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Solving the 1-, 2-, and 3-Dimensional Schrödinger Equation for Multiminima Potentials Using the Numerov–Cooley Method. An Extrapolation Formula for Energy Eigenvalues

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As demonstrated with examples the Numerov–Cooley algorithm can be applied to more complicated potentials (especially multiminima potentials). There are no stability problems in the classically forbidden regions. An extrapolation formula for energy eigenvalues is deduced, which gets an additional accuracy of $2 \cdots 4$ digits for energy eigenvalues. This formula is checked as follows: For one state of a double minimum potential (which is used to approximate hydrogen bond potentials) an analytical solution is given. This solution is compared with numerical results. Also the accuracy of the eigenfunctions is checked. Computer-dependent rounding errors (CDC Cyber 995) are estimated. The eigenfunctions corresponding to 1-dimensional potentials $V^x(x)$ and $V^y(y)$ are used as basis functions for a perturbed 2-dimensional multiminima potential $V^x(x) + V^y(y) + \Delta V(x, y)$. For a 63-minima potential as an example, the accuracy of the eigenvalues is $4 \cdots 6$ digits depending on the perturbation $\Delta V(x, y)$. The computer time, depending on the accuracy, is tabulated for different potentials. © 1989 Academic Press, Inc.

INTRODUCTION

The Cooley–Numerov algorithm [1, 2] is a 3-point shooting method with the recurrence formula

$$y_{n+1} = \left(1 - \frac{\Delta x^2}{12} u_{n+1}\right)^{-1} \left[\left(2 + \frac{10\Delta x^2}{12} u_n\right) y_n - \left(1 - \frac{\Delta x^2}{12} u_{n-1}\right) y_{n-1}\right] + O(\Delta x^6), \tag{1}$$

whereby

$$u(x) = \frac{2m}{\hbar^2} (V(x) - E),$$

solving the 1-dimensional stationary Schrödinger equation, whereby the energy E is an input parameter. This procedure was improved by various authors [3–7] and compared with other methods [8–10]. The boundary conditions $y_1 := y(x_1) = 0$

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and $y_2 := y(x_2) \neq 0$ are used to integrate with increasing index n up to a matching point y_k. In the same way the integration for decreasing n with the boundary conditions $\overline{y_N} := \overline{y(x_N)} = 0$ and $\overline{y_{N-1}} := \overline{y(x_{N-1})} \neq 0$ (N = total number of points) is done up to the matching point y_k. The function values $(y_1, y_2, ..., y_k)$ are adapted to $(\overline{y_k}, \overline{y_{k+1}}, ..., \overline{y_N})$ by the condition $y_k = \overline{y_k}$. If the slope at x_k is equal for left and right integration $(y'_k = \overline{y'_k})$, an eigenvalue E is found.

In the following only boundary conditions at one outer region are used (for example, at $x = x_1$ and $x = x_2$) [11–13]. In this modified method it is the goal to obtain good boundary conditions at the other side by varying the energy E.

To determine the eigenvalues E, the following criterion is used: a necessary condition that the solutions are eigenfunctions is that the obtained functions decrease with increasing x in the right outer region. This criterion is verified by minimizing $y(x_N)$.

Essential for this procedure is the fact that the linear independent solutions have opposite properties for each eigenvalue: The physical solution vanishes for large x values, whereas the second solution increases exponentially.

With $(y_n, n = 1, ..., N)$ also $(c \times y_n, n = 1, ..., N)$ is a solution. Therefore, without restriction, y_1 can be chosen as a fixed value, for instance, $y_1 = 1$.

