J Math Chem (2014) 52:1895–1920
DOI 10.1007/s10910-014-0354-9

ORIGINAL PAPER

An explicit linear six-step method with vanished phase-lag and its first derivative

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Received: 25 March 2014 / Accepted: 31 March 2014 / Published online: 3 May 2014

Abstract An explicit linear sixth algebraic order six-step method with vanished phase-lag and its first derivative is constructed in this paper. We will study the method theoretically and computationally. Theoretical investigation contains the building of the method, the calculation of the local truncation error, the comparative error analysis of the new method with the method with constant coefficients and the stability analysis of the new method using scalar test equation with different frequency than the frequency of the scalar test equation used for the development of the method. Computational investigation contains the application of the new obtained linear six-step method to the resonance problem of the radial time independent Schrödinger equation. The theoretical and computational study lead us to the summary that the new proposed linear scheme is computationally and theoretically more efficient than other well known methods for the numerical solution of the Schrödinger equation and related periodic initial or boundary value problems.

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

Mathematics Subject Classification: 65L05

1 Introduction

The approximate solution of special second-order periodic initial or boundary value problems is studied in this paper. The mathematical model of the previously mentioned problems can be written in the form

$$q''(x) = f(x, q), \quad q(x_0) = q_0 \ \ and \ \ q'(x_0) = q'_0. \tag{1}$$

The main characteristic of the above mentioned mathematical models is that are systems of second order ordinary differential equations in which the derivative q' does not appear explicitly see for more details [1–121] and references therein).

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

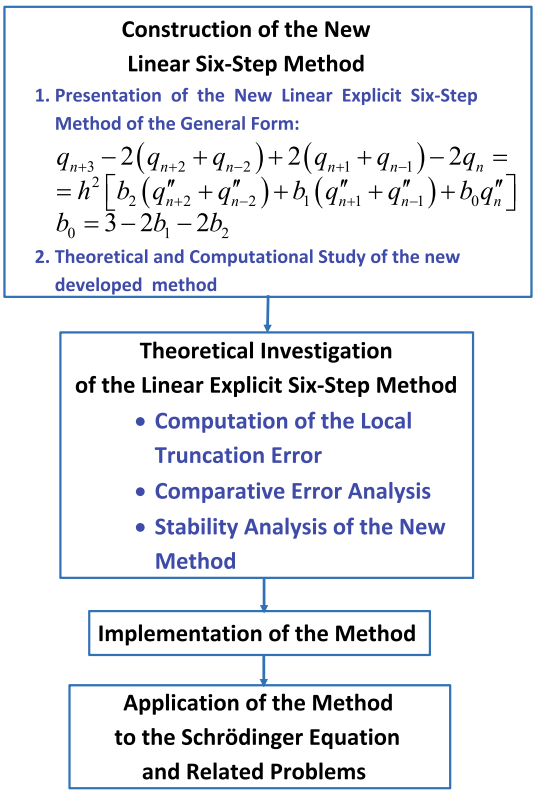

Fig. 1 Flowchart of the formulation of the present paper

A bibliography on the aims, scope and research of this paper is presented in Sect. 2. Theoretical results on the Phase-lag analysis of the Symmetric Multistep Methods are described in Sect. 3. The construction of the new Linear Explicit Six-Step Method is studied in Sect. 4. The Comparative Error Analysis is investigated in Sect. 5. The Stability Analysis using scalar test equation with different frequency than the frequency of the scalar test equation used for phase-lag analysis and construction of the method is presented in Sect. 6. Finally, in Sect. 7 we present the computational results obtained using the resonance problem of the radial time independent Schrödinger equation and the new proposed method together with several well known numerical methods. Concluding remarks on the efficiency of the methods used in this comparison are also finally analyzed in the same section.

2 Bibliography relevant on the subject of the paper

The last decades much research has been done on the numerical solution of the one-dimensional time independent Schrödinger equation and on the approximate solution of related periodic initial or boundary-value problems.

The categories of the finite difference methods which developed during these decades are presented in Fig. 2. The development of efficient, fast and reliable algorithms was the aim and scope of this research (see for example [1–114]).

Indicative bibliography on the above mentioned research 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.
- 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].

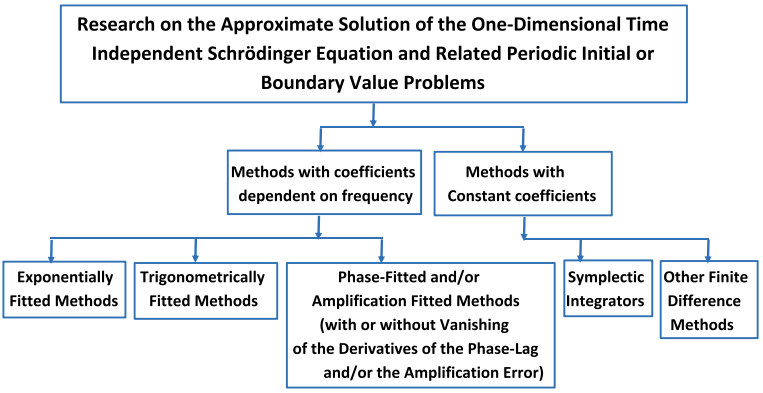

Fig. 2 Categories of the finite difference methods developed the last decades

– Nonlinear methods have been studied in [108] and [109]
– Review papers have been presented in [110–115]
– Special issues and Symposia in International Conferences have been developed on this subject (see [32,33])

3 Study of the phase-lag for the symmetric multistep finite difference methods

Consider the approximate solution of the periodic initial value problem (1).

