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The Numerical Solution of Coupled Differential Equations Arising From the Schrödinger Equation

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Several step-by-step methods for the numerical solution of coupled differential equations are given and compared under realistic circumstances. A variant of the Numerov method is found to be the most efficient. A novel method that consists of approximating the solutions by sets of Airy functions is investigated.

1. INTRODUCTION

Many problems in theoretical physics can be reduced to the solution of coupled differential equations. Within the last five years direct numerical integration of small sets of coupled equations has become practical on the available electronic computers [1–3]. The solution of large sets remains a time-consuming, expensive, and difficult operation, and it is of considerable interest to find the most efficient method. Solutions are often not required to very high accuracy, and it is possible to design methods that work very quickly for low accuracy although they may lose their advantages for higher accuracy [4, 5].

In this paper we assess several step-by-step methods based on well-known formulas and their comparison with the new method introduced by Gordon [4]. In Section 2 we stress some of the features of the numerical solution of a single second-order linear differential equation that we shall require for the extension, in Section 3, to a set of such equations. Section 4 compares the method of Gordon [4] with one of the methods of Section 3, and concluding remarks are made in Section 5.

2. SINGLE EQUATION

Several authors [6, 7] have noted that for the step-by-step integration of the single-channel radial Schrödinger equation,

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - V(r)\right] y(r) = 0, \tag{1}$$

the method of Numerov [8] is superior to any other that has been suggested. This is true if $k^2 < 0$ giving a closed channel or eigenvalue problem or if $k^2 > 0$ giving an open channel. The Numerov algorithm applies to a second-order linear differential equation with the first derivative absent, i.e.,

$$y'' + fy = g,$$

where f and g are functions of the independent variable. We may write

$$\left(1 + \frac{1}{12} h^2 f_{n+1}\right) y_{n+1} - \left(2 - \frac{10}{12} h^2 f_n\right) y_n + \left(1 + \frac{1}{12} h^2 f_{n-1}\right) y_{n-1}$$
$$= \frac{1}{12} h^2 (g_{n+1} + 10 g_n + g_{n-1}), \tag{2}$$

where h is the interval and the subscript n refers to the value of the function at the n-th mesh point. The truncation error is $1/240\ \delta^6 y_n$, which is the smallest error known for three-point methods. This method is also very stable although it can be shown that, for the equation

$$y'' + k^2 y = 0,$$

Numerov's method suffers from instability if the interval h is chosen such that $k^2 h^2 > 6$ [2, 6]. However, this condition is usually satisfied if the truncation error is made small enough and hence, for all practical purposes, it may be ignored.

Two disadvantages that are inherent in Numerov's method are the requirements of special procedures to (a) start the integration and (b) change the interval. Both these disadvantages can be readily overcome in the case of Eq. (1). Typical boundary conditions for this equation are, for $k^2 > 0$,

$$y(r) = 0 \qquad \text{at} \qquad r = 0,$$

$$y(r) \sim \sin(kr + \eta) \qquad \text{as} \qquad r \to \infty,$$

where η is the phase shift. Since Eq. (1) is linear and homogeneous, any solution with the correct behavior at the origin will be a multiple of any other solution with the same initial condition. Thus the second point in the solution may be chosen completely arbitrarily and the overall normalization determined by matching to the required form in the asymptotic region.

In many problems, the function $V(r)$ in Eq. (1) is a rapidly varying function for small r, gradually becoming smoother and finally tending to zero for large r. To integrate efficiently using such a function requires a steady increase in interval size. These increase can effectively be chosen to be multiples of the previous interval and,

in this case, there is no difficulty in increasing the interval within the Numerov algorithm.

From a programming point of view the number of arithmetic operations per step can be reduced by means of the substitution

$$Y_n = \left(1 + \frac{1}{12} h^2 f_n\right) y_n - \frac{1}{12} h^2 g_n . \tag{3}$$

Equation (2) then becomes

$$Y_{n+1} = 2Y_n + h^2(g_n - f_n y_n) - Y_{n-1} . \tag{4}$$

Admittedly, the mechanism for changing the interval is now more complicated since the Y_n are functions of the interval h, but as this routine is used very seldom compared with the total number of steps required, the overall effect is an increase in efficiency. This form is particularly amenable for extension to a set of coupled radial Schrödinger equations.

