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Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation

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In this paper some new eighth algebraic order symmetric eight-step methods are introduced. For these methods a direct formula for the computation of the phase-lag is given. Based on this formula, the calculation of free parameters is done in order the phase-lag to be minimal. The new methods have better stability properties than the classical one. Numerical illustrations on the radial Schrödinger equation indicate that the new method is more efficient than older ones.

KEY WORDS: symmetric methods, multistep methods, radial Schrödinger equation, resonance problems, scattering problems, phase shift problems, phase-lag

AMS subject classification: 65L05

1. Introduction

Many problems in theoretical physics, theoretical chemistry, quantum physics and physical chemistry (see, for example, [1–4]) consist of the radial Schrödinger equation. This equation has the form:

$$y''(x) = \left[\frac{l(l+1)}{x^2} + V(x) - k^2\right] y(x). \tag{1}$$

For the above reason the computational efficient solution of these types of equations via numerical methods has a great research activity the last decades. In (1) the function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, k^2 is a real number denoting *the energy*, l is a given integer, related to the

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angular momentum, and V is a given function representing the potential. The boundary conditions are:

$$y(0) = 0 \tag{2}$$

and a second boundary condition, for large values of x, determined by physical considerations.

Much research has been done on numerical methods for the numerical solution of the Schrödinger equation and related problems (see [2,5,6,10–15]. For detailed reviews see [16–18,22–27]). Most of the research has been made in symmetric two and four-step methods.

In the present paper we derive a family of eight-step symmetric methods of algebraic order eight with phase-lag of order ten, twelve and fourteen for the numerical solution of the Schrödinger equation. We note here that the cost of these methods is three, four and five function evaluations per step. In section 2 the phase-lag analysis of eight-step methods is described and a direct formula for the computation of the phase-lag for this type of methods is given. In section 3 the construction of the new method is given. Numerical illustrations are presented in section 4.

2. Phase-lag analysis of eight-step symmetric methods

Applying an eight-step symmetric method to the test equation $y'' = -s^2 y$ we obtain the following difference equation:

$$\begin{aligned} &A(H)y_{n+4} + B(H)y_{n+3} + C(H)y_{n+2} + D(H)y_{n+1} + E(H)y_n \\ &\quad + D(H)y_{n-1} + C(H)y_{n-2} + B(H)y_{n-3} + A(H)y_{n-4} = 0 \end{aligned} \tag{3}$$

and the associated characteristic equation:

$$\begin{aligned} P(z) = {} & A(H)z^8 + B(H)z^7 + C(H)z^6 + D(H)z^5 + E(H)z^4 \\ & + D(H)z^3 + C(H)z^2 + B(H)z + A(H) = 0, \end{aligned} \tag{4}$$

where $H = sh$.

Based on Lambert and Watson [7] we have the following definition.

Definition 1. A symmetric eight-step method with the characteristic equation given by (4) is said to have an *interval of periodicity* $(0, H_0^2)$ if, for all $H \in (0, H_0^2)$, the roots z_i, $i = 1(1)8$, satisfy

$$z_1 = \mathrm{e}^{\mathrm{i}\theta(H)}, \quad z_2 = \mathrm{e}^{-\mathrm{i}\theta(H)}, \quad \text{and} \quad |z_i| \leqslant 1,\ i = 3(1)8, \tag{5}$$

where $\theta(H)$ is a real function of H.

Definition 2. For any symmetric eight-step method with the characteristic equation given by (4) the phase-lag is equal to

$$t = H - \theta(H) = cH^{q+1} + \mathrm{O}\big(H^{q+2}\big), \tag{6}$$

where c is the *phase-lag constant* and q is *phase-lag order*.

Theorem 1. For all H in the interval of periodicity, the phase-lag of the eight-step method with stability polynomial given by (4) is $\mathrm{O}(H^Q)$ if:

$$\frac{2A(H)\cos(4H)+2B(H)\cos(3H)+2C(H)\cos(2H)+2D(H)\cos(H)+E(H)}{H[8A(H)\sin(4H)+6B(H)\sin(3H)+4C(H)\sin(2H)+2D(H)\sin(H)]} = \mathrm{O}\big(H^Q\big), \tag{7}$$

and we say that the phase-lag of the method is of order Q if (7) is valid.