Consider also that for this numerical approximation the multistep methods given by:

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

is used.

We note that for the above mentioned family of methods (2), the m steps can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)m-1$, where $|a_0| + |b_0| \neq 0$.

Remark 1 If $b_m = 0$ the method is explicit, otherwise it is implicit.

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

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

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

$$q'' = -\omega^2 q \tag{3}$$

a difference equation of the form

$$\sum_{i=1}^{k} A_i(v) \, (q_{n+i} + q_{n-i}) + A_0(v) \, q_n = 0 \tag{4}$$

is obtained. We note that in (4):

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

The characteristic equation associated with (4) is given by

$$\sum_{i=1}^{k} A_i(v)(\lambda^i + \lambda^{-i}) + A_0(v) = 0 \tag{5}$$

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

Definition 1 A symmetric $2k$-step method with characteristic equation given by (5) is said to have an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots $\lambda_i, i = 1(1)2k$ of Eq. (5) satisfy:

$$\lambda_1 = e^{i\theta(v)},\ \lambda_2 = e^{-i\theta(v)},\ \textit{and}\ |\lambda_i| \leq 1,\ i = 3(1)2k \tag{6}$$

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

Theorem 1 [24] *The symmetric $2k$-step method with characteristic equation given by (5) has phase-lag order q and phase-lag constant c given by:*

$$-cv^{q+2} + O(v^{q+4}) = \frac{2\sum_{j=1}^{k} A_j(v)\cos(jv) + A_0(v)}{2\sum_{j=1}^{k} j^2 A_j(v)} \tag{7}$$

Based on the above formula, we can produce a direct algorithm for the computation of the phase-lag of any symmetric $2k$- step method.

Remark 3 For the method to be developed in this paper, the symmetric six-step method has phase-lag order q and phase-lag constant c given by:

$$\begin{aligned} &-cv^{q+2} + O\left(v^{q+4}\right) \\ &\quad = \frac{2\,A_3(v)\,\cos(3v) + 2\,A_2(v)\,\cos(2v) + 2\,A_1(v)\,\cos(v) + A_0(v)}{18\,A_3(v) + 8\,A_2(v) + 2\,A_1(v)} \end{aligned} \tag{8}$$

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

We begin our study from the following explicit symmetric $2m$-step finite difference method:

$$\begin{aligned} &q_{n+m} + \sum_{i=0}^{m-1} c_i\ (q_{n+i} + q_{n-i}) + q_{n-m} \\ &\quad = h^2 \sum_{i=1}^{m-1} b_i\ \left[f(x_{n+i}, q_{n+i}) + f(x_{n-i}, q_{n-i})\right] b_0\ f(x_n, q_n) \end{aligned} \tag{9}$$

We investigate the specific case the above form (9) of $m = 3$.

As a result of the above study, we arrive to the following form of the explicit symmetric six-step finite difference methods:

$$\begin{aligned} &q_{n+3} + c_2\ (q_{n+2} + q_{n-2}) + c_1\ (q_{n+1} + q_{n-1}) + c_0\, q_n + q_{n-3} \\ &\quad = h^2\left[b_2\ (f_{n+2} + f_{n-2}) + b_1\ (f_{n+1} + f_{n-1}) + b_0\ f_n\right] \end{aligned} \tag{10}$$

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

Now we define the scheme which we will study. This is the above mentioned linear explicit symmetric six-step finite difference method with

$$c_2 = -2,\ c_1 = 2,\ c_0 = -2,\ b_0 = 3 - 2\,b_1 - 2\,b_2 \tag{11}$$

Demanding the above linear explicit symmetric six-step finite difference method (10) with coefficients given by (11) to have the phase-lag and its first derivative vanished, the following system of equations is produced:

$$\text{Phase} - \text{Lag(PL)} = \frac{T_0}{2\,v^2\,b_1 + 8\,v^2\,b_2 + 6} = 0$$
$$\text{First Derivative of PL} = \frac{T_1}{\left(v^2 b_1 + 4\,v^2 b_2 + 3\right)^2} = 0$$

