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Eigenvalue Correction Estimates for the One-dimensional Schrödinger Equation

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The problem of solving the Schrödinger equation and the more general Sturm–Liouville problem in the finite-difference approximation is considered with emphasis on the question of where to match inward and outward solutions. It is shown that the determination of the matching point is a variational problem. A modification of the usual energy correction method in which previously calculated eigenfunctions are projected out of the trial solution is described. An iterative scheme which should determine all eigenvalues below some prescribed upper limit is proposed, and its application in two sample cases is discussed.

1. INTRODUCTION

The problem of solving the Schrödinger equation and the more general Sturm–Liouville problem numerically is one that occurs commonly. The problem is usually solved either by replacing the equation with a finite-difference approximation, or by expanding the solutions in a finite basis and using algebraic techniques. Two recent applications of the latter method are in the work of Shore [1], using spline functions, and of Lin, using harmonic oscillator wave functions [2].

Various aspects of the finite-difference method have been discussed recently by Tobin and Hinze [3] and Wolniewicz and Orlikowski [4]. One approach to the finite-difference equation is to recognize that the basic equation (Eq. (3) below) is the algebraic eigenvalue problem for a tridiagonal matrix and use one of the highly developed matrix diagonalization methods to solve the problem.

The widely used method developed by Cooley [5] also treats the finite-difference equation as a matrix equation but uses a specific method of Löwdin [6] for obtaining an improved estimate for an eigenvalue from an initial estimate and emphasizes the use of the Numerov difference equation. The use of the various methods has been discussed and compared recently by Shore [1] and by Wicke and Harris [7].

If preliminary estimates of the eigenvalues are known, Cooley's method will, in general, be very effective. The purpose of this article is to discuss modifications of the

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method that can be made when no preliminary estimates are known, and to present a systematic way of obtaining the solutions.

In order to be specific, the dimensionless form of the Schrödinger equation on a finite interval $[0, a]$,

$$\begin{aligned} -\phi_n'' + V(x)\,\phi_n(x) &= e_n \phi_n(x), \\ \phi(0) = \phi(a) &= 0, \end{aligned} \tag{1}$$

will be discussed. The most general Sturm–Liouville problem can in fact be reduced by a change of independent variable to

$$-y_i'' + q(x)\,y_i = \lambda_i r(x)\,y_i, \tag{2}$$

where $r(x) > 0$ and y_i satisfies homogeneous boundary conditions $y'(0) = \alpha y(0)$, $y'(a) = \beta y(a)$. The modifications in the method needed to treat the general problem will be indicated briefly.

In practice, the problem is often on the interval $[0, \infty)$. This problem can usually be satisfactorily approximated by requiring $\phi(a) = 0$, where a is sufficiently large, or by matching the solution to the known asymptotic solution, e.g., either an exponential or a Coulombic wave function. This problem will not be discussed in this article except to note that if the approximation $\phi(a) = 0$ is used, the energy correction given in Eq. (8) below can be applied to show that the error in the eigenvalue decreases as e^{-2ka}, $k^2 = -e_i$, if a is large enough that $V(x)$ is negligible for $x > a$.

In a numerical calculation, Eq. (1) is replaced by a difference equation, e.g., the lowest-order equation

$$\phi_{n,i-1} - 2\phi_{n,i} + \phi_{n,i+1} = h^2(v_i - e_n)\,\phi_{n,i}, \tag{3}$$

where $\phi_{n,i}$, v_i are the values of $\phi_n(x)$, $V(x)$ at $N+1$ mesh points $0, h, \ldots, ih, \ldots, a$, $\phi_{n,0} = \phi_{n,N} = 0$ and $Nh = a$. The discussion here will primarily be based, however, on the differential equation (1); derivatives and integrals are then to be replaced in obvious ways.

The standard method of solving Eq. (1) is to consider the equation for a general e,

$$-y'' + V(x)\,y = ey, \tag{4}$$

and to obtain two solutions $y_1(x)$ and $y_2(x)$ satisfying the boundary conditions at 0 and a, respectively, and to match the solutions at some intermediate point X; i.e., y_1 and y_2 are multiplied by constants so that $y_1(X) = y_2(X)$. If e is close to an eigenvalue, a correction Δe can be estimated from the difference in the slopes of y_1 and y_2 at X. A simple calculation, similar to that given by Hartree [8] and Ridley [9], is as follows. Write

$$-y_1'' + V(x)\,y_1 = ey_1, \tag{5}$$

$$-y'' + V(x)\,y = (e + \Delta e)\,y, \tag{6}$$

where $y_A(x) = y_1(x)$, $x < X$ and $y_A(x) = y_2(x)$, $x > X$ and y is an exact eigenfunction. Multiply (5) by y, (6) by y_A, subtract and integrate over $[0, a]$. The result can be written

$$\int_0^a d(y'_A y - y' y_A) = \Delta e \int_0^a y(x)\, y_A(x)\, dx.$$

The second term under the differential on the left hand is continuous and integrates to 0. The first term is discontinuous at X and integrates to

$$y'_1(X)\, y(X) - y'_2(X)\, y(X) = \Delta e \int_0^a y(x)\, y_A(x)\, dx. \tag{7}$$

(The contributions to the integral at 0 and a cancel between the two terms because of the boundary conditions.) If $y(x)$ is approximated by $y_A(x)$ in (7) the energy correction estimate

$$\Delta e = y_1(X)[\, y'_1(X) - y'_2(X)] \Big/ \int_0^a y_A(x)^2\, dx \tag{8}$$

is obtained.

One purpose of this article is to discuss the best choice for X; this question seems not to have been thoroughly treated previously. It wil be shown that the choice of X can be regarded as a variational problem. That is, the problem of determining Δe is formulated variationally; X can then be chosen to minimize the energy functional for the problem. It will also be shown that if X is chosen in this way, successive iterations for the eigenvalue will in principle converge downward to the ground state. Excited states can then be calculated with lower-lying known states projected out. The projected energy corrections will be calculated and a method that should calculate systematically all eigenvalues below any fixed maximum will be described. This method does not require any preliminary estimates for the eigenvalues. Two examples of the application of the method to problems from the recent literature will be described.

A brief discussion of the use of the method with the Numerov difference equation has also been included.

