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ORIGINAL PAPER

A high algebraic order multistage explicit four-step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives for the numerical solution of the Schrödinger equation

Ibraheem Alolyan[1] · **T. E. Simos**[1,2,3]

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Abstract A new Multistage high algebraic order four-step method is obtained in this paper. It is the first time in the literature that a method of this category is developed and has vanishing of the phase-lag and its first, second, third, fourth and fifth derivatives. We study this new method by investigating: (1) the development of the new method, i.e. the calculation of the coefficients of the method in order the phase-lag and its first, second, third, fourth and fifth derivatives of the phase-lag to be vanished, (2) the determination of the formula of the Local Truncation Error, (3) the comparative analysis of the Local Truncation Error (with this we mean the application of the new method and similar methods on a test problem and the analysis of their behavior), (4) the stability of the new method, by applying the new obtained method to a scalar test equation with frequency different than the frequency of the scalar test equation for the phase-lag analysis and by studying the results of this application i.e. by investigating the interval of periodicity of the new obtained method. We finally study the computational behavior the new

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T. E. Simos: Highly Cited Researcher (http://isihighlycited.com/), Active Member of the European Academy of Sciences and Arts. Active Member of the European Academy of Sciences. Corresponding Member of European Academy of Arts, Sciences and Humanities.

✉ T. E. Simos
tsimos.conf@gmail.com

1 Department of Mathematics, College of Sciences, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

2 Laboratory of Computational Sciences, Department of Informatics and Telecommunications, Faculty of Economy, Management and Informatics, University of Peloponnese, 221 00 Tripolis, Greece

3 10 Konitsis Street, Amfithea - Paleon Faliron, 175 64 Athens, Greece

developed method by using the application of the new method to the approximate solution of the resonance problem of the radial Schrödinger equation. We prove the effectiveness of the new obtained method by comparing it with (1) well known methods of the literature and (2) very recently obtained methods.

Keywords Schrödinger equation · Multistep methods · Multistage methods · Explicit methods · Interval of periodicity · P-stability · Phase-lag · Phase-fitted · Derivatives of the phase-lag

Mathematics Subject Classification 65L05

1 Introduction

A new multistage explicit four-step method of tenth algebraic order is studied in this paper. For this category of methods, we have the following novelties:

- The explicitly type of this category of methods. Consequently, these methods can be easily applied to any kind of problem (linear or non-linear)
- The new category of methods are of tenth algebraic order
- The new category of methods is based on an explicit four-step method with optimum choice of parameters
- For the first time in the literature for these kind of methods, the new obtained method has vanished the phase-lag and its first, second, third, fourth and fifth derivatives

The new category of methods are for the numerical solution of problems which can be written as:

$$q''(x) = f(x, q(x)). \tag{1}$$

We study the special case of the above problems with periodical and/or oscillating solutions.

Remark 1 These problems consist of a system of second order ordinary differential equations (ODEs) in which the first derivative q' does not appear explicitly. There are many problems of this kind in astronomy, astrophysics, quantum mechanics, quantum chemistry, quantum physics, celestial mechanics, electronics, physical chemistry, chemical physics etc (see for more details in [1–4]).

Remark 2 The aim and scope of our study is the construction of an efficient algorithm for the above mentioned problems. With the term efficient we mean an algorithm which is effective, fast and reliable for the numerical solution of these kind of problems. A lot of research has been done on this subject (see for example [5–119]).

The main classes of the finite difference methods which was developed as a result of the above described research are presented in Fig. 1. It is obvious that much research is done on this subject.

The category of methods which will study in the paper has the following characteristics:

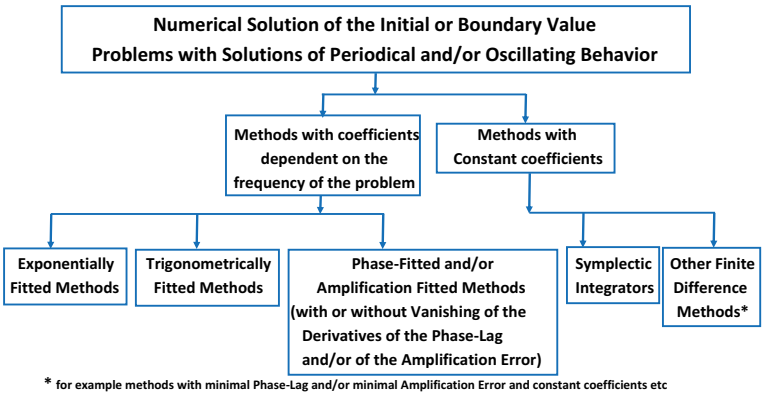

Fig. 1 Categories of finite difference methods developed in the last decades

1. The methods of this category have three stages (multistage method).
2. The basic idea for the development of the special methods of this category is the vanishing of the phase-lag and its derivatives. We will apply all the stages of the new method to the scalar test equation in order to define the phase-lag and its derivatives. It is the first time in the literature that for these kind of methods we will try to vanish the phase-lag and its first, second, third, fourth and fifth derivatives.
3. Our study will investigate how the vanish of the phase-lag and its derivatives affects the effectiveness of the new obtained method.
4. We will compare the finally developed methods with other well known methods of the literature and also with recently developed method in order to study its efficiency.