where $T_i,\ i = 1,\ 2$ are given by

$$\begin{aligned}
T_0 &= 2\,\cos(3\,v) + 2\,\left(v^2 b_2 - 2\right)\cos(2\,v) + 2\,\left(v^2 b_1 + 2\right)\cos(v)\\
&\quad -2 + v^2\,(-2\,b_1 - 2\,b_2 + 3)\\
T_1 &= 4\,\sin(v)\cos(v)\,v^4 b_1 b_2 + 16\,\sin(v)\cos(v)\,v^4 {b_2}^2\\
&\quad + \sin(v)\,v^4 {b_1}^2 + 4\,\sin(v)\,v^4 b_1 b_2 + 12\,(\cos(v))^2\sin(v)\,v^2 b_1\\
&\quad + 48\,(\cos(v))^2\sin(v)\,v^2 b_2 - 8\,\sin(v)\cos(v)\,v^2 b_1 - 20\,\sin(v)\cos(v)\,v^2 b_2\\
&\quad + 8\,(\cos(v))^3\,v\,b_1 + 32\,(\cos(v))^3\,v\,b_2 + 2\,\sin(v)\,v^2 b_1 - 4\,\sin(v)\,v^2 b_2\\
&\quad - 8\,(\cos(v))^2\,v\,b_1 - 44\,(\cos(v))^2\,v\,b_2\\
&\quad + 36\,\sin(v)\,(\cos(v))^2 - 8\,v\,b_1\cos(v)\\
&\quad - 8\,\cos(v)\,v\,b_2 - 24\,\sin(v)\cos(v) + 8\,v\,b_1 + 20\,v\,b_2 - 3\,\sin(v) - 9\,v
\end{aligned}$$

Solving the above system of equations, we obtain the coefficients of the new linear explicit six-step method:

$$\begin{aligned}
b_1 &= \frac{T_2}{4\,\cos(v)\,v^3 - v^3\cos(2\,v) - 3\,v^3}\\
b_2 &= \frac{T_3}{5\,v^3\sin(v) + v^3\sin(3\,v) - 4\,v^3\sin(2\,v)}
\end{aligned} \tag{12}$$

where $T_i,\ i = 5(1)10$ are given by:

$$\begin{aligned}
T_2 &= 6\,\cos(v)\,v^3 - 12\,\cos(v)\,v + 7\,v\,\cos(2\,v)\\
&\quad - v\,\cos(4\,v) + 2\,\sin(4\,v) - 4\,\sin(3\,v)\\
&\quad + 2\,\sin(2\,v) + 6\,v\\
T_3 &= -12\,v\,\sin(2\,v) - 2\,v\,\sin(4\,v) + 3\,v^3\sin(v)\\
&\quad + 8\,v\,\sin(v) + 8\,v\,\sin(3\,v) - 8 - 2\,\cos(4\,v)\\
&\quad - 14\,\cos(2\,v) + 16\,\cos(v) + 8\,\cos(3\,v)
\end{aligned}$$

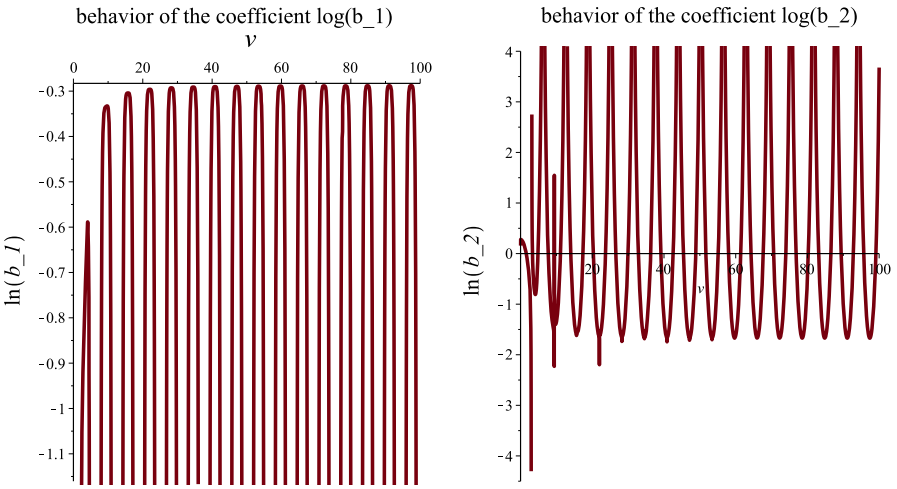

Fig. 3 Behavior of the coefficients of the new proposed method given by (12) for several values of $v = \omega h$

The following Taylor series expansions should be used in the cases that the formulae given by (12) are subject to heavy cancellations for some values of $|v|$:

$$
\begin{aligned}
b_1 \;=\; & -\frac{31}{30}+\frac{275}{504}v^2-\frac{6457}{75600}v^4+\frac{48119}{6652800}v^6 \\
& -\frac{19694243}{54486432000}v^8+\frac{7736587}{653837184000}v^{10}-\frac{30776419}{111152321280000}v^{12} \\
& +\frac{672850093}{141919283810304000}v^{14}-\frac{9357107237}{140500090972200960000}v^{16} \\
& +\frac{5782991749}{9232863121030348800000}v^{18}+\ldots \\
b_2 \;=\; & \frac{317}{240}-\frac{275}{2016}v^2+\frac{5203}{1209600}v^4-\frac{3833}{26611200}v^6 \\
& -\frac{2237189}{435891456000}v^8-\frac{1702639}{2615348736000}v^{10}-\frac{33561289}{508124897280000}v^{12} \\
& -\frac{3821843479}{567677135241216000}v^{14}-\frac{768195401381}{1124000727777607680000}v^{16} \\
& -\frac{17914211682931}{2585201673888497664000000}v^{18}+\ldots
\end{aligned}
\tag{13}
$$

The behavior of the coefficients is given in the following Fig. 3.