Proof. Putting $z = \mathrm{e}^{\mathrm{i}\theta(H)}$ we have:

$$2A(H)\cos\big(4\theta(H)\big)+2B(H)\cos\big(3\theta(H)\big)+2C(H)\cos\big(2\theta(H)\big) + 2D(H)\cos\big(\theta(H)\big)+E(H)=0. \tag{8}$$

Putting now $\theta(H) = H(1+T(H)+\mathrm{O}(H^{2Q}))$, where $T(H)=\sum_Q^{2Q-1} p_i H^i$, we have:

$$\begin{aligned} &2A(H)\big[\cos(4H)-4HT(H)\sin(4H)+\mathrm{O}\big(H^{2Q+2}\big)\big] \\ &+2B(H)\big[\cos(3H)-3HT(H)\sin(3H)+\mathrm{O}\big(H^{2Q+2}\big)\big] \\ &+2C(H)\big[\cos(2H)-2HT(H)\sin(2H)+\mathrm{O}\big(H^{2q+2}\big)\big] \\ &+2D(H)\big[\cos(H)-HT(H)\sin(H)+\mathrm{O}\big(H^{2Q+2}\big)\big]+E(H)=0. \end{aligned} \tag{9}$$

So, we have:

$$\begin{aligned} &2A(H)\cos(4H)+2B(H)\cos(3H)+2C(H)\cos(2H)+2D(H)\cos(H)+E(H) \\ &-HT(H)\big[8A(H)\sin(4H)+6B(H)\sin(3H)+4C(H)\sin(2H)+2D(H)\sin(H)\big] \\ &+\mathrm{O}\big(H^{2Q+2}\big)=0. \end{aligned} \tag{10}$$

It is obvious that the coefficient of $T(H)$ is of order $\mathrm{O}(H^2)$. Hence (10) implies that $T(H)$ and the expression in (7) only differ by $\mathrm{O}(H^{2Q})$ and the theorem follows from the definition of phase-lag. □

3. Derivation of the new method

For the numerical integration of the Schrödinger equation we consider the three-parameter family of eight-step methods, which is denoted as METH8(w_i, $i=0(1)3$):

$$\begin{aligned} y_{n,i} &= y_n - w_i h^2 (f_{n+3}+af_{n+2}+bf_{n+1} \\ &\qquad +cf_{n,i-1}+bf_{n-1}+af_{n-2}+f_{n+3}\big), \quad i=0(1)3, \\ y_{n+4}&-2y_{n+3}+2y_{n+2}-y_{n+1}-y_{n-1}+2y_{n-2}-2y_{n-3}+y_{n-4} \\ &= h^2(q_3f_{n+3}+q_2f_{n+2}+q_1f_{n+1}+q_0f_{n,3}+q_1f_{n-1}+q_2f_{n-2}+q_3f_{n+3}), \end{aligned} \tag{11}$$

where $f_{n,-1}=f(x_n,y_n)$, $f_{n+i}=f(x_{n+i},y_{n+i})$, $i=-4(1)4$, and $f_{n,i}=f(x_n,y_{n,i})$, $i=0(1)3$.

In order the above method has algebraic order eight, the following values of the parameters must hold:

$$\begin{aligned} &a=-6, \quad b=15, \quad c=-20, \\ &q_0=-\frac{12629}{3024}, \quad q_1=\frac{20483}{4032}, \quad q_2=-\frac{3937}{2016}, \quad q_3=-\frac{17671}{12096}. \end{aligned} \tag{12}$$

The local truncation error of the produced method is

$$LTE=\frac{h^{10}}{725760}\left(45767y_n^{(10)}+3030960w_3y_n^{(8)}\right), \tag{13}$$

so the method is of eight algebraic order.

When we apply the above method to the test equation $y''=-s^2y$ we obtain the difference equation (3) and the associated characteristic equation (4) with:

$$\begin{aligned} A(H)&=1, \\ B(H)&=-2+\frac{17671}{12096}H^2-\frac{12629}{3024}H^4w_3+\frac{63145}{756}H^6w_3w_2 \\ &\quad-\frac{315725}{189}H^8w_3w_2w_1+\frac{6314500}{189}H^{10}w_3w_2w_1w_0, \\ C(H)&=2-\frac{3937}{2016}H^2+\frac{12629}{504}H^4w_3-\frac{63145}{126}H^6w_3w_2 \\ &\quad+\frac{6315450}{63}H^8w_3w_2w_1-\frac{12629000}{63}H^{10}w_3w_2w_1w_0, \\ D(H)&=-1+\frac{20483}{4032}H^2-\frac{63145}{1008}H^4w_3+\frac{315725}{252}H^6w_3w_2 \\ &\quad-\frac{1578625}{63}H^8w_3w_2w_1+\frac{31572500}{63}H^{10}w_3w_2w_1w_0, \\ E(H)&=-\frac{12629}{3024}H^2+\frac{63145}{756}H^4w_3-\frac{315725}{189}H^6w_3w_2 \\ &\quad+\frac{6314500}{189}H^8w_3w_2w_1-\frac{126290000}{189}H^{10}w_3w_2w_1w_0. \end{aligned} \tag{14}$$