2. The Energy Correction

If e is an approximate value for an eigenvalue of Eq. (1) the correction to e of Eq. (8) can be obtained from the functions $y_1(x)$ and $y_2(x)$ in the following way. Define an approximate solution by

$$\begin{aligned} y_X(x) &= y_2(X)\, y_1(x), \qquad x \leqslant X, \\ &= y_1(X)\, y_2(x), \qquad x \geqslant X, \end{aligned} \tag{9}$$

where X is the matching point. The function y_X is continuous and satisfies Eq. (4) but has a discontinuous derivative at X. The eigenvalue problem can be derived as the problem of minimizing the energy functional

$$E[y] = \int_0^a [y'(x)^2 + V(x)\, y(x)^2]\, dx \Big/ \int_0^a y(x)^2\, dx. \tag{10}$$

To obtain an estimate of an eigenvalue of Eq. (1), the function $y_X(x)$ can be used as a trial function in Eq. (10). A straightforward calculation, making an integration by parts and using the fact that y_1 and y_2 satisfy Eq. (4), gives

$$E = e + W y_1(X)\, y_2(X)\, D^{-2}, \tag{11}$$

where $W = y_2(X)\, y_1'(X) - y_1(X)\, y_2'(X)$ is the (constant) Wronskian of y_2 and y_1 and

$$D^2 = y_2(X)^2 \int_0^X y_1(x)^2\, dx + y_1(X)^2 \int_X^a y_2(x)^2\, dx. \tag{12}$$

The second term in Eq. (11) is the energy correction given in Eq. (8) apart from multiplicative factors in the numerator and denominator. In the case of the more general Sturm–Liouville problem of Eq. (2), a factor $r(x)$ would also be included in the integrands in the denominator of Eq. (10) and in Eq. (12).

This derivation of the energy correction gives an indication of how the matching point X should be chosen. One can regard X as a variational parameter in the approximate solution $y_X(x)$, and, if the ground state solution of Eq. (1) is being sought, X should be chosen to minimize

$$\Delta e = W y_1(X)\, y_2(X)/D^2. \tag{13}$$

It should be remarked that the choice suggested by Cooley is to choose X at the first maximum of the inward solution. In many cases this is close to the optimum choice.

It is of interest to consider this result from a somewhat different aspect. It may be recognized that the function $y_X(x)$ in Eq. (9) is essentially the Green's function for the operator

$$e - V(x) + \frac{d^2}{dx^2}.$$

In fact,

$$y_X(x) = W G(x, X)$$

$$= W \sum_i (e_i - e)^{-1}\, \phi_i(x)\, \phi_i(X), \tag{14}$$

$$\Delta e = W^2 G(X, X)/D^2. \tag{15}$$

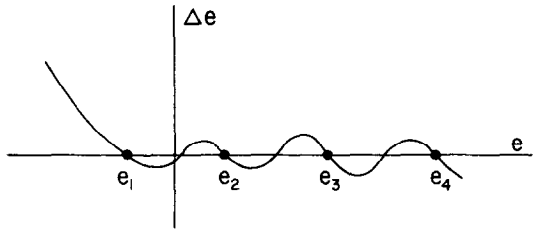

FIG. 1. A graph of Δe vs e at a fixed matching point. The slope is -1 at $e = e_i$ and is $+1$ at $\Delta e = 0$, $e \neq e_i$.

It is also straightforward to calculate

$$D^2 = \int_0^a G(X, x)\, G(x, X)\, dx$$
$$= W^2 \sum_i (e_i - e)^{-2}\, \phi_i(X)^2,$$

from which we find

$$\Delta e = \left[\sum_i (e_i - e)^{-1}\, \phi_i(X)^2\right]\left[\sum_i (e_i - e)^{-2}\, \phi_i(X)^2\right]^{-1}. \tag{16}$$

The denominator is the derivative of the numerator, suggesting that Eq. (16) is the Newton–Raphson estimate for Δe. That this is the case was shown by Cooley [5]. This is in the sense that a single of the Eqs. (3) fails to be satisfied at the i corresponding to X. The equation to be solved is then $F(e) = 0$, where $F(e)$ is the error in this equation.

It can be seen from (16) that if e is close to e_i, $\Delta e \approx e_i - e$ since one term dominates the sums. The qualitative behavior of Δe as a function of e is shown in Fig. 1 for fixed X; the graph passes through the e axis with slope -1 at the e_i; Δe is also zero at intermediate e values for which $y_1(X)$ or $y_2(X)$ is 0.

3. Calculation of Excited States

The variational method for calculating excited states is to find them in order of increasing energy eigenvalues by projecting out of the trial wave function at each step the assumed known eigenfunctions of lower energy. This approach to the present problem can be taken and the eigenfunctions calculated in order of increasing energy.

In order to project known solutions $\phi_i(x)$ out of $y_X(x)$ the overlap integral between them is required. It is seen from Eq. (14) that

$$\int_0^a \phi_i(x)\, y_X(x)\, dx = W(e_i - e)^{-1}\, \phi_i(X). \tag{17}$$

This result leads to a "projected" value for the energy correction,

$$\Delta e_p = \left[W y_1(X)\, y_2(X) - \sum_i{}'' W^2 (e_i - e)^{-1}\, \phi_i(X)^2 \right] D_p^{-2}, \tag{18}$$

where

$$D_p^2 = D^2 - W^2 \sum_i{}'' (e_i - e)^2\, \phi_i(X)^2. \tag{19}$$

We adopt the notation that $\sum_i''$ represents the sum over states i that are projected out, and $\sum_i'$ represents the sum over all states except the projected states. If known states $\phi_1, \phi_2, \ldots, \phi_{n-1}$ are projected out in Eqs. (18) and (19), $e + \Delta e_p$ provides a rigorous upper bound to e_n.

It is also possible to write Δe_P in a form analogous to Eq. (10):

$$\Delta e_p = \left[\sum_i{}' (e_i - e)^{-1}\, \phi_i(X)^2 \right] \left[\sum_i{}' (e_i - e)^{-2}\, \phi_i(X)^2 \right]^{-1}. \tag{20}$$

The behavior of Δe_P with e is qualitatively the same as that in Fig. 1 without the nodes at the projected e_i values.

4. Convergence of the Successive Iterations

It is seen from Eq. (13) that the sign of Δe is governed by $W y_1(X)\, y_2(X)$ and therefore for a fixed e, Δe changes sign at a node of y_1 or y_2. A diagram showing the nodes of $y_1(X)$ and $y_2(X)$ and regions of positive and negative Δe in the general situation is given in Fig. 2. It is known from the theory of ordinary differential equations

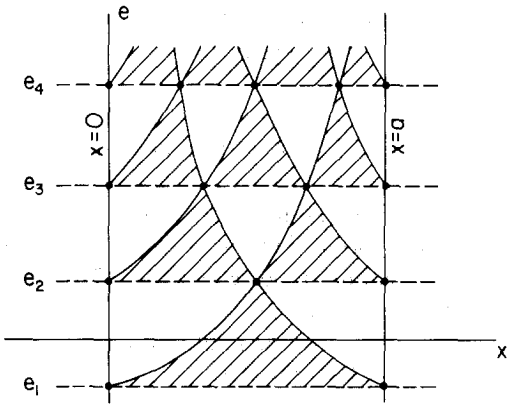

FIG. 2. The shaded regions in the X–e plane show where Δe is negative. The curves bounding the shaded regions are the nodes of $y_1(x)$ and $y_2(x)$.

that the nodes of $y_1(X)$ and $y_2(X)$ interlace, and that as e increases the nodes of $y_1(y_2)$ move to the left (right). The curves going upward to the left (right) in Fig. 2 show the nodes of $y_1(y_2)$. As e passes through an eigenvalue the nodes coincide at the nodes of the corresponding eigenfunction.

