Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem

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Received 29 January 1997; revised 18 June 1997

Two new hybrid eighth algebraic order two-step methods with phase-lag of order twelve and fourteen are developed for computing elastic scattering phase shifts of the radial Schrödinger equation. Based on these new methods we obtain a new variable-step procedure for the numerical integration of the Schrödinger equation. Numerical results obtained for the integration of the phase shift problem for the well known case of the Lennard–Jones potential show that these new methods are better than other finite difference methods.

1. Introduction

The radial Schrödinger equation has the form

$$y''(r) + f(r)y(r) = 0, \tag{1}$$

where $0 \leqslant r < \infty$ and $f(r) = E - l(l+1)/r^2 - V(r)$. We call the term $l(l+1)/r^2$ the *centrifugal potential*, and the function $V(r)$ the *potential*, where $V(r) \to 0$ as $r \to \infty$. According of the sign of the energy E there are two main categories of problems for (1) (see for details [19]).

In many scientific areas there is a real need for the numerical solution of the Schrödinger equation. Some of these areas are nuclear physics, physical chemistry, chemical physics, theoretical physics and chemistry (see [1,7,9]).

There is much activity in the area of the solution of the radial Schrödinger equation (1). The result of this activity is the development of a great number of methods. The most important characteristics of an efficient method for the solution of the problem (1) are the accuracy and the computational efficiency. The development of methods with the above mentioned characteristics is an open problem.

One of the most important properties for the numerical solution of the general second order differential equations with periodical solution is the algebraic order of the method. Another important new insight is the *phase-lag* first introduced by Bruca and Nigro [2]. The most widely used technique for the numerical integration of (1) is the *Numerov's method*, with interval of periodicity $(0, 6)$ and phase-lag of order four. Many authors [3–6,10,17–20] have developed methods with minimal phase-lag for the solution of general second-order differential equations with periodical solutions. All these methods have algebraic orders four and six.

The purpose of this paper is to introduce methods of algebraic order eight, with phase-lag of order twelve and fourteen, for the numerical solution of the phase shift problem of the radial Schrödinger equation. The phase shifts calculated by these methods are more accurate compared with those given by Riehl et al. [13], Hepburn et al. [8]. Based on these new methods, we introduce a new variable step method for the solution of (1). The numerical results given by this new variable-step method are better than those of the most well known variable-step method of Raptis and Cash [12]. For the production of the present methods the symbolic language manipulation package MAPLE is used. We note here that the new methods are based on the Runge–Kutta type (or hybrid) methods. The new methods are the first methods of algebraic order eight which have very large interval of periodicity and are also of very high phase-lag order.

2. Phase-lag analysis

We investigate the numerical integration of the problem

$$y'' = f(r, y), \qquad y(r_0) = y_0, \qquad y'(r_0) = y'_0. \tag{2}$$

To examine the stability properties of the methods for solving the initial-value problem (2) Lambert and Watson [11] introduce the scalar test equation

$$y'' = -w^2 y \tag{3}$$

and the *interval of periodicity*. When we apply a symmetric two-step method to the scalar test equation (3) we obtain a difference equation of the form

$$y_{n+1} - 2Q(s)y_n + y_{n-1} = 0, \tag{4}$$

where $s = wh$, h is the step length, $Q(s) = B(s)/A(s)$, where $B(s)$ and $A(s)$ are polynomials in s and y_n is the computed approximation to $y(nh)$, $n = 0, 1, 2, \ldots.$ For explicit methods $A(s) = 1$.

The characteristic equation associated with (4) is

$$z^2 - 2Q(s)z + 1 = 0. \tag{5}$$

We have the following definitions.

Definition 1 ([20]). The method (4) with the characteristic equation (5) is unconditionally stable if $|z_1| \leqslant 1$ and $|z_2| \leqslant 1$ for all values of wh, where z_1 and z_2 are the roots of (5).

Definition 2. Following Lambert and Watson [11], we say that the numerical method (4) has an interval of periodicity $(0, H_0^2)$, if, for all $s^2 \in (0, H_0^2)$, z_1 and z_2 satisfy

$$z_1 = \mathrm{e}^{\mathrm{i}\theta(s)} \quad \text{and} \quad z_2 = \mathrm{e}^{-\mathrm{i}\theta(s)}, \tag{6}$$

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

Definition 3 ([11]). The method (4) is *P-stable* if its *interval of periodicity* is $(0, \infty)$.

Based on the above we have the following theorems (for the proofs see [19]).

Theorem 1. A method which has the characteristic equation (5), has an interval of periodicity $(0, H_0^2)$, if for all $s^2 \in (0, H_0^2)$, $|Q(s)| < 1$.

