J Math Chem (2014) 52:2087–2118
DOI 10.1007/s10910-014-0364-7

ORIGINAL PAPER

A family of explicit linear six-step methods with vanished phase-lag and its first derivative

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Received: 4 May 2014 / Accepted: 19 May 2014 / Published online: 31 May 2014

Abstract A family of explicit linear sixth algebraic order six-step methods with vanished phase-lag and its first derivative is obtained in this paper. The investigation of the above family of methods contains:

– theoretical study of the new family of methods and
– computational study of the new family of methods.

The theoretical study of the above mentioned family of methods contains:

1. the development of the method,
2. the computation of the local truncation error,
3. the comparative local truncation error analysis. The comparison is taken place between the new family of methods with the corresponding method with constant coefficients and
4. the stability analysis of the new family of methods. The stability analysis is taken place using test equation with different frequency than the frequency of the test equation used for the phase-lag analysis of the methods.

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The application of the new family of linear six-step sixth algebraic order methods to the resonance problem of the one-dimensional time independent Schrödinger equation is used for the computational study of the new family of methods. The result of the above mentioned theoretical and computational investigation is that the new proposed family of linear explicit schemes are computationally and theoretically more effective than other well known methods for the approximate solution of the radial Schrödinger equation and related initial or boundary value problems with periodic and/or oscillating solutions.

Keywords Phase-lag · Derivatives of the phase-lag · Initial value problems · Oscillating solution · Symmetric · Multistep · Schrödinger equation

1 Introduction

There are many real problems in sciences and engineering for which the mathematical models can be expresses via special second-order periodic initial or boundary value problems. Therefore the numerical solution of the above mentioned problems is of great interest. The general form of the model of the above described problems can be expressed in the form

$$y''(x) = f(x, y), \quad y(x_0) = y_0 \ \ and \ \ y'(x_0) = y'_0. \tag{1}$$

Remark 1 It is easy for one to see that one the main characteristics of the above presented models is that these models consist of systems of second order ordinary differential equations for the first derivatives y' does not appear explicitly. (see for more details [1–121] and references therein).

In Fig. 1, we present the formulation of this paper. More specifically:

In Sect. 2, we present a bibliography on the aims, scope, research and innovation on the subject of this paper. In Sect. 3, a theoretical approach for the Phase-lag analysis of the Symmetric Multistep Methods is presented. A direct formula for the computation

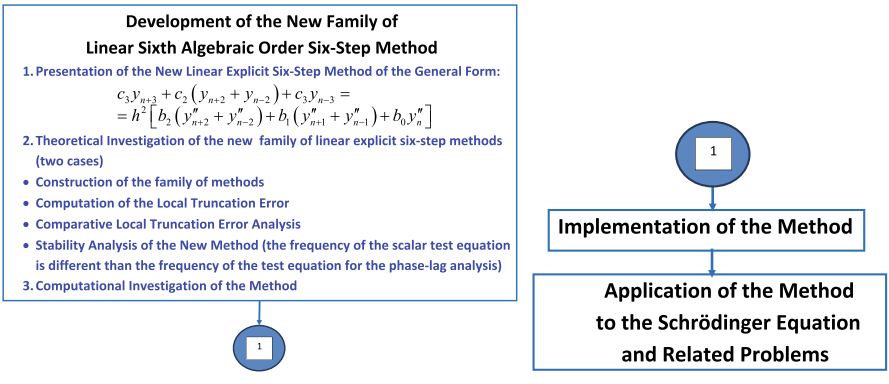

Fig. 1 Flowchart of the description of the form of the present paper

of the phase-lag is also obtained. In Sect. 4, we investigate the development of the new Family of Linear Explicit Six-Step Methods. We study two cases. In Sect. 5, we study the Comparative Error Analysis. In Sect. 6, we investigate the Stability Analysis. We use for this a scalar test equation with frequency different than the frequency of the scalar test equation used for phase-lag analysis. Finally, in Sect. 7, the numerical results produced using the resonance problem of the one-dimensional time independent Schrödinger equation and the new proposed family of methods together with several well known numerical algorithms are presented. In the same section, we describe concluding remarks on the effectiveness of the methods used in this comparison.

2 Bibliography relevant on the subject of the paper

On the approximate solution of the radial time independent Schrödinger equation and on the numerical solution of related initial or boundary-value problems with periodical and/or oscillating solutions, much research and innovation has been done on the last decades .

In Fig. 2, we present the main categories of finite difference methods on which the research and innovation was taken place during the last decades. The main aim and scope of this research and innovation was the production of effective, fast and reliable numerical methods (see for example [1–113]).

Indicative bibliography on the above mentioned research and innovation is given below :

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta Nyström type have been obtained in [1–7].
- In [8–13] exponentially and trigonometrically fitted Runge—Kutta and Runge–Kutta Nyström methods are constructed.

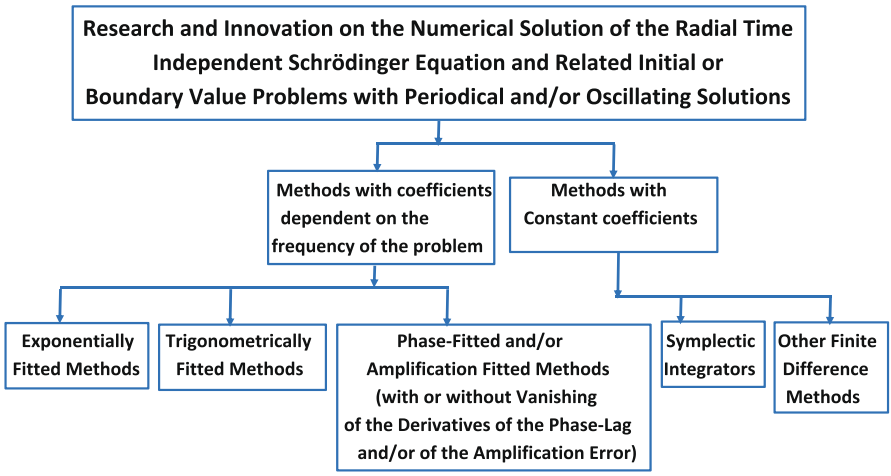

Fig. 2 Categories of the finite difference methods developed the last decades

– Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [26–55].
– Symplectic integrators are investigated in [56–84].
– Exponentially and trigonometrically multistep methods have been produced in [87–107].
– Nonlinear methods have been studied in [40] and [108]
– Review papers have been presented in [109–113]
– Special issues and Symposia in International Conferences have been developed on this subject (see [32,33])

3 Investigation on phase-lag for the symmetric multistep finite difference methods

We consider the initial value problem (1) with periodical and/or oscillating solution. We study the numerical solution of the above mentioned problem.

For the numerical solution of the problem (1), let us consider the multistep methods given by :

$$\sum_{i=0}^{m} a_i \, y_{n+i} = h^2 \sum_{i=0}^{m} b_i \, f(x_{n+i}, y_{n+i}) \tag{2}$$

where :

– m are the number of steps over the equally spaced intervals $[x_i, x_{i+1}], i = 0(1)m-1$, where $\{x_i\}_{i=0}^{m} \in [a, b]$
– $h = |x_{i+1} - x_i|, \;\; i = 0(1)m-1$, where h is called stepsize of integration
– $|a_0| + |b_0| \neq 0$

Remark 2 If $b_m = 0$ the method is explicit, otherwise it is implicit.

Remark 3 If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}, \;\; i = 0(1)\lfloor \frac{m}{2} \rfloor$.

Remark 4 The Multistep Finite Difference Method (2) is associated with the operator

$$L(x) = \sum_{i=0}^{m} c_i \, z(x + i\,h) - h^2 \sum_{i=0}^{m} b_i \, z''(x + i\,h) \tag{3}$$

where $z \in C^2$.

For the algebraic order and the conditions of consistency one can see [122].