For the above method and based on theorem 1 we have that the phase-lag is given by:

$$\begin{aligned} T(H)&=\left(-\frac{45767}{7257600}+\frac{12629}{30240}w_0\right)H^8+\left(-\frac{29851}{2661120}+\frac{138919}{181440}w_0\right)H^{10} \\ &\quad+\left(-\frac{138919}{9072}w_3w_2+\frac{467273}{483840}w_3-\frac{3318163483}{237758976000}+\frac{63145}{378}w_3w_2w_1\right)H^{12} \\ &\quad+\left(-\frac{166033967}{10973491200}+\frac{694595}{2268}w_3w_2w_1-\frac{631450}{189}w_3w_2w_1w_0\right. \\ &\qquad\left.+\frac{964085231}{914457600}w_3-\frac{467273}{24192}w_3w_2\right)H^{14} \end{aligned}$$

$$+\left[-\frac{964085231}{45722880}w_3w_2+\frac{1529334013}{1371686400}w_3-\frac{7152335079299}{447718440960000}\right.$$
$$+\frac{2336365}{6048}w_3w_2w_1-\frac{3472975}{567}w_3w_2w_1w_0$$
$$\left.+\frac{1}{10}\left(\frac{45767}{7257600}-\frac{12629}{30240}w_3\right)\left(\frac{278039}{181440}-\frac{12629}{504}w_3\right)\right]H^{16}+\cdots. \quad (15)$$

Based on (15) we have that in order the methods have minimal phase-lag the values of parameters given in table 1 must hold.

We note here that in table 1:

$$T_1=\frac{-520367H^{12}}{158505984000},\quad T_2=\frac{76873H^{14}}{896690995200},\quad T_3=\frac{-919071H^{16}}{32011868528640000}.$$

For the values of $w_i,\ i=0(1)3$, given in table 1, we determine the stability functions given in figure 1. Based on this figure we have that the interval of periodicity for the new methods is equal to: $(0, 0.64)$ (method I), $(0, 0.64)$ (method II) and $(0, 0.64)$ (method III), i.e., larger than the interval of periodicity of the classical method (developed by Quinlan and Tremaine [21]) which is equal to $(0, 0.56)$.

4. Numerical illustrations – Schrödinger equation

Consider the numerical solution of the radial Schrödinger equation (1). In the asymptotic region, the equation (1) effectively reduces to

$$y''(x)+\left(k^2-\frac{l(l+1)}{x^2}\right)y(x)=0, \quad (16)$$

for x greater than some value X, where X defines the asymptotic region.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx), n_l(kx)$ are the *spherical Bessel* and *Neumann functions*, respectively. Thus, the solution of equation (1) has the asymptotic form (when $x\to\infty$)

$$y(x)\sim Akxj_l(kx)-Bn_l(kx)$$
$$\sim D\left[\sin\left(kx-\frac{\pi l}{2}\right)+\tan\delta_l\cos\left(kx-\frac{\pi l}{2}\right)\right], \quad (17)$$

where δ_l is the *phase shift* which may be calculated from the formula

$$\tan\delta_l=\frac{y(x_i)S(x_{i+1})-y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i)-y(x_i)C(x_{i+1})} \quad (18)$$

for x_i and x_{i+1} distinct points on the asymptotic region (for which we have that x_{i+1} is the right-hand end point of the interval of integration and $x_i=x_{i+1}-h$, h is the stepsize) with $S(x)=kxj_l(kx)$ and $C(x)=kxn_l(kx)$.

We evaluate the phase shift δ_l from the above relation at x_i in the asymptotic region.

Table 1
Parameters of the new proposed methods.

Parameters	Method I	Method II	Method III
w_0	0	0	$\frac{538111}{412130664}$
w_1	0	$\frac{5724037}{11984845600}$	$\frac{5724037}{11984845600}$
w_2	$\frac{164627}{60412440}$	$\frac{164627}{60412440}$	$\frac{164627}{60412440}$
w_3	$\frac{45767}{3030960}$	$\frac{45767}{3030960}$	$\frac{45767}{3030960}$
Phase-lag	T_1	T_2	T_3