The new obtained method (10) (mentioned as $FourStepI$) with the coefficients given by (12)–(13) has a local truncation error which is given by:

$$
LTE_{Six\ Step\ New\ Linear} = \frac{275\,h^8}{4032}\left(q_n^{(8)}+2\,\omega^2\,q_n^{(6)}+\omega^4\,q_n^{(4)}\right)+O\left(h^{10}\right) \tag{14}
$$

5 Comparative error analysis

We continue the theoretical analysis of the method, studying the error of the new obtained linear six-step method and comparing this error with that of the linear six-step method with constant coefficients.

The investigation of the error will be focused on two methods:

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

Therefore, we will study the following methods:

5.1 The sixth algebraic order classical method [i.e. the method (10) with constant coefficients]

$$LTE_{CL} = \frac{275\,h^8}{4032}\,q_n^{(8)} + O\left(h^{10}\right) \tag{15}$$

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

$$LTE_{Six\ Step\ New\ Linear} = \frac{275\,h^8}{4032}\left(q_n^{(8)} + 2\,\omega^2\,q_n^{(6)} + \omega^4\,q_n^{(4)}\right) + O\left(h^{10}\right) \tag{16}$$

In order to study the error on the radial time independent Schrödinger equation, we follow the process mentioned below:

- The one-dimensional time independent Schrödinger equation can be written as:

$$q''(x) = f(x)\,q(x) \tag{17}$$

- We express the function $f(x)$ as mentioned below (see for more details at Ixaru and Rizea [87]):

$$f(x) = g(x) + G \tag{18}$$

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 analyze the Local Truncation Error Formulae (LTEF). In order to do this, we must substitute the derivatives $q_n^{(i)}$, $i = 2, 3, 4, \ldots$, with corresponding expression of the formula (18).

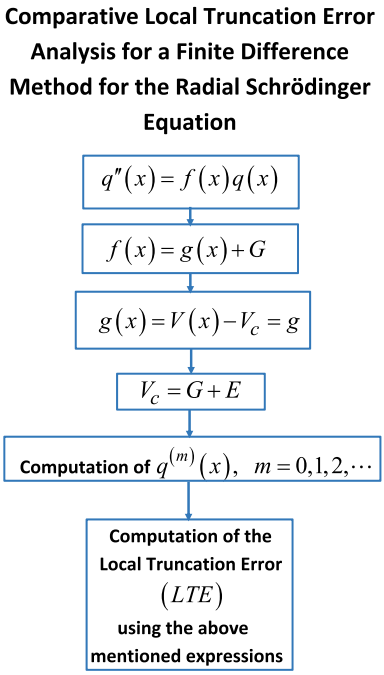

Fig. 4 Flowchart for the comparative error analysis

– Finally, the above mentioned (previous step) new expression of the derivatives are inserted into the LTEF. Therefore, the LTEF finally are expressed as polynomials of G.

The Flowchart of the Fig. 4 is used for the Local Truncation Error Analysis.

we compute the derivatives of the formulae of the Local Truncation Errors, based on the Eq. (18) and the procedure mentioned above:

$$
\begin{aligned}
q_n^{(2)} &= (V(x) - V_c + G)\, q(x) \\
q_n^{(3)} &= \left(\frac{d}{dx} g(x)\right) q(x) + (g(x) + G) \frac{d}{dx} q(x) \\
q_n^{(4)} &= \left(\frac{d^2}{dx^2} g(x)\right) q(x) + 2 \left(\frac{d}{dx} g(x)\right) \frac{d}{dx} q(x) \\
&\quad + (g(x) + G)^2 q(x) \\
q_n^{(5)} &= \left(\frac{d^3}{dx^3} g(x)\right) q(x) + 3 \left(\frac{d^2}{dx^2} g(x)\right) \frac{d}{dx} q(x) \\
&\quad + 4\,(g(x) + G)\, q(x) \frac{d}{dx} g(x) + (g(x) + G)^2 \frac{d}{dx} q(x) \\
q_n^{(6)} &= \left(\frac{d^4}{dx^4} g(x)\right) q(x) + 4 \left(\frac{d^3}{dx^3} g(x)\right) \frac{d}{dx} q(x)
\end{aligned}
$$

$$
\begin{aligned}
&+7\ (g(x)+G)\,q(x)\,\frac{d^2}{dx^2}g(x)+4\left(\frac{d}{dx}g(x)\right)^2 q(x)\\
&+6\ (g(x)+G)\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}g(x)\\
&+(g(x)+G)^3\,q(x)\\
q_n^{(7)} &= \left(\frac{d^5}{dx^5}g(x)\right)q(x)+5\left(\frac{d^4}{dx^4}g(x)\right)\frac{d}{dx}q(x)\\
&+11\ (g(x)+G)\,q(x)\,\frac{d^3}{dx^3}g(x)+15\left(\frac{d}{dx}g(x)\right)q(x)\,\frac{d^2}{dx^2}g(x)\\
&+13\ (g(x)+G)\left(\frac{d}{dx}q(x)\right)\frac{d^2}{dx^2}g(x)\\
&+10\left(\frac{d}{dx}g(x)\right)^2\frac{d}{dx}q(x)+9\ (g(x)+G)^2\,q(x)\,\frac{d}{dx}g(x)\\
&+(g(x)+G)^3\,\frac{d}{dx}q(x)\\
q_n^{(8)} &= \left(\frac{d^6}{dx^6}g(x)\right)q(x)+6\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}q(x)\\
&+16\ (g(x)+G)\,q(x)\,\frac{d^4}{dx^4}g(x)+26\left(\frac{d}{dx}g(x)\right)q(x)\,\frac{d^3}{dx^3}g(x)\\
&+24\ (g(x)+G)\left(\frac{d}{dx}q(x)\right)\frac{d^3}{dx^3}g(x)\\
&+15\left(\frac{d^2}{dx^2}g(x)\right)^2 q(x)+48\left(\frac{d}{dx}g(x)\right)\\
&\left(\frac{d}{dx}q(x)\right)\frac{d^2}{dx^2}g(x)+22\ (g(x)+G)^2\,q(x)\\
&\frac{d^2}{dx^2}g(x)+28\ (g(x)+G)\,q(x)\left(\frac{d}{dx}g(x)\right)^2\\
&+12\ (g(x)+G)^2\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}g(x)\\
&+(g(x)+G)^4\,q(x)\\
&\ldots
\end{aligned}
$$