Remark 3 The area of application of the methods belonging to the category which will be investigated in this paper is

– problems with periodic solution and/or,
– problems with oscillating solution,
– problems with solutions containing functions cos and sin,
– problems with solutions containing combination of the the functions cos and sin.

A description of the recent literature on the subject of the paper is presented in Sect. 2. In Sect. 3, we present an analysis of the category of the methods which will be studied in this paper. The phase-lag analysis together with the direct formula for the computation of the phase-lag for the symmetric $2k$ methods is presented in Sect. 4. In Sect. 5, we present the construction of the new obtained explicit three stages four-step method. An investigation of the local truncation error analysis (LTE) of the new developed multistage method is presented in Sect. 6. In the same section, we will compare the asymptotic behavior of the LTE of the new method with the asymptotic behavior of the LTE of other methods when we apply them to a scalar test problem. In Sect. 7, we investigate the stability (interval of periodicity) analysis of the new method. Numerical results on the numerical solution of the resonance problem of the

one dimensional time independent Schrödinger type are presented in Sect. 8. Finally, in Sect. 9, we present some remarks and conclusions.

2 Recent literature on the subject of the paper

Some recent literature on the subject 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 [5–14].
- In [15–20], 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 [25–61].
- Symplectic integrators are investigated in [62–91].
- Exponentially and trigonometrically multistep methods have been produced in [92–112].
- Nonlinear methods have been studied in [113] and [114]
- Review papers have been presented in [115–119]
- Special issues and Symposia in International Conferences have been developed on this subject (see [120–123])

3 Analysis of the new three-stage four-step method

The analysis of new three-stage four-step method is presented in Fig. 2.

The aim and scope of the above mentioned analysis are:

- The computation of the coefficients a_0, a_j, $j = 2(1)4$ of the new three stage method in order to achieve
  1. the highest possible algebraic order,
  2. the vanishing of the phase-lag,
  3. the vanishing of the first derivative of the phase-lag,
  4. the vanishing of the second derivative of the phase-lag,
  5. the vanishing of the third derivative of the phase-lag,
  6. the vanishing of the fourth derivative of the phase-lag,
  7. the vanishing of the fifth derivative of the phase-lag,
- The investigation of the obtained local truncation error. We will also compare the asymptotic behavior of the produced local truncation error of the new four-step method with the asymptotic behavior of other methods of the same form in the case of a scalar test problem.
- The investigation of the stability of the new method. The scalar test equation which will be used for this study has frequency different than the frequency of the scalar test equation used for the phase-lag analysis.
- The investigation of the effectiveness of the new four-step method using the resonance problem of the one-dimensional time independent Schrödinger equation.

Remark 4 It is the first time in the literature that for this kind of methods we achieve the vanishing of the phase-lag and its first, second, third, fourth and fifth derivatives.

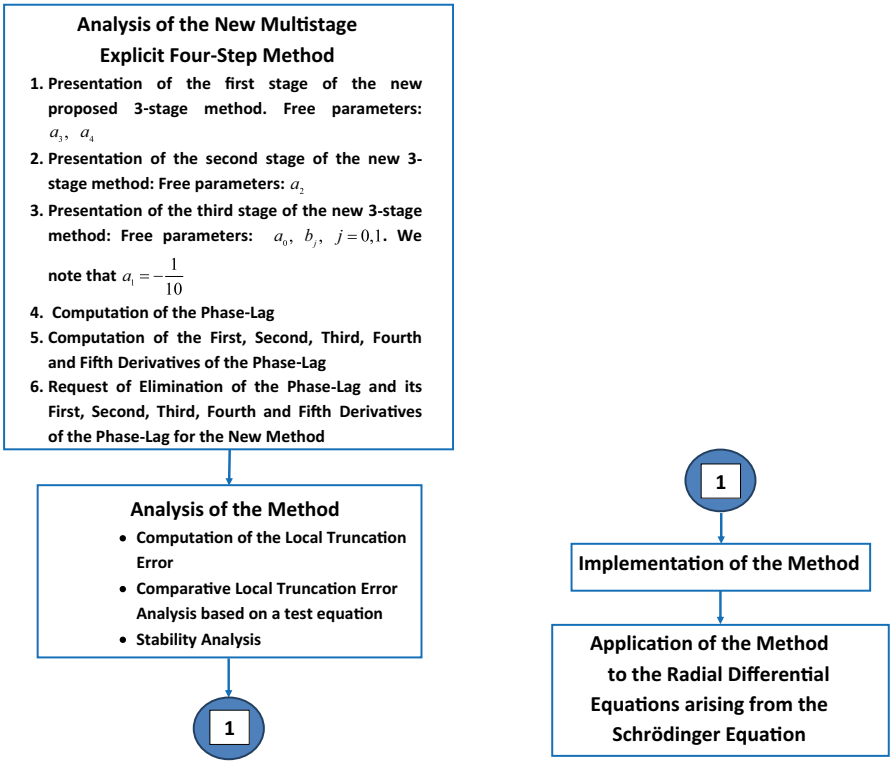

Fig. 2 Flowchart of the presentation of the analysis of the new obtained three-stage high algebraic order method

Remark 5 The direct formula for any $2k$ symmetric multistep method developed by Simos and his coworkers in [28] and [31] is used for the calculation of the phase-lag and its derivatives.

