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ORIGINAL PAPER

A new explicit four-step method with vanished phase-lag and its first and second derivatives

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Abstract A study on the vanishing of the phase-lag and its first and second derivatives for a family of explicit four-step methods first introduced by Anastassi and Simos (J Comput Appl Math 236:3880–3889, 2012) is presented in this paper. The methods investigated in this paper belongs to the category of methods with frequency dependent coefficients. For these methods we will investigate the procedure of vanishing of the phase-lag and its first and second derivatives. For the new proposed methods we will define the local truncation error and we will study an local truncation error analysis. Finally we will compare the results of the error analysis with other known methods of the literature. We will study also the stability analysis of the new proposed method. We will apply the new produced methods on the resonance problem of the Schrödinger equation in order to investigate their efficiency.

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

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1 Introduction

The approximate solution of special second-order initial- or boundary-value problems of the form

$$p''(x) = f(x, p), \quad p(x_0) = p_0 \quad and \quad p'(x_0) = p'_0 \tag{1}$$

is investigated in this paper. The main characteristics of the mathematical models of these type of problems are:

- the mathematical models of the above mentioned problems are systems of second order ordinary differential equations in which the first derivative p' does not appear explicitly
- the solutions of the the mathematical models of the above mentioned papers are of periodical and/or oscillatory behavior.

For numerical schemes for these problems see [1–17,19,21–34,37–59,61–130] and references therein.

The structure of the present paper is the following.

- Presentation of the new explicit linear four-step method
- Investigation of the new presented method (definition of the coefficients of the method which are based on the requirement of elimination of the phase-lag and its first and second derivatives)
- Analysis of the method
  1. Computation of the local truncation error
  2. Comparative local truncation error analysis
  3. Stability analysis
- Implementation of the method
- Application of the method to the Schrödinger equation and related problems

The paper is constructed as follows:

Some bibliography on the subject of this paper is presented in Sect. 2. The phase-lag analysis of the symmetric multistep methods is developed in Sect. 3. In Sect. 4 we present the construction of the new linear explicit symmetric four-step method with eliminated phase-lag and its first and second derivatives. The comparative local truncation error analysis is investigated in Sect. 5. In Sect. 6 the stability analysis (with frequency of scalar test equation different than the frequency of scalar test equation for phase-lag analysis) is presented. Finally, the numerical experiments obtained by the application of the new developed method to the resonance problem of the radial time independent Schrödinger equation is presented in Sect. 7. Some comments on the comparative application of the new obtained method with other well know methods in the literature are also presented in the same section.

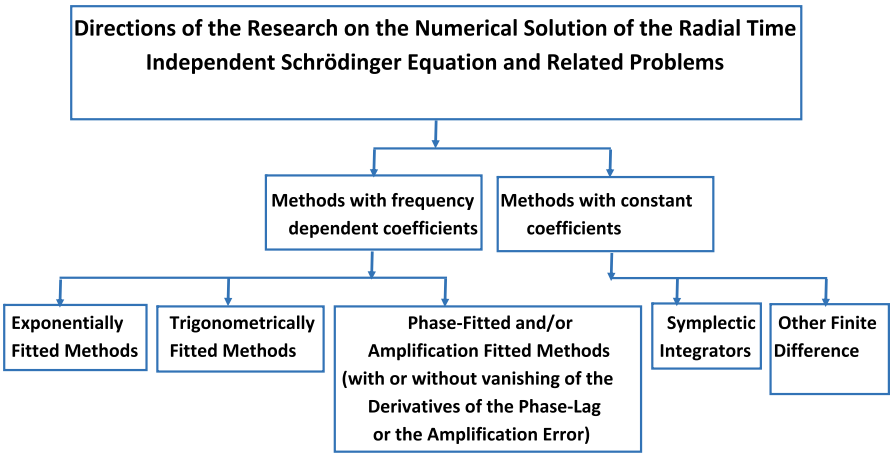

Fig. 1 The main categories of the methods developed the last decades

2 Literature related on the research subject of the paper

Extended research the last decades has been done on the numerical solution of the one-dimensional time independent Schrödinger equation and on the approximate solution of the related problems.

The main directions of this research are presented in Fig. 1. The aim and scope of this research was the construction of efficient, fast and reliable algorithms (see for example [1–17,19,21–34,37–59,61–130]).

Below we give some bibliography on this research:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta–Nyström type have been obtained in [5,28,32,33,47,57–59,86,119].
- In [4,6,24,85,87,121] 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 [1–3,10,11,13,14,30,31,48,51–56,68,69,71,75,82,88,90,102,106,107,109,111,112,128,129].
- Symplectic integrators are investigated in [23,25–27,38–46,70,73,74,91,96–100,103,104,108,110,117,118,120,123].
- Exponentially and trigonometrically multistep methods have been produced in [7,12,21,29,50,61–64,66,84,89,93–95,101,105,115,124,127,130].
- Nonlinear methods have been studied in [112] and [113]
- Review papers have been presented in [8,22,83,125,126]
- Special issues and Symposia in International Conferences have been developed on this subject (see [30,90]).