Figure 1a shows how the eigenvalues are systematically found. In this figure,

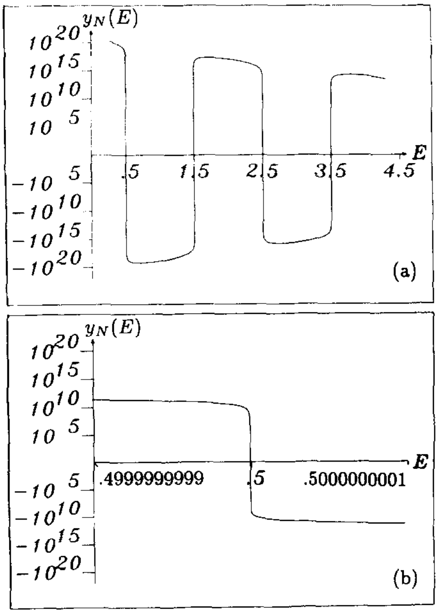

FIG. 1(a) $y_N(E)$ is the right function value $y(x_N)$ for the energy parameter E. $y_N(E)$ is logarithmic scaled in positive and negative direction. The zeros of $y_N(E)$ are the energy eigenvalues E of the harmonic oscillator. (b) Results from (a) with a stretching factor of about 2×10^{10} in E direction near $E = 0.5$. It demonstrates the large slope of $y_N(E)$ near an eigenvalue and the high accuracy of the method.

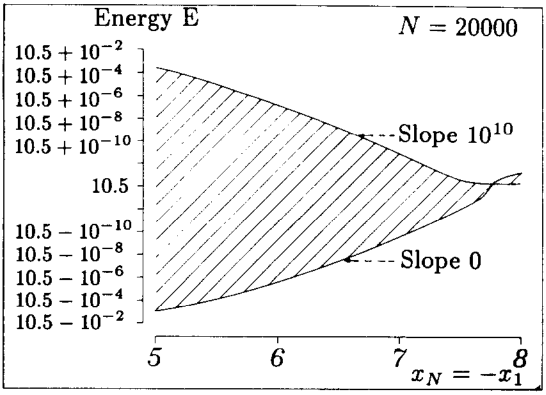

FIG. 2. Dependence of the eigenvalue of the 10th excited state of the harmonic oscillator ($E = 10.5$) on the boundaries $x_N = -x_1$ and the initial condition $y_1' = y'(x_1)$. Eigenvalues $E < 10.5$ and eigenvalues $E > 10.5$ are scaled logarithmic, respectively. The dashed area marks the eigenvalues corresponding to $0 < y'(x_1) < 10^{10}$.

$y_N := y(x_N)$ is shown as a function of the energy E (harmonic oscillator; $m = \omega = \hbar = 1$). The eigenvalues are the zeros of this function. The iteration algorithm works as follows: it counts the zeros of the functions $y(x)$ for every energy parameter E. If the number of zeros increases by one then the neighboring function values $y_N(E_i)$ and $y_N(E_{i+1})$ are connected by a cubic spline function. The zero of this interpolation function is the next iteration value for the energy parameter E.

Figure 1b shows a section of Fig. 1a in which the abscissa is expanded by a factor 2×10^{10}. This figure illustrates the very steep slope of this function near an eigenvalue. Therefore, the convergence of the iteration is very rapid.

Figure 2 shows the numerical eigenvalues of the tenth state of the harmonic oscillator as a function of x_N ($x_N = -x_1$). The lower curve represents values for a slope $(y_2 - y_1)/(x_2 - x_1) = 0$ and the upper one for a slope $(y_2 - y_1)/(x_2 - x_1) = 10^{10}$. This figure points out the connection between the accuracy of the calculated eigenvalues and the chosen boundaries $x_N = -x_1$. The accuracy decreases orders of magnitude if x_N is chosen too small. The eigenvalues in the dashed area correspond to a slope, which is greater than 0 but smaller than 10^{10}.

AN EXTRAPOLATION FORMULA FOR ENERGY EIGENVALUES

The Numerov algorithm is exact up to fourth order [1]. Therefore the deviation of the energy eigenvalues $E^{(N)}$ (using N points) from the exact (extrapolated) value E_{extr} should be $2^4 = 16$ times larger than for $E^{(2N)}$. More generally,

$$\frac{E_{\text{extr}} - E^{(M)}}{E_{\text{extr}} - E^{(N)}} = \left(\frac{N}{M}\right)^4 \qquad (N > M)$$

or

$$E_{\text{extr}} = \frac{E^{(M)} - E^{(N)}(N/M)^4}{1 - (N/M)^4}. \tag{2}$$

Herewith M and N are the step numbers of two calculations (Richardson extrapolation, [14]).