4 Phase-lag analysis of symmetric $2k$-step methods

Let us consider the multistep method with $2k$ steps for the numerical solution of the problem (1):

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

where:

- $2m$ are the number of steps over the equally spaced intervals $[x_{-i-1}, x_{i+1}]$, $i = 0(1)m-1$, where $\{x_i\}_{i=-m}^{m} \in [a,b]$
- $h = |x_{i+1} - x_i|$, $i = 0(1)m-1$, where h is called stepsize of integration
- $|a_0| + |b_0| \neq 0$

Remark 6 The method (2) with $b_k \neq 0$ is called implicit and with $b_k = 0$ is called explicit.

Remark 7 The method (2) is called symmetric if

$$a_{i-k} = a_{k-i}, \quad b_{i-k} = b_{k-i}, \quad i = 0(1)k \tag{3}$$

The application of a symmetric $2k$-step the method (2) to the scalar test equation

$$q'' = -w^2 q, \tag{4}$$

leads to the following difference equation

$$A_k(v)\, y_{n+k} + \cdots + A_1(v)\, y_{n+1} + A_0(v)\, y_n + A_1(v)\, y_{n-1} + \cdots + A_k(v)\, y_{n-k} = 0, \tag{5}$$

where $v = w\,h$, h is the step length and $A_0(v)$, $A_1(v)$, ..., $A_k(v)$ are polynomials of v.

The difference equation (5) leads to the following associated characteristic equation:

$$A_k(v)\,\lambda^k + \cdots + A_1(v)\,\lambda + A_0(v) + A_1(v)\,\lambda^{-1} + \cdots + A_k(v)\,\lambda^{-k} = 0 \tag{6}$$

Theorem 1 [28] *and* [31] *The symmetric* $2k$*-step method with characteristic equation given by* (6) *has phase-lag order m and phase-lag constant c given by:*

$$-c\,v^{m+2} + O\left(v^{m+4}\right) = \frac{2A_k(v)\cos(kv) + \cdots + 2A_j(v)\cos(jv) + \cdots + A_0(v)}{2k^2 A_k(v) + \cdots + 2j^2 A_j(v) + \cdots + 2A_1(v)} \tag{7}$$

Remark 8 For the category of methods investigated in this paper i.e. for a symmetric four-step method - the number $k = 2$ and the direct formula for the computation of the phase-lag is given by:

$$-c\,v^{m+2} + O(v^{m+4}) = \frac{2A_2(v)\cos(2v) + 2A_1(v)\cos(v) + A_0(v)}{8A_2(v) + 2A_1(v)} \tag{8}$$

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

5 The new multistage explicit four-step method

Let us consider the family of symmetric three stage explicit four-step methods for the numerical solution of problems of the form (1):

$$\begin{aligned}
\bar{q}_n &= q_n - a_3 h^2 \left(q''_{n+1} - 2q''_n + q''_{n-1}\right) - 2a_4 h^2 q''_n \\
\tilde{q}_n &= q_n - a_2 h^2 \left(q''_{n+1} - 2\bar{q}''_n + q''_{n-1}\right) \\
&q_{n+2} + a_1 q_{n+1} + a_0 q_n + a_1 q_{n-1} + q_{n-2}
\end{aligned} \tag{9}$$