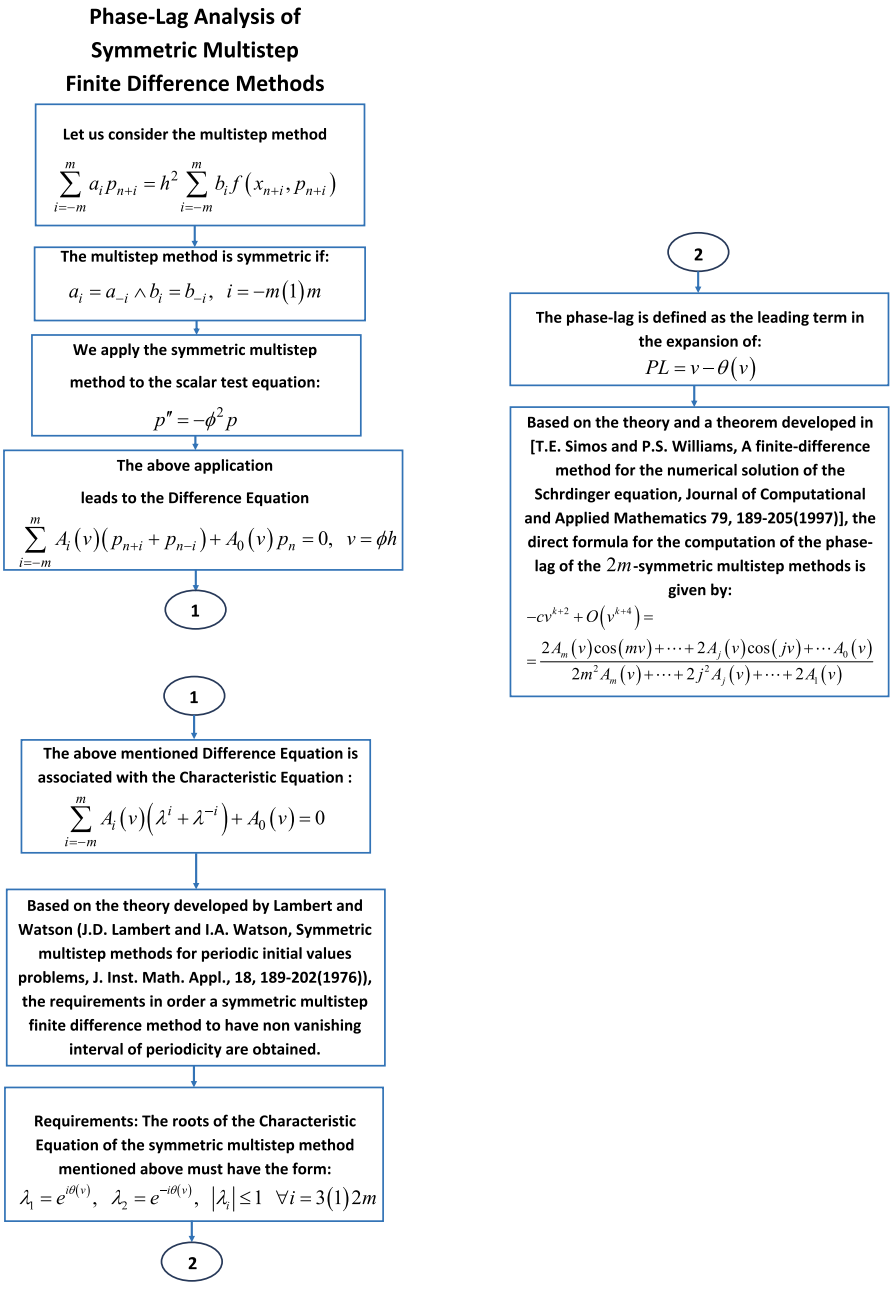

Fig. 2 Flowchart for the phase-lag analysis of $2m$-symmetric multistep methods. $v = \phi h$

3 Analysis of the phase-lag for symmetric multistep methods

The phase-lag analysis of the symmetric multistep methods is based on the flowchart of the Fig. 2.

Based on this flowchart we have the following algorithm for the phase-lag analysis of the symmetric $2m$-step methods

– Let us consider the $2m$—multistep methods of the form:

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

for the approximate solution of the periodic initial or boundary value problem of the form (1). In the above methods, m is the number of steps over the equally spaced intervals $\{x_i\}_{i=-m}^{m} \in [a, b]$, $h = |x_{i+1} - x_i|$, $i = -m + 1(1)m - 1$, where h is called stepsize of integration.

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

Remark 2 The operator

$$L(x) = \sum_{i=0}^{k} a_i \, u(x + ih) - h^2 \sum_{i=0}^{k} b_i \, u''(x + ih) \tag{3}$$

where $u \in C^2$, is associated with thr above mentioned $2m$—multistep method (2).

Definition 1 [9] We call that the multistep method (2) is of algebraic order q if its associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{q+1}$.

– We apply the symmetric $2m$-step method ($i = -m(1)m$), to the scalar test equation:

$$p'' = -\phi^2 \, p \tag{4}$$

– The following difference equation is obtained as a result of the above mentioned application:

$$\begin{aligned} &A_m(v) \, p_{n+m} + \cdots + A_1(v) \, p_{n+1} + A_0(v) \, p_n \\ &+ A_1(v) \, p_{n-1} + \cdots + A_m(v) \, p_{n-m} = 0 \end{aligned} \tag{5}$$

where $v = \phi \, h$, h is the stepsize of the integration and $A_j(v)$ $j = 0(1)m$ are polynomials of v.

– The obtained difference Eq. (5) is associated with the characteristic equation:

$$\begin{aligned} &A_m(v) \, \lambda^m + \cdots + A_1(v) \, \lambda + A_0(v) \\ &+ A_1(v) \, \lambda^{-1} + \cdots + A_m(v) \, \lambda^{-m} = 0 \end{aligned} \tag{6}$$

We have the definitions:

Definition 2 [34] 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:

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

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

Definition 3 [82,116] For any method corresponding to the characteristic Eq. (6) the phase-lag is defined as the leading term in the expansion of

$$t = v - \theta(v) \tag{8}$$

Then if the quantity $t = O(v^{k+1})$ *as* $v \to \infty$, the order of phase-lag is k.

Definition 4 [67] *Phase-fitted* is called a method with vanished phase-lag.

Remark 3 The phase-fitted methods are problem dependent methods, when the methods with minimal phase-lag are problem independent.

Theorem 1 [82] *The symmetric $2m$-step method with characteristic equation given by (6) has phase-lag order k and phase-lag constant c given by*

$$\begin{aligned} &-cv^{k+2} + O(v^{k+4}) \\ &= \frac{2A_m(v)\cos(mv) + \cdots + 2A_j(v)\cos(jv) + \cdots + A_0(v)}{2m^2 A_m(v) + \cdots + 2j^2 A_j(v) + \cdots + 2A_1(v)}. \end{aligned} \tag{9}$$

Remark 4 For the direct computation of any symmetric $2m$-step method we use the formula mentioned in above theorem.