Applying a symmetric $2k$-step method, that is for $i = -m(1)m$, to the scalar test equation

$$y'' = -\omega^2 \, y \tag{4}$$

a difference equation of the form

$$\sum_{i=1}^{m} A_i(v) \; (y_{n+i} + y_{n-i}) + A_0(v) \, y_n = 0 \tag{5}$$

is obtained. We note that in (5):

- $v = \omega h$,
- h is the step length and
- $A_i(v)\, i = 0(1)k$, are polynomials of v.

The characteristic equation associated with (5) is given by

$$\sum_{i=1}^{m} A_i(v)(\lambda^i + \lambda^{-i}) + A_0(v) = 0 \tag{6}$$

From Lambert and Watson [14], we have the following definition:

Definition 1 A symmetric $2m$-step method with characteristic equation given by (6) is said to have an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots $\lambda_i, i = 1(1)2m$ of Eq. (6) satisfy:

$$\lambda_1 = e^{i\theta(v)},\ \lambda_2 = e^{-i\theta(v)},\ \textit{and}\ |\lambda_i| \leq 1,\ i = 3(1)2m \tag{7}$$

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

Theorem 1 [24] *The symmetric $2m$-step method with characteristic equation given by (6) has phase-lag order q and phase-lag constant c given by:*

$$-cv^{q+2} + O(v^{q+4}) = \frac{2\sum_{j=1}^{m} A_j(v)\cos(jv) + A_0(v)}{2\sum_{j=1}^{k} j^2 A_j(v)} \tag{8}$$

If we know the number m, then we can produce the direct algorithm for the calculation of the phase-lag of the corresponding symmetric $2m$-step method.

Remark 5 In our case - for the family of linear explicit symmetric six-step methods - the number $m = 3$ and the direct formula for the computation of the phase-lag is given by:

$$-cv^{q+2} + O(v^{q+4}) = \frac{2A_3(v)\cos(3v) + 2A_2(v)\cos(2v) + 2A_1(v)\cos(v) + A_0(v)}{18A_3(v) + 8A_2(v) + 2A_1(v)} \tag{9}$$

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

4 The general family of linear explicit six-step methods

Our new proposed family of methods is belonged to the general explicit symmetric $2m$-step finite difference methods of the form:

$$y_{n+m} + \sum_{i=0}^{m-1} c_i\ (y_{n+i} + y_{n-i}) + y_{n-m} = h^2 \sum_{i=1}^{m-1} b_i\ \left[f(x_{n+i}, y_{n+i}) + f(x_{n-i}, y_{n-i})\right] + b_0\, f(x_n, y_n) \tag{10}$$

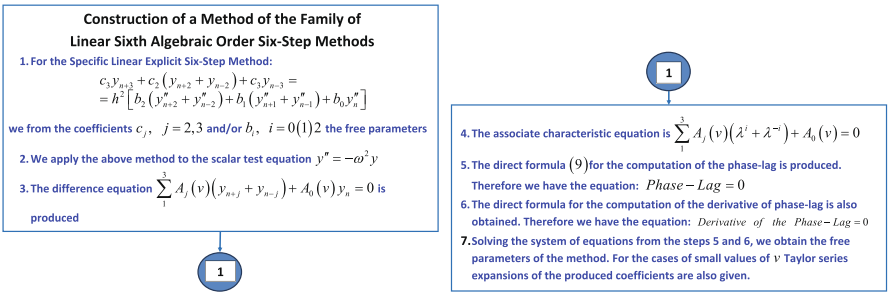

Fig. 3 Flowchart of the construction of any method of the family

where $f_i = y''(x_i, q_i)$, $i = n-2(1)n+2$.

Our studies refer to a special case of the above form (10) for $m = 3$.

More specifically, we will investigate the family of linear explicit symmetric six-step finite difference methods of the form:

$$\begin{aligned} &c_3\, y_{n+3} + c_2\, (y_{n+2} + y_{n-2}) + c_3\, y_{n-3} \\ &= h^2\Big[b_2\, (f_{n+2} + f_{n-2}) + b_1\, (f_{n+1} + f_{n-1}) + b_0\, f_n\Big] \end{aligned} \tag{11}$$

Remark 6 For the family of numerical methods (11) we have :

- the coefficients c_i, $j = 2, 3$ and b_j, $j = 0(1)2$ are our free parameters to be determined.
- h is the step size of the integration.
- the number of steps is defined to be n.
- y_n is defined as the approximation of the solution at the point x_n.
- $x_n = x_0 + n\,h$ and
- x_0 is the initial value point.

This family was first formed at [20].

In the flowchart of Fig. 3, we present the construction of any method of the family.

4.1 First method of the family

Let us consider the family of methods (11) with:

$$c_3 = 1,\ b_1 = -\frac{1}{6},\ b_2 = \frac{67}{48} \tag{12}$$

Application of the linear explicit six-step method (11) to the scalar test equation (4), leads to the difference equation (5) with $m = 3$ and :

$$A_3(v) = 1,\ \ A_2(v) = c_2 + \frac{67}{48}v^2,\ \ A_1(v) = -\frac{1}{6}v^2,\ \ A_0(v) = v^2\, b_0 \tag{13}$$

Based on the above polynomials $A_j(v)$, $j = 0(1)3$ and the formula (9), the following formula for the direct computation of the phase-lag is produced:

$$\text{Phase-Lag} = \frac{2\cos(3v) + 2\left(c_2 + \frac{67}{48}v^2\right)\cos(2v) - \frac{1}{3}v^2\cos(v) + v^2 b_0}{18 + 8c_2 + \frac{65}{6}v^2} = 0 \tag{14}$$

and the following formula for the direct computation of the first derivative of the phase-lag is also obtained:

$$\text{First Derivative Phase-Lag} = -\frac{T_0}{\left(65v^2 + 48c_2 + 108\right)^2} = 0 \tag{15}$$

where

$$\begin{aligned} T_0 = {} & 4355\sin(v)\cos(v)v^4 + 9360(\cos(v))^2\sin(v)v^2 \\ & + 6336\sin(v)\cos(v)v^2 c_2 - 130\sin(v)v^4 + 6240v(\cos(v))^3 \\ & + 6912(\cos(v))^2\sin(v)c_2 - 96(\cos(v))^2 v c_2 \\ & + 7236\sin(v)\cos(v)v^2 + 2304\sin(v)\cos(v){c_2}^2 \\ & - 96\sin(v)v^2 c_2 + 15552(\cos(v))^2\sin(v) \\ & - 7236(\cos(v))^2 v + 5184\sin(v)\cos(v)c_2 + 192\cos(v)v c_2 \\ & - 2556\sin(v)v^2 - 576v c_2 b_0 - 4248\cos(v)v - 1728\sin(v)c_2 + 48v c_2 \\ & - 1296v b_0 - 3888\sin(v) + 3618v \end{aligned}$$

Requesting the above mentioned family of methods (11) with coefficients given by (12), to have vanished phase-lag and its first derivative, the following coefficients are obtained :

$$\begin{aligned} c_2 &= \frac{T_1}{48v\sin(2v) + 48\cos(2v)} \\ b_0 &= \frac{T_2}{48v^2\sin(2v) + 48v\cos(2v)} \end{aligned} \tag{16}$$

where

$$\begin{aligned} T_1 &= -67v^3\sin(2v) + 4\sin(v)v^3 - 72v\sin(3v) - 48\cos(3v) \\ T_2 &= 4v^2\sin(3v) + 12v^2\sin(v) + 8v\cos(3v) - 67v\cos(4v) \\ &\quad + 8v\cos(v) + 24\sin(5v) + 120\sin(v) - 67v \end{aligned}$$

The formulae of the coefficients c_2 and b_0 which are given by (16) may subject to heavy cancellations for some values of $|v|$. In this case the following Taylor series expansions should be used :

$$c_2 = -1 + \frac{787}{8064}v^8 - \frac{647}{22680}v^{10}$$

$$
\begin{aligned}
&+\frac{1314347}{19160064}\,v^{12}-\frac{798220931}{21794572800}\,v^{14}\\
&+\frac{125596777}{2384363520}\,v^{16}-\frac{7455911565383}{200074178304000}\,v^{18}+\ldots\\
b_0 \;=\;&\frac{61}{24}-\frac{787}{3024}\,v^6+\frac{8377}{18144}\,v^8\\
&-\frac{611279}{1596672}\,v^{10}+\frac{3765304141}{9340531200}\,v^{12}\\
&-\frac{91439949493}{261534873600}\,v^{14}+\frac{15413620895639}{44460928512000}\,v^{16}\\
&-\frac{114092713192434497}{364935301226496000}\,v^{18}+\ldots
\end{aligned}
\tag{17}
$$

The behavior of the coefficients is given in Fig. 4.