Table I confirms that the extrapolated value E_{extr} is two to four digits more precise than $E^{(2N)}$. Table I(a) corresponds to the harmonic oscillator in atomic units, Table I(b) to the fourth eigenstate ($E_4 = 0$) of the double minimum potential (Fig. 3) which is calculated analytically as follows: To find the analytical solution, the shape of the potential is, first, not fixed. An answer of the following question is searched: What is the shape of the potential $V(x)$ if the wave function

$$\Psi(x) = f(x) \cdot e^{g(x)}; \qquad f, g \text{ polynomials} \quad g \leqslant c \in \mathbb{R} \tag{3}$$

is an analytical solution? From this formulation follows

$$\frac{(1/2m)\,\Psi''(x)}{\Psi(x)} = V(x) - E = \frac{1}{2m}\left(\frac{f'' + 2f'g'}{f} + g'' + g'^2\right). \tag{4}$$

TABLE I

The Use of Eq. (2) Increases the Accuracy of the Energy Eigenvalues by 2···4 Digits

state	N	$E^{(N)}$	2*N	$E^{(2*N)}$	E_{extr}
a 0	50	.499967959442	100	.499998016264	.500000020052
0	100	.499998016264	200	.499999876307	.500000000310
0	200	.499999876307	400	.499999992274	.500000000005
1	50	1.499774866318	100	1.499986101268	1.500000183598
1	100	1.499986101268	200	1.499999133956	1.500000002802
1	200	1.499999133956	400	1.499999945913	1.500000000043
2	50	2.499192106056	100	2.499950305663	2.500000852303
2	100	2.499950305663	200	2.499996906127	2.500000012825
2	200	2.499996906127	400	2.499999806819	2.500000000198
3	50	3.497952691725	100	3.499874606967	3.500002734650
3	100	3.499874606967	200	3.499992200942	3.500000040540
3	200	3.499992200942	400	3.499999513145	3.500000000625

state	N	$E^{(N)}$	2*N	$E^{(2*N)}$	E_{extr}
b 4	250	-.000008581487	500	-.000000536023	.000000000341
4	500	-.000000536023	1000	-.000000033497	.000000000005
4	1000	-.000000033497	2000	-.000000002094	.000000000000

Note. (a) Four lowest states of the harmonic oscillator. (b) Fourth state of a double minimum potential (see analytical solution in Fig. 3).

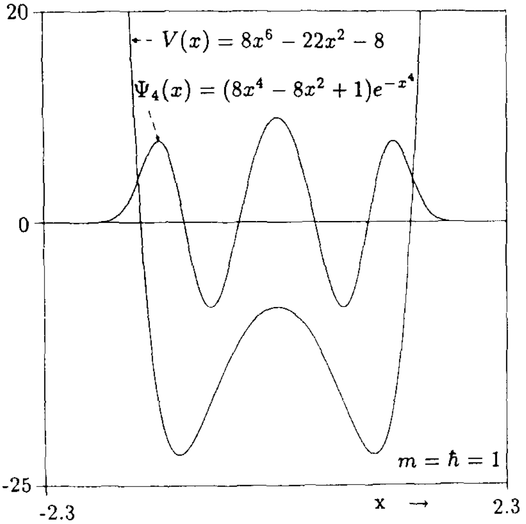

FIG. 3. $\Psi_4(x)$ is the analytical solution for the double minimum potential $V(x)$ ($m = \hbar = 1$; $E_4 = 0$).

The following special shape of the wave function is chosen

$$\Psi(x) = (a_4 x^4 + a_2 x^2 + a_0)\, e^{-x^4}. \tag{5}$$

The condition that the potential $V(x)$ should not have any singularities can only be fulfilled if the polynomial division $(f'' + 2f'g')/f$ (Eq. (4)) results again in a polynomial, i.e.,

$$f'' + 2f'g' = p \cdot f, \qquad c \in \mathbb{R},\ p \text{ polynomial}. \tag{6}$$

If Eq. (5) is inserted in Eq. (6) one obtains a system of equations for the coefficients of $f(x)$ and $p(x)$ and as result $\Psi_4(x)$ as well as $V(x)$. Parts of these calculations can be performed by the programming language REDUCE. In similar way an eigenfunction with eigenvalues to a multidimensional potential can be found analytically.