In our case, the symmetric four-step method has phase-lag order k and phase-lag constant c given by:

$$-cv^{k+2} + O(v^{k+4}) = \frac{2A_2(v)\cos(2v) + 2A_1(v)\cos(v) + A_0(v)}{8A_2(v) + 2A_1(v)}. \tag{10}$$

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

Let us consider, without loss of generality, from the family of methods (2) the case $a_m = a_{-m} = 1$. Then the family of methods (2) can be written as:

$$p_{n+m} + \sum_{i=-m+1}^{m-1} a_i\, p_{n+i} + p_{n-m} = h^2 \sum_{i=-m+1}^{m-1} b_i\, f(x_{n+i}, p_{n+i}), \tag{11}$$

In the case of symmetric multistep methods we have $a_i = a_{-i}$ and $b_i = b_{-i}, i = 0(1)m - 1$.

Using the family of methods (11) with $m = 2$ we can obtain the explicit symmetric four-step methods introduced in [9]:

$$\begin{aligned} &p_{n+2} + a_1\ (p_{n+1} + p_{n-1}) + a_0\, p_n + p_{n-2} \\ &= h^2\left[b_1\ (f_{n+1} + f_{n-1}) + b_0\, f_n\right] \end{aligned} \tag{12}$$

where $f_i = p''(x_i, p_i)\,, i = n - 1(1)n + 1.$

4.1 The new method

We consider (12) with the following coefficient:

$$b_1 = \frac{311}{240}. \tag{13}$$

Applying the method (12) with the coefficient given by (13) to the scalar test Eq. (4), we obtain the difference Eq. (5) with $m = 2$ and:

$$A_2(v) = 1, \quad A_1(v) = a_1 + \frac{311}{240}\, v^2, \quad A_0(v) = a_0 + v^2\, b_0. \tag{14}$$

Requiring the above method to have the phase-lag and its first and second derivatives vanished, the following system of equations is obtained:

$$\text{Phase-Lag(PL)} = \frac{2\cos(2v) + 2\left(a_1 + \frac{311\, v^2}{240}\right)\cos(v) + v^2 b_0 + a_0}{8 + 2\,a_1 + \frac{311}{120}\, v^2} = 0$$

$$\begin{aligned} \text{First Derivative of PL} = &\frac{-4\sin(2v) + \frac{311\, v\cos(v)}{60} - 2\left(a_1 + \frac{311\, v^2}{240}\right)\sin(v) + 2\, v\, b_0}{8 + 2\,a_1 + \frac{311}{120}\, v^2} \\ &- \frac{311}{60}\, v\, \frac{2\cos(2v) + 2\left(a_1 + \frac{311\, v^2}{240}\right)\cos(v) + v^2\, b_0 + a_0}{\left(8 + 2\,a_1 + \frac{311\, v^2}{120}\right)^2} = 0 \end{aligned}$$

$$\begin{aligned} \text{Second Derivative of PL} = &\frac{-8\cos(2v) + \frac{311\cos(v)}{60} - \frac{311\, v\sin(v)}{30} - 2\left(a_1 + \frac{311\, v^2}{240}\right)\cos(v) + 2\, b_0}{8 + 2\,a_1 + \frac{311\, v^2}{120}} \\ &- \frac{311}{30}\, v\, \frac{-4\sin(2v) + \frac{311\, v\cos(v)}{60} - 2\left(a_1 + \frac{311\, v^2}{240}\right)\sin(v) + 2\, v\, b_0}{\left(8 + 2\,a_1 + \frac{311\, v^2}{120}\right)^2} \\ &+ \frac{96721}{1800}\, v^2\, \frac{2\cos(2v) + 2\left(a_1 + \frac{311\, v^2}{240}\right)\cos(v) + v^2 b_0 + a_0}{\left(8 + 2\,a_1 + \frac{311\, v^2}{120}\right)^3} \end{aligned}$$

$$-\frac{311}{60}\frac{2\cos(2v)+2\left(a_1+\frac{311v^2}{240}\right)\cos(v)+v^2b_0+a_0}{\left(8+2a_1+\frac{311v^2}{120}\right)^2}=0. \tag{15}$$

The coefficients of the new proposed method are obtained solving the above system of equations:

$$\begin{aligned}
a_0 &= \frac{T_0}{240\,v\cos(v)-240\,\sin(v)}\\
a_1 &= \frac{-311\,\cos(v)\,v^3-960\,\cos(2v)\,v-933\,\sin(v)\,v^2+480\,\sin(2v)}{240\,v\cos(v)-240\,\sin(v)}\\
b_0 &= \frac{311\,\cos(2v)\,v-240\,\sin(3v)+311\,\sin(2v)+720\,\sin(v)-933\,v}{240\,v\cos(v)-240\,\sin(v)}
\end{aligned} \tag{16}$$

where

$$\begin{aligned}
T_0 = {} & -311\,v^3\cos(2v)+240\,v^2\sin(3v)+933\,\sin(2v)\,v^2\\
& -720\,\sin(v)\,v^2+933\,v^3+720\,v\cos(3v)+720\,v\cos(v)\\
& -240\,\sin(3v)-720\,\sin(v)
\end{aligned}$$

The following Taylor series expansions should be used in the cases that the formulae given by (16) are subject to heavy cancellations for some values of $|v|$:

$$\begin{aligned}
a_0 = {} & -\frac{11}{10}-\frac{987\,v^2}{200}+\frac{4271\,v^4}{5250}\\
& +\frac{359519\,v^6}{7560000}-\frac{230600219\,v^8}{11642400000}+\frac{414047801\,v^{10}}{275184000000}\\
& -\frac{187742245463\,v^{12}}{2860537680000000}+\frac{3452695838071\,v^{14}}{1945165622400000000}\\
& -\frac{4421834645959223\,v^{16}}{11383109222284800000000}\\
& +\frac{28209192944339923\,v^{18}}{6146878980033792000000000}+\cdots\\
a_1 = {} & -\frac{9}{20}+\frac{987\,v^2}{400}-\frac{4271\,v^4}{10500}\\
& +\frac{2479\,v^6}{236250}-\frac{103429\,v^8}{363825000}\\
& -\frac{5617\,v^{10}}{4299750000}-\frac{35089391\,v^{12}}{178783605000000}\\
& -\frac{266161457\,v^{14}}{30393212850000000}-\frac{1560599262793\,v^{16}}{3557221631964000000000}
\end{aligned}$$