The comparative error analysis, which is valid for any model of a problem which has the form of the Eq. (17), will be finished via the process mentioned below:

– The value of E within the Local Truncation Error analysis (via the parameters v and ω), is studied for two cases:

1. **First Case** : The Energy is close to the potential, i.e., $G = V_c - E \approx 0$. Therefore all the terms of the Local Truncation Error Formulae are vanished

except those which are the free terms of the polynomials in G. Consequently, the numerical methods are of comparable accuracy for these values of E. The explanation is that for these values of E all the terms the polynomials in G are equal to zero and only the free terms of the polynomials in G are not vanished. Tree 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 and the methods with vanished the phase-lag and its derivatives are of the same accuracy.

2. **Second Case** : $G \gg 0$ or $G \ll 0$. In this case the term $|G|$ is a large number.

– As final stage is the calculation of the asymptotic expansions of the Local Truncation Errors Formulae

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

5.3 Classical method

$$LTE_{CL} = h^8 \left(\frac{275}{4032} q(x)\ G^4 + \cdots \right) + O\left(h^{10}\right) \tag{19}$$

5.4 The method with vanished phase-lag and its first derivative produced in [50]

$$\begin{aligned} LTE_{Six\ Step\ New\ Linear} = h^8 \Bigg[& \left(\frac{275}{2016} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) \right. \\ & + \frac{275}{448} \left(\frac{d^2}{dx^2} g(x) \right) q(x) \\ & \left. + \frac{275}{4032} \left(g(x) \right)^2 q(x) \right) G^2 + \cdots \Bigg] + O\left(h^{10}\right) \end{aligned} \tag{20}$$

From the above equations 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 Method with Vanished Phase-lag and its First Derivative produced in this paper , the error increases as the second power of G.*

So, for the numerical solution of the time independent one-dimensional Schrödinger equation and related problems the Linear Six-Step Method developed in Sect. 4 with Vanished Phase-Lag and its First Derivative is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

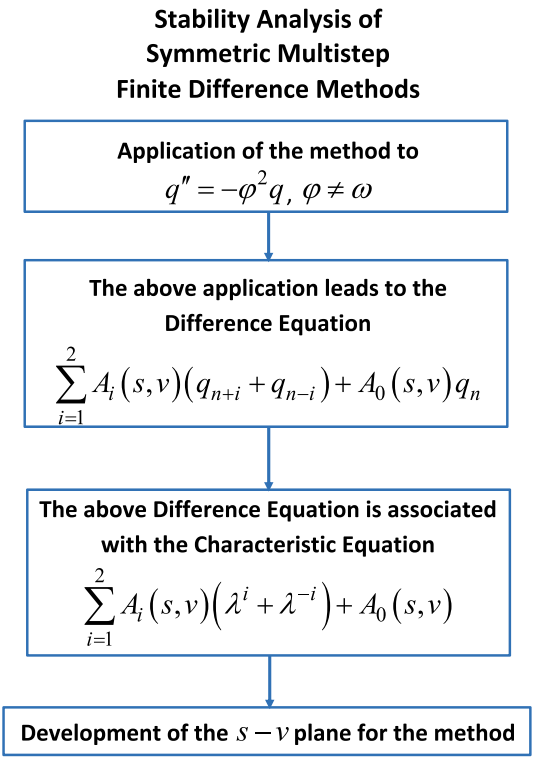

Fig. 5 Flowchart for the stability analysis of symmetric multistep finite difference methods

6 Stability analysis

The Flowchart of the Fig. 5, gives the procedure of the stability analysis for any of the new hybrid four-step explicit method is based on.