We present below the local truncation error of the new obtained method (11)–(12) (mentioned as $Linear\,Six\,Step\,I$) with the coefficients given by (16)–(17) is given by:

$$
LTE_{Linear\ Six\ Step\ I}=\frac{787\,h^8}{12096}\left(y_n^{(8)}+4\,\omega^6\,y_n^{(2)}+3\omega^8\,y_n\right)+O\left(h^{10}\right) \tag{18}
$$

4.2 Second method of the family

We consider again the family of methods (11) with different coefficients :

$$
b_0=\frac{61}{24},\;b_1=-\frac{1}{6},\;b_2=\frac{67}{48} \tag{19}
$$

If we apply the above linear explicit six-step method to the scalar test Eq. (4), we obtain the difference Eq. (5) with $m=3$ and :

$$
A_3(v)=a_3,\;\;A_2(v)=c_2+\frac{67}{48}\,v^2,\;\;A_1(v)=-\frac{1}{6}\,v^2,\;\;A_0(v)=\frac{61}{24}\,v^2 \tag{20}
$$

If we substitute the above mentioned polynomials $A_j(v)$, $j=0(1)3$ into the formula (9), we obtain the formula for the direct calculation of the phase-lag:

$$
\text{Phase-Lag}\;=\;\frac{T_3}{18\,c_3+8\,c_2+\frac{65}{6}\,v^2}=0 \tag{21}
$$

and the following formula for the direct calculation of the first derivative of the phase-lag:

$$
\text{First Derivative Phase-Lag}\;=\;-\frac{T_4}{\left(65\,v^2+48\,c_2+108\,c_3\right)^2}=0 \tag{22}
$$

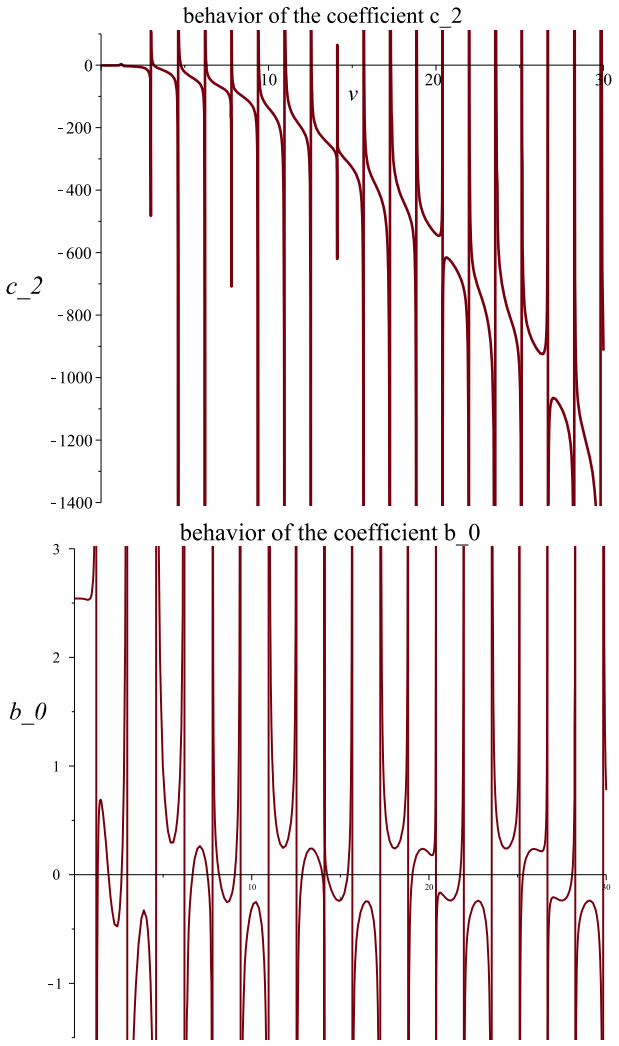

Fig. 4 Behavior of the coefficients of the new proposed method given by (16) for several values of $v = \omega h$

where

$$
\begin{aligned}
T_3 \;=\; & 2\,c_3 \cos(3\,v) + 2\left(c_2 + \frac{67}{48}\,v^2\right)\cos(2\,v) \\
& -1/3\,v^2\cos(v) + \frac{61}{24}\,v^2 \\
T_4 \;=\; & 9360\;(\cos(v))^2 \sin(v)\,v^2 c_3 \\
& + 4355\;\sin(v)\cos(v)\,v^4 + 6240\,v\,c_3\,(\cos(v))^3 \\
& + 6912\;(\cos(v))^2 \sin(v)\,c_2 c_3 \\
& + 15552\;(\cos(v))^2 \sin(v)\,{c_3}^2
\end{aligned}
$$

$$
\begin{aligned}
&+6336\,\sin(v)\cos(v)\,v^2c_2+7236\,\sin(v)\cos(v)\,v^2c_3\\
&-130\,\sin(v)\,v^4-96\,(\cos(v))^2\,v\,c_2\\
&-7236\,(\cos(v))^2\,v\,c_3+2304\,\sin(v)\cos(v)\,{c_2}^2\\
&+5184\,\sin(v)\cos(v)\,c_2c_3-96\,\sin(v)\,v^2c_2\\
&-2556\,\sin(v)\,v^2c_3+192\,\cos(v)\,v\,c_2-4248\,\cos(v)\,v\,c_3\\
&-1728\,\sin(v)\,c_2c_3-3888\,\sin(v)\,{c_3}^2-1416\,v\,c_2+324\,v\,c_3
\end{aligned}
$$

We request now the satisfaction of the above mentioned Eqs. (21) and (22). This satisfaction leads to the vanishing of the phase-lag and its first derivative. The request of vanished phase-lag and its first derivative leads to the method (11)–(19) with coefficients $c_j,\ j=2,3$ given by:

$$
\begin{aligned}
c_2 &= \frac{T_5}{240\,\sin(v)+48\,\sin(5\,v)}\\
c_3 &= \frac{T_6}{120\,\sin(v)+24\,\sin(5\,v)}
\end{aligned}
\tag{23}
$$

where

$$
\begin{aligned}
T_5 &= -366\,\sin(3\,v)\,v^2+32\,\sin(2\,v)\,v^2-335\,\sin(v)\,v^2\\
&\quad -67\,\sin(5\,v)\,v^2+16\,\sin(4\,v)\,v^2+16\,\cos(2\,v)\,v\\
&\quad -244\,\cos(3\,v)\,v-134\,\cos(v)\,v+16\,\cos(4\,v)\,v-134\,\cos(5\,v)\,v\\
T_6 &= -4\,\sin(3\,v)\,v^2+122\,\sin(2\,v)\,v^2-12\,\sin(v)\,v^2\\
&\quad +122\,\cos(2\,v)\,v-8\,\cos(3\,v)\,v-8\,\cos(v)\,v+67\,\cos(4\,v)\,v+67\,v
\end{aligned}
$$

The formulae of the coefficients c_2 and c_3 which are given by (23) may subject to heavy cancellations for some values of $|v|$. In this case the following Taylor series expansions should be used :

$$
\begin{aligned}
c_2 &= -1-\frac{787}{15120}\,v^6+\frac{1037}{13440}\,v^8\\
&\quad +\frac{6468857}{39916800}\,v^{10}+\frac{76974957359}{653837184000}\,v^{12}\\
&\quad -\frac{1872015347}{62270208000}\,v^{14}-\frac{59563385403889}{355687428096000}\,v^{16}\\
&\quad -\frac{2284124686606788527}{12772735542927360000}\,v^{18}+\cdots\\
c_3 &= 1+\frac{787}{15120}\,v^6+\frac{103}{5040}\,v^8\\
&\quad -\frac{1980527}{39916800}\,v^{10}-\frac{83521471}{928746000}\,v^{12}
\end{aligned}
$$

$$-\frac{3754449563}{62270208000}\,v^{14}+\frac{247049291327}{11115232128000}\,v^{16}+\frac{1203315005668907297}{12772735542927360000}\,v^{18}+\cdots \tag{24}$$

The behavior of the coefficients is given in Fig. 5.

