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Note

An Eighth-Order Formula for the Numerical Integration of the One-Dimensional Schrödinger Equation

1. INTRODUCTION

The numerical solution of the radial Schrödinger equation has attracted continuous interest over many years [1–20]. This equation has been subject of great activity, the aim being to achieve a fast and accurate algorithm that generates the numerical solution. The radial Schrödinger equation can be written

$$y'' = f(r)\, y, \tag{1.1}$$

where $f(r) = W(r) - E$ and $W(r) = l(l+1)/r^2 + V(r)$ is an effective potential with l a parameter of the problem and $V(r) \to 0$ as $r \to \infty$. E is a real number denoting the energy. The Schrödinger equation is normally posed in boundary value form, one boundary condition being $y(0) = 0$ and the other boundary condition for large values of r determined by physical considerations.

(1) For positive values of the energy, E, the solution is oscillatory for large r with asymptotic form:

$$y(r) \approx C \sin(\sqrt{E}\, r - l\pi/2 + \delta),$$

where δ, the *phase shift* is to be determined.

(2) For negative values of the energy, E, the solution for large values of r is a combination of increasing and decreasing exponential functions. Imposing the boundary condition $y(r) \to 0$ as $r \to \infty$ selects only the decreasing component leading to an eigenvalue problem; i.e., we have to find negative (discrete) values E_j of E for which a solution of Eq. (1.1), satisfying the boundary conditions, exists.

If we are interested in computing accurate values for the eigenvalues and the phase shifts it is necessary in general to use a small value for the steplength of the integration. Recent work seeks to improve the accuracy by: (1) using higher order difference equations (Cash and Raptis [1], Hajj *et al.* [10], Fack and Vanden Berghe [11, 12], Killingbeck [13]); (2) looking for other algorithms, such as methods based on an "eigenvalue function," methods such as those based on Rayleigh–Schrödinger perturbation theory and variational Rayleigh–Ritz methods (Shore [14], Kobessi [15], Cohen and Kais [16], Mitra [17]); and (3) constructing exact solutions for (1.1) for specific potentials (Razavy [18], Varma [19], Whitehead *et al.* [20]).

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So in view of accuracy, in category (1), we would expect a high order integration method to be more efficient than Numerov's method since it is generally the case that high order methods outperform lower order ones as increasing accuracy is requested. However, it is also important, since the solution is "nearly periodic" for large r, that the integration method being used should have a non-zero interval of periodicity [21]. It is well known that the interval of periodicity of Numerov's method is $[0, 6]$. It is, however, known that high order linear multistep methods with step number greater than 2 have a smaller interval of periodicity [21] which imposes constraints that can nullify the advantage of high order and lead to results which are generally no better than those obtained using the Numerov method. The purpose of this paper is to derive an eighth order, two-step method which has a larger interval of periodicity than Numerov's method and the sixth-order formula of Cash and Raptis [1] and to give some numerical results comparing these methods on three problems of practical interest which have been considered previously in the literature.

2. The Eighth-Order Method

We consider the method:

$$y_{n+1} - 2y_n + y_{n-1} = h^2[A(y''_{n+1} + y''_{n-1}) + B(y''_{n+1/2} + y''_{n-1/2}) + C(y''_{n+1/4} + y''_{n-1/4}) + Dy''_n] + \mathrm{LTE}(h), \tag{2.1}$$

where $\mathrm{LTE}(h)$ is the local truncation error.

To derive an eighth-order formula (i.e., $O(h^{10})$) we obtain the following linear system of equations:

$$\begin{aligned} 2A + 2B + 2C + D &= 1 \\ A + \frac{B}{4} + \frac{C}{16} &= \frac{1}{12} \\ \frac{A}{12} + \frac{B}{192} + \frac{C}{3072} &= \frac{1}{360} \\ \frac{A}{360} + \frac{B}{23040} + \frac{C}{1474560} &= \frac{1}{20160}. \end{aligned} \tag{2.2}$$

Solving this system we have

$$A = \frac{47}{3780}, \qquad B = \frac{332}{945}, \qquad C = \frac{-256}{945}, \qquad D = \frac{57}{70}$$

with

$$\mathrm{LTE}(h) = \frac{-1303}{9754214400} h^{10} y_n^{(10)} + O(h^{12}).$$

To obtain an eighth-order formula we need sixth-order (i.e., $O(h^8)$) approximations $\bar{y}_{n\pm 1/2}$ and $\bar{y}_{n\pm 1/4}$ for $y_{n\pm 1/2}$ and $y_{n\pm 1/4}$, respectively.