If $e_n < e < e_{n+1}$ there are $2n$ sign changes in Δe between $X = 0$ and $X = a$. For X close to 0, $\Delta e \sim y_1(X)\, y_1'(X)\, y_2(X)^2$ and since $y_1(X)$ and $y_1'(X)$ have the same sign ($y_1(X) \sim cX$), $\Delta e > 0$. Similarly, for X close to a, $\Delta e > 0$. The regions in which $\Delta e > 0$ are therefore as shown in Fig. 2. In the case of more general homogeneous boundary conditions, the nodal curves intersect the lines $X = 0$ and $X = a$ between the eigenvalues. The shaded regions then intersect the lines $X = 0$ and $X = a$ in open intervals.

It is seen from Fig. 2 that for a fixed $e > e_1$, Δe is negative for some X value, and hence if Δe is minimized on X, successive iterations must approach a limit. It must be recognized that the negative Δe is not sufficient to guarantee that the limit is an eigenvalue since Δe could conceivably approach 0 for e not an eigenvalue. If we recall, however, that Δe can be written $f(e)/f'(e)$ (see Eq. (16)) then

$$\frac{d\Delta e}{de} = 1 - \left(\frac{f}{f'}\right)\frac{f''}{f'},$$

which is 1 if Δe is close to 0 away from an eigenvalue. This indicates that a zero value of Δe away from an eigenvalue is unstable and, therefore, that successive iterations converge down to an eigenvalue.

This conclusion does not hold if the projected energy correction is used. If, for example, ϕ_1 is projected out, Δe_P is increased for $e > e_1$. This must decrease the shaded regions of Fig. 2, and the bottom shaded region disappears completely, since $\Delta e_P > 0$

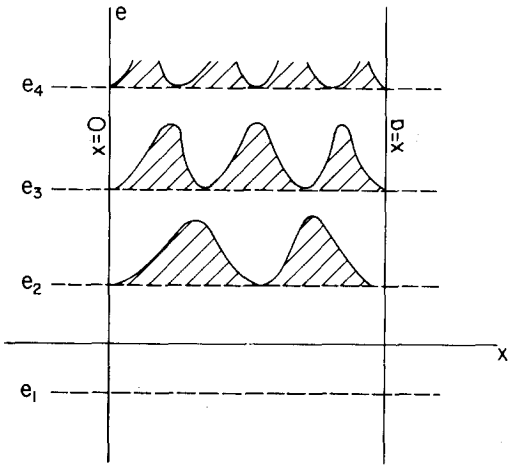

FIG. 3. The shaded regions in the X–e plane show where Δe_p is negative if ϕ is projected out. The shaded regions must be inside those of Fig. 2.

for $e < e_2$. A detailed analysis (see the Appendix) of the behavior near the nodes in Fig. 2 shows that the behavior of Δe_p must be as shown in Fig. 3 so that convergence downward cannot be guaranteed even when Δe_p is minimized on X.

The question of whether successive iterative values for e can cross an eigenvalue e_m is of interest. If e is slightly above e_m, it is seen from Fig. 1 that the next iterative value for e is below e_m if $\Delta e''(e) < 0$. This can be seen to be possible by considering Eq. (16) for e close to e_m. By picking the dominant terms $\phi_m(X)^2/(e_m - e)$ and $\phi_m(X)^2/(e_m - e)^2$ out of the numerator and denominator, and expanding the denominator, it is found that

$$\Delta e = e_m - e + (e_m - e)^2 \, \phi_m(X)^{-2} \sum_{i \neq m} (e_i - e)^{-1} \, \phi_i(X)^2 + O((e_m - e)^3).$$

Therefore, the sign of $\Delta e''(e)$ is governed by

$$G_m(X, X) = \sum_{i \neq m} (e_i - e_m)^{-1} \, \phi_i(X)^2.$$

This is given by [10]

$$G_m(X, X) = \phi_m(X) \, \psi_m(X) - 2\phi_m(X) \, \Psi_m(X) + C\phi_m(X)^2, \tag{21}$$

where $\psi_m(X)$ is a second solution of Eq. (1), satisfying $\phi_m \psi_m' - \psi_m \phi_m' = 1$ and

$$\Psi_m(X) = \phi_m(X) \int_0^X \phi_m(x) \, \psi_m(x) \, dx + \psi_m(X) \int_X^a \phi_m(x)^2 \, dx,$$

$$C = \int_0^a \phi_m(x) \, \Psi_m(x) \, dx.$$

It is seen from Eq. (21) that $G_m(X, X)$ vanishes at the nodes of ϕ_m. At a node

$$\frac{d}{dX} G_m(X, X) = \phi_m'(X) \, \psi_m(X) - 2\phi_m'(X) \, \Psi_m(X)$$

$$= 1 - 2 \int_X^a \phi_m(x)^2 \, dx.$$

The last quantity could vanish, but clearly only in special circumstances such as a symmetry in the problem and then only at one node. Therefore, normally $\Delta e''(e)$ changes sign at a node of ϕ_m and can be negative at $e = e_m$.

This result shows that in principle successive iterations for the energy, using the *unprojected* Δe and minimizing on X, will converge to e_1. In practice, of course, when e becomes slightly below e_m, Δe may not be negative because of the finite sampling of

X values. The result also shows that the usual technique of calculating the unprojected Δe at a fixed X value could possibly miss an eigenvalue.

The question of whether energy iterations given by Δe_P can also cross an eigenvalue e_m remains unresolved. It appears that this must be possible if e_m is large enough but no general results have been obtained.

5. A Possible Practical Strategy

In this section a method will be described that should permit the systematic calculation of all the eigenvalues below some upper bound E. It appears to be difficult to construct a procedure that will guarantee downward convergence to the successive eigenvalues of the problem because there is no control on the sign of Δe_p. However, we can combine the considerations of the previous section with bounds determined by node counting to formulate the procedure. There are, of course, other possibilities, and the choice of a suitable method will depend on the particular problem.

If $y_1(x)$ satisfies Eq. (4) for some e and has n nodes in $[0, a]$ apart from the node at $x = 0$, then e is an upper bound for $e_1, e_2, \ldots, e_n$, and a lower bound for $e_{n+1}, e_{n+2}, \ldots$. Therefore, intermediate results in an initial search for e_1 can be used to provide good starting estimates for the higher eigenvalues. This device of counting the nodes is the same as counting the sign changes in the Sturm sequence for the equation.