The method (11)–(19) (mentioned as $LinearSixStepII$) with the coefficients given by (23)–(24) has a local truncation error given by :

$$LTE_{Linear\ Six\ Step\ II}=\frac{787\,h^8}{12096}\left(y_n^{(8)}+4\,\omega^6\,y_n^{(2)}+3\omega^8\,y_n\right)+O\left(h^{10}\right) \tag{25}$$

5 Comparative error analysis

Based on the flowchart of Fig. 1, continuing the theoretical investigation for the new methods, we will study the local truncation error of the new obtained linear six-step methods. We will compare this local truncation error with that of the linear six-step method with constant coefficients.

We will study the local truncation error for the following methods:

- Explicit Linear Six-Step Methods with constant coefficients and of Algebraic Order Six
- The New Linear Explicit Six-Step Method of Algebraic Order Six with Vanished the Phase-Lag and its First Derivative Developed in Sect. 4.1 and
- The New Linear Explicit Six-Step Method of Algebraic Order Six with Vanished the Phase-Lag and its First Derivative Developed in Sect. 4.2.

Therefore, we will study the following methods:

5.1 The sixth algebraic order classical method (i.e. the method (11) with constant coefficients)

$$LTE_{CL}=\frac{787\,h^8}{12096}\,y_n^{(8)}+O\left(h^{10}\right) \tag{26}$$

5.2 The sixth algebraic order linear six-step method with vanished phase-lag and its first derivative produced in Sect. 4.1

$$LTE_{Linear\ Six\ Step\ I}=\frac{787\,h^8}{12096}\left(y_n^{(8)}+4\,\omega^6\,y_n^{(2)}+3\omega^8\,y_n^{(2)}\right)+O\left(h^{10}\right) \tag{27}$$

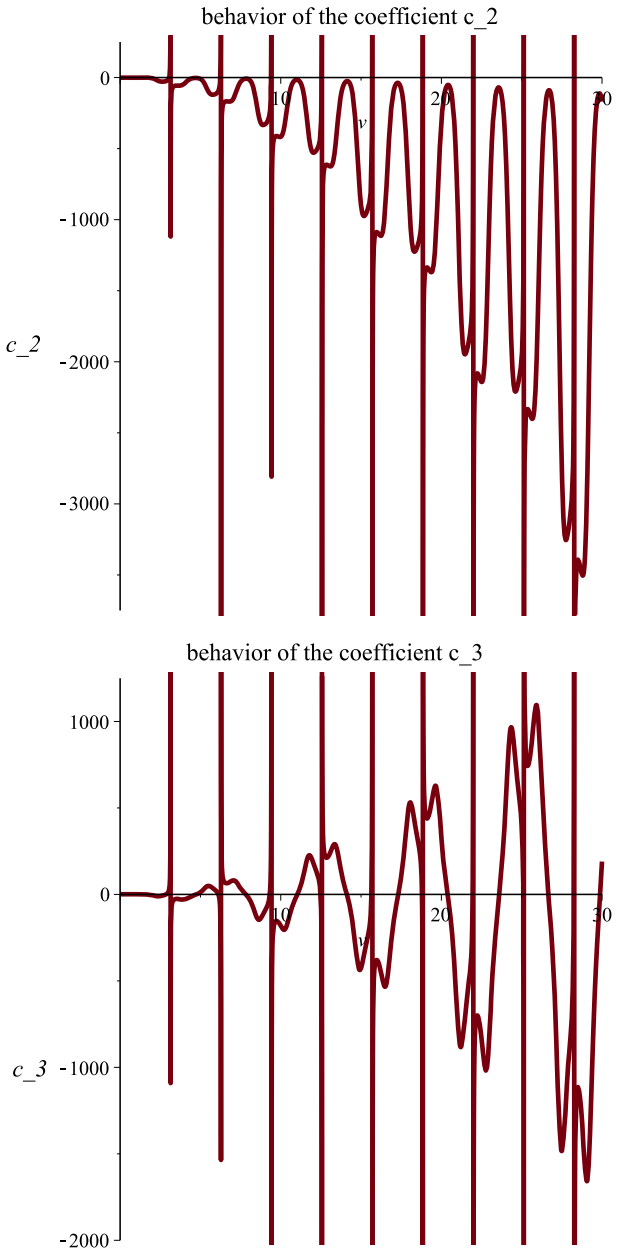

Fig. 5 Behavior of the coefficients of the new proposed method given by (23) for several values of $v = \omega h$

5.3 The sixth algebraic order linear six-step method with vanished phase-lag and its first derivative produced in Sect. 4.2

$$LTE_{Linear\ Six\ Step\ II} = \frac{787\,h^8}{12096}\left(y_n^{(8)} + 4\,\omega^6\,y_n^{(2)} + 3\omega^8\,y_n^{(2)}\right) + O\left(h^{10}\right) \quad (28)$$

Remark 7 It is easy to see that the local truncation errors (27) and (28) are exactly the same. Therefore we will investigate the local truncation errors (26) and (27).

The investigation of the local truncation error of the one-dimensional time independent Schrödinger equation, is based on the following procedure :

– We write the radial time independent Schrödinger equation in the following form:

$$y''(x) = f(x)\ y(x) \quad (29)$$

– The function $f(x)$ is expressed as (see for more details at Ixaru and Rizea [87]):

$$f(x) = g(x) + G \quad (30)$$

where:
1. $g(x) = V(x) - V_c = g$,
2. V_c is the constant approximation of the potential and
3. $G = \omega^2 = V_c - E$.

– We substitute the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \ldots$, with corresponding expressions of the formula (30).
– Based on the above expressions we analyze the Local Truncation Error Formulae (LTEF).
– The above mentioned analysis leads to new formulae of the LTEF which are expressed as polynomials of G.

The Local Truncation Error Analysis is based on the Flowchart of the Fig. 6.

Based on the above mentioned flowchart, we calculate the derivatives in the formulae of the Local Truncation Errors. The computations are based on the Eq. (30) (i.e. on the formula: $y''(x) = f(x) = g(x) + G$). Therefore we can now calculate the formulae of $y_n^{(j)}$, $j = 2, 3, 4, \ldots$.

$$\begin{aligned}
y_n^{(2)} &= (V(x) - V_c + G)\ y(x) \\
y_n^{(3)} &= \left(\frac{d}{dx}g\,(x)\right) y\,(x) + (g\,(x) + G)\,\frac{d}{dx}y\,(x) \\
y_n^{(4)} &= \left(\frac{d^2}{dx^2}g\,(x)\right) y\,(x) + 2\left(\frac{d}{dx}g\,(x)\right)\frac{d}{dx}y\,(x) \\
&\quad + (g\,(x) + G)^2\,y\,(x)
\end{aligned}$$