3. Coupled Equations

The set of coupled differential equations may be written

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i(l_i+1)}{r^2} - V_{ii}\right] y_{ij} = \sum_{\substack{k=1 \\ k \neq i}}^{N} V_{ik} y_{kj} \tag{5}$$

for $1 \leqslant i \leqslant N$, $1 \leqslant \gamma \leqslant N$.

We restrict attention to the case in which all channels are open so that the boundary conditions are

$$y_{ij} = 0 \qquad \text{at} \qquad r = 0, \tag{6}$$

$$y_{ij} \sim k_i r j_{l_i}(k_i r)\, \delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} R_{ij} k_i r n_{l_i}(k_i r), \tag{7}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively.

If the matrix elements V_{ij} have no singularities of order two or higher at the origin, then for small R the solutions of (5) that satisfy (6) are given by

$$w_{ij} = \alpha_{ij} r^{l_q+1},$$

where α is a matrix of constants. The solutions thus obtained will not, in general,

satisfy the asymptotic boundary conditions (7). Thus N linearly independent solutions of (5) must be found and a suitable linear combination of them matched to the correct asymptotic form.

The criterion for linearly independent solutions of this equation is that the phase shifts must themselves be markedly different and independent as noted by Buckingham [9]. We make the assumption that if the rows of α are linearly independent then the respective asymptotic forms will also be linearly independent. Thus the solutions y_{ij} may be expanded as

$$y_{ij} = \sum_{k=1}^{N} w_{ik} c_{kj} ,$$

or

$$y = w \cdot c.$$

The solutions y may be matched to the boundary conditions at two values of r large enough so that the terms V_{ij} are negligible. Then, defining a matrix R' and diagonal matrices M^r, N^r by

$$R'_{ij} = \left(\frac{k_i}{k_j}\right)^{1/2} R_{ij} ,$$

$$M^r_{ij} = k_i r j_{l_i}(k_i r) \cdot \delta_{ij} ,$$

$$N^r_{ij} = k_i r n_{l_i}(k_i r) \cdot \delta_{ij} ,$$

the asymptotic condition (7) may be written

$$y \sim M + N \cdot R'.$$

Following Barnes, Lane, and Lin [1], and writing

$$w = M \cdot A + N \cdot B,$$

we obtain the relations

$$c = A^{-1},$$

$$R' = B \cdot A^{-1},$$

which lead directly to the formation of the R matrix.

Eq. (5) may be rewritten in matrix form as

$$y'' + F \cdot y = 0, \tag{8}$$

where

$$F_{ij} = \left(-\frac{l_i(l_i+1)}{r^2} + k_i^2\right) \cdot \delta_{ij} - V_{ij}\,, \tag{9}$$

and $V_{ij} \to 0$ as $r \to \infty$.

The Numerov formula (2) immediately generalizes to

$$y_{n+1} = \left(I + \frac{1}{12}\,h^2F_{n+1}\right)^{-1}\left\{\left(2I - \frac{10}{12}\,h^2F_n\right)y_n - \left(I + \frac{1}{12}\,h^2F_{n-1}\right)y_{n-1}\right\}, \tag{10}$$

where I is a unit matrix.

Using matrices 0 and α as starting conditions, we may integrate step by step into the asymptotic region and match to the boundary conditions at two points. Note that in this form each step requires a matrix inversion. This is the method used by Barnes, Lane, and Lin [1] and Smith, Henry, and Burke [10]. Now the matrix that is inverted at each step,

$$I + \frac{1}{12}\,h^2F_{n+1}\,,$$

is strongly diagonally dominant, save possibly for small r, and tends to a diagonal matrix as r increases. This suggests that an iterative method would converge very rapidly and Allison [2] has proposed such a method based on the extension of Eq. (4) to the set of Eqs. (5). Eq. (4) immediately generalizes to

$$Y_{i,n+1} = 2Y_{i,n} + h^2(g_{i,n} - f_{i,n}y_{i,n}) - Y_{i,n-1}\,, \tag{11}$$

where

$$y_{i,n} = \frac{Y_{i,n} + 1/12\;h^2g_{i,n}}{1 + 1/12\;h^2f_{i,n}} \qquad \text{for} \quad 1 \leqslant i \leqslant N, \tag{12}$$

and, in the notation of Eq. (5),

$$f_{i,n} = \left(k_i^2 - \frac{l_i(l_i+1)}{r^2} - V_{ii}\right)_n\,, \tag{13}$$

$$g_{i,n} = \sum_{\substack{k=1 \\ k\neq i}}^{N} V_{ik}y_{i,n}\,. \tag{14}$$

A great advantage of using the equations in this form is that $Y_{i,n+1}$ is independent of the coupling between the equations and can be found immediately from Eq. (11). The coupling only enters through the term $g_{i,n+1}$ in Eq. (12).