Using similar techniques, we can show that the following formulae are sixth-order approximations of $y_{n\pm 1/2}$ and $y_{n\pm 1/4}$:

$$\bar{y}_{n+1/2} = \frac{1}{128}(-25y_{n+1} + 205y_n - 15y_{n-1} - 37y_{n-2}) + \frac{h^2}{1536}(23y''_{n+1} + 761y''_n + 509y''_{n-1} + 27y''_{n-2})$$

$$\bar{y}_{n-1/2} = \frac{1}{128}[37(y_{n+1} + y_{n-2}) + 27(y_n + y_{n-1})] + \frac{h^2}{512}[-9(y''_{n+1} + y''_{n-2}) - 171(y''_n + y''_{n-1})] \tag{2.3}$$

$$\bar{y}_{n+1/4} = \frac{1}{4096}[605y_{n+1} + 4070y_n - 579y_{n-1} - 160(\bar{y}_{n+1/2} - \bar{y}_{n-1/2})] + \frac{h^2}{49152}[113y''_{n+1} - 1390y''_n - 103y''_{n-1} + 1944(\bar{y}''_{n+1/2} + \bar{y}''_{n-1/2})]$$

$$\bar{y}_{n-1/4} = -\frac{1}{4096}[579y_{n+1} - 4070y_n - 605y_{n-1} - 160(\bar{y}_{n+1/2} - \bar{y}_{n-1/2}) - \frac{h^2}{49152}[103y''_{n+1} + 1390y''_n - 113y''_{n-1} + 1944(\bar{y}''_{n+1/2} + \bar{y}''_{n-1/2})]. \tag{2.4}$$

So, the final integration formula is

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{3780}[47(y''_{n+1} + y''_{n-1}) + 1328(\bar{y}''_{n+1/2} + \bar{y}''_{n-1/2}) - 1024(\bar{y}''_{n+1/4} + \bar{y}''_{n-1/4}) + 3078y''_n] + \mathrm{LTE}^*(h), \tag{2.5}$$

where $y_{n\pm 1/2}$ and $y_{n\pm 1/4}$ are given by (2.3) and (2.4). The modified truncation error is now:

$$\mathrm{LTE}^*(h) = -\frac{h^{10}}{9754214400}(8854y_n^{(8)} + 1303y_n^{(10)}) + O(h^{12}). \tag{2.6}$$

Note that, in practice, this is a three-step method, since the value y_{n-2} is required in calculations (2.3) and (2.4).

3. Interval of Periodicity

To determine the interval of periodicity of this method we apply it to the scalar test equation $y'' = -k^2 y$ to obtain the difference equation:

$$\left(1+\frac{11}{252}H^2+\frac{13}{15120}H^4\right)y_{n+1}-2\left(1-\frac{115}{252}H^2+\frac{313}{15120}H^4\right)y_n$$
$$+\left(1+\frac{11}{252}H^2+\frac{13}{15120}H^4\right)y_{n-1}=0, \tag{3.1}$$

where $H^2 = h^2k^2$. The stability polynomial associated with (3.1) is

$$P(\lambda) = A(H)\lambda^2 - 2B(H)\lambda + A(H), \tag{3.2}$$

where

$$A(H)=\left(1+\frac{11}{252}H^2+\frac{13}{15120}H^4\right) \quad \text{and} \quad B(H)=\left(1-\frac{115}{252}H^2+\frac{313}{15120}H^4\right). \tag{3.3}$$

Letting $\lambda = (1+z)/(1-z)$ and solving the equation $P(\lambda)=0$, we obtain

$$2[A(H)+B(H)]z^2+2[A(H)-B(H)]=0. \tag{3.4}$$

Clearly the roots of (3.4) are purely imaginary if $[A(H)+B(H)]\cdot[A(H)-B(H)]>0$. But $A(H)+B(H)>0$ for all $H\in(0,\infty)$, while $A(H)-B(H)>0$ for all $H\in(0, 25.2)$. Thus the interval of periodicity of this method is $(0, 25.2)$. To start this method we compute y_2 with a special strategy. We compute first $y_{3/2}$ with stepsize $h/2$ using the sixth-order formula of Cash and Raptis [1] and then we compute y_2 using the same steplength and the above method. We give some numerical results illustrating the performance of this new method in the next section.

4. Numerical Illustration

In this section we present some numerical results to illustrate the performance of our method on the classes of problems described in Section 1. We consider first the case of positive energy.