ACCURACY OF EIGENFUNCTIONS AND EIGENVALUES

A measure of accuracy for *eigenfunctions* is

$$F = \int_{x_1}^{x_N} |\Psi_1(x) - \Psi_2(x)|\, dx \tag{7}$$

whereby $\Psi_1(x)$ is the normalized analytical and $\Psi_2(x)$ the normalized numerical eigenfunction.

TABLE II

Measure of Accuracy (Eq. (7)) for the 4th eigenfunction of the double minimum potential in Fig. 3 depending on the number N of function values.

N	E	F
125	-.0001376322	.0000219367
250	-.0000085815	.0000013644
500	-.0000005360	.0000000852
1000	-.0000000335	.0000000052
2000	-.0000000021	.0000000003
4000	-.0000000001	.0000000000

Table II shows this measure of accuracy for the fourth eigenstate of the above double minimum potential depending on the number of function values N. For $N = 1000$ the accuracy is better than 10^{-6} %, for $N = 4000$ better than 10^{-8} %.

In contrast to usual numerical methods with the above treatment very high eigenfunctions and eigenvalues also can be calculated precisely. This is demonstrated in Table III in which the *eigenvalues* of the 1000th, 3000th, and 10,000th excited state of the harmonic oscillator are given as a function of the number of points N. The table shows the convergence of the eigenvalues to the analytical values $(k + \frac{1}{2})$ with an increasing number of points N.

The right side of Table III shows that the extrapolation formula (2) also gives

TABLE III

Accuracy of the 1000th, 3000th, and 10000th States of the Harmonic Oscillator $(m = \omega = \hbar = 1)$ Depending on the Number N of Calculated Function Values y_n $(n = 1, \ldots, N)$

N	state	E	2*N	E_{extr}
8000	1000	1000.399597	16000	1000.500049
16000	1000	1000.493771	32000	1000.500000
32000	1000	1000.499611	64000	1000.500000
64000	1000	1000.499976	128000	1000.500000
128000	1000	1000.499998	256000	1000.500000
256000	1000	1000.500000		
32000	3000	3000.411601	64000	3000.500023
64000	3000	3000.494497	128000	3000.500000
128000	3000	3000.499656	256000	3000.500000
256000	3000	3000.499979	512000	3000.500000
512000	3000	3000.499999		
128000	10000	10000.369712	256000	10000.500022
256000	10000	10000.491878	512000	10000.500001
512000	10000	10000.499493		

Note. The eigenfunctions corresponding to these states have 1000, 3000, and 10,000 zeros. The analytical energy value of the kth state is $E = k + \frac{1}{2}$. The right side shows results obtained by the extrapolation formula (2).

results which are three to four orders of magnitude more precise for very high states.

MULTIMINIMA POTENTIALS

Some authors [4, 10] have reported stability problems in the classically forbidden regions and difficulties with multiminima potentials. The following 40-minima potential and other calculated examples show that the (modified) Cooley–Numerov algorithm is particularly suitable for multiminima potentials and can therefore also be used in solid state physics. The potential

$$V(x)=\begin{cases} 0.5\cdot(x-a)^2 & \text{for } -\infty<x\leqslant 2a \\ 0.5\cdot(x-(2k-1)a)^2 & \text{for } 2(k-1)a<x\leqslant 2ka;\ 2\leqslant k\leqslant M-1 \\ 0.5\cdot(x-(2M-1)a)^2 & \text{for } 2(M-1)a<x<\infty \end{cases} \tag{8}$$

$$m=\hbar=1, \qquad M=\text{number of minima } (=40)$$

is a parabolic 40-minima potential. With increasing a, the barriers and the classical forbidden regions increase.