Theorem 2. About the method which has an interval of periodicity $(0, H_0^2)$ we can write

$$\cos\left[\theta(s)\right] = Q(s), \tag{7}$$

where $s^2 \in (0, H_0^2)$.

Definition 4 ([10]). For any method corresponding to the characteristic equation (5) the quantity

$$t = s - \cos^{-1}\left[B(s)/A(s)\right] \tag{8}$$

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

Based on the above definition Coleman [6] arrived to the following remark. If the order of dispersion is $2r$ then we have

$$\begin{aligned} t &= cs^{2r+1} + \mathrm{O}(s^{2r+3}) \\ &\Rightarrow \cos(s) - Q(s) = \cos(s) - \cos(s-t) = cs^{2r+2} + \mathrm{O}(s^{2r+4}), \end{aligned} \tag{9}$$

where t is the *phase-lag of the method*.

3. The new eighth order methods

3.1. Some basic formulae

Consider the following formulae given by

$$y_{n+s} + y_{n-s} = a_0(y_{n+1} + y_{n-1}) + a_1 y_n + h^2\left[a_2(f_{n+1} + f_{n-1}) + a_3 f_n\right], \tag{10}$$

$$y_{n+s} - y_{n-s} = b_0(y_{n+1} - y_{n-1}) + h^2 b_1(f_{n+1} - f_{n-1}). \tag{11}$$

Using the Taylor series expansions and requiring approximations of order O(h^7), we have the following system of equations:

$$\begin{aligned} 2a_0 + a_1 &= 2, \\ a_0 + 2a_2 + a_3 &= s^2, \\ a_0 + 12a_2 &= s^4, \\ a_0 + 30a_2 &= s^6, \\ b_0 &= s, \\ b_0 + 6b_1 &= s^3, \\ b_0 + 20b_1 &= s^5. \end{aligned} \tag{12}$$

Solving the above system of equations and after some straightforward manipulations we have the following approximations:

$$\begin{aligned} \bar{y}_{n+s} = {} & \frac{1}{486}\bigl[3\sqrt{7}y_{n+1}\bigl(7\sqrt{7} + 27\sqrt{3}\bigr) + 192y_n + 3\sqrt{7}y_{n-1}\bigl(7\sqrt{7} - 27\sqrt{3}\bigr) \\ & + h^2\bigl[2\sqrt{7}f_{n+1}\bigl(9\sqrt{3} + 7\sqrt{7}\bigr) + 224f_n + 2\sqrt{7}f_{n-1}\bigl(7\sqrt{7} - 9\sqrt{3}\bigr)\bigr]\bigr], \end{aligned} \tag{13}$$

$$\bar{f}_{n+s} = f(r_{n+s}, \bar{y}_{n+s}), \quad s = \frac{\sqrt{21}}{3},$$

$$\begin{aligned} \bar{y}_{n-s} = {} & \frac{1}{486}\bigl[3\sqrt{7}y_{n+1}\bigl(7\sqrt{7} - 27\sqrt{3}\bigr) + 192y_n + 3\sqrt{7}y_{n-1}\bigl(7\sqrt{7} + 27\sqrt{3}\bigr) \\ & + h^2\bigl[2\sqrt{7}f_{n+1}\bigl(9\sqrt{3} - 7\sqrt{7}\bigr) + 224f_n + 2\sqrt{7}f_{n-1}\bigl(7\sqrt{7} + 9\sqrt{3}\bigr)\bigr]\bigr], \end{aligned} \tag{14}$$

$$\bar{f}_{n-s} = f(r_{n-s}, \bar{y}_{n-s}), \quad s = \frac{\sqrt{21}}{3}.$$

Consider, now, the following formulae given by

$$\begin{aligned} y_{n+q} + y_{n-q} = {} & c_0(y_{n+1} + y_{n-1}) + c_1 y_n \\ & + h^2\bigl[c_2(f_{n+1} + f_{n-1}) + c_3 f_n + c_4(f_{n+s} + f_{n_s})\bigr], \end{aligned} \tag{15}$$

$$y_{n+q} - y_{n-q} = d_0(y_{n+1} - y_{n-1}) + h^2\bigl[d_1(f_{n+1} - f_{n-1}) + d_2(f_{n+s} - f_{n-s})\bigr]. \tag{16}$$