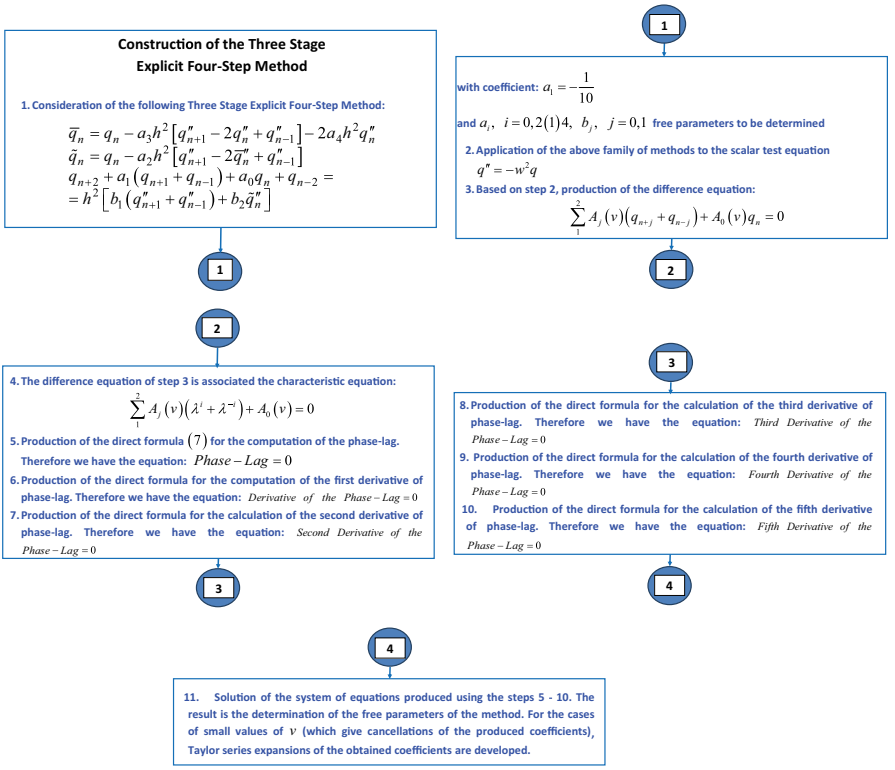

Fig. 3 Flowchart of the construction of any method of the family

$$= h^2 \left[b_1 \left(q''_{n+1} + q''_{n-1} \right) + b_0 \tilde{q}''_n \right], \tag{10}$$

where

$$a_1 = -\frac{1}{10} \tag{11}$$

and the coefficients $a_i,\ i = 0,\ 2(1)4$ and $b_j,\ j = 0,\ 1$ are free parameters, h is the step size of the integration, n is the number of steps, q_n is the approximation of the solution on the point x_n, $x_n = x_0 + n\,h$ and x_0 is the initial point of integration.

In Fig. 3, we present the flowchart for the development of the new three stages symmetric four-step method.

Based on the flowchart of Fig. 3, application of the new proposed method (10) to the scalar test equation (4) leads to the difference equation (5) with $k = 2$ and $A_j\,(v),\ j = 0,\ 1,\ 2$ given by:

$$A_2\,(v) = 1,\ A_1\,(v) = -\frac{1}{10} + v^2 \left(b_1 + b_0\, a_2\, v^2 \left(-2\, a_3\, v^2 + 1 \right) \right)$$

$$A_0(v) = a_0 + v^2 b_0 \left(1 + a_2 v^2 \left(4 a_3 v^2 - 4 a_4 v^2 - 2\right)\right) \tag{12}$$

Requesting vanishing of the phase-lag and its first, second, third, fourth and fifth derivatives and using the formulae (8) and (12), we obtain the following system of equations:

$$\text{Phase-lag} = -\frac{T_0}{T_{denom1}} = 0 \tag{13}$$

$$\text{First derivative of the phase-lag} = \frac{T_1}{T_{denom}^2} = 0 \tag{14}$$

$$\text{Second derivative of the phase-lag} = \frac{T_2}{T_{denom}^3} = 0 \tag{15}$$

$$\text{Third derivative of the phase-lag} = \frac{T_3}{T_{denom}^4} = 0 \tag{16}$$

$$\text{Fourth derivative of the phase-lag} = \frac{T_4}{T_{denom}^5} = 0 \tag{17}$$

$$\text{Fifth derivative of the phase-lag} = \frac{T_5}{T_{denom}^6} = 0 \tag{18}$$

where $T_j,\ j = 0(1)5$, T_{denom1} and T_{denom} are given in Supplement Material A.

Solving the above system of equations (13)–(18) we obtain the coefficients of the new three stage symmetric explicit four-step method:

$$\begin{aligned} a_4 &= -\frac{1}{6}\frac{T_6}{T_7}, \quad a_3 = \frac{1}{2}\frac{T_8}{T_7}, \quad a_2 = -\frac{1}{2}\frac{T_9}{T_{10}} \\ a_0 &= -\frac{1}{15}\frac{T_{11}}{T_{12}}, \quad b_1 = \frac{1}{10}\frac{T_{13}}{v^2\, T_{12}}, \quad b_0 = \frac{1}{5}\frac{T_{14}}{v^2\, T_{12}} \end{aligned} \tag{19}$$

where $T_i,\ i = 6(1)14$ are given in Supplement Material B.

In order to avoid cancellations for small values of $|w|$, the following Taylor series expansions should be used:

$$\begin{aligned} a_4 = {} & \frac{109}{4072} - \frac{353395\, v^2}{22799128} + \frac{200277123529\, v^4}{61273112482560} - \frac{30009157545747761\, v^6}{56194564082177993472} \\ & + \frac{19214311632778175467441 7\, v^8}{256740825265629501726978048 0} - \frac{78686963396032760519753182 21\, v^{10}}{81937037197748796069652955172864 0} \\ & + \frac{89141161880357589687343690165925 29\, v^{12}}{75334119492789999404486269240007393280 00} \\ & - \frac{25121809273709926121027044209858669323\, v^{14}}{17715420871685510679960182101941658588938240 0} \\ & + \frac{99977457332742623657560083565950430294731956 27\, v^{16}}{59804138224624634956196387128056537146568221392896 0000} \\ & - \frac{11719756436469341111074277273344053199471808607449 11\, v^{18}}{60070900563589395602881996732479946136164203601241151897600 0} + \cdots \end{aligned}$$