4.1. *Phase Shift Problem*

If we assume that the potential $V(r)$ dies away faster than the term $l(l+1)/r^2$ then Eq. (1.1) becomes, for large values of r,

$$y''(r) = [l(l+1)/r^2 - k^2]\, y(r). \tag{4.1}$$

This has the linearly independent solutions $kr.j_l(kr)$ and $kr.n_l(kr)$, where $j_l(r)$ and $n_l(r)$ are the spherical Bessel and Neumann functions, respectively. We thus have, for large r,

$$\begin{aligned} y(r) &\approx Akr.j_l(kr) - Bkr.n_l(kr) \\ &\approx A\sin(kr - l\pi/2) - B\cos(kr - l\pi/2) \\ &\approx C\sin(kr - l\pi/2 + \delta_l), \end{aligned}$$

where δ_l is the *real scattering phase shift* of the lth partial wave induced by the potential $V(r)$. The value of δ_l can be computed using the formula:

$$\tan\delta_l = [y(r_n)\,J(r_{n-1}) - y(r_{n-1})\,J(r_n)]/[y(r_{n-1})\,N(r_n) - y(r_n)\,N(r_{n-1})], \tag{4.2}$$

where r_{n-1}, r_n are two distinct step points in the asymptotic region, $J(r) = kr.j_l(kr)$ and $N(r) = kr.n_l(kr)$. Here we follow the usual practice of introducing a term $l\pi/2$ in the expression for $y(r)$ so that all phase shifts vanish when the potential, $V(r)$, vanishes. For the purpose of our numerical comparison we consider the Lennard–Jones potential,

$$V(r) = M(1/r^{12} - 1/r^6) \tag{4.3}$$

with $M = 500$ and the problem considered is to compute the phase shift to three decimal places. We solve this problem as an initial value one and, in order to be able to use the new method, we need two extra initial conditions y_1 and y_2 to be specified. Since Eq. (1.1) is linear and homogeneous then y_1 can be chosen arbitrarily. For convenience we use $y_1 = h^{l+1}$. To compute the other extra condition y_2 we follow the special strategy described in previous section. In Table I we list the accuate values of the phase shifts obtained from the perturbative numerical

TABLE I

Computed Phase Shifts Using Numerov's Method, the Cash and Raptis Method [1], and Our New Method

	Exact values			Numerov			Cash and Raptis			New		
$l\backslash k$	1	5	10	1	5	10	1	5	10	1	5	10
0	0.154	−0.484	0.431	0.163	−0.479	0.419	0.159	−0.484	0.432	0.154	−0.484	0.431
1	1.233	0.928	1.045	1.241	0.939	1.056	1.238	0.927	1.044	1.233	0.928	1.045
2	−1.430	−0.964	−0.716	−1.419	−0.960	−0.704	−1.423	−0.964	−0.716	−1.430	0.964	−0.716
3	0.783	0.120	0.568	0.790	0.124	0.580	0.788	0.120	0.568	0.783	0.120	0.568
4	0.126	1.032	−1.387	0.126	1.036	−1.375	0.126	1.032	−1.386	0.126	1.032	−1.387
5	0.036	−1.379	−0.299	0.037	−1.376	−0.288	0.037	−1.379	−0.299	0.036	−1.379	−0.299
6	0.015	−0.845	0.686	0.015	−0.842	0.696	0.015	−0.845	0.686	0.015	−0.845	0.686
7	0.007	−0.526	1.566	0.007	−0.523	1.566	0.007	−0.525	1.567	0.007	−0.526	1.566
8	0.003	−0.458	−0.806	0.003	−0.456	−0.797	0.003	−0.458	−0.805	0.003	−0.458	−0.806
9	0.002	−0.758	0.153	0.002	−0.756	0.145	0.002	−0.758	0.152	0.002	−0.758	0.153
10	0.001	1.414	0.377	0.001	1.415	0.389	0.001	1.414	0.378	0.001	1.414	0.377

method CPM(2) [22] and the phase shifts obtained from the Numerov method, the Cash and Raptis method [1], and our new method. The energy relates to $k = 1$, 5, and 10 with appropriate interval size of 0.08, 0.06, and 0.05, respectively.

It is clear that the new method gives more reliable results than the other two methods, particularly at the higher energies. For low energy and high l values, where the phase shift is small, there is little to choose between them.

4.2. *Resonance Problem*

We consider the numerical integration of the Schrödinger equation,

$$y''(r) = [W(r) - E]\, y(r), \tag{4.4}$$

in the case where the potential $V(r)$ is the Woods–Saxon potential,

$$V(r) = u_0/(1+t) - u_0 t/[a(1+t)^2] \tag{4.5}$$

TABLE II

Deviations of the Computed Eigenenergies from the Exact Values, in 10^{-6} Units, for Various Choices of Step Size Shown in the Second Column

