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New Variable-Step Procedure for the Numerical Integration of the One-Dimensional Schrödinger Equation

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A new variable-step procedure is developed for the numerical integration of the one-dimensional Schrödinger equation. The new variable-step method is based on two P-stable methods of order eight and ten. Numerical results indicate that the new procedure is more efficient than similar variable-step procedures.

1. INTRODUCTION

In the last few years there has been considerable interest in the numerical solution of the initial-value problems of the form

$$y''(x) = f(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \quad (1.1)$$

involving ordinary differential equations of second order in which the derivative does not appear explicitly. Equations having oscillatory solutions are of particular interest. Examples occur in celestial mechanics, in quantum mechanical scattering problems, and elsewhere. The one-dimensional Schrödinger equation is a member of this family of equations.

The numerical solution of this equation is discussed by several authors (see Cash *et al.* [4]). We refer to the works of Allison [1], Raptis and Cash [17], Raptis and Allison [18], and Ixaru and Berceanu [14].

Until 1980 the most important property for the numerical solution of the problem (1.1) was the interval of periodicity and the P-stability. Another related concept, which is important when solving problems of the form (1.1), is *the phase-lag of the method.* This property was introduced by Brusa and Nigro [3].

Recently, several methods with minimal phase-lag have been proposed for the numerical integration of the initial-value problem (1.1). Chawla and Rao [6–9] have developed methods with phase-lag of order six and eight. Also, Thomas [22] has given a two-step sixth-order method with phase-lag of order eight. Van der Houwen and Sommeijer [23, 24] have derived some methods with minimal phase-lag.

Coleman [11] has given a new approach to construct methods for the numerical integration of $y'' = f(x, y)$ via rational approximation for the cosine.

Simos and Raptis [20] have proposed P-stable methods with minimal phase-lag. Also, Raptis and Simos [16] have given the *required conditions* to construct four-step methods with minimal phase-lag with large interval of periodicity and they have produced a four-step *phase-fitted* method. Finally Simos [21] has produced a two-step method with algebraic order six and phase-lag order infinity.

The purpose of this paper is to develop two-step *predictor-corrector P-stable* methods of order eight and ten. Based on these methods a new variable-step procedure is developed for the numerical integration of the one-dimensional Schrödinger equation.

Numerical results presented in Section 3 show that this new variable-step procedure is much more efficient than other variable-step procedures.

It must be noted that this new method can be useful in cases where a large step-size is to be used; that is, where a modest accuracy is sufficient or in case of problems where the solution consists of a slowly varying oscillation with a high-frequency oscillation superimposed, having a small amplitude.

2. THE NEW METHODS

2.1. *Basic Theory*

When we apply any direct two-step integration method to the scalar test equation

$$y'' = -w^2 y, \quad (2.1)$$

we obtain the difference equation,

$$Q_2(H)\, y_{n+1} + Q_1(H)\, y_n + Q_0(H)\, y_{n-1} = 0, \qquad H = iwh, \quad (2.2)$$

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where Q_j, $j=0, 1, 2$, are polynomials in H, h is the integration step, and y_n is the numerical approximation to $y(x_n)$ $(n=0, 1, ...)$. The general solution to the difference equation (2.2) is

$$y_n = B_1 z_1^n + B_2 z_2^n, \tag{2.3}$$

where B_j $(j=1, 2)$ are constants which may be determined from the initial conditions and z_1 and z_2 are the zeros of the *stability polynomial*:

$$P(c, H) = Q_2(H)\, c^2 + Q_1(H)\, c + Q_0(H). \tag{2.4}$$

DEFINITION 1 [15]. A method to solve the problem (1.1) is said to have a *periodicity interval* $(0, H_0)$ if, for all $H \in (0, H_0)$, the roots of the stability polynomial (2.4) satisfy

$$\begin{aligned} c_1 &= e^{i\vartheta(H)} \\ c_2 &= e^{-i\vartheta(H)}, \end{aligned} \tag{2.5}$$

where ϑ is a real function of $H = wh$.

DEFINITION 2 [15]. A method is said to be *P-stable* if its interval of periodicity is $(0, \infty)$.

DEFINITION 3 [13]. The solution of the characteristic equation $P(c, H)=0$ is said to be *of order p* $(p \geqslant 1)$, if one of the roots of $P(c, H)$ (i.e., one of the roots (2.5)) satisfies

$$e^H - c_1(H) = CH^{p+1} + O(H^{p+2}) \quad \text{for} \quad H \to 0, \tag{2.6}$$

where C $(\neq 0)$ is the error constant of $c_1(H)$.