$$
\begin{aligned}
a_3 = {} & \frac{799}{24432} - \frac{3988315\,v^2}{957563376} + \frac{1509609104713\,v^4}{2573470724267520} - \frac{59202693865264847\,v^6}{842918461232669902080} \\
& + \frac{9154701375368361077188 9\,v^8}{10783114661156439072533078 0160} \\
& - \frac{43328885930767733916648936 3047\,v^{10}}{43016944528818117936567801 4657536000} \\
& + \frac{70400529150776823378697690015 5542947\,v^{12}}{60116627355246419524780042853525899837 44000} \\
& - \frac{48117034538886122823491369910 2260397381\,v^{14}}{35342264639012593806520563293373608884931788800} \\
& + \frac{38876201598049401809534307597479985412699390 2673\,v^{16}}{24758913224994598871865304271015406378679243656658 9440000} \\
& - \frac{17225033777387249011347701365942076060745792065 2781\,v^{18}}{95406724424524334192812583045703443863319617484324182425 6000} + \cdots \\
a_2 = {} & -\frac{509}{10500} - \frac{439\,v^2}{161700} + \frac{1142177\,v^4}{2716560000} - \frac{1719589\,v^6}{444972528000} + \frac{549495505483\,v^8}{349481423491200000} \\
& - \frac{9728550433298707\,v^{10}}{17430385996623600000000} - \frac{8312639070239291\,v^{12}}{58566096948655296000000 0} \\
& + \frac{3829577952958885716143\,v^{14}}{50563771876833407992800000 0000} \\
& - \frac{3331261723711479450871 1\,v^{16}}{54366167521971280273858560000000} \\
& + \frac{4675187425885382368186753\,v^{18}}{57084475898069844287551488000000000} + \cdots \\
\\
a_0 = {} & -\frac{9}{5} + \frac{439\,v^{12}}{186278400} - \frac{175933\,v^{14}}{782369280000} + \frac{802609\,v^{16}}{85434725376000} \\
& - \frac{103982671867\,v^{18}}{201301299930931200000} + \cdots \\
b_1 = {} & \frac{53}{40} - \frac{439\,v^8}{12418560} + \frac{110009\,v^{10}}{43464960000} - \frac{3074651\,v^{12}}{37970989056000} \\
& + \frac{21712832027\,v^{14}}{3727801850572800000} - \frac{14959758133\,v^{16}}{72116021254717440000} \\
& + \frac{101577877872907\,v^{18}}{16867035921212725248000000} + \cdots \\
b_0 = {} & \frac{5}{4} + \frac{439\,v^8}{6209280} - \frac{139103\,v^{10}}{7244160000} + \frac{78077647\,v^{12}}{56956483584000} - \frac{80230299949\,v^{14}}{1397925693964800000} \\
& + \frac{865900562837\,v^{16}}{2745956193929625600 00} - \frac{3851702611693273\,v^{18}}{33734071842425450496000000} \\
& + \frac{6219373210461308269\,v^{20}}{14911863091740694017972633600 00} + \cdots
\end{aligned}
\tag{20}
$$

In Fig. 4 the behavior of the coefficients $a_0,\ b_j,\ j = 0, 2(1)4$ is presented.