E_j	h	Numerov	Cash/Raptis	Ref. [24]	New
53.588872	1/16	228323	108	110	6
		(0.090)	(0.095)	(0.195)	(0.110)
	1/32	14059	18	2	0
		(0.191)	(0.200)	(0.385)	(0.220)
	1/64	870	3	0	0
163.215341	1/16	—	6825	85	36
			(0.100)	(0.191)	(0.111)
	1/32	476488	208	11	1
		(0.191)	(0.198)	(0.380)	(0.219)
	1/64	29378	55	1	0
341.495874	1/16	—	174675	103	977
			(0.098)	(0.195)	(0.110)
	1/32	—	3354	13	70
			(0.202)	(0.385)	(0.220)
	1/64	435752	438	2	1
		(0.362)	(0.398)	(0.720)	(0.430)
989.701916	1/16	—	—	2089	98623
				(0.198)	(0.109)
	1/32	—	—	117	3044
				(0.390)	(0.220)
	1/64	—	10685	4	44
			(0.400)	(0.720)	(0.430)

Note. Units of time required to calculate the final results are given in parentheses below the appropriate entry. The empty entries indicate that the corresponding deviations are larger than the allowed format of the table.

$= \exp[(r - R_0)/a]$, $u_0 = -50$, $a = 0.6$, and $R_0 = 7.0$. We chose $l = 0$. In order
ve this problem numerically we need to approximate the true (infinite) range
egration $[0, \infty)$ by a finite range. For the purpose of our numerical computa-
ve take the domain of integration to be $0 \leqslant r \leqslant 15$. The problem we consider
so-called resonance problem. That is, we wish to find those eigenenergies E_j
n the range $1 \leqslant E \leqslant 1000$ for which the phase shift $\delta(E_j)$ is equal to $\pi/2$.
our numerical experiments we compute the eigenenergy by splitting up the
lary value problem into two separate initial value problems. Having chosen a
igenenergy, the process is to integrate forwards from the origin using starting
tions as described in Section 4.1 and then integrate backwards from $r = 15$
the known asymptotic form $y \sim \cos(\sqrt{E}\, r)$ to match up the solution at some
al point in the range of integration. The iterative process used to compute a
tion to the eigenvalue is the one originally proposed by Cooley [23] and
quently improved by Blatt [4].
our numerical example we have computed eigenenergies E_j to six decimal
and compared the Numerov method, the method of Cash and Raptis [1],
ponentially fitted scheme of Ixaru and Rizea [24], and our new method. The
ions of the computed values from the exact eigenenergies together with the
of time required to calculate the final results are given in Table II.
te that the new algorithm is much superior to the Numerov and the Cash-
s methods, while incurring only a 20% increase in computing cost. The new
od outperforms the maximally adapted two-step scheme of Ixaru and Rizea
being comparable to it at low energies for approximately half the cost. At
energy, the exponentially fitted method gives higher accuracy, as expected,
ill incurs a significant cost penalty.

Eigenvalue Problem

the case of negative E the problem is an eigenvalue one. We wish to find
ive (discrete) values E_j of E which are such that the eigenfunction vanishes at
ends of the integration range. We use the same technique described in 4.2
ugh the asymptotic boundary condition must now be changed to
$\exp(-\sqrt{E}\, r)$.
the purpose of obtaining our numerical results we consider the integration
1) using the Woods–Saxon potential. For this problem we have computed the
ximations to the eigenvalues E_j, $j = 0(2)\,12$, using Numerov's method, the
and Raptis method [1], a four-step method developed by Ixaru and Rizea
and our new method.
Table III we list the true eigenvalues correct to nine decimal places and the
ute errors obtained by the above methods. Note the significant improvements
ved by the method presented in this paper, particularly at the higher eigen-
s.
hough the formulae presented in this paper may appear complicated, they are
o implement in a compact fashion and the extra computational resource is
by the increased reliability of the results at higher energies. All computations

TABLE III

Deviations of the Computed Eigenvalues from the Exact Values, in 10^{-9} Units for Various Choices of Step Size Shown in the Second Column

E_j	h	Numerov	Cash/Raptis	Ref. [25]	New
−49.457788728	1/8	238	12	0	1
	1/16	15	0	0	0
	1/32	1	0	0	0
−46.290753954	1/8	39012	85	9	1
	1/16	2434	0	0	0
	1/32	152	0	0	0
−41.232607772	1/8	494856	737	513	0
	1/16	30803	15	8	0
	1/32	1923	1	0	0
−34.672313205	1/8	2617703	3649	4696	1
	1/16	162470	34	74	0
	1/32	10137	1	1	0
−26.873448915	1/8	29911087	10083	21617	87
	1/16	549709	170	364	0
	1/32	34267	2	6	0
−18.094688282	1/8	22817487	15745	69943	615
	1/16	1405771	236	1364	0
	1/32	87545	3	24	0
−8.676081670	1/8	47213825	13280	247862	504
	1/16	549709	321	4298	5
	1/32	34267	4	73	0

were carried out on a computer Micro-Vax II of the Department of Mathematics of the National Technical University of Athens, using double precision arithmetic with 16 significant digit accuracy.

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