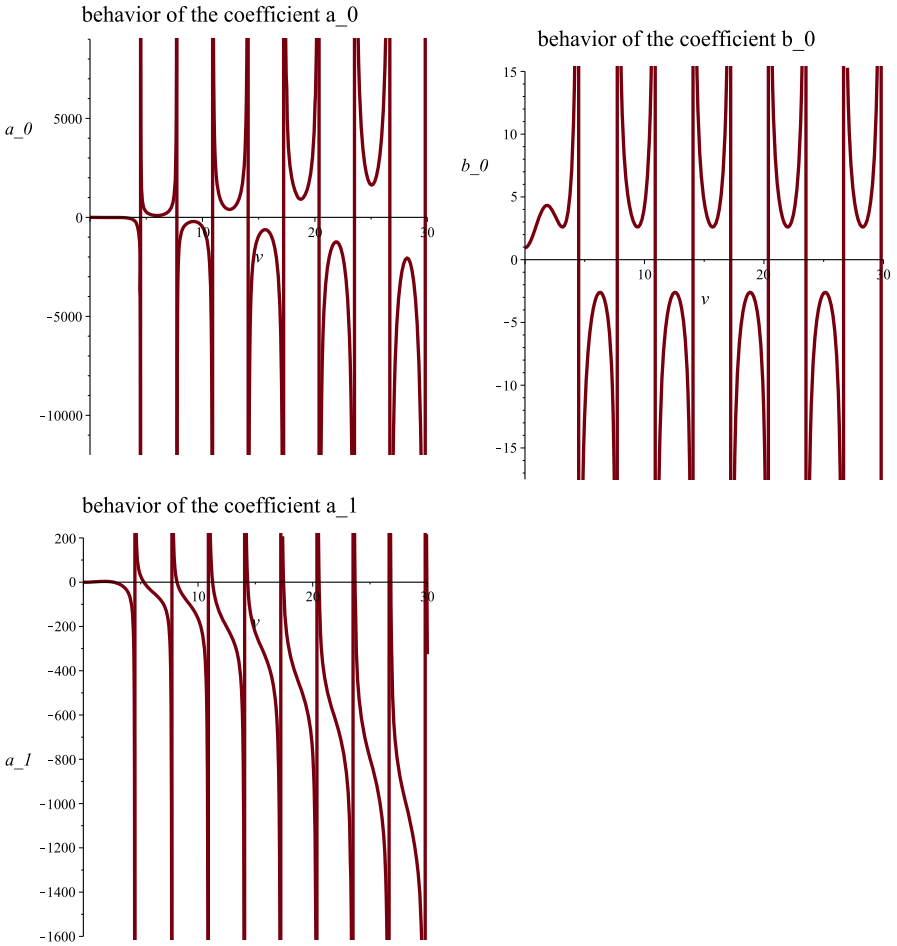

Fig. 3 Behavior of the coefficients of the new proposed method given by (16) for several values of $v = \phi h$

$$b_0 = \frac{23}{24} + \frac{987\,v^2}{400} - \frac{102881\,v^4}{168000} + \frac{45031\,v^6}{720000} - \frac{17661053\,v^8}{5174400000} + \frac{2228607707\,v^{10}}{18162144000000} - \frac{23030031811\,v^{12}}{7628100480000000} + \frac{25545357151\,v^{14}}{432259027200000000} - \frac{333812746110859\,v^{16}}{455324368891392000000000} + \frac{585466706807639\,v^{18}}{4097919320022528000000000} + \cdots - \frac{20847247620191\,v^{18}}{960449840630280000000000} + \cdots \tag{17}$$

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

The local truncation error of the new obtained method (12) (mentioned as *Expl FourStep*) with the coefficients given by (16)–(17) is given by:

$$LTE_{ExplFourStep} = \frac{329\,h^6}{4800}\left(p_n^{(6)} + 3\,\phi^2\,p_n^{(4)} + 3\,\phi^4\,p_n^{(2)} + \phi^6\,p_n\right) + O\left(h^8\right) \tag{18}$$

5 Comparative local truncation error analysis

We will investigate the following methods:

5.1 Classical method (i.e. the method (12) with constant coefficients of the case I)

$$LTE_{CL} = \frac{329\,h^6}{4800}\,p_n^{(6)} + O\left(h^8\right) \tag{19}$$

5.2 The method with vanished phase-lag produced in [8]

$$LTE_{MethAnasSim} = \frac{161\,h^6}{2400}\left(p_n^{(6)} + \phi^2\,p_n^{(4)}\right) + O\left(h^8\right) \tag{20}$$

5.3 The method with vanished phase-lag and its first derivative produced in [111]

$$LTE_{FourStep} = \frac{161\,h^6}{2400}\left(p_n^{(6)} + 2\,\phi^2\,p_n^{(4)} + \phi^4\,p_n^{(2)}\right) + O\left(h^8\right) \tag{21}$$

5.4 The new obtained method with vanished phase-lag and its first and second derivatives produced in Sect. 4

$$LTE_{ExplFourStep} = \frac{329\,h^6}{4800}\left(p_n^{(6)} + 3\,\phi^2\,p_n^{(4)} + 3\,\phi^4\,p_n^{(2)} + \phi^6\,p_n\right) + O\left(h^8\right). \tag{22}$$