Using the Taylor series expansions and requiring to have approximations of order O(h^7), we have the following system of equations:

$$\begin{aligned} 2c_0 + c_1 &= 2, \\ c_0 + 2c_2 + c_3 + 2c_4 &= q^2, \\ c_0 + 12c_2 + 28c_4 &= q^4, \\ 3c_0 + 90c_2 + 490c_4 &= 3q^6, \\ 27c_0 + 1152c_2 + 19208c_4 &= 27q^8, \\ d_0 &= q, \\ d_0 + 6d_1 + 2\sqrt{21}d_2 &= q^3, \\ 3\sqrt{3}d_0 + 60\sqrt{3}d_1 + 140\sqrt{7}d_2 &= 3\sqrt{3}q^5, \end{aligned} \tag{17}$$

$$3\sqrt{3}d_0 + 126\sqrt{3}d_1 + 686\sqrt{7}d_2 = 3\sqrt{3}q^7.$$

Solving the above system of equations and after some straightforward manipulations we have the following approximations:

$$\begin{aligned}
\bar{y}_{n+q} = {} & \frac{1}{171360}\bigl[1680qy_{n+1}(9q^7 - 56q^5 + 98q^3 + 51) - 3360y_n(9q^8 - 56q^6 \\
& + 98q^4 - 51) + 1680qy_{n-1}(9q^7 - 56q^5 + 98q^3 - 51) \\
& - h^2q\bigl[7f_{n+1}(261q^7 - 1318q^5 + 459q^4 + 1057q^3 - 3570q^2 + 3111) \\
& + 16qf_n(747q^6 - 4801q^4 + 9409q^2 - 5355) \\
& + 7f_{n-1}(261q^7 - 1318q^5 - 459q^4 + 1057q^3 + 3570q^2 - 3111) \\
& - 9\sqrt{3}\bar{f}_{n+\sqrt{21}/3}\bigl(9\sqrt{3}q^7 - 22\sqrt{3}q^5 + 51\sqrt{7}q^4 + 13\sqrt{3}q^3 \\
& - 170\sqrt{7}q^2 + 119\sqrt{7}\bigr) - 9\sqrt{3}\bar{f}_{n-\sqrt{21}/3}\bigl(9\sqrt{3}q^7 - 22\sqrt{3}q^5 - 51\sqrt{7}q^4 \\
& + 13\sqrt{3}q^3 + 170\sqrt{7}q^2 - 119\sqrt{7}\bigr)\bigr]\bigr], \\
\bar{f}_{n+q} = {} & f(r_{n+q}, \bar{y}_{n+q}),
\end{aligned} \tag{18}$$

$$\begin{aligned}
\bar{y}_{n-q} = {} & \frac{1}{171360}\bigl[1680qy_{n+1}(9q^7 - 56q^5 + 98q^3 - 51) - 3360y_n(9q^8 - 56q^6 \\
& + 98q^4 - 51) + 1680qy_{n-1}(9q^7 - 56q^5 + 98q^3 + 51) \\
& - h^2q\bigl[7f_{n+1}(261q^7 - 1318q^5 - 459q^4 + 1057q^3 + 3570q^2 - 3111) \\
& + 16qf_n(747q^6 - 4801q^4 + 9409q^2 - 5355) \\
& + 7f_{n-1}(261q^7 - 1318q^5 + 459q^4 + 1057q^3 - 3570q^2 + 3111) \\
& - 9\sqrt{3}\bar{f}_{n+\sqrt{21}/3}\bigl(9\sqrt{3}q^7 - 22\sqrt{3}q^5 - 51\sqrt{7}q^4 + 13\sqrt{3}q^3 \\
& + 170\sqrt{7}q^2 - 119\sqrt{7}\bigr) - 9\sqrt{3}\bar{f}_{n-\sqrt{21}/3}\bigl(9\sqrt{3}q^7 - 22\sqrt{3}q^5 + 51\sqrt{7}q^4 \\
& + 13\sqrt{3}q^3 - 170\sqrt{7}q^2 + 119\sqrt{7}\bigr)\bigr]\bigr], \\
\bar{f}_{n-q} = {} & f(r_{n-q}, \bar{y}_{n-q}).
\end{aligned} \tag{19}$$

Finally, consider the method

$$\begin{aligned}
y_{n+1} - 2y_n + y_{n-1} = {} & h^2\bigl[t_0(f_{n+1} + f_{n-1}) + t_1f_n \\
& + t_2\bigl(f_{n+\sqrt{21}/3} + f_{n-\sqrt{21}/3}\bigr) + t_3(f_{n+q} + f_{n-q})\bigr].
\end{aligned} \tag{20}$$

To have the above method (20), the maximal algebraic order we have the following system of equations:

$$\begin{aligned}
2t_0 + t_1 + 2t_2 + 2t_3 &= 1, \\
12t_0 + 28t_2 + 12q^2t_3 &= 1, \\
90t_0 + 490t_2 + 90q^4t_3 &= 3, \\
1512t_0 + 19208t_2 + 1512q^6t_3 &= 27.
\end{aligned} \tag{21}$$