Figure 4a shows this potential for $a=3$. In the Figs. 4b–d the wave functions of

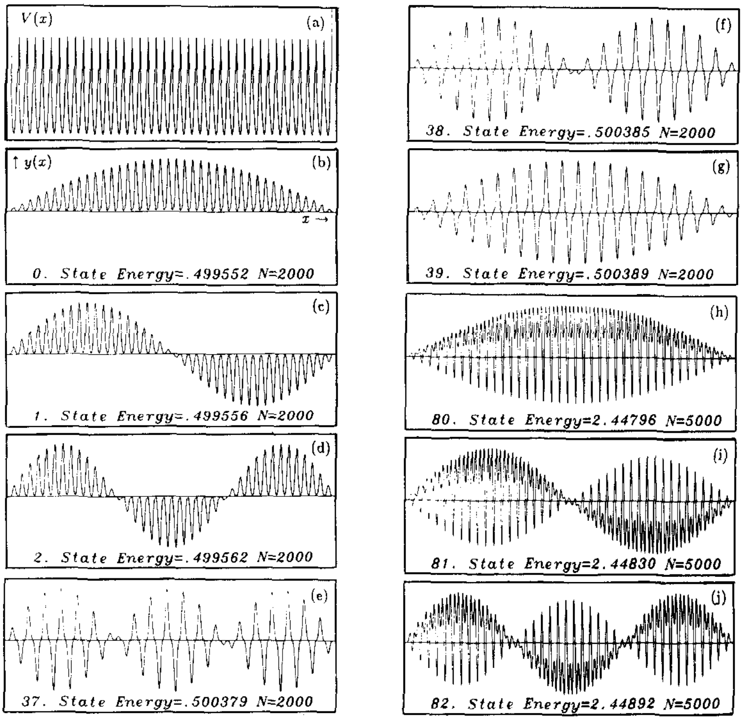

FIG. 4. Eigenfunctions and eigenvalues to the 40-minima potential, represented in Fig. 4a; $-3.5\leqslant x\leqslant 243.5$, $a=3$.

the three lowest states are given. Figs. 4e–g show the three highest states of the lowest energy band. Finally, Figs. 4h–j show the three lowest states of the third energy band.

For $a = 2$; 3; 4; 5 the height of the potential barriers amounts to 2; 4.5; 8; 12.5 and the width of the energy band $\Delta E = E_{39} - E_0$ amounts to 0.082987; 0.000837; 0.00000102; 0.000000000156 for $N = 5000$ steps, respectively.

The accuracy of the energy eigenvalues of this potential is limited to $6 \cdots 8$ digits by the peaks at $x = 2 \times k \times a$ $(k = 1, ..., 39)$.

In Fig. 5 the function $y_N(E)$ for $a = 5$ and $N = 5000$ is shown (see Fig. 1). The deviation of the energy band from the theoretical center $E = 0.5$ (harmonic oscillator) decreases with increasing N. The accuracy of the differences $E_i - E_j$ $(i, j = 0, ..., 39)$ is much higher than the absolute values E_i and E_j. The energy levels are not homogeneously distributed in the band: The density at the boundaries is higher.

Only in a small energy section $y_N(E) < y_{\max}$ is true, whereby $y_{\max}$ has a size of about 10^{300} (dependent on the computer used). An arithmetic overflow error $(y_N(E) > y_{\max})$ can be avoided by stopping the calculation if $y_i(E) > y_{\max}$ $(3 \leqslant i \leqslant N)$. The procedure to find an energy value E without arithmetic overflow is similar to the algorithm described in the introduction.

Table IV shows the convergence of the three lowest energy eigenvalues for a 40-, 100-, and 1000-minima parabolic potential (Eq. (8)) for $a = 3$ as a function of the number of steps N. For $N = 18{,}000$ the accuracy amounts to 8 (40 minima), 7 (100 minima), and 3 (1000 minima) digits. The extrapolated energy for the 1000-minima potential amounts to 0.49955 and is precise up to five digits. In the case of 1000-minima the distance of the lowest energy levels is of the order of magnitude of 10^{-10}.