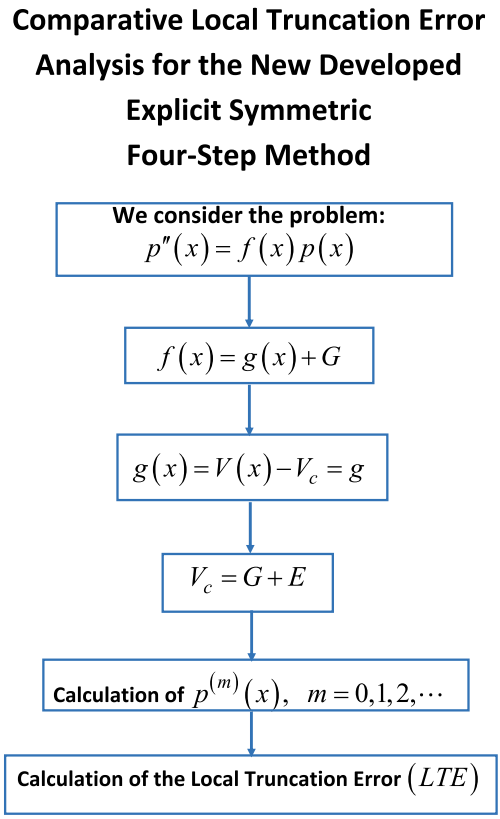

Fig. 4 Flowchart for the Local Truncation Error Analysis of $2m$-symmetric multistep methods

The comparative local truncation error analysis is based on the flowchart of the Fig. 4.

Based on the above mentioned flowchart we have the following procedure

- We consider the problem: $p''(x) = f(x)\,p(x)$.
- We calculate the derivatives which are presented in the formulae of the Local Truncation Errors:

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

$$
\begin{aligned}
p_n^{(6)} = & \left(\frac{d^4}{dx^4}g\left(x\right)\right)p\left(x\right) + 4\left(\frac{d^3}{dx^3}g\left(x\right)\right)\frac{d}{dx}p\left(x\right) \\
& + 7\left(g\left(x\right)+G\right)p\left(x\right)\frac{d^2}{dx^2}g\left(x\right) + 4\left(\frac{d}{dx}g\left(x\right)\right)^2 p\left(x\right) \\
& + 6\left(g\left(x\right)+G\right)\left(\frac{d}{dx}p\left(x\right)\right)\frac{d}{dx}g\left(x\right) \\
& + \left(g\left(x\right)+G\right)^3 p\left(x\right) \\
p_n^{(7)} = & \left(\frac{d^5}{dx^5}g\left(x\right)\right)p\left(x\right) + 5\left(\frac{d^4}{dx^4}g\left(x\right)\right)\frac{d}{dx}p\left(x\right) \\
& + 11\left(g\left(x\right)+G\right)p\left(x\right)\frac{d^3}{dx^3}g\left(x\right) + 15\left(\frac{d}{dx}g\left(x\right)\right)p\left(x\right) \\
& \times \frac{d^2}{dx^2}g\left(x\right) + 13\left(g\left(x\right)+G\right)\left(\frac{d}{dx}p\left(x\right)\right)\frac{d^2}{dx^2}g\left(x\right) \\
& + 10\left(\frac{d}{dx}g\left(x\right)\right)^2\frac{d}{dx}p\left(x\right) + 9\left(g\left(x\right)+G\right)^2 p\left(x\right) \\
& \times \frac{d}{dx}g\left(x\right) + \left(g\left(x\right)+G\right)^3\frac{d}{dx}p\left(x\right)
\end{aligned}
$$

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

– The above procedure (substitution of the derivatives in the Local Truncation Errors with the above mentioned formulae) leads to formulae of the Local Truncation Error which are dependent from the energy E.
– Two cases in terms of the value of E are investigated for the Local Truncation Error analysis :

1. The Energy is close to the potential, i.e., $G = V_c - E \approx 0$. In this case we consider only the free terms of the polynomials in G (since all the other terms are equal to 0—due to dependence on G). Therefore, the methods are of comparable accuracy (for the specific value of G, i.e. for $G = 0$). The reason is that in the case of $G = 0$ the the free terms of the polynomials in G are the same for the classical method and for the methods with vanished the phase-lag and its derivatives.
2. $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number.

– The asymptotic expansions of the Local Truncation Errors are finally determined.

The following asymptotic expansions of the Local Truncation Errors are obtained based on the analysis presented above :

5.5 Classical method

$$LTE_{CL} = h^6 \left(\frac{329}{4800} \, p\,(x) \; G^3 + \cdots \right) + O\left(h^8\right) \tag{23}$$

5.6 The method with vanished phase-lag produced in [9]

$$LTE_{MethAnasSim} = h^6 \left(\frac{161}{2400} \, g\,(x) \; p\,(x) \; G^2 + \cdots + \right) + O\left(h^8\right) \tag{24}$$

5.7 The method with vanished phase-lag and its first derivative produced in [111]

$$\begin{aligned} LTE_{FourStep} = h^6 \Bigg[& \left(\frac{161}{2400} \; (g\,(x))^2 \; p\,(x) \right. \\ & + \frac{161}{1200} \left(\frac{d}{dx} g\,(x) \right) \frac{d}{dx} y\,(x) + \frac{161}{480} \\ & \left. \times \left(\frac{d^2}{dx^2} g\,(x) \right) p\,(x) \right) G + \cdots \Bigg] + O\left(h^8\right) \end{aligned} \tag{25}$$

5.8 The new obtained method with vanished phase-lag and its first and second derivatives produced in Sect. 4

$$LTE_{ExplFourStep} = h^6 \left(\frac{329}{1200} \left(\frac{d^2}{dx^2} g\,(x) \right) p\,(x) \; G + \cdots \right) + O\left(h^8\right) \tag{26}$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Four-Step Explicit Method, the error increases as the third power of G. For the Four-Step Explicit Phase-Fitted Method developed in* [9]*, the error increases as the second power of G. For the Four-Step Explicit Method with Vanished Phase-lag and its First Derivative developed in* [111]*, the error increases as the first power of G. Finally, for Four-Step Explicit Method with Vanished Phase-lag and its First and Second Derivatives developed in Sect.* 4*, the error increases as the first power of G but with coefficient lower than the coefficient of the method developed in* [111]*. So, for the numerical solution of the time independent one-dimensional Schrödinger equation the New Obtained Method with Vanished Phase-Lag and its First and Second Derivatives is 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 is based on the flowchart of the Fig. 5.