Solving the above system of equations we have

$$t_0 = \frac{406q^2 - 151}{3360(q^2 - 1)}, \quad t_1 = \frac{2324q^2 - 255}{2940q^2},$$
$$t_2 = \frac{9(42q^2 - 13)}{7840(7 - 3q^2)}, \quad t_3 = \frac{17}{56q^2(q^2 - 1)(3q^2 - 7)}. \tag{22}$$

3.2. *The new eighth order method with phase-lag of order twelve*

Consider the two parameter family of methods $M_8(w_0, q)$:

$$\bar{y}_n = y_n + w_0 h^2 \big[f_{n+1} - 2f_n + f_{n-1} + z_2\big(\bar{f}_{n+\sqrt{21}/3} + \bar{f}_{n-\sqrt{21}/3} - 2f_n\big) + z_3\big(\bar{f}_{n+q} + \bar{f}_{n-q} - 2f_n\big)\big], \tag{23}$$
$$y_{n+1} - 2y_n + y_{n-1} = h^2\big[t_0(f_{n+1} + f_{n-1}) + t_1\bar{f}_n + t_2\big(\bar{f}_{n+\sqrt{21}/3} + \bar{f}_{n-\sqrt{21}/3}\big) + t_3\big(\bar{f}_{n+q} + \bar{f}_{n-q}\big)\big], \tag{24}$$

where t_i, $i = 0(1)3$, are given by (22), $z_2 = 9(1-q^2)/(7(3q^2-7))$, $z_3 = 4/(q^2(3q^2-7))$, w_0 and q are free parameters. The approximations $\bar{f}_{n\pm\sqrt{21}/3}$ and $\bar{f}_{n\pm q}$ are given by the formulae (13), (14) and (18), (19), respectively.

The local truncation error (LTE) of the new method (13), (14), (18), (19), (23) and (24), is given by

$$\mathrm{LTE} = \frac{h^{10}}{152409600(7 - 3q^2)}\big[3y_n^{(10)}(765q^4 - 2007q^2 + 518) + 8y_n^{(8)}F_n\big[24w_0(q^2 - 1)(3q^2 - 7)(2324q^2 - 255) - 792(42q^2 - 13)\big]\big] + \mathrm{O}(h^{12}), \tag{25}$$

where $F_n = (\partial f/\partial y)_n$, $y_n^{(8)} = (\mathrm{d}^8 y/\mathrm{d}r^8)_n$ and $y_n^{(10)} = (\mathrm{d}^{10} y/\mathrm{d}r^{10})_n$.

We apply this method to the scalar test equation (3). Setting $s = wh$ we obtain the *difference equation* (4) and the corresponding characteristic equation (5) with

$$A(s) = 1 + s^2\frac{27q^4 + 27q^2 - 154}{504(3q^2 - 7)} + s^4\frac{T_1}{1799280q^2(7 - 3q^2)} + s^6\frac{T_2}{21591360q^2(7 - 3q^2)} + s^8\frac{w_0(2324q^2 - 255)(9q^4 - 22q^2 + 13)}{5783400(7 - 3q^2)}, \tag{26}$$
$$B(s) = 1 + s^2\frac{27q^4 - 729q^2 + 1610}{504(3q^2 - 7)} + s^4\frac{T_3}{1799280q^2(7 - 3q^2)} + s^6\frac{T_4}{2698920q^2(3q^2 - 7)} + s^8\frac{w_0(2324q^2 - 255)(9q^4 - 22q^2 + 13)}{5060475(3q^2 - 7)}, \tag{27}$$

where $T_1,\ T_2,\ T_3$ and T_4 are given in appendix A.

Theorem 3 ([19]). The phase-lag of a symmetric two-step method with characteristic equation (5) is the leading term in the expansion of

$$\left[\cos(s) - Q(s)\right]/s^2, \quad Q(s) = B(s)/A(s). \tag{28}$$

Theorem 4. The method, $M_8(w_0, q)$, where $w_0 = 0.00126588252227788819$ and $q = 1.24832627500665355549$, has phase-lag of order twelve and an interval of periodicity equal to $(0, 32.5779)$.