PROPOSITION 1 [13]. *If the solution of the equation* $P(c, H)=0$ *is of order p* $(p \geqslant 1)$ *with error constant C, then*

$$P(e^H, H) = \partial^2 P(1, 0)/\partial c^2 CH^{p+1} + O(H^{p+3}) \quad \textit{for} \quad H \to 0. \tag{2.7}$$

Consider the algebraic equation

$$\begin{aligned} P(c, r) = {} & [T_m(r)\, T_m(-r)]\, c^2 - [T_m^2(r) + T_m^2(-r)]\, c \\ & + [T_m(r)\, T_m(-r)] \end{aligned} \tag{2.8}$$

with $r \in \mathbb{C}$ and T_m given by

$$\begin{aligned} T_m(r) = 1 + \frac{mr}{2m} + \frac{m(m-1)\, r^2}{2m(2m-1)\, 2!} + \cdots \\ + \frac{m(m-1)\cdots 1 r^m}{2m(2m-1)\cdots(m+1)\, m!}. \end{aligned} \tag{2.9}$$

The roots of (2.8) are given by

$$c_1(r) = c_2(r)^{-1} = T_m(r)/T_m(-r); \tag{2.10}$$

i.e., we are dealing with the (m, m) Padé approximant to $\exp(H)$. So, if we take $H = iwh$, those roots are going to be conjugate complex numbers and always lie in the unit circle. They are the solution of order $2m$ of Eqs. (2.8):

$$e^H - c_1(H) = CH^{2m+1} + O(H^{2m+2}) \quad \text{for} \quad H \to 0.$$

2.2. *Construction of the New Pairs*

For the numerical integration of the initial-value problem (1.1) consider the family of two-step methods:

$$\begin{aligned} y_{n,m-j} = {} & y_n - h^2(b_{0j+1} f_{n+1} + b_{1j+1} f_{n,m-j-1} \\ & + b_{0j+1} f_{n-1}) \end{aligned} \tag{2.11}$$

$$\begin{aligned} & a_0 y_{n+1} + a_1 y_n + a_0 y_{n-1} \\ & \quad = h^2(b_0 f_{n+1} + b_1 f_{n,m} + b_0 f_{n-1}), \end{aligned} \tag{2.12}$$

where

$$\begin{aligned} f_{n+1} &= f(x_{n+1}, y_{n+1}), \\ f_{n-1} &= f(x_{n-1}, y_{n-1}), \\ f_{n,i} &= f(x_n, y_{n,i}), \\ f_{n,0} &= f(x_n, y_n), \qquad j = m-1, m-2, ..., 0. \end{aligned} \tag{2.13}$$

We investigate the cases $m=3$ and $m=4$. Applying (2.11)–(2.13) to (2.1) we have the *stability polynomial of the new methods*:

$$Q_0(H)\, c^2 + Q_1(H)\, c + Q_0(H), \qquad H = iwh, \tag{2.14}$$

where:

(1) *Case* $m=3$:

$$\begin{aligned} Q_0(H) = {} & a_0 - b_0 H^2 + b_1 b_{01} H^4 - b_1 b_{11} b_{02} H^6 \\ & + b_1 b_{11} b_{12} b_{03} H^8, \\ Q_1(H) = {} & a_1 - b_1 H^2 + b_1 b_{11} H^4 - b_1 b_{11} b_{12} H^6 \\ & + b_1 b_{11} b_{12} b_{13} H^8. \end{aligned} \tag{2.15}$$

(2) *Case* $m=4$.

$$\begin{aligned} Q_0(H) = {} & a_0 - b_0 H^2 + b_1 b_{01} H^4 - b_1 b_{11} b_{02} H^6 \\ & + b_1 b_{11} b_{12} b_{03} H^8 - b_1 b_{11} b_{12} b_{13} b_{04} H^{10} \\ Q_1(H) = {} & a_1 - b_1 H^2 + b_1 b_{11} H^4 - b_1 b_{11} b_{12} H^6 \\ & + b_1 b_{11} b_{12} b_{13} H^8 - b_1 b_{11} b_{12} b_{13} b_{14} H^{10}. \end{aligned} \tag{2.16}$$

Based on (2.8)–(2.10), if we impose the conditions

$$\begin{aligned} Q_0(H) &= T_{m+1}(H)\, T_{m+1}(-H) \\ Q_1(H) &= -[T^2_{m+1}(H) + T^2_{m+1}(-H)], \end{aligned} \tag{2.17}$$

identifying terms in both of them, we obtain a system of $2(m+2)$ equations and $2(m+2)$ unknowns. Its solution determines the coefficients of a linear symmetric method of two-step, m stages and P-stability of order $2(m+1)$.

