A: Math. Gen.* **18** 1389
- [22] Witwit M R M 1995 *Ind. J. Pure Appl. Phys.* **33** 179