The number of eigenvalues below E can first be determined by counting the nodes in y_1 (or y_2) calculated at $e = E$.

The ground state energy e_1 can then be found iteratively by beginning at E and using the energy correction Δe. This sequence must converge downward but can possibly converge to an eigenvalue $e_m \neq e_1$ (even though theoretically it should not) because of the finite sampling of X values. If this occurs it is not serious; m can be determined by node counting and the search for e_1 continued starting slightly below e_m and projecting out ϕ_m.

It may be remarked in passing that projecting out a known ϕ_m *repels* $e + \Delta e$ from e_m. To see this write $\Delta e = n/d$ and

$$\Delta e_p = [n - (e - e_m)^{-1} a^2][d - (e - e_m)^{-2} a^2]^{-1},$$

where $a^2 = [W\phi_m(X)]^2$. Then

$$\Delta e_p - \Delta e = a^2(e_m - e)^{-2}[d - (e_m - e)^{-2} a^2]^{-1}(e + \Delta e - e_m).$$

The coefficient of $(e + \Delta e - e_m)$ is positive. Therefore, if $e + \Delta e > e_m$, $\Delta e_P > \Delta e$, and if $e + \Delta e < e_m$, $\Delta e_P < \Delta e$. Therefore, to increase the rate of downward convergence, known states of energy $e_m > e$ should be projected out.

When e_1 and ϕ_1 have been obtained, the remaining eigenvalues can be obtained iteratively as follows. Suppose at some step eigenvalues $e_1, e_2, \ldots, e_{n-1}$, together with other possible eigenvalues $e_{m_1}, e_{m_2}, \ldots$ have been obtained. Then upper and lower

bounds for e_n are known. These can be averaged to provide an initial estimate e for e_n. The search for e_n can then be carried out projecting out any known eigenfunctions ϕ_m, $m > n$. If at some step e becomes less than e_m as determined by node counting, the calculation is repeated with the immediately preceding value of e but also projecting out the known ϕ_m, $m < n$ in this and subsequent steps.

It can possibly happen that $\Delta e_p > 0$, if as shown in Fig. 3, e is just below an e_i. In this case, the average of the current upper and lower bounds should be used for the next iteration rather than $e + \Delta e_p$. If this is done whenever $e + \Delta e_p$ exceeds the current upper bound for e_n, a convergent sequence must in principle be obtained.

When an eigenvalue e_n has been obtained to the desired degree of accuracy, $\phi_m(x)$ is obtained as $y_X(x)$ and normalized. The accuracy of $\phi_m(x)$ can be perhaps improved by making one "inverse iteration," i.e., by calculating

$$\int_0^a G(x, y)\, \phi_m(y)\, dy = y_2(x) \int_0^x y_1(t)\, \phi_m(t)\, dt + y_1(x) \int_x^a y_2(t)\, \phi_m(t)\, dt \tag{22}$$

and renormalizing. This essentially multiples any erroneous component ϕ_n in ϕ_m by $(e - e_m)/(e_n - e_m)$.

6. Numerical Examples

The procedure outlined in the previous section has been applied to two examples that have been considered recently in the literature. The results of these calculations will be described to illustrate some of the points that have been made in the discussion. In both cases, $y = 0$ at the end points.

One problem is essentially the same as the example of Wicke and Harris [7] (WH) for which the potential has two minima with a large repulsive region between them which may complicate the solution of the problem. The equation can be placed in the dimensionless form of Eq. (1) with

$$V(x) = 3906.25(1 - \exp(2.3237 - x))^2 + 1250 \exp(-83.363(x - 2.47826)^2), \tag{23}$$

$1.5489 < x < 3.87227$. In comparison with the WH example, the variable x is $1.5489R$ (R in Å), and the eigenvalues are one-eighth the WH energies (expressed in cm^{-1}). However, the energies are not strictly comparable, because the potentials are not exactly the same.

The problem was solved on this interval with 201 uniformly spaced mesh points using the lowest-order integration formula Eq. (3) to calculate y_1 and y_2 for each e value. The energy correction Δe (or Δe_p) was calculated at each mesh point and the

TABLE I

Successive Iterations for the Eigenvalues in the WH Problem with the Potential of Eq. (23)[a]

	e	Δe	NN	MPT		e	Δe	NN	MPT
1	1200.000	−60.99	9	39	40	626.272	16.22	3	45
2	1139.012	−6.374	9	41	41	642.494	−0.8941	4	45
3	1132.638	−0.7758	8	82	42	641.600	−0.3198*D*-02	4	45
4	1131.862	−1.601	8	82	43	641.597	−0.4054*D*-07	4	45
5	1130.260	−2.973	8	82					
6	1127.287	−4.979	8	96		$N=4$	$E=641.59686$		
7	1122.308	−7.240	8	51					
8	1115.068	−3.821	8	42	44	772.402	−79.99	5	66
9	1111.247	−0.7281	7	95	45	772.402	−11.98	5	110
10	1110.519	−1.572	7	95	46	760.422	−0.6635	5	110
11	1108.947	−3.371	7	95	47	759.758	−0.1785*D*-02	5	110
12	1105.576	−7.470	7	95	48	759.756	−0.1282*D*-07	5	110
13	1098.105	−17.24	7	95					
14	1080.869	−38.17	7	95		$N=5$	$E=759.75628$		
15	1042.699	−63.85	7	42					
16	978.845	−72.13	7	69	49	887.102	−29.55	6	109
17	906.719	−39.23	6	110	50	887.102	−3.526	6	41
18	867.485	−60.14	5	97	51	883.576	−0.5862*D*-01	6	41
19	807.345	−69.89	5	66	52	883.518	−0.1554*D*-04	6	41
20	737.458	−78.38	4	66	53	883.518	−0.1145*D*-11	6	41
21	659.077	−65.61	4	101					
22	593.468	−49.72	3	101		$N=6$	$E=883.51759$		
23	543.747	−74.11	3	63					
24	469.641	−61.57	2	63	54	942.782	10.58	6	118
25	408.067	−7.919	2	61	55	953.363	−0.4980	7	118
26	400.148	0.2133	1	59	56	952.865	−0.1264*D*-02	7	118
27	400.361	0.1418*D*-02	1	59	57	952.864	−0.8082*D*-08	7	118
28	400.363	0.5814*D*-07	1	59					
						$N=7$	$E=952.86362$		
	$N=2$	$E=400.36260$							
					58	1113.158	−1.377	8	42
29	396.359	−60.14	1	62	59	1113.158	−1.137	8	80
30	336.216	−82.45	1	62	60	1112.021	−0.6116*D*-01	8	79
31	253.767	−68.04	1	62	61	1111.959	−0.1573*D*-03	8	79
32	185.730	−21.39	1	62	62	1111.959	−0.1034*D*-08	8	79
33	164.342	−1.295	1	62					
34	163.046	−0.4141*D*-02	1	62		$N=8$	$E=1111.95934$		
35	163.042	−0.4200*D*-07	1	62					
					63	1135.825	−1.957	9	51
	$N=1$	$E=163.04226$			64	1135.825	−1.612	9	126
					65	1134.213	−0.2948*D*-01	9	126
36	506.694	25.52	2	100	66	1134.184	−0.9456*D*-05	9	126
37	532.217	−1.533	3	100					
38	530.684	−0.6748*D*-02	3	100		$N=9$	$E=1134.18358$		
39	530.677	−0.1291*D*-06	3	100					