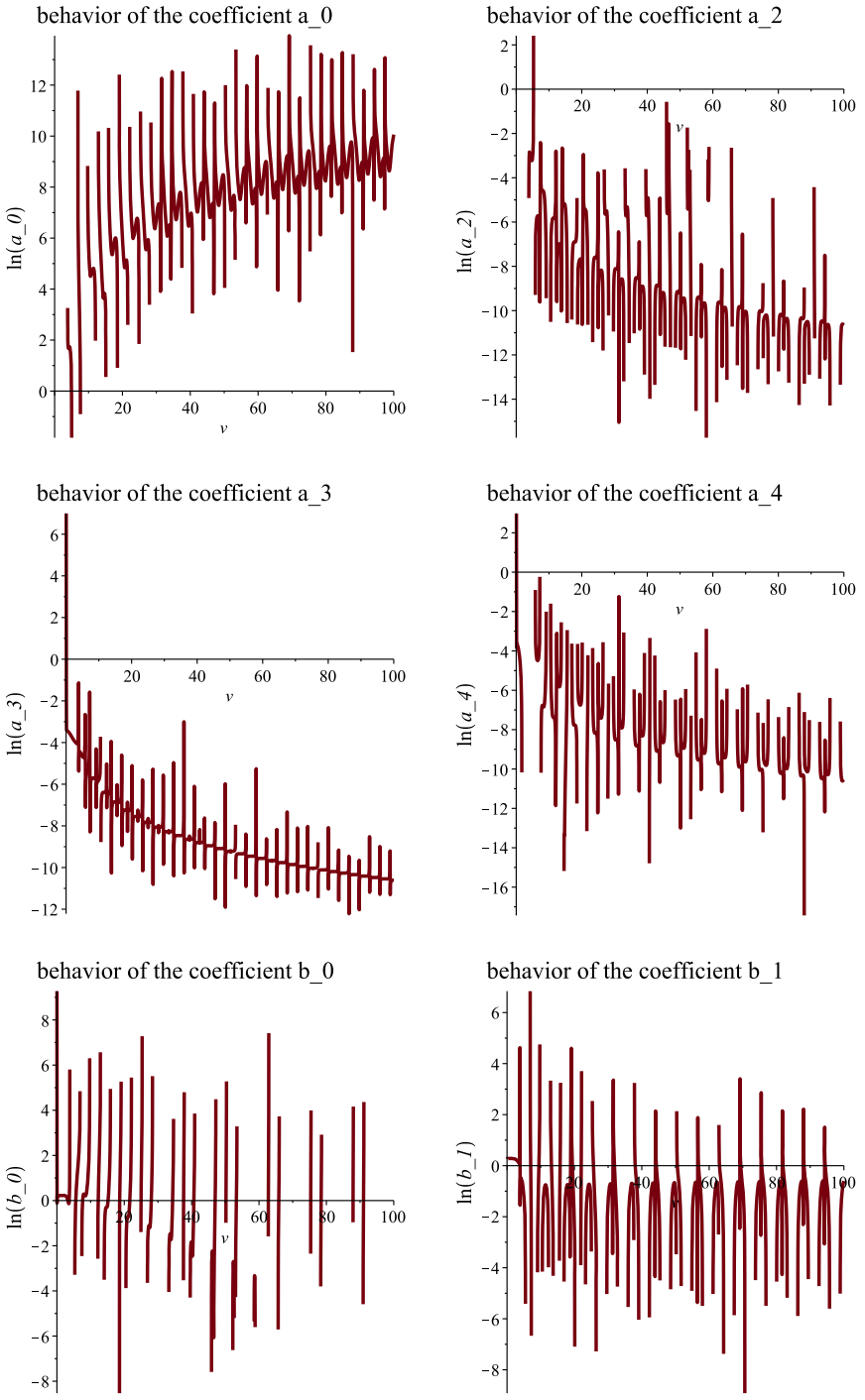

Fig. 4 Behavior of the coefficients of the new obtained three stages method given by (19) for several values of $v = w\,h$

Remark 9 The new developed three stages method is the the symmetric four-step method (10) with the coefficients given by (19)–(20).

The local truncation error of this new obtained three stages symmetric explicit four-step method (mentioned as $MuSMeth10$) is given by:

$$LTE_{MuSMeth10} = \frac{439\,h^{12}}{186278400}\left(q_n^{(12)} + 6\,w^2\,q_n^{(10)} + 15\,w^4\,q_n^{(8)} + 20\,w^6\,q_n^{(6)} + 15\,w^8\,q_n^{(4)} + 6w^{10}\,q_n^{(2)} + w^{12}\,q_n\right) + O\left(h^{14}\right) \tag{21}$$

where $q_n^{(j)}$ is the jth derivative of q_n.

6 Comparative error analysis

The following methods will be investigated:

6.1 Classical predictor–corrector explicit four-Step method, i.e., the method (10) with constant coefficients

$$LTE_{CL} = \frac{439\,h^{12}}{186278400}\,q_n^{(12)} + O\left(h^{14}\right) \tag{22}$$

6.2 The three stages explicit symmetric four-step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives developed in Sect. 5

$$LTE_{MuSMeth10} = \frac{439\,h^{12}}{186278400}\left(q_n^{(12)} + 6\,w^2\,q_n^{(10)} + 15\,w^4\,q_n^{(8)} + 20\,w^6\,q_n^{(6)} f + 15\,w^8\,q_n^{(4)} + 6w^{10}\,q_n^{(2)} + w^{12}\,q_n\right) + O\left(h^{14}\right) \tag{23}$$

The study of the Local Truncation Error Analysis is based on the flowchart presented in the Fig. 5.

Based on the scalar test equation (which is mentioned in the flowchart) which is used for the comparative local truncation error analysis, we calculate the derivatives $q_n^j,\ j = 2, 3, \ldots$. These formulae of the derivatives are given by:

$$q_n^{(2)} = (V(x) - V_c + G)\ q(x)$$
$$q_n^{(3)} = \left(\frac{d}{dx}g\,(x)\right) q\,(x) + (g\,(x) + G)\,\frac{d}{dx}q\,(x)$$
$$q_n^{(4)} = \left(\frac{d^2}{dx^2}g\,(x)\right) q\,(x) + 2\left(\frac{d}{dx}g\,(x)\right)\frac{d}{dx}q\,(x)$$