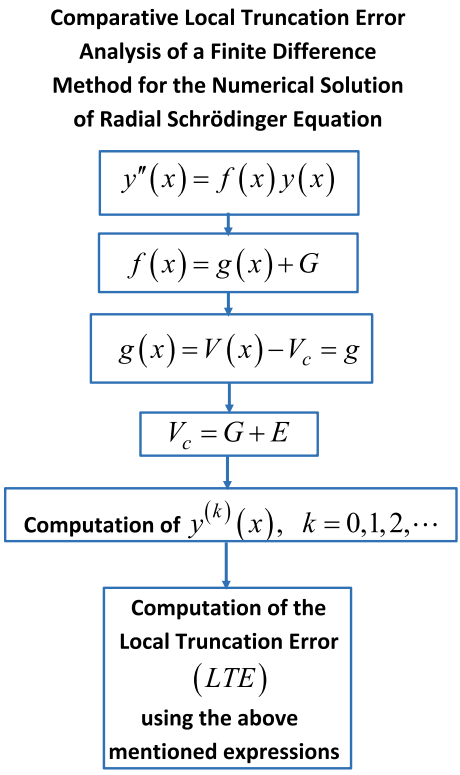

Fig. 6 Flowchart for the comparative error analysis

$$
\begin{aligned}
y_n^{(5)} &= \left(\frac{d^3}{dx^3}g(x)\right) y(x) + 3\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}y(x) \\
&\quad + 4\,(g(x)+G)\,y(x)\,\frac{d}{dx}g(x) + (g(x)+G)^2\,\frac{d}{dx}y(x) \\
y_n^{(6)} &= \left(\frac{d^4}{dx^4}g(x)\right) y(x) + 4\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}y(x) \\
&\quad + 7\,(g(x)+G)\,y(x)\,\frac{d^2}{dx^2}g(x) + 4\left(\frac{d}{dx}g(x)\right)^2 y(x) \\
&\quad + 6\,(g(x)+G)\left(\frac{d}{dx}y(x)\right)\frac{d}{dx}g(x) \\
&\quad + (g(x)+G)^3\,y(x) \\
y_n^{(7)} &= \left(\frac{d^5}{dx^5}g(x)\right) y(x) + 5\left(\frac{d^4}{dx^4}g(x)\right)\frac{d}{dx}y(x) \\
&\quad + 11\,(g(x)+G)\,y(x)\,\frac{d^3}{dx^3}g(x) + 15\left(\frac{d}{dx}g(x)\right) y(x) \\
&\quad \frac{d^2}{dx^2}g(x) + 13\,(g(x)+G)\left(\frac{d}{dx}y(x)\right)\frac{d^2}{dx^2}g(x)
\end{aligned}
$$

$$
\begin{aligned}
&+10\left(\frac{d}{dx}g\left(x\right)\right)^{2}\frac{d}{dx}y\left(x\right)+9\left(g\left(x\right)+G\right)^{2}y\left(x\right)\\
&\frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^{3}\frac{d}{dx}y\left(x\right)\\
y_{n}^{(8)} &= \left(\frac{d^{6}}{dx^{6}}g\left(x\right)\right)y\left(x\right)+6\left(\frac{d^{5}}{dx^{5}}g\left(x\right)\right)\frac{d}{dx}y\left(x\right)\\
&+16\left(g\left(x\right)+G\right)y\left(x\right)\frac{d^{4}}{dx^{4}}g\left(x\right)+26\left(\frac{d}{dx}g\left(x\right)\right)y\left(x\right)\\
&\frac{d^{3}}{dx^{3}}g\left(x\right)+24\left(g\left(x\right)+G\right)\left(\frac{d}{dx}y\left(x\right)\right)\frac{d^{3}}{dx^{3}}g\left(x\right)\\
&+15\left(\frac{d^{2}}{dx^{2}}g\left(x\right)\right)^{2}y\left(x\right)+48\left(\frac{d}{dx}g\left(x\right)\right)\\
&\left(\frac{d}{dx}y\left(x\right)\right)\frac{d^{2}}{dx^{2}}g\left(x\right)+22\left(g\left(x\right)+G\right)^{2}y\left(x\right)\\
&\frac{d^{2}}{dx^{2}}g\left(x\right)+28\left(g\left(x\right)+G\right)y\left(x\right)\left(\frac{d}{dx}g\left(x\right)\right)^{2}\\
&+12\left(g\left(x\right)+G\right)^{2}\left(\frac{d}{dx}y\left(x\right)\right)\frac{d}{dx}g\left(x\right)\\
&+\left(g\left(x\right)+G\right)^{4}y\left(x\right)\\
&\ldots
\end{aligned}
$$

The current investigation for the local truncation error analysis is finalized via the procedure mentioned below:

- We investigate the value of E within the Local Truncation Error analysis (we note that the value of E is included in parameters v and ω), for two cases :
  1. **First Case** : The Energy is close to the potential, i.e., $G = V_c - E \approx 0$. Consequently all the terms of the Local Truncation Error Formulae are vanished (since they have terms of G^q, $q = 1, 2, \ldots$) except those which are the free terms of the polynomials in G (since they have terms of G^0). Therefore, all numerical methods of the same family of methods have comparable accuracy for these values of E. The reason is that in the formulae of Local Truncation Error for these values of E, the terms of power of G , say q , not equal to zero, are equal to zero and only the terms of zero power of G are not vanished. As a summary : The free from G terms of polynomials are the same for the cases of the same family of methods and therefore for the same family of methods: the classical method - i.e. the method with constant coefficients - and the methods with vanished phase-lag and its derivatives are of the same accuracy.

2. **Second Case** : $G >> 0$ or $G << 0$. In this case the term $|G|$ is a large number. Consequently, the methods of the family which have lower power of $|G|$ are more accurate than the methods of the family which have larger power of $|G|$.

– The computation of the asymptotic expansions of the Local Truncation Errors Formulae is the final stage of the comparative error analysis

Remark 8 We note that the above mentioned procedure for the comparative local truncation error analysis is valid for any model of a problem which has the form of the Eq. (29)

The asymptotic expansions of the Local Truncation Errors Formulae mentioned below is the result of the theoretical analysis presented above :

5.4 Classical method

$$LTE_{CL} = h^8 \left(\frac{787}{12096} \, y(x) \, G^4 + \cdots \right) + O\left(h^{10}\right) \tag{31}$$

5.5 The sixth algebraic order linear six-step methods with vanished phase-lag and its first derivative produced in Sects. 4.1 and 4.2

$$\begin{aligned} LTE_{Linear\ Six\ Step\ I\&II} = h^8 \Bigg[& \left(\frac{8657}{6048} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \right. \\ & + \frac{787}{1008} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} y(x) \\ & \left. + \frac{787}{2016} \left(g(x) \right)^2 y(x) \right) G^2 + \cdots \Bigg] + O\left(h^{10}\right) \end{aligned} \tag{32}$$

Based on the above analysis, we have the following theorem:

Theorem 2 – *For the Classical Linear Six-Step Explicit Method, the error increases as the fourth power of G.*

– *For the Linear Six-Step Explicit Methods with Vanished Phase-lag and its First Derivative produced in this paper (Sects. 4.1, 4.2), the error increases as the second power of G.*

Therefore, for the numerical solution of the time independent radial Schrödinger equation and related problems the Linear Six-Step Methods developed in Sects. 4.1 and 4.2 with Vanished Phase-Lag and its First Derivative are the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

6 Stability analysis

The stability—interval of periodicity analysis of any symmetric multistep finite difference method for the problems of the form of the radial Schrödinger equation is based on the Flowchart of Fig. 7.