Proof. Substituting (26) and (27) into (28), and expanding via Taylor series $\cos(s)$ and after straightforward manipulation we get the following system of equations in order to have the maximal order of the phase-lag:

$$\begin{aligned}&9q^6(148736w_0 + 255) - 3q^4(1536320w_0 + 1223)\\&\quad + 2q^2(1806528w_0 + 413) - 342720w_0 = 0,\end{aligned} \tag{29}$$

$$\begin{aligned}&2673q^{10}(297472w_0 + 255) + 1782q^8(765 - 1090112w_0)\\&\quad - 9q^6(569647232w_0 + 1288537) + 12q^4(1463144672w_0 + 1103207)\\&\quad - 112q^2(111112584w_0 + 20909) + 1161135360w_0 = 0.\end{aligned} \tag{30}$$

It therefore follows that for $w_0 = 0.00126588252227788819$ and $q = 1.24832627500665355549$ the phase-lag is given by

$$t = 5.3458610^{-11}s^{12}. \tag{31}$$

To prove the property of non-empty interval of periodicity, we note first that considering (5) it is clear that the roots $z_{1,2}$ will be distinct, complex conjugate and each of modulus one for $s^2 \in (0, H_0^2)$ provided $|Q(s)| < 1$ for all $s^2 \in (0, H_0^2)$. Considering (5) and theorem 1 and for a given above we have that, $|Q(s)| < 1$ for all $s^2 \in (0, 32.5779)$. Thus the theorem is proved. □

3.3. The new eighth order method with phase-lag of order fourteen

Consider the three parameter family of methods $M_8(w_0, w_1, q)$:

$$\bar{y}_n = y_n + w_0h^2\left[f_{n+1} - 2f_n + f_{n-1} - \frac{3}{7}\left(\bar{f}_{n+\sqrt{21}/3} + \bar{f}_{n-\sqrt{21}/3} - 2f_n\right)\right], \tag{32}$$

$$\begin{aligned}\bar{\bar{y}}_n = y_n + w_1h^2\big[&f_{n+1} - 2\bar{f}_n + f_{n-1} + z_2\left(\bar{f}_{n+\sqrt{21}/3} + \bar{f}_{n-\sqrt{21}/3} - 2\bar{f}_n\right)\\&+ z_3\left(\bar{f}_{n+q} + \bar{f}_{n-q} - 2\bar{f}_n\right)\big],\end{aligned} \tag{33}$$

$$\begin{aligned}y_{n+1} - 2y_n + y_{n-1} = h^2\big[&t_0(f_{n+1} + f_{n-1}) + t_1\bar{\bar{f}}_n + t_2\left(\bar{f}_{n+\sqrt{21}/3} + \bar{f}_{n-\sqrt{21}/3}\right)\\&+ t_3\left(\bar{f}_{n+q} + \bar{f}_{n-q}\right)\big],\end{aligned} \tag{34}$$

where t_i, $i = 0(1)3$, are given by (22), $z_2 = 9(1-q^2)/(7(3q^2-7))$, $z_3 = 4/(q^2(3q^2-7))$, w_i, $i = 0, 1$, and q, are free parameters. The approximations $\bar{f}_{n\pm\sqrt{21}/3}$ and $\bar{f}_{n\pm q}$ are given by the formulae (13), (14) and (18), (19), respectively.

The local truncation error (LTE) of the new method (13), (14), (18), (19), (32)–(34), is given by

$$\begin{aligned}\mathrm{LTE} = {} & \frac{h^{10}}{1066867200q^4(7-3q^2)}\big[21q^4y_n^{(10)}(765q^4-2007q^2+518)\\ & + 8\big[5760w_1w_0y_n^{(6)}F_nF_n'(q^2-1)(3q^2-7)(2324q^2-255)\\ & + 7y_n^{(8)}F_n\big[24w_1(q^2-1)(3q^2-7)(2324q^2-255)\\ & - 7q^2(42q^2-13)\big]\big]\big] + \mathrm{O}(h^{12}), \end{aligned} \tag{35}$$

where $F_n = (\partial f/\partial y)_n$, $F_n' = \mathrm{d}F_n/\mathrm{d}r$, $y_n^{(6)} = (\mathrm{d}^6y/\mathrm{d}r^6)_n$, $y_n^{(8)} = (\mathrm{d}^8y/\mathrm{d}r^8)_n$ and $y_n^{(10)} = (\mathrm{d}^{10}y/\mathrm{d}r^{10})_n$.

We apply this method to the scalar test equation (3). Setting $s = wh$ we obtain the *difference equation* (4) and the corresponding characteristic equation (5) with

$$\begin{aligned} A(s) = {} & 1 + s^2\frac{27q^4+27q^2-154}{504(3q^2-7)} + s^4\frac{T_1}{1799280q^2(7-3q^2)}\\ & + s^6\frac{T_2}{151139520q^4(7-3q^2)} + s^8\frac{w_1(2324q^2-255)T_3}{40483800q^4(7-3q^2)}, \end{aligned} \tag{36}$$

$$\begin{aligned} B(s) = {} & 1 + s^2\frac{27q^4-729q^2+1610}{504(3q^2-7)} + s^4\frac{T_4}{1799280q^2(7-3q^2)}\\ & + s^6\frac{T_5}{2698920q^2(3q^2-7)} + s^8\frac{w_1(2324q^2-255)T_3}{35423325q^4(3q^2-7)}, \end{aligned} \tag{37}$$

where T_1, T_2, T_3, T_4 and T_5 are given in appendix B.