(1) *Case* $m=3$. In this case, from (2.17) with $m=3$, we have a system of 10 equations with 10 unknowns from which we find that

$$\begin{aligned} &a_0 = 1, \quad b_0 = 1/28, \quad b_{01} = 3/3640, \\ &b_{02} = -1/3468, \quad b_{03} = 1/1520, \\ &a_1 = -2, \quad b_1 = 13/14, \quad b_{11} = -289/5460, \\ &b_{12} = -19/1734, \quad b_{13} = -1/760. \end{aligned} \tag{2.18}$$

(2) *Case* $m=4$. From (2.17) with $m=4$ we have a system of 12 equations with 12 unknowns from which we find that

$$\begin{aligned} &a_0 = 1, \quad b_0 = 1/36, \quad b_{01} = 1/2142, \\ &b_{02} = -1/10240, \quad b_{03} = 1/13608, \quad b_{04} = -1/3480, \\ &a_1 = -2, \quad b_1 = 17/18, \quad b_{11} = -64/1071, \\ &b_{12} = -81/5120, \quad b_{13} = -29/6804, \\ &b_{14} = -1/1740. \end{aligned} \tag{2.19}$$

Based on (2.18) and (2.19) we have the next theorem.

THEOREM 1. *The methods* (2.11)–(2.13) *with coefficients given by* (2.18) *and* (2.19) *are P-stable, are of order eight and ten, and have phase-lag of order eight and ten, respectively.*

Proof. The methods are of order eight and ten as we proved by previous analysis (see Definition 3 and (2.7)–(2.19)).

If we apply the method (2.1)–(2.3) to the scalar test equation (2.1) with coefficients given by (2.18) and (2.19) we obtain the *characteristic polynomial*:

$$S_0(H)\, c^2 - 2S_1(H)\, c + S_0(H), \tag{2.20}$$

where

(1) *Case* $m=3$.

$$\begin{aligned} S_0(H) &= 1 + H^2/28 + 3H^4/3920 \\ &\quad + H^6/70560 + H^8/2822400 \end{aligned}$$

and

$$\begin{aligned} S_1(H) &= 1 - 13H^2/28 + 289H^4/11760 - 19H^6/70560 \\ &\quad + H^8/2822400; \end{aligned} \tag{2.21}$$

(2) *Case* $m=4$.

$$\begin{aligned} S_0(H) &= 1 + H^2/36 + H^4/2268 + H^6/181440 \\ &\quad + H^8/15240960 + H^{10}/914457600 \end{aligned}$$

and

$$\begin{aligned} S_1(H) &= 1 - 17H^2/36 + 16H^4/567 - H^6/2240 \\ &\quad + 29H^8/15240960 - H^{10}/914457600. \end{aligned} \tag{2.22}$$

A symmetric two-step method is P-stable if for all $H \in (0, \infty)$ $S_0(H) \pm S_1(H) \geqslant 0$. From (2.21) and (2.22) is obvious that the new methods are P-stable.

DEFINITION 4 [23]. For any method corresponding to the characteristic polynomial (2.20), the quantity

$$t(H) = H - \cos^{-1}[S_1(H)/S_0(H)] \tag{2.23}$$

is called the *dispersion* or *phase error* or *phase-lag*. If $t(H) = O(H^{q+1})$ as $H \to 0$ the order of *dispersion* is q.

Remark 1 [11]. If the order of dispersion is $q=2r$, so that

$$t(H) = cH^{2r+1} + O(H^{2r+3}), \tag{2.24}$$

then

$$\begin{aligned} \cos(H) - S_1(H)/S_0(H) &= \cos(H) - \cos(H - t) \\ &= cH^{2r+2} + O(H^{2r+4}). \end{aligned} \tag{2.25}$$

So we have

(1) *Case* $m=3$.

$$\cos(H) - S_1(H)/S_0(H) = H^{10}/25401600 + O(H^{12});$$

i.e., the method has phase-lag of order eight and

(2) *Case* $m=4$.

$$\cos(H) - S_1(H)/S_0(H) = H^{12}/10059033600;$$

i.e., the method has phase-lag of order ten.