Based on the above flowchart we have the following procedure in order to investigate the stability of the new obtained method.

– We apply the new constructed method to the scalar test equation:

$$p'' = -\omega^2 p. \tag{27}$$

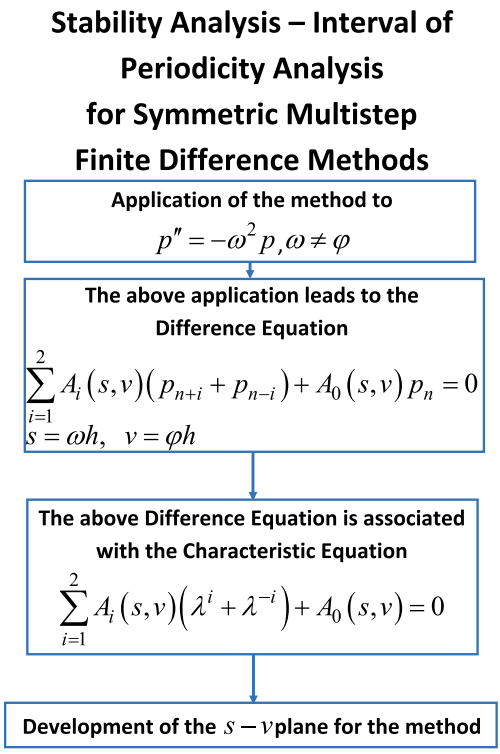

Fig. 5 Flowchart for the stability (interval of periodicity) analysis of 2 *m*-symmetric multistep methods

– The above application leads to the following difference equation:

$$A_2(s,v)\ (p_{n+2}+p_{n-2})+A_1(s,v)\ (p_{n+1}+p_{n-1})+A_0(s,v)\ p_n=0 \tag{28}$$

where

$$A_2(s,v)=1,\quad A_1(s,v)=-\frac{T_1}{240\,v\cos(v)-240\,\sin(v)}$$
$$A_0(s,v)=\frac{T_2}{120\,v\cos(v)-120\,\sin(v)} \tag{29}$$

where

$$\begin{aligned}T_1=&-311\cos(v)\,s^2v+311\cos(v)\,v^3+1920\,v\,(\cos(v))^2\\&+311\sin(v)\,s^2+933\sin(v)\,v^2-960\sin(v)\cos(v)-960\,v\\T_2=&-480\,(\cos(v))^2\sin(v)\,s^2+480\,(\cos(v))^2\sin(v)\,v^2\\&+311\,(\cos(v))^2\,s^2v-311\,(\cos(v))^2\,v^3\\&+1440\,v\,(\cos(v))^3+311\sin(v)\cos(v)\,s^2\\&+933\sin(v)\cos(v)\,v^2-480\sin(v)\,(\cos(v))^2\\&+480\sin(v)\,s^2-480\sin(v)\,v^2-622\,s^2v+622\,v^3\\&-720\,v\cos(v)-240\sin(v)\end{aligned}$$

and $s=\omega h$.

Remark 5 The frequency of the scalar test Eq. (27), ω, is not equal with the frequency of the scalar test Eq. (4), ϕ, i.e., $\omega\neq\phi$.

The following definitions are produced based on the analysis which has been presented in Sect. 2:

Definition 5 (See [34]) A method is called P-stable if its interval of periodicity is equal to $(0,\infty)$.

Definition 6 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., $s=v$.

The $s-w$ plane for the method obtained in this paper is presented in Fig. 6.

Remark 6 The method is stable on the shadowed area denoted on the $s-v$ region. The method is unstable on the white area on the $s-v$ region.

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

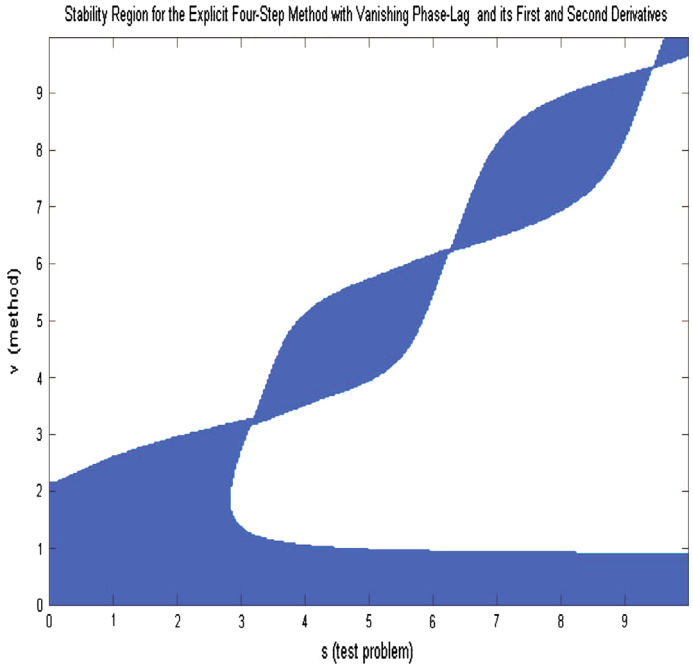

Fig. 6 $s-v$ plane of the the new obtained method with vanished phase-lag and its first and second derivatives

Remark 7 For the application of the methods on the mathematical models of some problems, it is interesting to observe *the surroundings of the first diagonal of the* $s-v$ *plane*. This is happened when we have problems with mathematical models where in order to apply the new obtained 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. We have many problems in sciences and engineering in this category (for example the time independent Schrödinger equation).

Based on the above remark, the case where 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 is now investigated , i.e. 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 the results that the interval of periodicity of the new explicit four-step method with minimal phase-lag and its first and second derivatives developed in Sect. 4 is equal to: $(0, 256)$.