Based on the analysis presented in previous section we have the following theorem:

Theorem 5. The method, $M_8(w_0, w_1, q)$, where $w_0 = 0.00864946221830391659$, $w_1 = 0.00186967764609313898$ and $q = 1.30364491397327910153$, has phase-lag of order fourteen and an interval of periodicity equal to $(0, 62.7458)$.

Proof. Substituting (36)–(37) into (28), expanding $\cos(s)$ in a Taylor series, and after straightforward manipulation we get the system of equations in order to have the maximal order of the phase-lag given in the appendix C.

It therefore follows that for

$$w_0 = 0.00864946221830391659, \qquad w_1 = 0.00186967764609313898$$

and $q = 1.30364491397327910153$ the phase-lag is given by

$$t = 1.2458510^{-13}s^{14}. \tag{38}$$

To prove the property of non-empty interval of periodicity, we note first that considering (5) it is clear that the roots $z_{1,2}$ will be distinct, complex conjugate and each of modulus one for $s^2 \in (0, H_0^2)$ provided $|Q(s)| < 1$ for all $s^2 \in (0, H_0^2)$.

Considering (5) and theorem 1 and for a given above we have that, $|Q(s)| < 1$ for all $s^2 \in (0, 62.7458)$. Thus the theorem is proved. □

4. Numerical illustration

The methods developed in section 3 can be applied in both the open channel problem and the bound states problem. We investigate in this paper the case of open channel problem, i.e., the case $E = k^2 > 0$.

In this case, in general, the potential function $V(r)$ dies away much faster than $l(l+1)/r^2$ so the latter is the predominant term. Then, equation (1) effectively reduces to: $y''(r) + (k^2 - l(l+1)/r^2)y(r) = 0$, for large r. It is well known that the equation (1) has two linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions, respectively. Thus the asymptotic solution of (1) (i.e., for $r \to \infty$) has the form of

$$\begin{aligned} y(r) &\cong Akrj_l(kr) - Bkrn_l(kr) \\ &\cong AD\big[\sin(kr - l\pi/2) + \tan\delta_l \cos(kr - l\pi/2)\big], \end{aligned} \tag{39}$$

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

$$\tan\delta_l = \frac{y(r_b)S(r_a) - y(r_a)S(r_b)}{y(r_a)C(r_b) - y(r_b)C(r_a)}, \tag{40}$$

where r_a and r_b are two distinct points in the asymptotic region, $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$.

The term $l\pi/2$ in (39) is conventional. The reason for inserting it is that, with this definition, all phase shifts vanish when the potential function vanishes itself.

Based on (39) and (40), we have that the normalization factor D is given by (see [15] for details)

$$D \approx \frac{y(r_a)}{kr_a[\cos(\delta_l)S(r_a) + (-1)^l \sin(\delta_l)C(r_a)]}. \tag{41}$$

In this section we present some numerical results to illustrate the performance of our methods on a problem of practical interest. We consider the numerical integration of the Schrödinger equation (1) in the well known case where the potential $V(r)$ is the Lennard–Jones potential:

$$V(r) = 500\big(1/r^{12} - 1/r^6\big). \tag{42}$$

In table 1 we present the calculated phase shifts of the Schrödinger equation (1) for $k = 10$ and for $l = 0(10)50$ using the present methods, the method of Riehl et al. [13] and the method of Hepburn et al. [8]. From the results presented it is obvious

Table 1
Phase shifts computed for $k = 10$ and for $l = 0(10)50$ using the method of Riehl et al. [13] (which is indicated as method [a]), the method of Hepburn et al. [8] (which is indicated as method [b]), the method with phase-lag of order twelve which is developed in section 3.2 (which is indicated as method [c]), and the method with phase-lag of order fourteen which is developed in section 3.3 (which is indicated as method [d]).

l	Method [a]	Method [b]	Method [c]	Method [d]
0	−0.4310577165	−0.4310042854	−0.4310043414	−0.4310043352
10	0.3778467885	0.3779001026	0.3779001472	0.3779001525
20	0.4658914343	0.4659447864	0.4659447394	0.4659447440
30	0.0565858728	0.0566390782	0.0566390823	0.0566390817
40	0.0135267163	0.0135797673	0.0135797535	0.0135797453
50	0.0045124372	0.0044944721	0.0044945198	0.0044945241

that our new methods are much more accurate than the other methods for the same computational cost.