Our investigation is based on the above described procedure (see flowchart in Fig. 5). In order to analyze the stability of the new linear six-step symmetric method developed in Sect. 4, we apply it to the scalar test equation:

$$q'' = -\phi^2 q. \tag{21}$$

Then, the following difference equation is obtained:

$$\begin{aligned} &A_3(s,v)\ (q_{n+3} + q_{n-3}) + A_2(s,v)\ (q_{n+2} + q_{n-2}) \\ &+A_1(s,v)\ (q_{n+1} + q_{n-1}) + A_0(s,v)\ q_n = 0 \end{aligned} \tag{22}$$

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

$$A_3(s,v) = 1,\quad A_2(s,v) = -\frac{1}{4}\frac{T_4}{\left((\cos(v))^3 - (\cos(v))^2 - \cos(v) + 1\right) v^3}$$

$$A_1(s,v) = \frac{T_5}{\left((\cos(v))^2 - 2\cos(v) + 1\right) v^3}$$
$$A_0(s,v) = -\frac{1}{2}\frac{T_6}{\left((\cos(v))^3 - (\cos(v))^2 - \cos(v) + 1\right) v^3} \quad (23)$$

where

$$\begin{aligned}
T_4 &= 16(\cos(v))^4 vs^2 - 16(\cos(v))^3 \sin(v) s^2 + 8v^3(\cos(v))^3 \\
&\quad -16vs^2(\cos(v))^3 - 3\cos(v) v^3 s^2 \\
&\quad +16(\cos(v))^2 \sin(v) s^2 - 8(\cos(v))^2 v^3 \\
&\quad -16(\cos(v))^2 vs^2 - 3v^3 s^2 + 4\cos(v)\sin(v) s^2 \\
&\quad -8\cos(v) v^3 + 16\cos(v) vs^2 - 4\sin(v) s^2 + 8v^3 \\
T_5 &= 4(\cos(v))^4 vs^2 - 8(\cos(v))^3 \sin(v) s^2 - 3\cos(v) v^3 s^2 \\
&\quad +8(\cos(v))^2 \sin(v) s^2 + 2(\cos(v))^2 v^3 \\
&\quad -11(\cos(v))^2 vs^2 + 2\cos(v)\sin(v) s^2 - 4\cos(v) v^3 \\
&\quad +6\cos(v) vs^2 - 2\sin(v) s^2 + 2v^3 + vs^2 \\
T_6 &= 16(\cos(v))^5 vs^2 - 6(\cos(v))^3 v^3 s^2 - 32(\cos(v))^4 \sin(v) s^2 \\
&\quad -6(\cos(v))^2 v^3 s^2 + 16(\cos(v))^3 \sin(v) s^2 + 4v^3(\cos(v))^3 \\
&\quad -28vs^2(\cos(v))^3 - 3\cos(v) v^3 s^2 + 24(\cos(v))^2 \sin(v) s^2 \\
&\quad -4(\cos(v))^2 v^3 - 4(\cos(v))^2 vs^2 - 3v^3 s^2 - 4\cos(v)\sin(v) s^2 \\
&\quad -4\cos(v) v^3 + 12\cos(v) vs^2 - 4\sin(v) s^2 + 4v^3 + 4vs^2
\end{aligned}$$

Remark 4 It is important to note that the frequency of the scalar test Eq. (3), ω (which was used for the phase-lag analysis), is not equal with the frequency of the scalar test Eq. (21) (which was used for the stability analysis), ϕ, i.e. $\omega \neq \phi$.

We give the following definitions:

Definition 2 (*see* [14]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$[1] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $s = v$.

In Fig. 6 we present the $s - w$ plane for the method developed in this paper.

Remark 5 A shadowed region declares the $s - v$ area where the method is stable, while a white area declares the area where the method is unstable.

Remark 6 From the $s - v$ area one can chose several parts depending on mathematical model of the specific problem. The time independent Schrödinger equation belongs to a

[1] Where S is a set of distinct points.

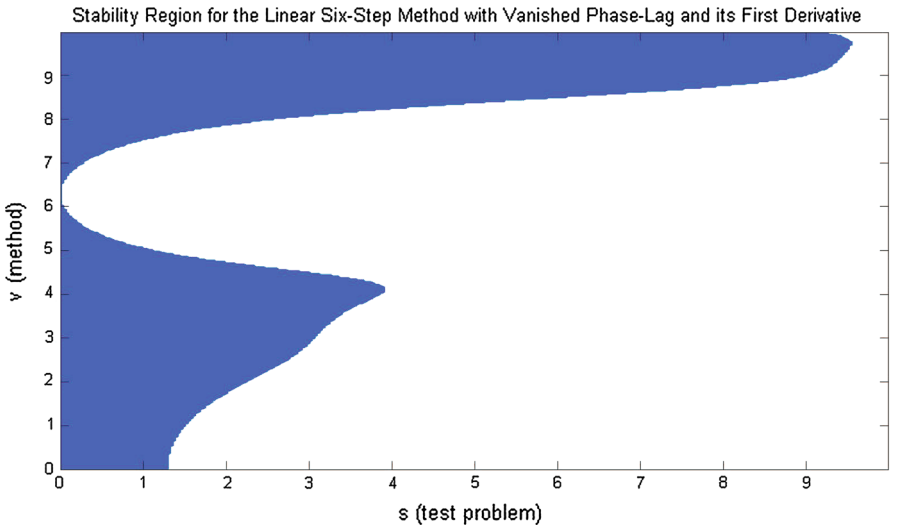

Fig. 6 $s - v$ Plane of the the new obtained method with vanished phase-lag and its first and second derivatives

category of mathematical models where it is appropriate to observe **the surroundings of the first diagonal of the $s - v$ plane**. In these categories of mathematical models in order to apply the new obtained methods, the frequency of the phase fitting must be equal to the frequency of the scalar test equation.