Eqs. (12) and (14) may be rewritten

$$y_{i,n+1}^{(m+1)} = \frac{Y_{i,n+1} + 1/12\, h^2 g_{i,n+1}^{(m)}}{1 + 1/12\, h^2 f_{i,n}} \tag{15}$$

and

$$g_{i,n+1}^{(m)} = \sum_{k>i} V_{ik} y_{i,n+1}^{(m)} + \sum_{k<i} V_{ik} y_{i,n+1}^{(m+1)} \tag{16}$$

to define an iterative scheme that converges to the solution. In practice very few iterations are required, and in the asymptotic region this method settles down very quickly, depending on the value of the convergence parameter, to an estimation by Eq. (15) and a single correction by use of Eq. (16). The integration over the entire range is repeated N times, corresponding to N different columns of the matrix α and the resultant solution matrices used in the matching process.

As a result of the extra work required to handle the coupling it is not clear that Numerov's method is the most efficient for the set of equations defined by (5).

Lester [11] has suggested the use of De Vogelaere's method, a hybrid method for solving a second-order equation

$$y'' = f(r, y),$$

in which the first derivative is absent. Generalizing to a set of such equations,

$$y_i'' = f(r, y_1, \ldots, y_N), \qquad 1 \leqslant i \leqslant N, \tag{17}$$

De Vogelaere's algorithm becomes

$$y_{i,1/2} = y_{i,0} + \frac{1}{2} h y'_{i,0} + \frac{h^2}{24} (4f_{i,0} - f_{i,-1/2}),$$

$$y_{i,1} = y_{i,0} + h y'_{i,0} + \frac{h^2}{6} (f_{i,0} + 2f_{i,1/2}),$$

$$y'_{i,1} = y'_{i,0} + \frac{h}{6} (f_{i,0} + 4f_{i,1/2} + f_{i,1}),$$

where

$$y_{i,s} = y_i(r + sh),$$

$$f_{i,s} = f(r + sh, y_{1,s}, \ldots, y_{N,s}),$$

and h is the interval. The neglected terms are of order h^4, h^5, and h^5, respectively,

and the method is comparable in accuracy with the fourth-order Runge–Kutta process. To start the integration it is necessary to know not only $y_{i,0}$, $y'_{i,0}$ but also $f_{i,-1/2}$. However, this quantity is readily obtained from $y_{i,-1/2}$, given to sufficient accuracy by

$$y_{i,-1/2} = y_{i,0} - \tfrac{1}{2}hy'_{i,0} + \tfrac{1}{8}h^2 f_{i,0}.$$

The N equations given in (17) may then be integrated into the asymptotic region N times, each time corresponding to a different column of the matrix α that, in this case, may be regarded as a linearly independent set of initial derivatives. Usually a unit matrix is a satisfactory choice for these nonsingular starting matrices.

These then are the three methods we shall compare using an example from theoretical physics. To summarize:

Method 1. The matrix Numerov method, in which we use matrices 0 and α to start the step-by-step integration out to the matching points. The integration over the entire range is performed only once but matrix operations are used throughout.

Method 2. De Vogelaere's method, where the initial conditions are specified by a column of zeros and successive columns of a nonsingular matrix of initial derivatives. The integration over the range of r must be performed N times for a set of N coupled equations.

Method 3. The iterative Numerov method, in which a column of zeros and successive columns of α are used to start the integration. Again the integration is repeated N times over the entire range.

It is difficult to establish precise criteria for the comparison of the speed and efficiency of different numerical methods. Comparison between different programs run on different computers is at best a rough estimate and at worst misleading. Perhaps the best that can be done to compare different methods is to use procedures written by the same programmer in the same language and run on the same computer under the same operating system and with the same compiler.