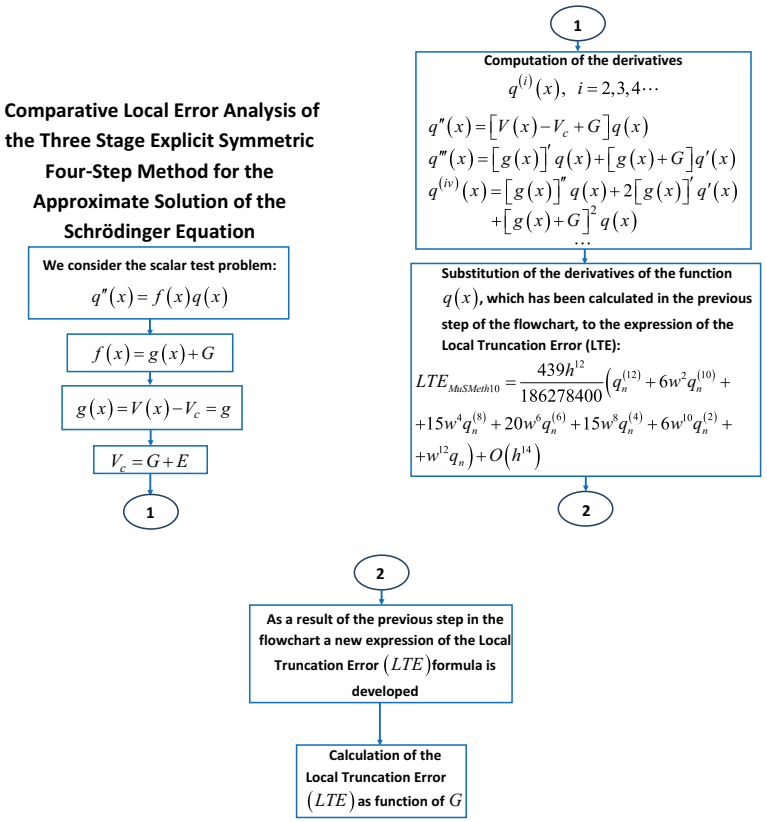

Fig. 5 Flowchart for the calculations on the comparative local truncation error analysis

$$
\begin{aligned}
&+ (g(x)+G)^2 q(x)\\
q_n^{(5)} &= \left(\frac{d^3}{dx^3}g(x)\right)q(x)+3\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}q(x)\\
&+4(g(x)+G)q(x)\frac{d}{dx}g(x)+(g(x)+G)^2\frac{d}{dx}q(x)\\
q_n^{(6)} &= \left(\frac{d^4}{dx^4}g(x)\right)q(x)+4\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}q(x)\\
&+7(g(x)+G)q(x)\frac{d^2}{dx^2}g(x)+4\left(\frac{d}{dx}g(x)\right)^2 q(x)\\
&+6(g(x)+G)\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}g(x)+(g(x)+G)^3 q(x)\\
q_n^{(7)} &= \left(\frac{d^5}{dx^5}g(x)\right)q(x)+5\left(\frac{d^4}{dx^4}g(x)\right)\frac{d}{dx}q(x)
\end{aligned}
$$

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

Using the new formulae of the derivatives q_n^j, $j = 2, 3, \ldots$, we produce the new formulae of the Local Truncation Error.

We study two cases (based on the value of E):

1. *The Energy* (E) *is closed to the potential*, i.e., $G = V_c - E \approx 0$. Therefore, all the non zero powers of G (i.e. G^j, $j \neq 0$) are equal to zero and consequently all the terms of the formulae of the Local Truncation Error which include G^j, $j \neq 0$ are approximately equal to zero (since $G \approx 0$). Therefore, in this case the formulae of the Local Truncation Error consist only from the free of G terms.

Remark 10 Multistep methods belonging in the same class of methods with different coefficients have the same free of G terms in the formulae of the Local Truncation Error

Therefore, for this case (energy (E) close to the potential) and based on the above investigation, the formulae of the Local Truncation Error for both methods (i.e. classical methods (methods with constant coefficients) and methods with vanished the phase-lag and its derivatives) are the same. Consequently, the error for these two kind of methods: (1) classical methods (methods with constant coefficients) and (2) methods with vanished the phase-lag and its derivatives, will be approximately the same.

2. *The Energy* (E) *is much bigger or smaller than the potential i.e. for the quantity* G *we have* $G >> 0$ *or* $G << 0$. Then $|G|$ is a big number. Consequently, the formulae of the Local Truncation Error are not the same for the numerical methods

of the same family [(1) classical methods (methods with constant coefficients) and (2) methods with vanished the phase-lag and its derivatives].