For the time independent Schrödinger equation and due to the above mentioned remark, the frequency of the scalar test equation is equal with the frequency of phase fitting. Therefore, we study 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 method produced in Sect. 4 are equal to: $(0, 9.9)$.

The above investigation leads to the following theorem:

Theorem 3 *The method produce in Sect. 4:*

- *is of sixth algebraic order,*
- *has the phase-lag and its first derivative equal to zero*
- *has an interval of periodicity equals to:* $(0, 9.9)$ *when the frequency of the scalar test equation is equal with the frequency of phase fitting*

7 Numerical results

The examination of the effectiveness of the new obtained method is the scope of this section. In order to achieve the above, we will apply the new constructed sixth algebraic order explicit linear six-step method on the numerical approximation of the radial time-independent Schrödinger equation.

The model of the radial time independent Schrödinger equation is given by (see [123–125] for details):

$$q''(r) = \left[l(l+1)/r^2 + V(r) - k^2 \right] q(r). \tag{24}$$

This model belongs to the special boundary value problems. The boundary conditions are given by:

$$q(0) = 0. \tag{25}$$

The second boundary condition, for large values of r, is determined using the physical characteristics of the specific problem.

Below we give some definitions of the functions, quantities and parameters for the above mathematical model (24):

- The function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(x) \to 0$ as $x \to \infty$,
- The quantity k^2 is a real number denoting *the energy*,
- The quantity l is a given integer representing the *angular momentum*,
- V is a given function which denotes the *potential*.

As we have mentioned previously the finite difference methods for the numerical solution of problems of the form of the radial time independent Schrödinger equation, can be divided into two categories:

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

Our new obtained method belongs to the CATEGORY B. Therefore the frequency ω, from which are depended the coefficients of new constructed method, must be defined. The definition of the frequency ω is necessary in order to be possible the coefficients of the method to be determined and therefore in order the method to be possible to be applied to any problem (see for example the formulae in Sect. 4). This frequency ω for the case of the one-dimensional time independent Schrödinger equation is given by (for $l = 0$):

$$\omega = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{26}$$

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

7.1 Woods–Saxon potential

The application of any finite difference methods to the numerical approximation of the radial time independent Schrödinger equation requires the determination of a potential. For our computational purpose on the numerical applications of this paper, we will use the well known Woods–Saxon potential, which can be written as:

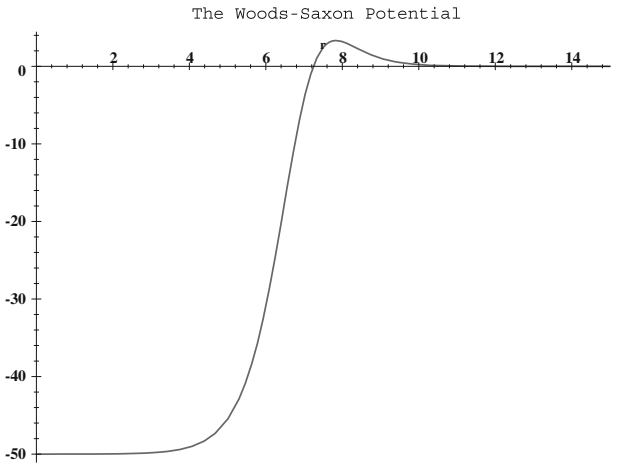

Fig. 7 The Woods–Saxon potential

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{27}$$

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

The behavior of Woods–Saxon potential is shown in Fig. 7.

There are investigations where present the discrete approximations of several potentials. These approximations are based on the computation of some critical points of a potential, the knowledge of which gives a very good picture of the potential. We have selected the the discrete approximation of the parameter ω, and therefore we use such critical points for the Woods–Saxon potential which are based on specific studies (see for details [113]).

Based on the studies mentioned above and for the purpose of our numerical computations, we choose ω as follows (see for details [126] and [87]):

$$\phi = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{28}$$

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

7.2 Radial Schrödinger equation: the resonance problem

The approximate solution of the one-dimensional time independent Schrödinger equation (24), with the Woods–Saxon potential (27), is investigated. The purpose of this study is the examination of the effectiveness of the new developed method.

7.3 Procedure for the numerical solution

The procedure for the approximate solution is based on the following algorithm:

- A basic part of the algorithm for the approximate solution of the one-dimensional time independent Schrödinger equation is the reduction of the infinite interval of integration (which is the true interval of integration) into a finite one. For our computational example we choose the integration interval $r \in [0, 15]$.
- We will investigate the case of Eq. (24) in a rather large domain of energies, i.e., $E \in [1, 1000]$.

In the case of positive energies, $E = k^2$, the potential decays faster than the term $\frac{l(l+1)}{r^2}$ and the radial time independent Schrödinger equation effectively reduces to

$$y''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) y(r) = 0 \tag{29}$$

for r greater than some value R.

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. (24) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} y(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{30}$$

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

$$\tan \delta_l = \frac{y(r_2) S(r_1) - y(r_1) S(r_2)}{y(r_1) C(r_1) - y(r_2) C(r_2)} \tag{31}$$

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 $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need $y_j,\ j = 0, (1)3$ before starting a four-step method. 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.