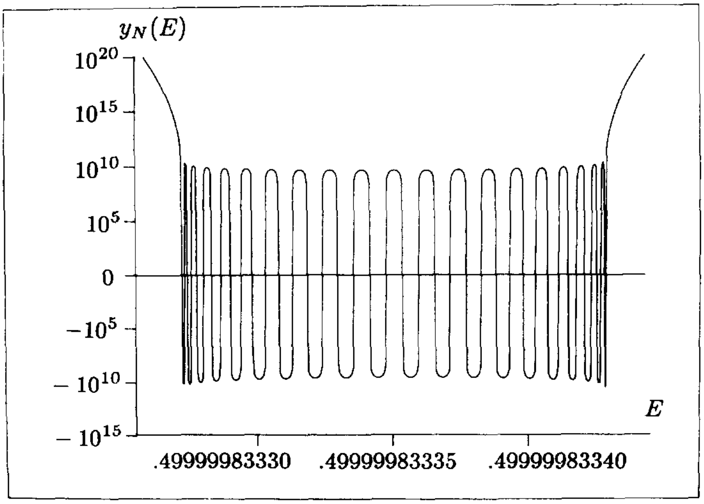

FIG. 5. $y_N(E)$ for $a = 5$ and $N = 5000$. For $E < E_0$ and $E > E_{39}$, $y_N(E)$ is increasing very quickly.

TABLE IV

The Three Lowest Energy Eigenvalues of a 40-, 100-, and 1000-minima potential depending on *N*.

N	40 Minima, E_0	N	100 Minima, E_0	N	1000 Minima, E_0
2000	.499552012	2000	.499519042	12000	.499292503
4000	.499552852	4000	.499549844	14000	.499410954
6000	.499552896	6000	.499551476	16000	.499468546
8000	.499552903	8000	.499551743	18000	.499499444
10000	.499552904	10000	.499551823		
12000	.499552907	12000	.499551849		
14000	.499552906	14000	.499551861		
16000	.499552906	16000	.499551866		
18000	.499552907	18000	.499551869		
N	40 Minima, E_1	N	100 Minima, E_1	N	1000 Minima, E_1
2000	.499555693	2000	.499519651	12000	.499292503
4000	.499556549	4000	.499550455	14000	.499410954
6000	.499556592	6000	.499552085	16000	.499468546
8000	.499556602	8000	.499552354	18000	.499499445
10000	.499556596	10000	.499552432		
12000	.499556604	12000	.499552458		
14000	.499556606	14000	.499552469		
16000	.499556606	16000	.499552474		
18000	.499556604	18000	.499552478		
N	40 Minima, E_2	N	100 Minima, E_2	N	1000 Minima, E_2
2000	.499561878	2000	.499520668	12000	.499292503
4000	.499562695	4000	.499551475	14000	.499410954
6000	.499562736	6000	.499553099	16000	.499468546
8000	.499562746	8000	.499553374	18000	.499499446
10000	.499562776	10000	.499553446		
12000	.499562748	12000	.499553472		
14000	.499562748	14000	.499553483		
16000	.499562749	16000	.499553488		
18000	.499562748	18000	.499553491		

There are no stability problems in the classically forbidden regions of such multiminima potentials.

A similar, but differentiable potential is

$$V(x)=\begin{cases} a_1\cdot x^4, & \text{for } x<0,\\ a_2\cdot\sin^{2n_1}\left(\pi\cdot\dfrac{x}{a_3}\right), & \text{for } 0\leqslant x<(n_2-1)\,a_3,\\ a_4(x-(n_2-1)\,a_3)^4, & \text{for } (n_2-1)\,a_3\leqslant x<\infty, \end{cases}$$
$$+a_5\cdot\exp[-a_6(x-a_7)^2]+a_8\cdot x$$
$$n_1, n_2\in\mathbb{N};\qquad a_i\in\mathbb{R},\qquad i=1,\ldots,8. \tag{9}$$

n_1 determines the width of the barriers and n_2 the number of minima. a_3 is the distance of two minima; a_5, a_6, and a_7 correspond to a Gaussian function simulating a local perturbation. a_8 corresponds to a term simulating a constant external electrical field. Such a potential (including eigenvalues) is illustrated in Fig. 6.