TABLE II

Successive Iterations for the Eigenvalues in the WO Problem with the Potential of Eq. (24), Using the Lowest-Order Difference Equation

	e	Δe	NN	MPT		e	Δe	NN	MPT
1	−500.000	−17.96	6	139	30	−751.581	−.1442D-09	2	142
2	−517.964	−27.47	6	158	31	−751.581	−.1390D-09	2	142
3	−545.430	−20.01	6	45	32	−751.581	.9254D-13	1	154
4	−565.436	−.6466	6	47					
5	−566.082	.1892D-01	4	47		$N=2$	$E=-751.5805105919111$		
6	−566.063	.1984D-04	4	47					
7	−566.063	−.1354D-06	5	101	33	−660.934	4.087	2	143
8	−566.063	−.9787D-07	5	101	34	−656.847	−.1421	4	143
9	−566.063	−.2862D-07	5	101	35	−656.989	−.1899D-03	4	143
10	−566.063	−.1690D-08	5	101	36	−656.989	−.9090D-09	3	101
11	−566.063	−.5410D-11	5	138	37	−656.989	−.8525D-09	3	101
12	−566.063	.1798D-13	4	142	38	−656.989	−.3999D-09	3	101
					39	−656.989	−.5430D-10	3	101
	$N=5$	$E=-566.0633800189521$			40	−656.989	−.8351D-12	3	163
					41	−656.989	.1019D-13	2	160
13	−571.724	−4.946	4	58					
14	−576.670	−9.754	4	58		$N=3$	$E=-656.9889664473616$		
15	−586.425	−18.68	4	47					
16	−605.103	−28.75	4	47	42	−656.989	−.9509D-14	4	52
17	−633.848	−20.62	4	47	43	−656.989	−.9493D-04	4	143
18	−654.465	−12.94	4	52	44	−656.989	−.1687D-09	4	137
19	−667.403	−23.81	2	52	45	−656.989	−.3426D-13	4	58
20	−691.212	−31.89	2	52					
21	−723.106	−22.93	2	52		$N=4$	$E=-656.9889664436041$		
22	−746.039	−5.351	2	52					
23	−751.390	−.1899	2	52	46	−565.750	−.3189	6	155
24	−751.580	−.2186D-03	2	52	47	−565.750	−.3117	6	138
25	−751.581	−.2887D-09	2	62	48	−566.061	−.2183D-02	6	138
26	−751.581	−.2926D-11	1	101	49	−566.063	−.1054D-06	6	55
27	−751.581	−.2376D-11	1	101	50	−566.063	−.6043D-13	6	41
28	−751.581	−.9633D-12	1	154					
29	−751.581	−.6553D-13	1	153		$N=6$	$E=-566.0633794769586$		
	$N=1$	$E=-751.5805105919228$							

Wolniewicz and Orlikowski suggest that the symmetry condition $\phi_n(x) = \pm \phi_n(-x)$ provides a good test of the accuracy of the computed eigenfunctions. The solutions found satisfied this condition to better than 5 % at the maxima of $|\phi_n|$. The degree to which it is satisfied seems to be governed by the degree of precision in the determination of the eigenvalues.

Wolniewicz and Orlikowski recommend that for a double minimum potential one should integrate through the barrier in the direction of increasing $|y|$. The results of

the WH problem confirm this. In every case except $n=9$, X is on the side of the barrier in which $|y|$ increases. In the case $n=9$, the recommendation is not applicable because ϕ_9 has a node very close to the maximum. The recommendation does not apply to the WO problem because of the symmetry of the potential.

The calculations in these examples are subject to technical problems because the very strong repulsive regions cause very rapid exponential growth and possible overflows. These are readily avoided by scaling the solution for $y_{1,n}$ or $y_{2,n}$ down if $|y_{i,n}|$ becomes too large and setting any exceedingly small values to 0. Normally, the integration is in the direction of exponential increase and is stable. However, when e is very close to an eigenvalue, the solutions y_1 and y_2 may become very close to zero at a and 0, respectively, and loss of significant digits can cause spurious values for Δe. This problem can be avoided by calculating W afresh at each mesh point rather than treating it as a constant.

The value of D_p^2 in Eqs. (18) and (19) is in theory positive. However, it can happen that rounding errors can give slightly negative values at certain X values and completely spurious Δe_p; these should be checked for and rejected.

7. The Numerov Equation

A widely used improvement on the lowest-order recurrence relation, Eq. (3), is the Numerov equation, which can be written

$$z_{i-1} - 2z_i + z_{i+1} = h^2(v_i - e)\, y_i, \tag{25}$$

$$z_i = \{1 - h^2(v_i - e)/12\}\, y_i. \tag{26}$$

This can be expressed in the form of a generalized eigenvalue problem

$$A\mathbf{y} = eB\mathbf{y}, \tag{27}$$

where A and B are both tridiagonal, and B is symmetric and positive definite. The Numerov equation is an improvement on the lowest-order equation because the error is of order h^6 rather than h^4. In the work of Cooley an explicit correction Δe for the Numerov equation is developed. This differs from the correction of Eq. (8) by a term of order h^4. The error in the eigenvalues is of order h^4 rather than h^2 [1].

The methods described have been applied also to the Numerov equation. There are two ways to do this. One is to solve Eqs. (25) and (26) and calculate Δe or Δe_p in the same way as before. This is straightforward and the only change is that the Wronskian W is no longer constant because of the change in difference equation, and must be calculated at each mesh point. The second way is to solve instead for z_i:

$$z_{i-1} - 2z_i + z_{i+1} = h^2(v_i - e)\{1 - h^2(v_i - e)/12\}^{-1} z_i. \tag{28}$$

This is of the form of Eq. (3) with e regarded as a nonlinear parameter.