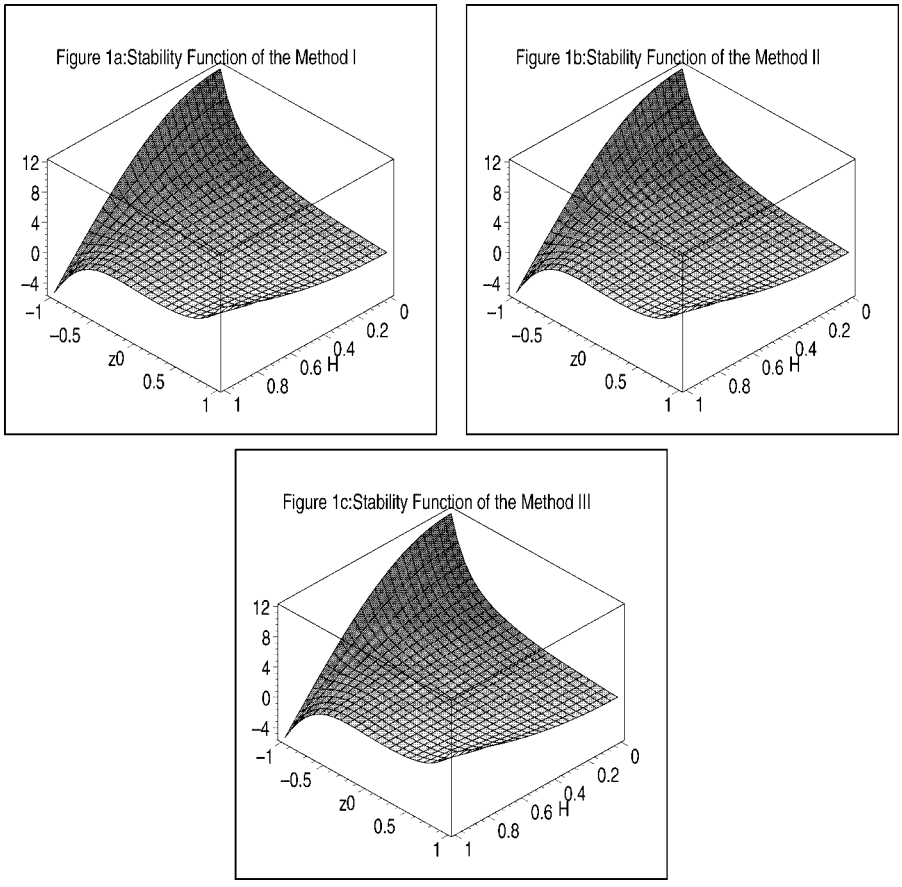

Figure 1. Stability functions for the new methods.

4.1. The Woods–Saxon potential

As a test for the accuracy of our methods we consider the numerical integration of the one-dimensional Schrödinger equation (1) with $l = 0$ in the case where $V(x)$ is the Woods–Saxon potential:

$$V(x) = V_{\mathrm{W}}(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{a(1+z)^2} \tag{19}$$

with $z = \exp[(x - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$.

For positive energies one has the so-called resonance problem. This problem consists either of finding the *phase shift* $\delta(E) = \delta_l$ or of finding those $E \in [1, 1000]$, at which δ equals $\pi/2$. We actually solve the latter problem, using the technique fully described in [1], when *the positive eigenenergies lie under the potential barrier*.

The boundary conditions for this problem are:

$$\begin{aligned} &y(0) = 0, \\ &y(x) \sim \cos\left[\sqrt{E}x\right] \quad \text{for large } x. \end{aligned}$$

The domain of numerical integration is [0, 15].

For comparison purposes in our numerical illustration we use the explicit Numerov-type method with phase-lag of order six developed by Chawla et al. in [19] (labelled as method [a]), the four-step method of Henrici [8] (labelled as method [b]), the classical eight-step method developed by Quinlan et al. in [21] (labelled as method [c]), the new method I (labelled as method [d]), the new method II (labelled as method [e]) and the new method III (labelled as method [f]).

The numerical results obtained by the above four methods, with stepsizes $h = 1/2^n, n = 4(1)7$, were compared with the analytic solution of the resonance problem with the Woods–Saxon potential, rounded to six decimal places. Figure 2 shows the errors $-\log(\mathit{Error})$ where $\mathit{Error} = |E_{\mathrm{calculated}} - E_{\mathrm{analytical}}|/E_{\mathrm{analytical}}$ for the highest eigenenergy $E_3 = 989.701916$ using several values of n.

4.2. Modified Woods–Saxon potential

A second example of this method is illustrated by solving a similar problem using the modified Woods–Saxon potential, given by

$$V(x) = V_{\mathrm{W}}(x) + \frac{D}{x}, \tag{20}$$

where V_{W} is the Woods–Saxon potential (19). For the purpose of our numerical experiments we use the same parameters as in [2], i.e., $D = 20$, $l = 2$. Figure 3 shows the errors $-\log(\mathit{Error})$ where $\mathit{Error} = |E_{\mathrm{calculated}} - E_{\mathrm{analytical}}|/E_{\mathrm{analytical}}$ of the highest eigenenergy $E_3 = 1002.768393$, for several values of n.