The stability investigation is based on the flowchart of Fig. 7. Application of the new linear six-step symmetric methods developed in Sects. 4.1 and 4.2 to the scalar test equation:

$$y'' = -\phi^2 y. \tag{33}$$

leads to the following difference equation:

$$\begin{aligned} &A_3(s,v)\ (y_{n+3} + y_{n-3}) + A_2(s,v)\ (y_{n+2} + y_{n-2}) \\ &+A_1(s,v)\ (y_{n+1} + y_{n-1}) + A_0(s,v)\ y_n = 0 \end{aligned} \tag{34}$$

where $s = \phi h$, $v = \omega h$ and

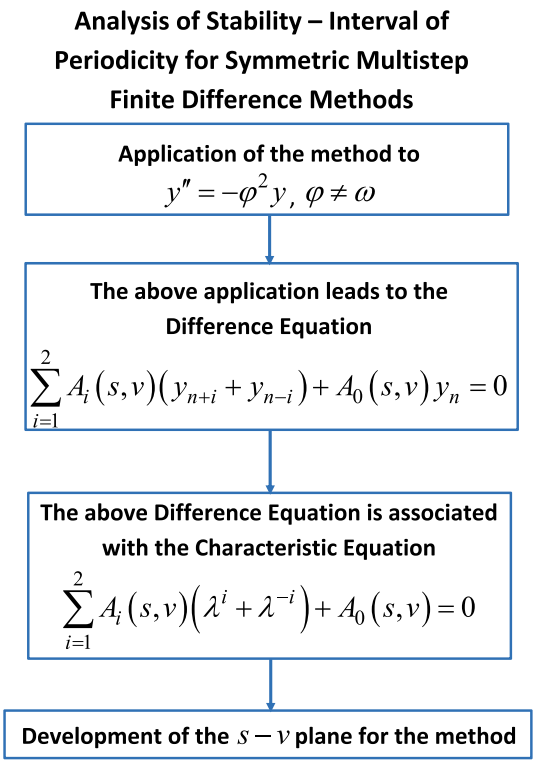

Fig. 7 Flowchart for the stability—interval of periodicity analysis of symmetric multistep finite difference methods

6.1 First method of the family

$$A_3(s,v) = 1,\quad A_2(s,v) = -\frac{1}{48}\,\frac{T_7}{v\,\sin(2v)+\cos(2v)}$$
$$A_1(s,v) = -\frac{1}{6}s^2,\ A_0(s,v) = \frac{1}{24}\,\frac{T_8}{v\,(v\,\sin(2v)+\cos(2v))} \tag{35}$$

where

$$\begin{aligned}
T_7 &= 134\,\sin(v)\,v^3\cos(v) - 134\,\sin(v)\cos(v)\,v\,s^2\\
&\quad +288\,\sin(v)\,(\cos(v))^2\,v - 4\,\sin(v)\,v^3\\
&\quad -134\,s^2\,(\cos(v))^2 + 192\,(\cos(v))^3\\
&\quad -72\,v\,\sin(v) + 67\,s^2 - 144\,\cos(v)\\
T_8 &= s^2\Big(192\,\sin(v)\,(\cos(v))^4 + 8\,\sin(v)\\
&\quad (\cos(v))^2\,v^2 - 268\,v\,(\cos(v))^4\\
&\quad +16\,v\,(\cos(v))^3 - 144\,\sin(v)\,(\cos(v))^2\\
&\quad +4\,v^2\sin(v) + 268\,v\,(\cos(v))^2 - 8\,v\,\cos(v)\\
&\quad +72\,\sin(v) - 67\,v\Big)
\end{aligned}$$

6.2 Second method of the family

$$A_3(s,v) = \frac{T_9}{120\,\sin(v)+24\,\sin(5v)}$$
$$A_2(s,v) = -\frac{1}{48}\,\frac{T_{10}}{\left(8\,(\cos(v))^4 - 6\,(\cos(v))^2 + 3\right)\sin(v)}$$
$$A_1(s,v) = -\frac{1}{6}s^2,\ A_0(s,v) = \frac{61}{24}s^2 \tag{36}$$

where

$$\begin{aligned}
T_9 &= -4\,v^2\sin(3v) + 122\,v^2\sin(2v) - 12\,v^2\sin(v)\\
&\quad +122\,v\,\cos(2v) - 8\,v\,\cos(3v) - 8\,v\,\cos(v) + 67\,v\,\cos(4v) + 67\,v\\
T_{10} &= 536\,\sin(v)\,(\cos(v))^4\,v^2\\
&\quad -536\,\sin(v)\,(\cos(v))^4\,s^2\\
&\quad -64\,\sin(v)\,(\cos(v))^3\,v^2\\
&\quad +1072\,v\,(\cos(v))^5 + 330\,\sin(v)\,(\cos(v))^2\,v^2\\
&\quad +402\,\sin(v)\,(\cos(v))^2\,s^2
\end{aligned}$$

$$
\begin{aligned}
&-64\,v\,(\cos(v))^4 - 852\,v\,(\cos(v))^3 \\
&+18\,v^2\sin(v) - 201\,s^2\sin(v) \\
&+48\,v\,(\cos(v))^2 + 36\,v\,\cos(v)
\end{aligned}
$$

Remark 9 The frequency of the scalar test Eq. (33) (which is used for the stability-interval of periodicity analysis), ϕ is different from the frequency of the scalar test Eq. (4), ω (which was used for the phase-lag analysis), i.e. $\omega \neq \phi$.

We give the following definitions:

Definition 2 (see [14]) If a Symmetric Multistep Method has an interval of periodicity equal to $(0, \infty)$, then is called P-stable.

Definition 3 In the case where the frequency of the scalar test equation for the phase-lag analysis is the same as the frequency of the scalar test equation for the stability analysis, i.e. in the case where $s = v$, then a method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$.[1]

In Figs. 8 and 9 we present the $s - w$ plane for the methods developed in this paper.

Remark 10 A shadowed region declares the $s - v$ area where the methods are stable, while a white area declares the area where the methods are unstable.

Remark 11 Depending on mathematical model of the specific problem one can chose different parts of the $s - v$ area. The mathematical model of the time independent radial Schrödinger equation belongs to a category for which it is necessary to observe *the surroundings of the first diagonal of the $s - v$ plane*. For these cases of mathematical models in order to apply the new produced methods, the frequency of the scalar test equation for the phase-lag analysis must be equal to the frequency of the scalar test equation for the stability analysis.

For the time independent radial Schrödinger equation and due to the above mentioned remark, the frequency of the scalar test equation for the phase-lag analysis is equal to the frequency of the scalar test equation for the stability analysis. Therefore, we investigate the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s - v$ plane). Based on this investigation we obtain that the interval of periodicity of the new methods produced in Sects. 4.1 and 4.2 are equal to: $(0, 0.7)$.

The above investigation leads to the following theorem:

Theorem 3 *The methods produced in Sects. 4.1 and 4.2:*

- *are of sixth algebraic order,*
- *have the phase-lag and its first derivative equal to zero*
- *have an interval of periodicity equals to:* $(0, 0.7)$ *the frequency of the scalar test equation for the phase-lag analysis must be equal to the frequency of the scalar test equation for the stability analysis*