In the two examples considered the second approach proved to be somewhat better

TABLE III

Successive Iterations for the Eigenvalues in the WH Problem
Using the Numerov Equation in the Form of Eq. (28)

	e	Δe	NN	MPT		e	Δe	NN	MPT
1	1200.000	−58.21	9	39	40	667.909	−70.82	4	101
2	1141.789	−5.091	9	41	41	667.909	−22.34	4	46
3	1136.699	0.2790D-01	8	82	42	645.574	−2.322	4	45
4	1136.727	0.5441D-01	8	82	43	643.251	−0.3486D-01	4	45
5	1136.781	0.1035	8	82	44	643.216	−0.2403D-03	4	45
6	1136.884	0.1851	8	82	45	643.216	−0.1628D-05	4	39
7	1137.070	0.2787	8	82					
8	1137.348	0.2442	8	82		$N = 4$	$E = 643.21619$		
9	1137.593	0.4685D-01	8	119					
10	1137.639	0.86.29D-03	8	119	46	744.114	16.97	4	110
11	1137.640	0.8677D-05	8	119	47	761.089	−0.8286	5	110
					48	760.260	−0.5312D-02	5	110
	$N = 9$	$E = 1137.64026$			49	760.255	−0.1834D-04	5	110
					50	760.255	−0.6299D-07	5	88
12	1126.264	−26.79	8	95					
13	1099.475	−51.92	7	95		$N = 5$	$E = 760.25458$		
14	1047.555	−82.70	7	69					
15	964.854	−56.72	7	70	51	881.301	5.353	5	40
16	908.135	−53.67	6	110	52	886.654	−0.6106D-01	6	40
17	854.468	−64.98	5	97	53	886.593	−0.5876D-03	6	40
18	789.487	−90.75	5	66	54	886.593	−0.5509D-05	6	39
19	698.740	−61.66	4	101					
20	637.077	−67.55	3	101		$N = 6$	$E = 886.59269$		
21	569.529	−78.88	3	63					
22	490.649	−76.17	2	63	55	836.494	18.74	6	118
23	414.482	−13.91	2	61	56	955.235	−1.330	7	118
24	400.567	0.4131	1	59	57	953.905	−0.1581D-01	7	118
25	400.981	0.7734D-02	1	59	58	953.889	−0.8127D-04	7	118
26	400.988	0.3310D-04	1	59	59	953.889	-0.4113D-06	7	117
27	400.988	0.1337D-06	1	74					
						$N = 7$	$E = 953.88877$		
	$N = 2$	$E = 400.98827$							
					60	1112.889	2.127	7	37
28	396.978	−11.30	1	60	61	1114.997	−0.2927D-01	8	37
29	385.678	−48.04	1	62	62	1114.967	−0.2488D-03	8	37
30	337.636	−86.87	1	63	63	1114.967	−0.2035D-05	8	130
31	250.765	−67.78	1	63					
32	182.984	−18.85	1	62		$N = 8$	$E = 1114.96708$		
33	164.134	−0.9552	1	62					
34	163.179	−0.3459D-02	1	62					
35	163.175	−0.4847D-05	1	64					
36	163.175	−0.6754D-08	1	73					
	$N = 1$	$E = 163.17518$							
37	530.089	0.7349	2	100					
38	530.824	−0.3717D-03	3	100					
39	530.823	−0.5249D-06	3	89					
	$N = 3$	$E = 530.82344$							

in that it required a smaller total number of iterations. The results of applying the second approach to the WH problem are given in Table III and the results for the WO problem are given in Table IV.

The theory that has been developed does not apply strictly to the Numerov equation because the matrix A in Eq. (27) has a small antisymmetric part and therefore

TABLE IV

Successive Iterations for the Eigenvalues of the WO Problem
Using the Numerov Equation in the Form of Eq. (28)

	e	Δe	NN	MPT		e	Δe	NN	MPT
1	−500.000	−18.38	6	139	31	−751.522	−0.1259D-08	2	44
2	−518.381	−27.82	6	158	32	−751.522	−0.1253D-08	2	148
3	−546.201	−18.79	6	45	33	−751.522	−0.2788D-11	2	134
4	−564.988	−0.4107	6	47	34	−751.522	0.3861D-13	1	155
5	−565.399	0.5226D-02	4	47					
6	−565.394	0.4024D-04	4	47		$N=2$	$E=-751.5224551804963$		
7	−565.394	0.4542D-07	4	62					
8	−565.394	−0.2606D-08	5	101	35	−659.629	2.978	2	143
9	−565.394	−0.3260D-10	5	132	36	−656.652	−0.6214D-01	4	143
10	−565.394	−0.2461D-12	5	44	37	−656.714	−0.3235D-03	4	143
					38	−656.714	−0.1500D-05	4	46
	$N=5$	$E=-565.3936452093306$			39	−656.714	−0.6187D-08	4	63
					40	−656.714	−0.6525D-09	3	101
11	−571.048	−4.680	4	144	41	−656.714	−0.8351D-09	3	101
12	−575.728	−9.309	4	144	42	−656.714	−0.7033D-09	3	101
13	−585.037	−17.80	4	155	43	−656.714	−0.2739D-09	3	101
14	−602.839	−28.31	4	155	44	−656.714	−0.2795D-10	3	142
18	−688.859	−31.63	2	150					
19	−720.484	−24.33	2	150	46	−656.714	−0.2648D-08	4	63
20	−744.809	−6.422	2	150	47	−656.714	−0.2195D-08	4	63
21	−751.231	−0.2908	2	150	48	−656.714	−0.9180D-11	4	140
22	−751.521	−0.9810D-03	2	52	49	−656.714	−0.1409D-12	4	163
23	−751.522	−0.1573D-05	2	48					
24	−751.522	−0.2514D-08	2	49		$N=4$	$E=-656.7143143062440$		
25	−751.522	−0.8831D-12	1	101					
26	−751.522	−0.1419D-11	1	101	50	−565.191	−0.2034	6	47
27	−751.522	−0.2142D-11	1	101	51	−565.191	−0.1989	6	138
28	−751.522	−0.2431D-11	1	101	52	−565.390	−0.3783D-02	6	138
29	−751.522	−0.1654D-11	1	101	53	−565.394	−0.5555D-04	6	64
30	−751.522	−0.4445D-12	1	153	54	−565.394	−0.8054D-06	6	65
					55	−565.394	−0.6738D-08	6	44
	$N=1$	$E=-751.5224551805060$			56	−565.394	−0.4935D-10	6	164
					57	−565.394	−0.3366D-12	6	71
						$N=6$	$E=-565.3936446872576$		

the Numerov equation cannot be derived variationally in any simple way. This problem can be avoided by arbitrarily symmetrizing A, i.e., by replacing A by $\bar{A} = (A + A^T)/2$. This introduces changes of order h^4 in the coefficients in Eq. (25) and the property that the error in the equation is of order h^6 is unaffected because the equation is of order h^2 overall. The symmetrized difference equation is