- In the case of positive energies, we have the so-called resonance problem. This problem consists either of finding the phase-shift δ_l or 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:

$$y(0) = 0,\ \ y(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{32}$$

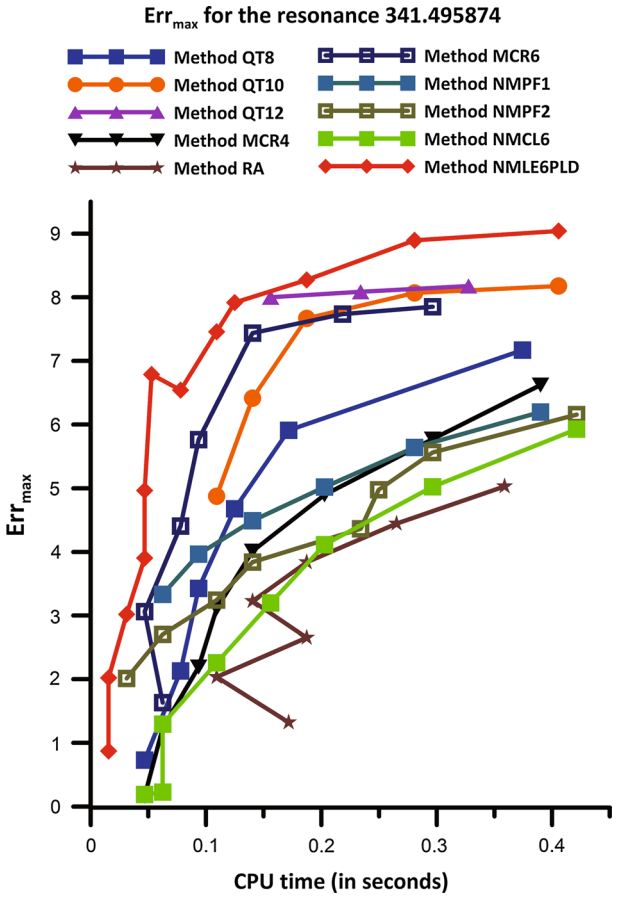

Fig. 8 Accuracy (Digits) for several values of CPU time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is <0

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**

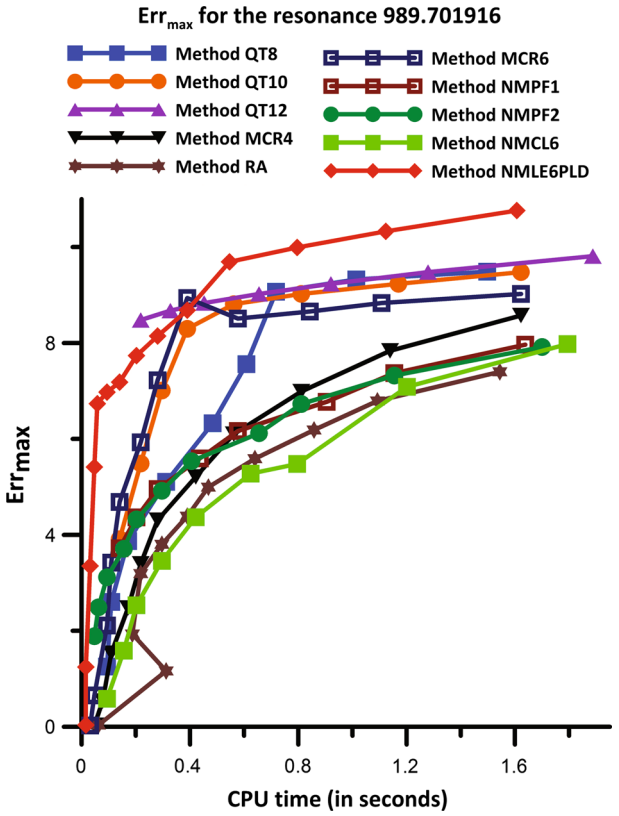

Fig. 9 Accuracy (Digits) for several values of CPU Time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is <0

- 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**
- The New Linear Sixth Algebraic Order Six-Step Explicit Method developed in Sect. 4, which is indicated as **Method NMLE6PLD**

The approximate calculated eigenenergies are compared with reference values.[3] In Figs. 8 and 9, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

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

[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.

$$Err = |E_{calculated} - E_{accurate}| \tag{33}$$

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

The development and the investigation for an explicit linear sixth algebraic order six-step method with vanished phase-lag and its first derivative is presented in this paper.

For this method we have described the following

1. Construction of the method which was based on
   - Maximization of the algebraic order of the linear six-step method
   - Vanishing of the phase-lag
   - Vanishing of the first derivative of the phase-lag
2. Theoretical Study of the methods which was based on
   - Comparative Local Truncation Error Analysis
   - Stability Analysis
3. Verification of the Theoretical Study via the numerical approximation of the resonance problem of the radial time independent Schrödinger equation and related problems.

The following conclusions are extracted from the numerical results presented above:

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 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 Obtained Linear Explicit Sixth Algebraic Order Six-Step Method with vanished phase-lag and its first derivative developed in Sect. 4, which is indicated as **Method NMLE6PLD** 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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