The above research leads to the following theorem:

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

- *is of fourth algebraic order,*
- *has the phase-lag and its first and second derivatives equal to zero*

– *has an interval of periodicity equals to:* $(0, 256)$ *when 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.*

7 Numerical results

The effectiveness of the new obtained explicit linear four-step method is studied via the numerical solution of the radial time-independent Schrödinger equation (see for details [36]), which has a model of the form :

$$p''(r) = \left[l(l+1)/r^2 + V(r) - k^2 \right] p(r). \tag{30}$$

Remark 8 We note that the model (30) presents a boundary value problem which has the following boundary conditions :

$$y(0) = 0 \tag{31}$$

and another boundary condition, for large values of r, determined by physical properties of the specific problem.

For the above mathematical model (30) we have the following definitions of the functions, quantities and parameters :

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

Since the obtained method is of the class of frequency - problem dependent method, the value of parameter ϕ (see for example the notation after (4) and the formulae in Sect. 4) must be defined in order the new obtained method to be applied to any problem. The parameter ϕ for the case of the one-dimensional time independent Schrödinger equation is given by (for $l = 0$):

$$\phi = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{32}$$

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

7.1 Woods–Saxon potential

For our numerical experiments the well known Woods-Saxon potential is used. This can be written as :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{33}$$

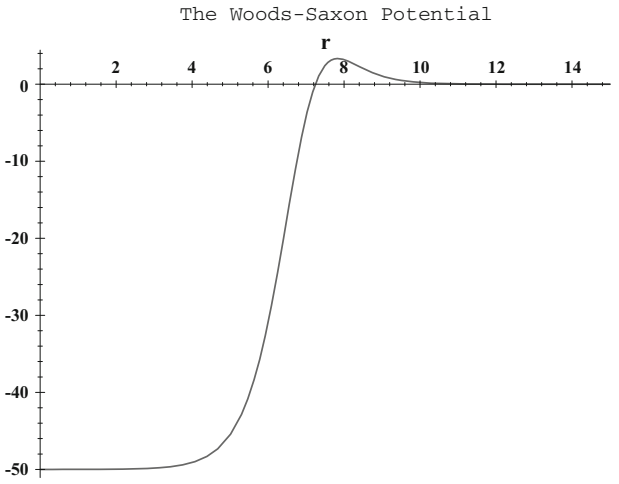

Fig. 7 The Woods–Saxon potential

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.

A methodology for the definition of the parameter ϕ into the new obtained method, contains for some potentials, such as the Woods–Saxon potential, the definition of some critical points (which are determined after study of the potentials—see for details [22]).

For the purpose of our experiments, it is appropriate to choose ϕ as follows (see for details [20] and [21]):

$$\phi = \begin{cases} \sqrt{-50+E}, & \text{for} \quad r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for} \quad r = 6.5-h \\ \sqrt{-25+E}, & \text{for} \quad r = 6.5 \\ \sqrt{-12.5+E}, & \text{for} \quad r = 6.5+h \\ \sqrt{E}, & \text{for} \quad r \in [6.5+2h, 15] \end{cases} \tag{34}$$

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

7.2 Radial Schrödinger equation: the resonance problem

We will investigate the approximate solution of the one-dimensional time independent Schrödinger equation (30) with the Woods–Saxon potential (33) in order to study the effectiveness of the new obtained method.

In order to proceed with the numerical solution of the above mentioned problem it is necessary to define a finite interval of integration. Therefore, we have to approximate the true (infinite) interval of integration. We determine for the specific integration the

interval $r \in [0, 15]$ for the purposes of our numerical tests. We consider Eq. (30) in a rather large domain of energies, i.e., $E \in [1, 1{,}000]$.

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

$$p''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) p(r) = 0 \tag{35}$$

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

$$\begin{aligned} p(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{36}$$

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

$$\tan \delta_l = \frac{y(r_2) S(r_1) - y(r_1) S(r_2)}{y(r_1) C(r_1) - y(r_2) C(r_2)} \tag{37}$$

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 $p_j,\ j = 0, (1)3$ before starting a four-step method. From the initial condition, we obtain p_0. The values $p_i,\ i = 1(1)3$ are obtained by using high order Runge–Kutta–Nyström methods(see [16] and [15]). With these starting values, we evaluate at r_2 of the asymptotic region the phase shift δ_l.

For 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 $E \in [1, 1{,}000]$, 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:

$$p(0) = 0,\ \ p(r) = \cos\left(\sqrt{E}r\right) \quad \text{for} \quad \text{large } r. \tag{38}$$

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

- The eighth order multi-step method developed by Quinlan and Tremaine [65], which is indicated as *Method QT8*.
- The tenth order multi-step method developed by Quinlan and Tremaine [65], which is indicated as *Method QT10*.
- The twelfth order multi-step method developed by Quinlan and Tremaine [65], which is indicated as *Method QT12*.