4.1. Error estimation

For the integration of systems of initial-value problems, several methods have been proposed for the estimation of the local truncation error (LTE) (see, for example, [14] and references therein).

In this paper we base our local error estimation technique on an embedded pair of integration methods and on the fact that when the local phase-lag error is of higher order then the approximation of the solution for the problems with a periodical solution is better.

We denote the solution obtained with high phase-lag order as y_{n+1}^H and the solution obtained with low phase-lag order as y_{n+1}^L and then, we have the following definition.

Definition 5. We define the *local phase-lag error* estimate in the lower phase-lag order solution y_{n+1}^L by the quantity

$$\mathrm{LPLE} = \left|y_{n+1}^H - y_{n+1}^L\right|. \tag{43}$$

Under the assumption that h is sufficiently small, the *local phase-lag error* in y_{n+1}^H can be neglected compared with that in y_{n+1}^L.

We assume that the solution y_{n+1}^H is obtained using the method described in section 3.3 and the solution y_{n+1}^L is obtained using the method described in section 3.2.

If the local phase-lag error of acc is requested and the step size of the integration used for the nth step length is h_n the estimated step size for the $(n+1)st$ step, which would give a local error of acc, must be

$$h_{n+1} = h_n \left(\frac{\mathrm{acc}}{\mathrm{LPLE}} \right)^{1/q}, \tag{44}$$

where q is the order of the local phase-lag error.

However, for ease of programming we have restricted all step changes to halving and doubling. Thus, based on the procedure developed in [12] for the local truncation error, the step control procedure which we have actually used is

$$\text{If LPLE} < \text{acc}, \;\; h_{n+1} = 2h_n,$$

$$\text{If } 100\text{acc} > \text{LPLE} \geqslant \text{acc}, \;\; h_{n+1} = h_n, \tag{45}$$

$$\text{If LPLE} \geqslant 100\text{acc}, \;\; h_{n+1} = h_n/2, \text{ and repeat the step.} \tag{46}$$

We note that the local phase-lag error estimate is in the lower phase-lag order solution y^L_{n+1}. However, if this error estimate is acceptable, i.e., less than acc, we adopt the widely used procedure of performing local extrapolation. Thus, although we are actually controlling an estimate of the local phase-lag error in lower phase-lag order solution y^L_{n+1}, it is the higher phase-lag order solution y^H_{n+1} which we actually accept at each point.

We investigate now the computational cost of the application of the new embedded method. The new embedded method is a variable-step method. So, for comparison purposes we could apply only variable-step methods. Such method in the literature is the methods developed by the Raptis and Cash [12].

Table 2
Computed phase shifts and real time of computation for variable-step method of Raptis et al. [12] and for our new embedded variable-step method.

l	Method of [12]		New embedded variable-step method	
	Phase-shift	Real time of computation	Phase-shift	Real time of computation
0	−0.4311	0.330	−0.431004335	0.043
1	1.0449	0.330	1.045008966	0.043
2	0.7158	0.330	−0.715807299	0.043
3	0.5687	0.340	0.568807035	0.043
4	−1.3858	0.340	−1.385766256	0.040
5	−0.2984	0.340	−0.298342153	0.043
6	0.6867	0.340	0.686829438	0.042
7	1.5662	0.340	1.566303108	0.040
8	−0.8060	0.330	−0.805939712	0.038
9	−0.1525	0.330	−0.152407691	0.040
10	0.3778	0.335	0.377900152	0.035

In table 2 we present the phase shifts for $k = 10$ and for acc $= 10^{-6}$ using the variable-step algorithm described above and the variable-step method presented in [12].

In all cases the embedded variable step method developed in this paper is more accurate and requires smaller time of computation.

All computations were carried out on an PC-AT 80486 using double precision arithmetic of 16 digits accuracy.

5. Conclusions

In this paper some new Runge–Kutta type (or hybrid) methods are developed. The new methods are the first methods of algebraic order eight which have very large interval of periodicity and are also of very high phase-lag order. From the numerical results it is obvious that the new methods and the new variable step procedure are more efficient than other well known methods in the literature.

Acknowledgements

The author wishes to thank the anonymous referees for their careful reading of the manuscript and their fruitful comments and suggestions.