$$q_i y_{i-1} - 2p_i y_i + q_{i+1} y_{i+1} = h^2(v_i - e) y_i, \tag{29}$$

where

$$p_i = 1 - h^2(v_i - e)/12, \tag{30}$$

$$q_i = (p_i + p_{i-1})/2. \tag{31}$$

The methods that have been developed can now be applied to the variational quotient $(\mathbf{y}, A'\mathbf{y})/(\mathbf{y}, B\mathbf{y})$. The only significant change is that inner products $(\mathbf{y}, \mathbf{z})$ that were calculated using the trapezoidal rule when the lowest-order Eq. (3) was used, must now be calculated with a rule appropriate to the quadratic form B. The elements of B are $B_{i,i} = 5h^2/6$, $b_{i,i+1} = b_{i+1,i} = h^2/12$. The result is that the Δe of Eq. (13) at mesh point M is given by

$$\Delta e_M = W y_{1,M} y_{2,M} / D_M^2, \tag{32}$$

where

$$W = q_M(y_{1,M} y_{2,M-1} - y_{2,M} y_{1,M-1})/h \tag{33}$$

and

$$D_M^2 = y_{2,M}^2 s_{1,M} + y_{1,M}^2 s_{2,M}. \tag{34}$$

The "Wronskian" W is again independent of M. The quantities $s_{1,M}$ and $s_{2,M}$ represent the indefinite integrals in Eq. (12) and satisfy the recurrence relations

$$s_{1,M+1} = s_{1,M} + (h/12)|5(y_{1,M+1}^2 + y_{1,M}^2) + 2y_{1,M+1} y_{1,M}|, \tag{35}$$

$$s_{2,M-1} = s_{2,M} + (h/12)|5(y_{2,M}^2 + y_{2,M-1}^2) + 2y_{2,M-1} y_{2,M}|, \tag{36}$$

$$s_{1,0} = s_{2,N} = 0. \tag{37}$$

Normalization integrals must be calculated as

$$(\mathbf{y}, B\mathbf{y}) = (h/6) \sum_{i=1}^{N} (5y_i^2 + y_{i-1} y_i). \tag{38}$$

Equations (17)–(19) for Δe_p remain unchanged.

The results of applying this method to the WH problem are given in Table V. The remarks that have been made for the solution of the lowest-order difference equation can be seen to apply also to these results. The symmetrized Numerov method has

TABLE V

Successive Iterations for the Eigenvalues in the WH Problem
Using the Symmetrized Numerov Equation

	e	Δe	NN	MPT		e	Δe	NN	MPT
1	1200.000	–58.72	9	39	36	675.804	–69.87	4	101
2	1141.280	–4.449	9	41	37	675.804	–28.68	4	46
3	1136.831	0.1463	8	82	38	647.128	–3.859	4	45
4	1136.977	0.2436	8	82	39	643.269	–0.5351*D*-01	4	45
5	1137.221	0.2910	8	82	40	643.216	–0.9935*D*-05	4	45
6	1137.512	0.1241	8	82	41	643.216	–0.2117*D*-12	4	47
7	1137.636	0.3612*D*-02	8	119					
8	1137.640	0.2271*D*-05	8	119		$N = 4$	$E = 643.21554$		
	$N = 9$	$E = 1137.63956$			42	754.180	6.204	4	110
					43	760.384	–0.1293	5	110
9	1126.263	–31.80	8	95	44	760.254	–0.5944*D*-04	5	110
10	1094.466	–56.44	7	95	45	760.254	–0.1252*D*-10	5	110
11	1038.025	–87.74	7	69					
12	950.280	–35.71	6	44		$N = 5$	$E = 760.25429$		
13	914.567	–51.21	6	110					
14	863.361	–63.94	5	97	46	888.964	–25.31	6	109
15	799.420	–90.48	5	46	47	888.964	–2.349	6	40
16	708.940	–66.27	4	85	48	886.615	–0.2329*D*-01	6	40
17	642.668	–26.37	3	98	49	886.592	–0.2228*D*-05	6	40
18	616.299	–62.45	3	101					
19	553.847	–84.42	3	63		$N = 6$	$E = 886.59180$		
20	469.427	–63.99	2	63					
21	405.439	–4.571	2	60	50	994.152	–85.70	7	69
22	400.868	0.1194	1	59	51	994.152	–31.08	7	118
23	400.987	0.4593*D*-03	1	59	52	963.069	–8.744	7	118
24	400.988	0.6539*D*-08	1	59	53	954.325	–0.4357	7	118
					54	953.889	–0.9628*D*-03	7	118
$N = 2$	$E = 400.98789$				55	953.888	–0.4875*D*-08	7	118
25	396.978	–75.86	1	63		$N = 7$	$E = 953.88840$		
26	321.118	–89.96	1	63					
27	231.160	–56.45	1	63	56	1110.365	4.827	7	37
28	174.708	–11.22	1	62	57	1115.191	–0.2245	8	37
29	163.487	–0.3114	1	62	58	1114.967	–0.5458*D*-03	8	37
30	163.175	–0.2242*D*-03	1	62	59	1114.966	–0.3208*D*-08	8	37
31	163.175	–0.1161*D*-09	1	62					
						$N = 8$	$E = 1114.96635$		
	$N = 1$	$E = 163.17503$							
32	511.637	20.11	2	100					
33	531.744	–0.9187	3	100					
34	530.825	–0.2221*D*-02	3	100					
35	530.823	–0.1289*D*-07	3	100					
	$N = 3$	$E = 530.82327$							

required somewhat fewer iterations, but this is at least partially offset by the greater complexity of each iteration. The results for the eigenvalues are seen to differ from the results of Table I by about one part in 10^3. On the other hand, they agree with the results of the Numerov equation to about one part in 10^6.

The results of applying the symmetrized Numerov equation to the WO problem are given in Table VI. The above comments on the WH problem apply also to these results.

The above equations are valid only for the boundary conditions $y(0) = y(a) = 0$. A boundary condition of the form $y'(0) = \alpha y(0)$ can be invoked with an error of order h^4 by following a procedure similar to that used in deriving the Numerov equation.