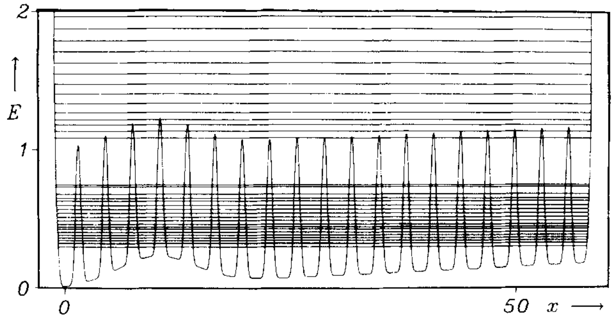

FIG. 6. 20-minima potential (Eq. (9)) with energy eigenvalues in atomic units. The $0 \cdots 19$th state are building up an energy band. The distance between states 1 and 2 is very small and cannot be represented in this figure ($m = \hbar = 1$; $n_1 = 10, n_2 = 20$; $a_1 = 1$, $a_2 = 1$, $a_3 = 3$, $a_4 = 1$, $a_5 = 0.2$, $a_6 = 0.028$ (half width $= 5$), $a_7 = 10$, $a_8 = 0.003$).

For such potentials the accuracy of eigenfunctions was checked. But $\Psi_1(x)$ in (7) is now the normalized numerical eigenfunction to $N = 4000$ and $\Psi_2(x)$ to $N = 8000$. With $n_2 = 10$ minima and $n_1 = 1, \ldots, 5$ the measure of accuracy F is about 10^{-8} (10^{-6} %); for 30 minima, 10^{-7}; for 60 minima, 10^{-6}; and for 100 minima, 10^{-5}.

2- AND 3-DIMENSIONAL SCHRÖDINGER EQUATION

For the potential

$$V(x, y) = V^x(x) + V^y(y) + \Delta V(x, y) \tag{10}$$

(in the same way: $V(x, y, z)$), the Schrödinger equation can only be separated for $\Delta V(x, y) = 0$ and then it can be solved by the shooting procedure [11–13]. The 2-dimensional eigenfunctions are products of the 1-dimensional ones. Figure 7 shows for the 2-dimensional case a 63-minima potential (9 minimas corresponding to $V^x(x)$, 7 minimas corresponding to $V^y(y)$). Additionally in the center of this figure a perturbation term $\Delta V(x, y)$ (for example a product of two Gaussian functions) is introduced. To obtain the eigenvalues of this perturbed system, the 2-dimensional basis functions are built up by products of 1-dimensional eigenfunctions of the unperturbed systems (corresponding $V^x(x)$ and $V^y(y)$). Also additional functions (for example, oscillator functions) can be used as basis functions. The eigenfunctions of the perturbed systems are a linear combination of these basis functions. The coefficients of the basis functions are determined by solving a matrix eigenvalue problem. All integrals can be reduced to 1-dimensional integrals, if

$$\Delta V(x, y) = \sum_i V_i^x(x) \cdot V_i^y(y). \tag{11}$$

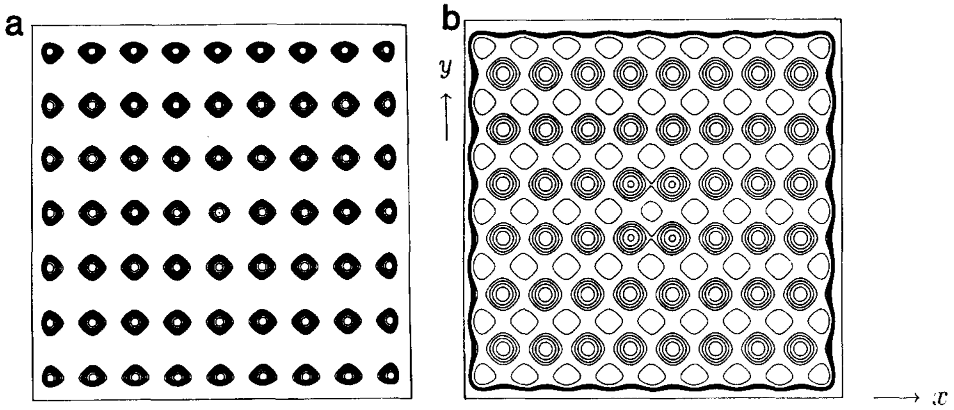

FIG. 7. Multiminima potential $V^x(x)+V^y(y)+\Delta V(x, y)$: (a) only minima; (b) only maxima. Perturbation $\Delta V(x, y)$ in the center.