[1] where S is a set of distinct points

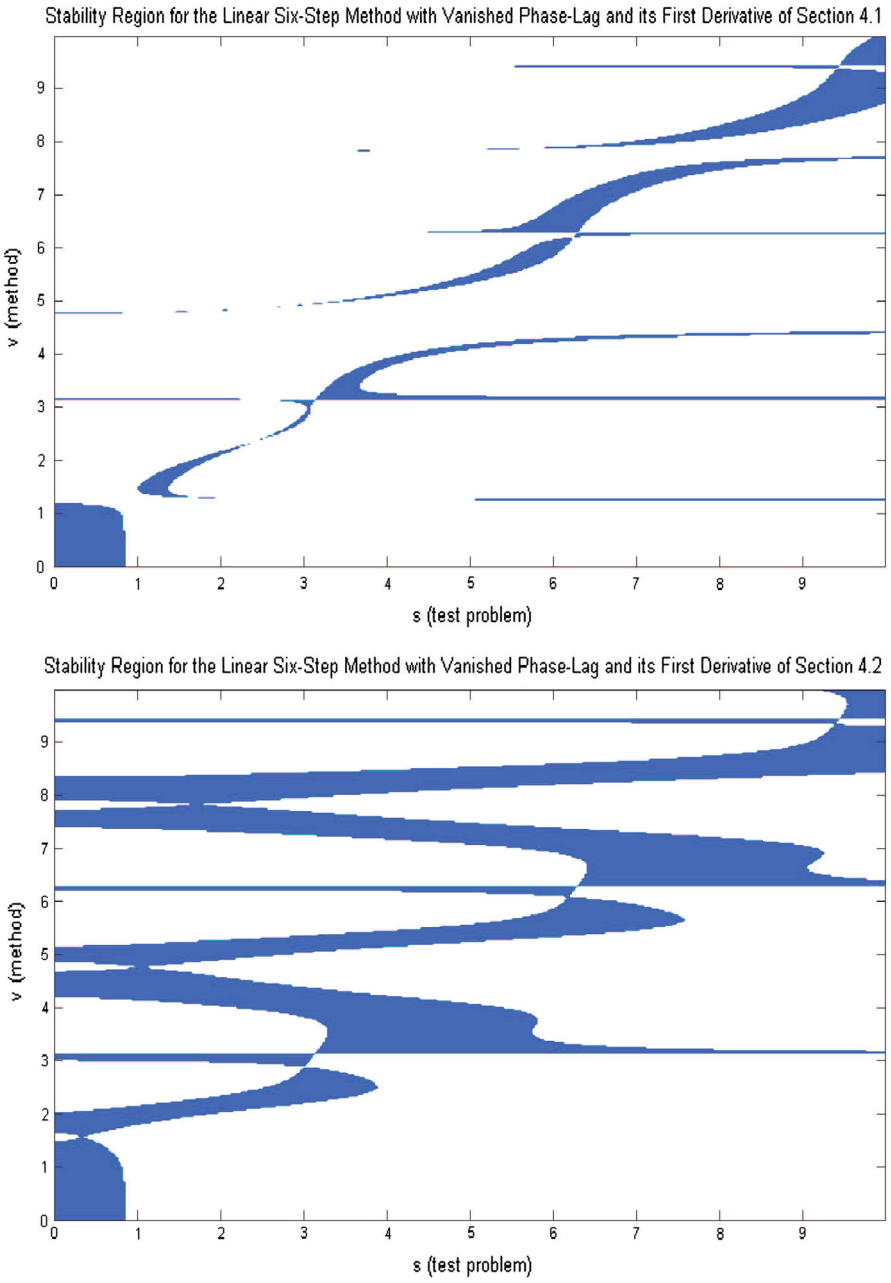

Fig. 8 $s - v$ plane of the the new developed methods in Sects. 4.1 and 4.2 with vanished phase-lag and its first derivatives

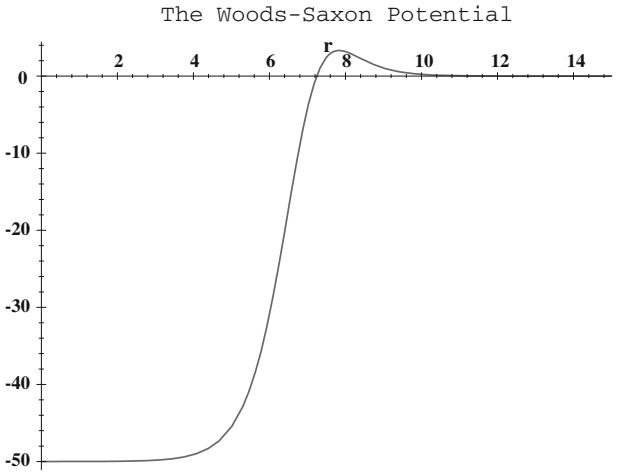

Fig. 9 The Woods-Saxon potential

7 Numerical results

In this section, we will investigate the effectiveness of the new produced methods in Sects. 4.1 and 4.2.

The investigation consists the application of the new obtained sixth algebraic order explicit linear six-step methods (of Sects. 4.1, 4.2) on the numerical solution of the radial time-independent Schrödinger equation (see more information in [123–125]).

We base our study on the following mathematical model of the one-dimensional time independent Schrödinger equation :

$$y''(r) = [l(l+1)/r^2 + V(r) - k^2]\, y(r). \tag{37}$$

The above mathematical model belongs to the special second order boundary value problems. The boundary conditions are given by:

$$y(0) = 0. \tag{38}$$

In order to determine the second boundary condition, for large values of r, the characteristics of the physical properties of the specific mathematical model are taken into account.

The above mathematical model of (37) has some functions, quantities and parameters which are defined below :

- We call the function $W(r) = l(l+1)/r^2 + V(r)$ *the effective potential*. One basic characteristic of the above mentioned function is: $W(x) \to 0$ as $x \to \infty$,
- We call the quantity k^2 *the energy* and it is a real number,
- We call the quantity l *angular momentum* and it is a given integer,
- The function V denotes the *potential*.

It is known (see Fig. 2) that we have two categories of finite difference methods for the numerical solution of problems with mathematical model of the form of the radial time independent Schrödinger equation :

- Methods with constant coefficients. We call this category: **CATEGORY I**
- Methods with coefficients dependent on the frequency of the problem. We call this category: **CATEGORY II**

The new constructed methods obtained in Sects. 4.1 and 4.2 belong to the **CATEGORY II**.

In this category of methods (CATEGORY II), in order the methods to be possible to be applied to any problem, the coefficients of the methods must be defined. In order these coefficients to be defined, the frequency of the specific problem must be defined.

Therefore in our new obtained methods the frequency ω, (from which are depended the coefficients of new developed methods), must be defined. Defining the frequency ω, we can determine the coefficients of the new produced methods. Therefore, it will be possible the new developed methods to be applied to any problem (see for example the formulae in Sects. 4.1, 4.2). In the case of the radial time independent Schrödinger equation the frequency ω (for $l = 0$) is given by :

$$\omega = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{39}$$

where $V(r)$ is the potential and E is the energy.

7.1 Woods-Saxon potential

In order to apply a finite difference method to the numerical solution of the radial time independent Schrödinger equation, the definition of a potential is required. For our investigations on the numerical applications of this paper, the well known Woods-Saxon potential is used. The Woods-Saxon potential has the form :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{40}$$

with $q = \exp\left[\frac{r-X_0}{a}\right]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

In Fig. 9 we present the behavior of Woods-Saxon potential.

In the literature that are studies in which discrete approximations of several potentials are shown. These investigations are based on the idea that some potentials (like Woods-Saxon potential) have some critical points, the knowledge of which give us the opportunity to have a very good picture of the potential. Based on the investigations presented in [111,126] and [87] we can define the discrete approximation of the the Woods-Saxon potential. Via this approximation we can define the parameter ω.

The above mentioned study leads us to the following values of the parameter ω (see for details [126] and [87]):

$$\phi = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{41}$$

For example, in the point of the integration region $r = 6.5 - h$, the value of ω is equal to: $\sqrt{-37.5+E}$. So, $w = \omega\, h = \sqrt{-37.5+E}\, h$. In the point of the integration region $r = 6.5 - 3\,h$, the value of ω is equal to: $\sqrt{-50+E}$, etc.

7.2 Radial Schrödinger equation—the resonance problem

In this Section we study the numerical solution of the radial time independent Schrödinger equation (37), using as potential the above described Woods-Saxon potential (40). The purpose of this investigation is the examination of the efficiency of the new obtained methods.

7.3 The numerical solution

In the following we describe the process for the numerical approximation of the solution :

- Since the real interval of integration for the numerical solution of the radial time independent Schrödinger equation is equal to $[0, +\infty)$, it is important this infinite integration interval to be reduced a finite one. For the specific numerical example we choose the interval of integration $r \in [0, 15]$.
- Our study will take into account a rather large domain of energies, i.e., $E \in [1, 1000]$ within of which we will solve numerically the Eq. (37) The one-dimensional time independent Schrödinger equation reduces to

$$y''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) y(r) = 0 \tag{42}$$

for r greater than some value R, in the case of positive energies, $E = k^2$, since the potential decays faster than the term $\frac{l(l+1)}{r^2}$.
The above equation has 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 solution of Eq. (37) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} y(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{43}$$

where δ_l is the phase shift that may be calculated from the formula

$$\tan \delta_l = \frac{y(r_2)\, S(r_1) - y(r_1)\, S(r_2)}{y(r_1)\, C(r_1) - y(r_2)\, C(r_2)} \tag{44}$$

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. With the above technique we transferred the boundary-value problem into an initial-value problem. For this reason and in order to be possible the application of the new obtained six-step methods, we need the values of $y_j,\ j = 0(1)5$. From the initial condition, we obtain y_0. The values $y_i,\ i = 1(1)5$ are obtained by using high order Runge–Kutta–Nyström methods (see [119] and [120]). With these starting values, we evaluate at r_6 of the asymptotic region the phase shift δ_l.