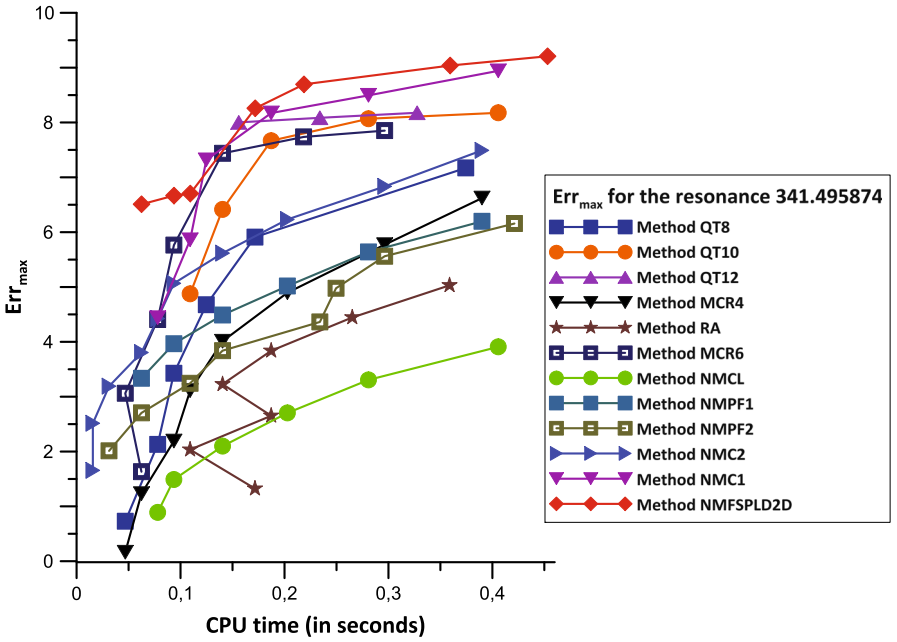

Fig. 8 Accuracy (digits) for several values of CPU Time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [13], which is indicated as *Method MCR4*
- The exponentially-fitted method of Raptis and Allison [66], which is indicated as *Method MRA*
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [14], which is indicated as *Method MCR6*
- The classical form of the fourth algebraic order four-step method developed in Sect. 4, which is indicated as *Method NMCL*.[2]
- The Phase-Fitted Method (Case 1) developed in [9], which is indicated as *Method NMPF1*
- The Phase-Fitted Method (Case 2) developed in [9], which is indicated as *Method NMPF2*
- The Explicit Symmetric Four-Step Method with Vanished Phase-Lag and its First Derivative (Case 2) developed in [111], which is indicated as *Method NMC2*
- The Explicit Symmetric Four-Step Method with Vanished Phase-Lag and its First Derivative (Case 1) developed in [111], which is indicated as *Method NMC1*
- The New Obtained Method developed in Sect. 4, which is indicated as *Method NMFSPLD2D*

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

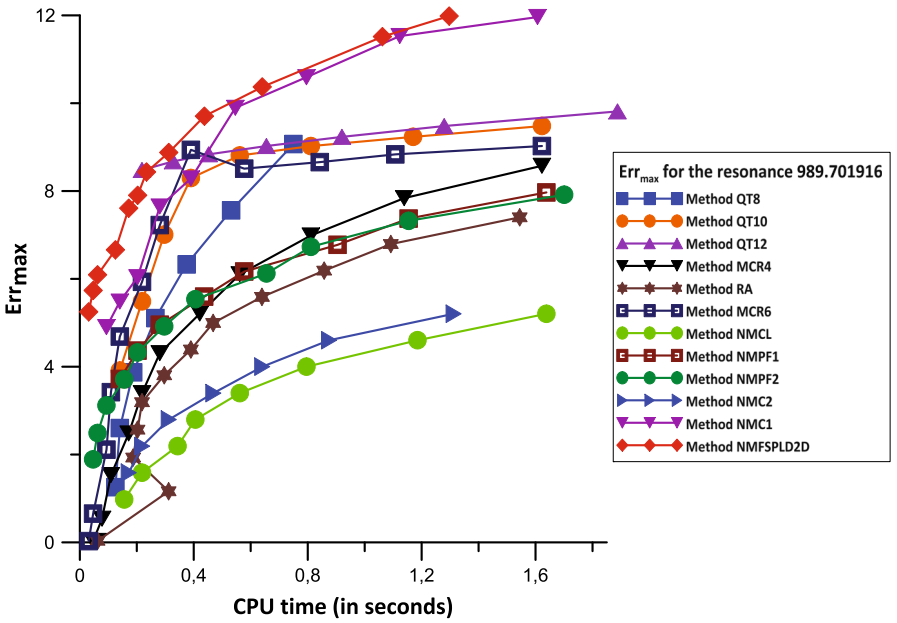

Fig. 9 Accuracy (digits) for several values of CPU Time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

The numerically 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

$$Err = |E_{calculated} - E_{accurate}| \tag{39}$$

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

A family of explicit four-step methods was investigated in this paper. The aim and scope of this research was the study of the vanishing of the phase-lag and its first and second derivatives for the above mentioned family of the explicit symmetric four-step methods. We presented for the specific obtained methods a comparative local truncation error and stability analysis. We studied also the effect of the elimination of the phase-lag and its first and second derivatives on the effectiveness of the produced method for the numerical solution of the one-dimensional Schrödinger equation and related problems.

[3] The reference values are computed using the well known two-step method of Chawla and Rao [14] with small step size for the integration.

From the results presented above, we can make the following remarks:

1. The classical form of the four-step method developed in Sect. 4, which is indicated as *Method NMCL* is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [13], which is indicated as *Method MCR4*. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [66], which is indicated as *Method MRA*.
2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [65], which is indicated as *Method QT10* is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [13], 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 [65], 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 [14], 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 [65], which is indicated as *Method QT12* is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [65], which is indicated as *Method QT10*
4. The Phase-Fitted Method (Case 1) developed in [9], which is indicated as *Method NMPF1* is more efficient than the classical form of the fourth algebraic order four-step method developed in Sect. 4, which is indicated as *Method NMCL*, the exponentially-fitted method of Raptis and Allison [66] and the Phase-Fitted Method (Case 2) developed in [9], which is indicated as *Method NMPF2*
5. The Explicit Symmetric Four-Step Method with Vanished Phase-Lag and its First Derivative (Case 2) developed in [111], which is indicated as *Method NMC2* is more efficient than the classical form of the fourth algebraic order four-step method developed in Sect. 4, which is indicated as *Method NMCL*, the exponentially-fitted method of Raptis and Allison [66] and the Phase-Fitted Method (Case 2) developed in [9], which is indicated as *Method NMPF2* and the Phase-Fitted Method (Case 1) developed in [9], which is indicated as *Method NMPF1*
6. The Explicit Symmetric Four-Step Method with Vanished Phase-Lag and its First Derivative (Case 1) developed in [111], which is indicated as *Method NMC21* is more efficient than all the above mentioned methods.
7. The New Obtained Method developed in Sect. 4, which is indicated as *Method NMFSPLD2D* 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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