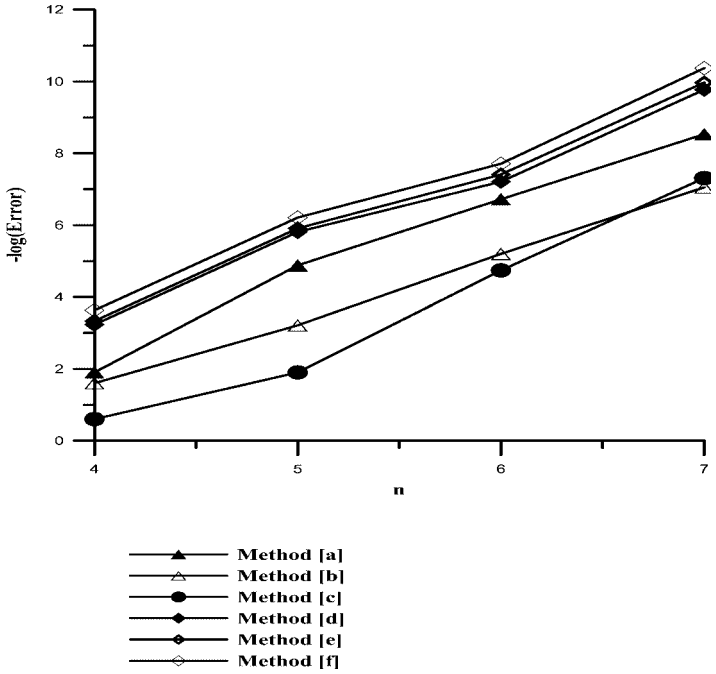

Figure 2. Values of $-\log(Error)$ for several values of n for the resonance $E_3 = 989.7019159$.

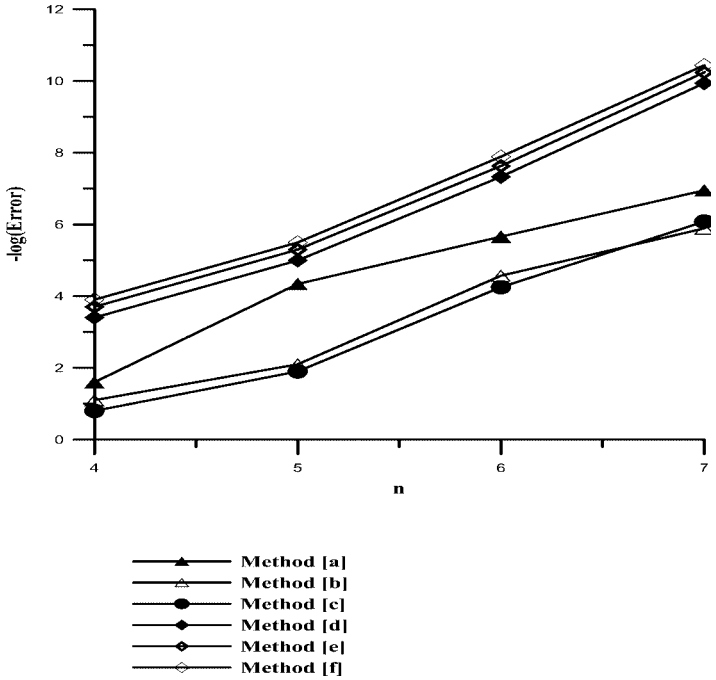

Figure 3. Values of $-\log(Error)$ for several values of n for the resonance $E_3 = 1002.768393$.

Since $V(x)$ is singular at the origin, we use the special strategy of [2]. We start the integration from a point $\varepsilon > 0$ and the initial values $y(\varepsilon)$ and $y(\varepsilon + h)$ for the integration scheme are obtained using a perturbative method (see [1]). As in [2] we use the value $\varepsilon = 1/4$ for our numerical experiments.

From the above results it follows that the new method is much more accurate than the other well-known methods of the same kind.

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

5. Conclusions

In this paper a family of eight-step eighth order symmetric methods is introduced. For these methods a direct formula for the computation of the phase-lag is obtained. Based on this formula, some eight-step symmetric methods with minimal phase-lag are developed. The new methods have a larger interval of periodicity than the classical one. Numerical illustrations on the radial Schrödinger equation indicate that the new methods are more efficient than older ones.

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