Appendix A

$$\begin{aligned}
T_1 &= 1003968q^8 w_0 - 6q^6(1059512w_0 + 1785) + 7q^4(2111168w_0 + 1547)\\
&\quad + 17q^2(637 - 611536w_0) + 971040w_0,\\
T_2 &= 1338624q^8 w_0 - q^6(7211840w_0 + 7497) + q^4(15351328w_0 + 10829)\\
&\quad - 10449152q^2 w_0 + 971040w_0,\\
T_3 &= 1003968q^8 w_0 + 3q^6(12495 - 2119024w_0) + 14q^4(1055584w_0 - 11849)\\
&\quad + 17q^2(15337 - 611536w_0) + 971040w_0,\\
T_4 &= 585648q^8 w_0 - 7q^6(552332w_0 + 153) + q^4(9164716w_0 + 1547)\\
&\quad - 6490940q^2 w_0 + 606900w_0.
\end{aligned}$$

Appendix B

$$\begin{aligned}
T_1 &= 1003968q^8 w_1 - 6q^6(1059512w_1 + 1785) + 7q^4(2111168w_1 + 1547)\\
&\quad + 17q^2(637 - 611536w_1) + 971040w_1,
\end{aligned}$$

$$\begin{aligned}
T_2 &= 9370368q^{10}w_1 - 7q^8(7211840w_1 + 7497) + 7q^6(43345920w_0w_1 \\
&\quad + 15351328w_1 + 10829) - 4352q^4w_1(240050w_0 + 16807) \\
&\quad + 2720q^2w_1(301088w_0 + 2499) - 77683200w_0w_1, \\
T_3 &= 63q^8 - 154q^6 + q^4(8160w_0 + 91) - 27200q^2w_0 + 19040w_0, \\
T_4 &= 1003968q^8w_1 + 3q^6(12495 - 2119024w_1) + 14q^4(1055584w_1 - 11849) \\
&\quad + 17q^2(15337 - 611536w_1) + 971040w_1, \\
T_5 &= 4099536q^{10}w_1 - 49q^8(552332w_1 + 153) - 7q^6(5418240w_0w_1 \\
&\quad - 9164716w_1 - 1547) + 340q^4w_1(384080w_0 - 133637) \\
&\quad + 340q^2w_1(12495 - 301088w_0) + 9710400w_0w_1.
\end{aligned}$$

Appendix C

$$\begin{aligned}
&63q^8(148736w_1 + 255) + 21q^6(15298560w_0w_1 - 1536320w_1 - 1223) \\
&\quad + 2q^4\big(7(1806528w_1 + 413) - 553075200w_0w_1\big) \\
&\quad + 2880q^2w_1(301088w_0 - 833) - 82252800w_0w_1 = 0, \qquad (47)
\end{aligned}$$

$$\begin{aligned}
&18711q^{12}(297472w_1 + 255) + 1247q^{10}(7649280w_0w_1 - 1090112w_1 + 765) \\
&\quad + 9q^8\big(40066329600w_0w_1 - 7(569647232w_1 + 1288537)\big) \\
&\quad - 84q^6(48151192320w_0w_1 - 1463144672w_1 - 1103207) \\
&\quad + 16q^4\big(529944465600w_0w_1 - 49(111112584w_1 + 20909)\big) \\
&\quad + 887040q^2w_1(9163 - 6070116w_0) + 494010316800w_0w_1 = 0, \qquad (48)
\end{aligned}$$

$$\begin{aligned}
&2189187q^{18}\big(22122397696w_1^2 + 113783040w_1 + 65025\big) \\
&\quad + 243243q^{16}\big(45895680w_0w_1(148736w_1 + 255) - 2410789240832w_1^2 \\
&\quad - 255(22453568w_1 + 7395)\big) + 11583q^{14}\big(7\big(37049889665024w_1^2 \\
&\quad + 41661700352w_1 + 22806435\big) - 46080w_0w_1(37668581888w_1 + 7696665)\big) \\
&\quad + 27q^{12}\big(26357760w_0w_1(144726131504w_1 + 41732807) \\
&\quad - 7\big(43534809545756672w_1^2 + 46110919547264w_1 + 53567638877\big)\big) \\
&\quad + 18q^{10}\big(119\big(5898059640332288w_1^2 + 10603437370240w_1 + 10405509373\big) \\
&\quad - 6589440w_0w_1(2378431465568w_1 + 4161680631)\big) \\
&\quad + 36q^8\big(37340160w_0w_1(322227908672w_1 + 1374717115) \\
&\quad - 7\big(416999131341844448w_1^2 + 123642410203312w_1 + 67886300447\big)\big) \\
&\quad + 8q^6\big(833\big(632555278198272w_1^2 + 2457461758752w_1 + 359067443\big) \\
&\quad - 823680w_0w_1(54676459529088w_1 + 402178416997)\big)
\end{aligned}$$

$$+ 196035840q^4 w_1\big(16w_0(46077744624w_1 + 443277779) - 2499(1238192w_1 + 2961)\big) + 5598783590400q^2 w_1\big(4998w_1 - w_0(3714576w_1 + 21973)\big) + 959407556050944000w_0 w_1^2 = 0. \quad (49)$$

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