Rotational excitation of a diatomic molecule by neutral particle impact is one problem in theoretical physics that may be described in terms of coupled differential equations. Using the notation of Arthurs and Dalgarno [12], denoting the entrance channel by the quantum numbers (j, l), the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$, we obtain

$$\left[\frac{d^2}{dr^2} + k^2_{j'j} - \frac{l'(l'+1)}{r^2}\right] y^{Jjl}_{j'l'}(r) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l'; J \mid V \mid j''l''; J \rangle\, y^{Jjl}_{j''l''}(r),$$

where

$$k_{j'j}^2 = \frac{2\mu}{\hbar^2}\left[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}\right],$$

E is the kinetic energy of the incident particle in the center-of-mass system, I is the moment of inertia of the rotator, and μ is the reduced mass of the system.

The potential V may be expanded as

$$V(r, \hat{\mathbf{k}}_{j'j} \cdot \hat{\mathbf{k}}_{jj}) = V_0(r)\, P_0(\hat{\mathbf{k}}_{j'j} \cdot \hat{\mathbf{k}}_{jj}) + V_2(r)\, P_2(\hat{\mathbf{k}}_{j'j} \cdot \hat{\mathbf{k}}_{jj}),$$

where $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$.

The coupling matrix element can then be written

$$\langle j'l'; J \mid V \mid j''l''; J\rangle = \delta_{j'j''}\delta_{l'l''}V_0(r) + f_2(j'l', j''l''; J)\, V_2(r),$$

where the f_2 coefficients can be evaluated from formulas given by Bernstein et al. [13]. The boundary conditions are

$$y_{j'l'}^{jjl}(r) = 0 \quad \text{at} \quad r = 0, \tag{18}$$

$$y_{j'l'}^{jjl}(r) \sim \delta_{jj'} \cdot \delta_{ll'} \exp\left[-i\left(k_{jj}r - \frac{1}{2}l\pi\right)\right] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l')\exp\left[+i\left(k_{j'j}r - \frac{1}{2}l'\pi\right)\right], \tag{19}$$

where the scattering S matrix is related to the R matrix of Eq. (5) by the relation

$$S = (I + iR)(I - iR)^{-1}. \tag{20}$$

A program has been written to solve this problem and has been used to calculate cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles [2, 14]. This program has a subroutine that deals exclusively with the step-by-step integration from the initial value to the matching points. Originally method 3 was used, but recently the author has programmed method 1 to fit this structure and also, using the routine given by Lester [15], modified the program to accept method 2.

As noted by several authors [2, 3], a good check on the calculation is furnished by inspection of the symmetry of the calculated R matrix, which, in turn, guarantees the unitarity of the S matrix. Note that this check gives no information about the convergence of the R matrix but shows only that numerical errors are not swamping the required solutions.

Several S matrices have already appeared in the literature [16, 17] and, for the sake of consistency, we choose one of these as the example on which we shall test the above three methods. The parameters are

$$\frac{2\mu}{\hbar^2} = 1000.0, \qquad \frac{\mu}{I} = 2.351, \qquad E = 1.1,$$

$$V_0(r) = r^{-12} - 2r^{-6},$$

and

$$V_2(r) = 0.2283\ V_0(r).$$

We take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$, and 6 giving rise to sets of four, nine, and sixteen coupled equations, respectively. Following the procedure developed by Bernstein [18] we assumed the potential infinite for values of r less than some r_0. The wavefunctions will then be zero in this region and effectively the boundary condition (18) may be modified to

$$y_{j'l'}^{Jjl}(r_0) = 0.$$

Using a single channel phase shift program with the same potential and parameters corresponding to the smallest wavenumber we found that successive values of the phase shift had converged to within 0.0001 around $r = 6.2$. We make the assumption that, for the coupled equations, the R matrix elements will have converged by the same radial distance, a situation that has been verified in practice.

The range of integration was chosen to be

r_0	0.75
100 steps at 0.007	0.7
350 steps at 0.014	4.9
Final matching point	6.35.

The times, in seconds, required by the three methods to calculate the square of the modulus of the S matrix for sets of four, nine, and sixteen coupled equations are shown in Table I. The iterative Numerov method is much the fastest, a factor of two over the matrix Numerov method, and slightly less over De Vogelaere's method. This factor did not vary significantly with the number of equations solved.