TABLE VI

Successive Iterations for the Eigenvalues in the WO Problem Using the Symmetrized Numerov Equation

	e	Δe	NN	MPT		e	Δe	NN	MPT
1	−500.000	−18.52	6	139	26	−751.523	−0.2932*D*-09	2	52
2	−518.515	−28.07	6	158	27	−751.523	−0.2867*D*-09	2	52
3	−546.588	−18.61	6	157	28	−751.523	0.2259*D*-12	1	52
4	−565.202	−0.1940	6	47					
5	−565.396	0.1954*D*-02	4	47		$N = 2$	$E = -751.5225188235487$		
6	−565.394	−0.4539*D*-07	5	101					
7	−565.394	−0.4787*D*-08	5	101	29	−660.097	3.487	2	59
8	−565.394	−0.4481*D*-10	5	101	30	−656.610	−0.1042	4	59
9	−565.394	0.4171*D*-13	4	58	31	−656.714	−0.1014*D*-03	4	59
					32	−656.714	−0.8429*D*-09	3	101
	$N = 5$	$E = -565.3939164025170$			33	−656.714	−0.6806*D*-09	3	101
					34	−656.714	−0.2430*D*-09	3	101
10	−571.048	−4.712	4	58	35	−656.714	−0.2042*D*-10	3	101
11	−575.760	−9.396	4	58	36	−656.714	−0.1053*D*-12	3	99
12	−585.156	−18.10	4	47					
13	−603.258	−28.59	4	47		$N = 3$	$E = -656.7144914463989$		
14	−631.849	−21.78	4	47					
15	−653.827	−12.94	4	52	37	−656.714	−0.5074*D*-04	4	52
16	−666.587	−23.43	2	52	38	−656.714	−0.5070*D*-04	4	59
17	−689.992	−31.87	2	52	39	−656.714	−0.4752*D*-10	4	143
18	−721.859	−23.62	2	52	40	−656.714	−0.4955*D*-13	4	61
19	−745.480	−5.816	2	52					
20	−751.296	−0.2264	2	52		$N = 4$	$E = -656.7144914430166$		
21	−751.522	−0.3113*D*-03	2	52					
22	−751.523	−0.5865*D*-09	2	150	41	−565.298	−0.9651*D*-01	6	47
23	−751.223	−0.2451*D*-11	1	101	42	−565.298	−0.9581*D*-01	6	64
24	−751.523	−0.1847*D*-11	1	101	43	−565.394	−0.2030*D*-03	6	64
25	−751.523	−0.6293*D*-12	1	101	44	−565.394	−0.9070*D*-09	6	138
					45	−565.394	−0.5880*D*-13	6	137
	$N = 1$	$E = -751.5225188235584$							
						$N = 6$	$E = -565.3939158804475$		

Write

$$y(h) = y(0) + hy'(0) + 1/2h^2y''(0) + 1/6h^3y'''(0) ...,$$
$$y''(h) = y''(0) + hy'''(0) ... .$$

Eliminating $y''(0)$ and $y'''(0)$ by using the differential equation gives

$$[1 - h^2(v_1 - e)/6]\, y_1 = [1 + \alpha h + h^2(v_0 - e)/3]\, y_0$$

as the relation for beginning the numerical solution. To put this into the symmetrized form, it should be replaced by

$$q_1 y_1 = [1 + \alpha h + h^2(7v_0 + 3v_1 - 10e)/24]\, y_0 . \tag{39}$$

Similarly, a boundary condition $y'(a) = \beta\, y(a)$ can be imposed in the form

$$q_{N-1} y_{N-1} = [1 - \beta h + h^2(7v_N + 3v_{N-1} - 10e)/24]\, y_N. \tag{40}$$

Also, the initial conditions of Eqs. (37) should then be replaced by

$$s_{1,0} = hy_{1,0}^2/6, \qquad s_{2,N} = hy_{2,N}^2/6. \tag{41}$$

The more general case, for which $r(x)$ in Eq. (2) is not constant, can be symmetrized and treated in a similar way.

8. Discussion

It is clear that if reliable preliminary estimates of the eigenvalues are available, the elaborate improvements suggested here are unnecessary. If e is close to an eigenvalue, it is found that Δe is almost constant close to its minimum over most of the interval and Cooley's recommendation for the choice of X cannot be far from optimum. The factor of 2 increase in time required to integrate y_1 and y_2 over the whole interval probably cannot be recovered by the optimum choice of Δe.

On the other hand, the methods described here should be effective and systematic in problems in which there are no good estimates for the eigenvalues. With the use of automatic computers, it may be worthwhile to sacrifice some speed in order to ensure reliability, and while it would be foolhardy to assert that the method is infallible, it should be more systematic than other procedures. Cooley [5] has noted that convergence problems may arise because e may jump between eigenvalues and that eigenvalues may be missed and that these problems are related to the choice of X. The variational approach to the choice of X and the use of the projected Δe should eliminate these possible difficulties.

It is possible that the methods discussed here can be adopted to finding low-lying eigenvalues of other large symmetric tridiagonal matrices.

APPENDIX

We are interested in the behavior of Δe_p given by Eq. (18) when e is close to an eigenvalue e_n and X is close to a node x_0 of the corresponding eigenfunction ϕ_n. The solutions of the difference equation (3) are clearly differentiable functions of e and in the neighborhood in question can be approximated linearly:

$$y_i(x) = C_i(x - x_0) + \alpha_i(e - e_n), \qquad i = 1, 2. \tag{A1}$$

(When $e = e_n$, $y_i(x_0) = 0$.)

The Wronskian W is then

$$W = (C_1\alpha_2 - C_2\alpha_1)(e - e_n). \tag{A2}$$

The second term in D_p^2 in Eq. (19) is then negligible with respect to the first term D^2, which can be regarded as a constant in the neighborhood in question. Therefore, we can write

$$\Delta e_p = \lambda\eta[(C_1\xi + \alpha_1\eta)(C_2\xi + \alpha_2\eta) + A\lambda\eta]\, D^{-2}, \tag{A3}$$

where $\xi = X - x_0$, $\eta = e - e_n$, $\lambda = C_1\alpha_2 - C_2\alpha_1$, and

$$A = \sum{}'' (e - e_i)^{-1}\, \phi_i(x_0)^2.$$

If only eigenfunctions below e are projected out, $A > 0$.

It is seen from Eq. (A3) that $\Delta e_p = 0$ along the line $\eta = 0$, or $e = e_n$ as it must be. It is also zero along the branches of the hyperbola

$$(C_1\xi + \alpha_1\eta)(C_2\xi + \alpha_2\eta) + A\lambda\eta = 0. \tag{A4}$$

The top branch of the hyperbola passes through $(0, 0)$ with zero slope as shown in Fig. 3. The bottom branch of the hyperbola is pushed away from $(0, 0)$. Along any line through $(0, 0)$ of the form $\xi = b\eta$,

$$\Delta e_p = \lambda\eta[(C_1 b + \alpha_1)(C_2 b + \alpha_2)\,\eta^2 + A\lambda\eta]\, D^{-2}. \tag{A5}$$

For small η, the dominant term is $A\lambda^2\eta^2 D^{-2} \geqslant 0$. This shows that no line through a node at an eigenvalue in Fig. 3 can pass through a shaded area for small η.

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