– We will solve the known as resonance problem. For this problem we have positive energies. We can have two caees:
  1. Finding the phase-shift δ_l or
  2. Finding those E, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$.

  We actually solve the latter problem, known as *the resonance problem*.
– The boundary conditions for this problem are:

$$y(0) = 0,\ \ y(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{45}$$

We compute the approximate positive eigenenergies of the Woods-Saxon resonance problem using:

– The eighth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT8**.
– The tenth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT10**.
– The twelfth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT12**.
– The fourth algebraic order method of Chawla and Rao with minimal phase-lag [28], which is indicated as **Method MCR4**
– The exponentially-fitted method of Raptis and Allison [88], which is indicated as **Method MRA**
– The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [27], which is indicated as **Method MCR6**
– The classical form of the sixth algebraic order six-step method developed in Sect. 4, which is indicated as **Method NMCL6**.[2]
– The Phase-Fitted Method (Case 1) developed in [21], which is indicated as **Method NMPF1**
– The Phase-Fitted Method (Case 2) developed in [21], which is indicated as **Method NMPF2**

[2] With the term classical we mean the method of Sect. 4 with constant coefficients.

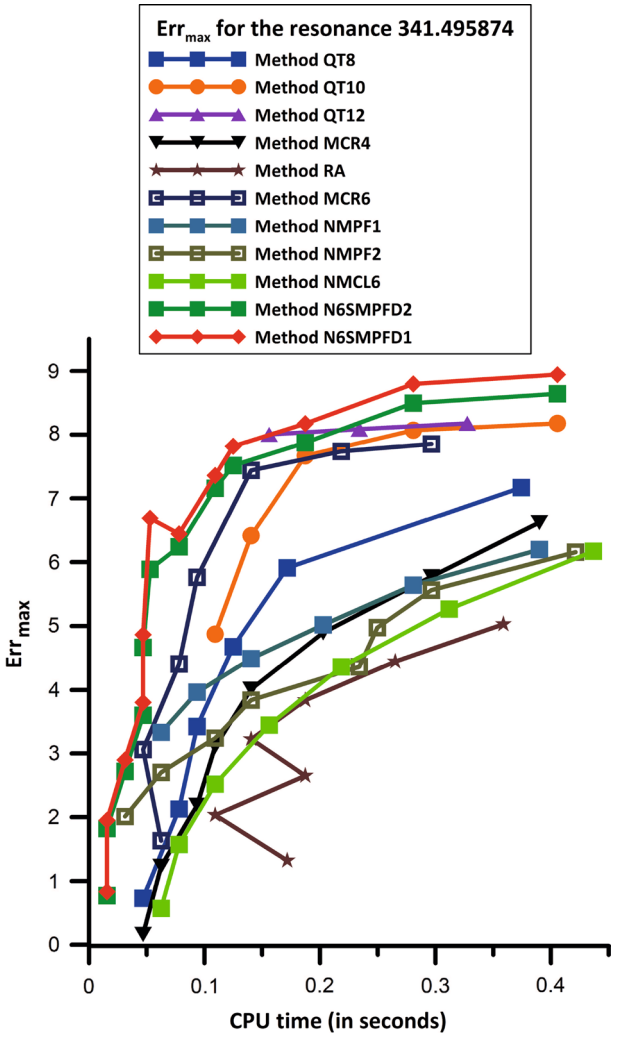

Fig. 10 Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (Digits) indicates that for this value of CPU, accuracy (Digits) is less than 0

– The New Linear Sixth Algebraic Order Six-Step Explicit Method developed in Sect. 4.1, which is indicated as **Method N6SMPFD1**
– The New Linear Sixth Algebraic Order Six-Step Explicit Method developed in Sect. 4.2, which is indicated as **Method N6SMPFD2**

The computed eigenenergies are compared with reference values. [3] In Figs. 10 and 11, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

[3] The reference values are computed using the well known two-step method of Chawla and Rao [27] with small step size for the integration.

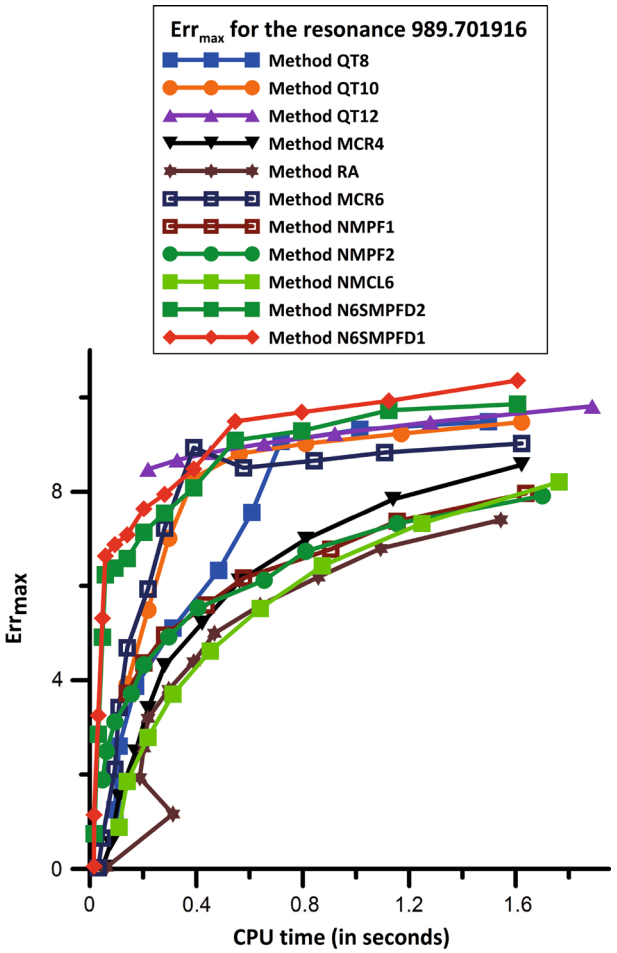

Fig. 11 Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (Digits) indicates that for this value of CPU, accuracy (Digits) is less than 0

$$Err = |E_{calculated} - E_{accurate}| \tag{46}$$

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of CPU time (in seconds). We note that the CPU time (in seconds) counts the computational cost for each method.

8 Conclusions

In the present paper we have developed and studied a family of explicit linear sixth algebraic order six-step methods with vanished phase-lag and its first derivative.

The study of the method consisted:

1. the construction of the method,
2. the calculation of the local truncation error,
3. the comparative error analysis.
4. the stability analysis of the new family of methods. We note here that the frequency of the test equation was different from the frequency of the test equation for the phase-lag analysis of the methods.
5. The application of the new family of linear six-step sixth algebraic order methods to the resonance problem of the radial time independent Schrödinger equation.

The computational results give us the following conclusions:

1. The classical form of the sixth algebraic order six-step method developed in Sect. 4, which is indicated as **Method NMCL6** has approximately the same efficiency than the exponentially-fitted method of Raptis and Allison [88], which is indicated as **Method MRA**.
2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [15], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [28], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [27], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.
3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [15], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [15], which is indicated as **Method QT10**
4. The Phase-Fitted Method (Case 1) developed in [21], which is indicated as **Method NMPF1** is more efficient than the classical form of the sixth algebraic order six-step method developed in Sect. 4, which is indicated as **Method NMCL6**, the exponentially-fitted method of Raptis and Allison [88] and the Phase-Fitted Method (Case 2) developed in [21], which is indicated as **Method NMPF2**
5. The New Linear Sixth Algebraic Order Six-Step Explicit Method developed in Sect. 4.2, which is indicated as **Method N6SMPFD2** has generally better behavior that all the above methods
6. The New Linear Sixth Algebraic Order Six-Step Explicit Method developed in Sect. 4.1, which is indicated as **Method N6SMPFD1** is the most efficient one

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

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