From the above relations it is obvious that *the new methods are P-stable and have phase-lag of much higher order than the known P-stable methods.*

The new schemes are:

(1) *Case* $m=3$.

$$y_{n,1}=y_n-h^2/1520(f_{n+1}-2f_n+f_{n-1})$$
$$y_{n,2}=y_n+h^2/3468(f_{n+1}+38f_{n,1}+f_{n-1})$$
$$y_{n,3}=y_n-h^2/10920(3f_{n+1}-578f_{n,2}+3f_{n-1})$$
$$y_{n+1}-2y_n+y_{n-1}=h^2/28(f_{n+1}+26f_{n,3}+f_{n-1}).$$

(2) *Case* $m=4$.

$$y_{n,1}=y_n+h^2/3480(f_{n+1}+2f_n+f_{n-1})$$
$$y_{n,2}=y_n-h^2/13608(f_{n+1}-58f_{n,1}+f_{n-1})$$
$$y_{n,3}=y_n+h^2/10240(f_{n+1}+162f_{n,2}+f_{n-1})$$
$$y_{n,4}=y_n-h^2/2142(f_{n+1}-128f_{n,3}+f_{n-1})$$
$$y_{n+1}-2y_n+y_{n-1}=h^2/36(f_{n+1}+34f_{n,4}+f_{n-1})$$

3. NUMERICAL ILLUSTRATION

The radial or one-dimensional Schrödinger equation may be written as

$$y''(x)=f(x)\cdot y(x), \qquad x\in[0,\infty), \tag{3.1}$$

where $f(x)=W(x)-E$, and $W(x)=l(l+1)/x^2+V(x)$ is an effective potential with $W(x)\to 0$ as $x\to\infty$, l is an integer, and E is a real number denoting the energy.

The problem is one of the boundary-value type, with $y(0)=0$, and a second boundary condition for large values of x determined by physical considerations.

If $E=p^2>0$, then, in general, the potential function $V(x)$ dies away faster than the term $l(l+1)/x^2$; then Eq. (3.1) effectively reduces to $y''(x)+(E-l(l+1)/x^2)\,y(x)=0$, for x which is greater than some value R depends on the potential function $V(x)$. The above equation has linearly independent solutions $pxj_l(px)$ and $pxn_l(px)$, where $j_l(px)$ and $n_l(px)$ are the spherical Bessel and Neumann functions, respectively. Thus the solution of Eq. (3.1) has the asymptotic form

$$y(x) \underset{x\to\infty}{\cong} Apxj_l(px)-Bpxn_l(px)$$
$$\underset{x\to\infty}{\cong} C[\sin(px-l\pi/2)+\tan d_l\cos(px-l\pi/2)],$$

where d_l is the phase shift which may be calculated from the formula

$$\tan d_l=\frac{[y(x_2)\,S(x_1)-y(x_1)\,S(x_2)]}{[y(x_1)\,C(x_2)-y(x_2)\,C(x_1)]} \tag{3.2}$$

for x_1 and x_2 distinct points on the asymptotic region with $S(x)=pxj_l(px)$ and $C(x)=-pxn_l(px)$.

When the potential becomes very small (i.e., in our numerical example $|V(x)|<0.01$) then, if we have a change of the sign of the function $y(x)$ we calculate the phase shift d_l from (3.2). Then, we repeat the calculation of the phase shift until $|d_l^{\text{old}}-d_l^{\text{new}}|<\text{ACC}$, where ACC is the wanted accuracy of the calculated phase shifts, d_l^{old} is the previous value of the phase shift, and d_l^{new} is the new value of the phase shift (for full details see [5]).

We illustrate the new methods derived in Section 2 by applying them to the solution of (3.1), where $V(x)$ is the *Lenard–Jones* potential which has been widely discussed in the literature. For this problem the potential $V(x)$ is given by

$$V(x)=m(1/x^{12}-1/x^6), \qquad \text{where} \quad m=500. \tag{3.3}$$

The problem we consider is the computation of the relevant phase shifts correct to four decimal places (analogous conclusions we have with the calculation of phase shifts correct to three decimal places). We will consider three separate approaches:

(1) based on the combination of the "classical" method described in [19] and the exponential fitting method described in [17].

(2) based on the combination of the "classical" method described in [19] and the Bessel fitting method described in [17].

(3) based on the two methods described in Section 2.

We note that the procedures (1) and (2) consist of methods in which the coefficients must be calculated in each step-size change (Procedure (1)), or in each step (Procedure (2)). Our new procedure consists of methods with *constant* coefficients.

We will describe the numerical integration procedure and the associate local error estimation for the new procedure. Procedures (1) and (2) are exactly described in [17] and are used without modification.