They are evaluated by Simpsons rule. The error caused by Simpson integration is in orders of magnitude smaller than the error caused by the finite (uncomplete) set of basis functions. The accuracy of the energy eigenvalues is $4 \cdots 6$ digits depending on the perturbation potential and the number of 2-dimensional basis functions $(n = 25 \cdots 49)$.

Only $N = 400$ eigenfunction values y_i $(i = 1, ..., N)$ are needed. This is one reason why the calculation time including the matrix eigenvalue problem amounts to only $0.2 \cdots 0.7$ s (CDC Cyber 995).

COMPARISON TO THE CONVENTIONAL COOLEY ALGORITHM

The algorithm used here (described in the Introduction) was compared to the conventional Cooley algorithm. Especially for higher states the curvature of the eigenfunction at the matching point may be very strong (see Figs. 4h–j). If, however, precise formulas for the slopes y'_k and $\overline{y'_k}$ at the matching point x_k are used, for example,

$$y'_k \approx \frac{1}{\Delta x}\left(2.45y_k - 6y_{k-1} + 7.5y_{k-2} - \frac{20}{3}\, y_{k-3} + 3.75y_{k-4} - 1.2y_{k-5} + \frac{1}{6}\, y_{k-6}\right) \tag{12}$$

$$\overline{y'_k} \approx -\frac{1}{\Delta x}\left(2.45y_k - 6y_{k+1} + 7.5y_{k+2} - \frac{20}{3}\, y_{k+3} + 3.75y_{k+4} - 1.2y_{k+5} + \frac{1}{6}\, y_{k+6}\right), \tag{13}$$

TABLE VI

Calculation Time in Seconds (CDC Cyber 995) for Six Potentials

No. of exact digits	Potential	Harmonic oscillator (10 states)	40-minima potential (10 states)	Hydrogen bond double minimum (10 states)	Morse (10 states)	Extended Morse potential (10 states)	Proton–Neutron interaction: Deuterium (1 state)
4		0.16	0.6	0.11	0.10	0.10	0.02
6		0.42	4.0	0.24	0.21	0.21	0.05
8		1.16	—	0.58	0.61	0.61	0.11
10		3.34	—	1.78	1.76	1.76	0.34

Note. The calculation time corresponds to the ten lowest levels. (For Deuterium only the ground state exists.) The calculation time depends on the number of correct digits (4, 6, 8, and 10) of the highest (9th excited) state.

TABLE V

Energy Eigenvalues E Depending on the Internal Accuracy (normal, 14 digits; double, 28 digits) and the Number of Steps N

N	E (DOUBLE)	E (NORMAL)
1000	.499999999919	.499999999906
2000	.499999999995	.499999999954
4000	.500000000000	.499999999812
8000	.500000000000	.499999999180

Note. Only in the case of double precision rounding errors can be neglected.

the Cooley algorithm yields the same results. The coefficients c_i of (12) and (13) were derived by solution of a system of linear equations

$$y_k^{(j)\prime} = \frac{1}{\Delta x} \sum_{i=0}^{n-1} c_i y_{k-i}^{(j)}; \qquad n = 7; \quad j = 1, ..., n. \tag{14}$$

$y_k^{(j)}$ are values of a given polynomial of $(n-1)$th order.

Computerdependent Accuracy

In the case of the Numerov–Cooley algorithm the propagation of error caused by rounding errors (Cyber 995, 14 digits in FORTRAN 77) yields only about nine digits for the energy eigenvalues. Table V shows the energy eigenvalue of the ground state (harmonic oscillator) for various step numbers N in the case of usual precision (14 digits) and double precision (28 digits). The convergence to the precise eigenvalue is only given with double precision.

Computer Time

In Table VI the computer time in seconds (CDC Cyber 995) for different potentials and various accuracy (number of exact digits for the highest state) is summarized.

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