This increase in speed for the iterative Numerov method is due entirely to the ability to vary the size of the convergence parameter ϵ, consistent with obtaining results correct to some predetermined figure. In fact, picking $\epsilon = 10^{-14}$, the limit of the precision of the CDC 6400 computer that was used for these calculations, the iterative Numerov method took longer than the other two. Even when ϵ was increased to a value of 10^{-2}, the elements of the matrix $|S|^2$ had varied by at most

TABLE I

Time, in Seconds, to Calculate $|S|^2$

Method	N		
	4	9	16
1. Matrix Numerov	5	38	186
2. De Vogelaere	5	35	162
3. Iterative Numerov	3	20	94

TABLE II

$|S|^2$ Calculated by Method 3 for $N = 9$ with $\epsilon = 10^{-2}$

		Values of j and l																	
j'	l'	0	6	2	4	2	6	2	8	4	2	4	4	4	6	4	8	4	10
0	6	0.4353		0.1538		0.1244		0.2045		0.0153		0.0122		0.0128		0.0151		0.0266	
2	4	0.1538		0.3768		0.0974		0.0301		0.2317		0.0823		0.0189		0.0071		0.0019	
2	6	0.1244		0.0974		0.4737		0.0561		0.0156		0.0208		0.0910		0.1103		0.0107	
2	8	0.2044		0.0300		0.0561		0.3780		0.0014		0.0012		0.0030		0.0241		0.3017	
4	2	0.0153		0.2317		0.0156		0.0014		0.6513		0.0759		0.0080		0.0007		0.0001	
4	4	0.0122		0.0823		0.0208		0.0012		0.0759		0.7001		0.1017		0.0058		0.0001	
4	6	0.0128		0.0189		0.0910		0.0030		0.0080		0.1016		0.7039		0.0602		0.0006	
4	8	0.0152		0.0071		0.1102		0.0241		0.0007		0.0058		0.0602		0.7668		0.0099	
4	10	0.0266		0.0019		0.0107		0.3016		0.0001		0.0001		0.0006		0.0099		0.6485	

one in the fourth decimal place. In the comparisons that follow a value of 10^{-2} was chosen for ϵ.

The symmetry of the square of the modulus of the S matrix is best for the matrix Numerov method where, for this example, the maximum difference between corresponding matrix elements is two in the sixth decimal place. For De Vogelaere's method and the iterative Numerov method the symmetry is still good, the discrepancy being one in the fourth decimal place. The matrix $|S|^2$ for $N = 9$ calculated by the iterative Numerov method is shown in Table II.

4. Gordon's Method

Gordon [4] has developed a novel method based on approximate fits to the potential function over various sections of the range and their subsequent analytical solution. He has implemented this method using linear fits to the potential

curve and efficient routines for the calculation of the resultant Airy functions. In many problems the potential functions are not very accurately known and, in such cases, a linear fit over fairly large regions will give a good representation. Gordon's program was run on an IBM 360-65 and a large increase of speed over the only other published timings was claimed [17]. This program has been adapted to run on the CDC 6400.

The great advantage of Gordon's method over the step-by-step methods is that once an approximate fit has been established for a particular effective potential characterised by a fixed value of the total angular momentum J and a calculation for some energy value performed, further calculations for different energies and the same value of J can be repeated very quickly. Repeated calculations were found to be a factor of five faster in all cases.

Thus, in the calculation of cross sections for rotational excitation of a molecule by neutral particle impact, a whole set of energies corresponding to a single value of J could be used, the resultant S matrices stored on a magnetic tape or disk, and the calculation repeated for consecutive values of J. At the end of the calculation it is a matter of housekeeping to read the S matrices off the storage device, sum over the various channels, and print out the required cross sections.

In Gordon's program there are several small convergence parameters, suitable values of which are given in terms of a variable labelled TOLLHI, the largest allowed perturbation correction. These values were varied to study the convergence of the elements of the matrix $|S|^2$. It was found to be very rapid for the off-diagonal elements agreeing to one in the third decimal place with the matrix elements calculated by the step-by-step methods. The convergence of the diagonal elements was slow and appeared to convergence to values that differed by up to three in the third decimal place. The results of the timings for the same calculation as before are shown in Table III. Note the large increase in speed for the repeated calculation over the first one.