Denoting the solution obtained using the eighth-order formula as y^N and the solution obtained using the tenth-order formula as y^H and under the assumption that h is sufficiently small so that the local error in y_{n+1}^H can be neglected compared with that in y_{n+1}^N, an estimate of the local truncation error in y_{n+1}^N is

$$\text{LTE}=y_{n+1}^H-y_{n+1}^N \tag{3.4}$$

So, our variable-step procedure is

(1) if $|\text{LTE}|<\text{TOL}$, $h_{n+1}=2h_n$

(2) if $100\,\text{TOL}>|\text{LTE}|>\text{TOL}$, $h_{n+1}=h_n$

(3) if $|\text{LTE}|>100\,\text{TOL}$, $h_{n+1}=h_n/2$ and repeat the step.

TABLE I

		TOL = 10^{-8}		TOL = 10^{-6}		TOL = 10^{-8}	
		Exponential fitting method		Bessel fitting method		New method	
l	Phase shift	No steps	Time	No steps	Time	No steps	Time
0	0.1544	102	0.95	79	0.72	83	0.66
1	1.2328	119	1.06	79	0.98	86	0.75
2	−1.4297	124	1.10	80	1.04	88	0.80
3	0.7832	117	1.09	69	0.85	85	0.75
4	0.1258	103	0.95	64	0.85	83	0.67
5	0.0366	108	0.95	68	0.93	84	0.69
6	0.0147	117	1.04	68	1.11	85	0.75
7	0.0068	105	0.91	62	0.96	83	0.66
8	0.0036	115	0.99	64	0.92	85	0.75
9	0.0020	128	1.10	71	1.07	89	0.82
10	0.0012	144	1.25	75	1.15	92	0.87

Note. $k = 1.0$ and $h_0 = 0.04$, accuracy in phase shifts four decimal places. h_0 = initial interval.

TABLE III

		TOL = 10^{-8}		TOL = 10^{-6}		TOL = 10^{-8}	
		Exponential fitting method		Bessel fitting method		New method	
l	Phase shift	No steps	Time	No steps	Time	No steps	Time
0	−0.4331	229	1.92	155	1.45	175	1.30
1	1.0449	218	1.88	162	1.85	170	1.55
2	−0.7159	280	2.26	160	1.85	175	1.55
3	0.5687	283	2.35	161	1.94	173	1.52
4	−1.3858	285	2.50	157	1.95	170	1.50
5	−0.2984	286	2.52	157	1.95	174	1.55
6	0.6868	287	2.45	156	1.92	172	1.55
7	1.5662	281	2.42	152	1.98	170	1.48
8	−0.8060	324	2.71	154	2.04	170	1.52
9	−0.1525	336	2.82	152	1.97	168	1.47
10	0.3778	348	2.97	152	2.22	168	1.47

Note. $k = 10.0$ and $h_0 = 0.01$, accuracy in phase shifts four decimal places. h_0 = initial interval.

In Tables I–III we present the phase shifts correct to four decimal places, the number of step, and the real time of computation.

It is easy for one to see that the new variable-step method is much more efficient than other variable-step procedures. It must be noted that the computational cost is smaller because the new procedure has constant coefficients while the other procedure have variable coefficients which must be recalculated in every step change (exponentially fitting procedure) or in every step (Bessel fitting procedure).

All computations were carried out on an IBM PC AT 386 with 387 mathcoprossesor with double precision arithmetic in 16 digits accuracy.

TABLE II

		TOL = 10^{-8}		TOL = 10^{-6}		TOL = 10^{-8}	
		Exponential fitting method		Bessel fitting method		New method	
l	Phase shift	No steps	Time	No steps	Time	No steps	Time
0	−0.4831	176	1.50	147	1.30	162	1.22
1	0.9282	206	1.75	147	1.70	180	1.50
2	−0.9637	202	1.68	145	1.58	178	1.50
3	0.1206	208	1.78	146	1.65	180	1.50
4	1.0328	216	1.82	147	1.67	182	1.50
5	−1.3785	229	1.97	146	1.68	185	1.52
6	−0.8441	226	1.93	147	1.78	184	1.52
7	−0.5256	192	1.74	112	1.37	137	1.21
8	−0.4575	274	2.25	108	1.34	135	1.18
9	−0.7571	188	1.68	109	1.56	136	1.18
10	1.4148	183	1.66	106	1.48	133	1.17

Note. $k = 5.0$ and $h_0 = 0.01$, accuracy in phase shifts four decimal places. h_0 = initial interval.

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