These comparisons assume that the calculation of the potential energy curve for a particular value of the internuclear separation is not a significant proportion

TABLE III

Gordon's Methods for $N = 9$

TOLLHI	Time for first calculation (sec)	Time for repeated calculation (sec)
3×10^{-3}	14.1	2.6
1×10^{-3}	19.4	3.4
5×10^{-4}	27.0	4.5

TABLE IV

Time, in Seconds, to Calculate $|S|^2$

Iterative Numerov,		fine interval	2.9	20.4	94.3
		coarse interval[a]	1.4	10.4	48.8
Gordon,	first calculation	TOLLHI $= 10^{-3}$	3.3	19.4	65.8
	repeated calculation		0.7	3.4	11.5

[a] The coarse integration interval that was used for the iterative Numerov method consisted of 60 steps of interval 0.015 followed by 150 steps of interval 0.03. A value of 0.75 was used for r_0 and the final matching took place at 5.85.

TABLE V

Comparison of $|S|^2$ Between Iterative Numerov Method with Coarse Interval and Gordon's Method with TOLLHI $= 10^{-3}$ [a]

		Values of j and l								
j'	l'	0 6	2 4	2 6	2 8	4 2	4 4	4 6	4 8	4 10
0	6	0.435	0.153	0.125	0.204	0.015	0.012	0.013	0.015	0.027
		0.438	0.154	0.124	0.203	0.015	0.012	0.013	0.015	0.026
2	4	0.154	0.376	0.098	0.030	0.232	0.082	0.019	0.007	0.002
		0.154	0.381	0.096	0.029	0.230	0.082	0.019	0.007	0.002
2	6	0.125	0.098	0.472	0.056	0.016	0.021	0.091	0.110	0.011
		0.124	0.096	0.477	0.056	0.015	0.021	0.091	0.110	0.011
2	8	0.205	0.030	0.057	0.376	0.001	0.001	0.003	0.024	0.303
		0.203	0.029	0.056	0.379	0.001	0.001	0.003	0.024	0.303
4	2	0.015	0.232	0.016	0.001	0.651	0.076	0.008	0.001	0.000
		0.015	0.230	0.015	0.001	0.654	0.076	0.008	0.001	0.000
4	4	0.012	0.082	0.021	0.001	0.076	0.701	0.101	0.006	0.000
		0.012	0.082	0.021	0.001	0.076	0.701	0.102	0.006	0.000
4	6	0.013	0.019	0.091	0.003	0.008	0.101	0.705	0.060	0.001
		0.013	0.019	0.091	0.003	0.008	0.102	0.704	0.060	0.001
4	8	0.015	0.007	0.110	0.024	0.001	0.006	0.060	0.767	0.010
		0.015	0.007	0.110	0.024	0.001	0.006	0.060	0.767	0.010
4	10	0.027	0.002	0.011	0.302	0.000	0.000	0.001	0.010	0.647
		0.026	0.002	0.011	0.302	0.000	0.000	0.001	0.010	0.648

[a] Upper entries Numerov, lower entries Gordon.

of the time required to calculate the S matrix. If this were not the case, then a method requiring fewer mesh points would be favored.

It is only fair to point out that most users of the conventional step-by-step methods have a tendency to overcompute. For example, for the integration of an oscillatory function a well-known criterion for the choice of step size is approximately one tenth of a wavelength. In fact, this criterion corresponds to fairly accurate computation and if less accuracy is required it can be drastically reduced. The usual equations corresponding to $N = 9$ have been solved by the iterative Numerov method using a very coarse interval division that corresponds to the use of about three or four intervals per wavelength in the region in which the solutions are oscillatory. The results are shown in Table IV, together with the corresponding results from Gordon's method using a value of TOLLHI $= 10^{-3}$. The time required is less than that required for a first calculation using Gordon's method, but slower than the repeated calculation by a factor that increases with N. The calculated $|S|^2$ matrices for $N = 9$, from the iterative Numerov with coarse interval and from Gordon's result for TOLLHI $= 10^{-3}$, are given in Table V.

It should be stressed here that determination of the accuracy of the S matrix obtained from a step-by-step integration involves different choices of integration mesh, and these may have to be adjusted for different energies.

5. Conclusion

If one is faced with the problem of solving large sets of coupled second-order linear differential equations for a set of energies or associated parameters using potential functions that are known only to a few per cent accuracy, then full consideration should be given to the recent method of Gordon [4]. On the other hand, if the potential functions are known more accurately and higher precision is required, or if it is not convenient to repeat the calculation immediately for different energies, then the established step-by-step methods and, in particular, the iterative Numerov variant are still very satisfactory and of comparable speed.

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