The asymptotic expressions of the Local Truncation Errors (based on the flowchart and study presented above) are given by:

6.3 Classical method

$$LTE_{CL} = h^{12}\left(\frac{439\ q\ (x)}{186278400}\right) G^6 + \cdots + O\left(h^{14}\right) \tag{24}$$

6.4 The three stages explicit symmetric four-step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives developed in Sect. 5

$$\begin{aligned} LTE_{MuSMeth10} = \frac{439\,h^{12}}{11642400}\Bigg(&15\left(\frac{\mathrm{d}}{\mathrm{d}x}g\ (x)\right) q\ (x)\ \frac{\mathrm{d}^3}{\mathrm{d}x^3}g\ (x) \\ &+ 6\,g\ (x)\,q\ (x)\ \frac{\mathrm{d}^4}{\mathrm{d}x^4}g\ (x) + 5\left(\frac{\mathrm{d}^6}{\mathrm{d}x^6}g\ (x)\right) q\ (x) \\ &+ 2\left(\frac{\mathrm{d}^5}{\mathrm{d}x^5}g\ (x)\right)\frac{\mathrm{d}}{\mathrm{d}x}q\ (x) \\ &+ 10\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}g\ (x)\right)^2 q\ (x)\Bigg) G^2 + \cdots + O\left(h^{14}\right) \end{aligned} \tag{25}$$

We have the following theorem:

Theorem 2 – *For the Classical Three Stage Explicit Symmetric Four-Step Method the error increases as the sixth power of G.*
– *For the Three Stages Explicit Symmetric Four-Step Method with Vanished Phase-Lag and its First, Second, Third, Fourth and Fifth Derivatives developed in Sect. 5, the error increases as the second power of G.*

So, for the numerical solution of the Schrödinger equation the New Three Stages Explicit Symmetric Four-Step Method with Vanished Phase-Lag and its First, Second, Third, Fourth and Fifth Derivatives developed in Sect. 5 is the most efficient, from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

7 Stability analysis

The flowchart given in Fig. 6 is the basis of the interval of periodicity analysis for the new three stage explicit symmetric four-step method (10) with the coefficients (11) and (19).

Application of the above mentioned method to the scalar test equation:

$$q'' = -z^2\,q \tag{26}$$

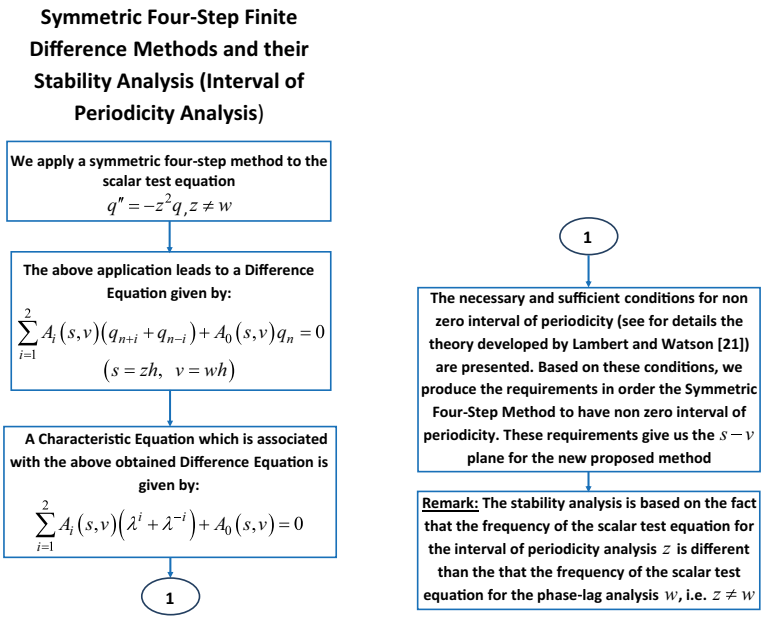

Fig. 6 Flowchart for the stability analysis of the new low cost hybrid explicit four-step method

leads to the difference equation:

$$A_2(s, v)\ (q_{n+2} + q_{n-2}) + A_1(s, v)\ (q_{n+1} + q_{n-1}) + A_0(s, v)\ q_n = 0 \tag{27}$$

where

$$A_2(s, v) = 1,\ A_1(s, v) = -\frac{1}{10}\frac{T_{15}}{T_{16}},\ A_0(s, v) = -\frac{1}{15}\frac{T_{17}}{T_{16}} \tag{28}$$

where $s = z\,h$ and $T_j,\ j = 15(1)17$ are given in Supplement Material C.

Remark 11 It is noted that the frequency of the scalar test equation (26) used for the stability analysis, z is not equal to the frequency of the scalar test equation (4) used for the phase-lag analysis, w, i.e. $w \neq z$.

The difference equation (27) is associated with a characteristic equation which is given by:

$$A_2(s, v)\ \left(\lambda^4 + 1\right) + A_1(s, v)\ \left(\lambda^3 + \lambda\right) + A_0(s, v)\ \lambda^2 = 0 \tag{29}$$

Definition 1 (see [21]) A symmetric $2\,m$-step method with the characteristic equation given by (29) is said to have an *interval of periodicity* $\left(0, v_0^2\right)$ if, for all $s \in \left(0, s_0^2\right)$, the roots $\lambda_i,\ i = 1(1)4$ satisfy

$$\lambda_{1,2} = e^{\pm i\,\zeta(s)}, \quad |\lambda_i| \leq 1, \quad i = 3, 4, \ldots \tag{30}$$

where $\zeta(s)$ is a real function of $z\,h$ and $s = z\,h$.

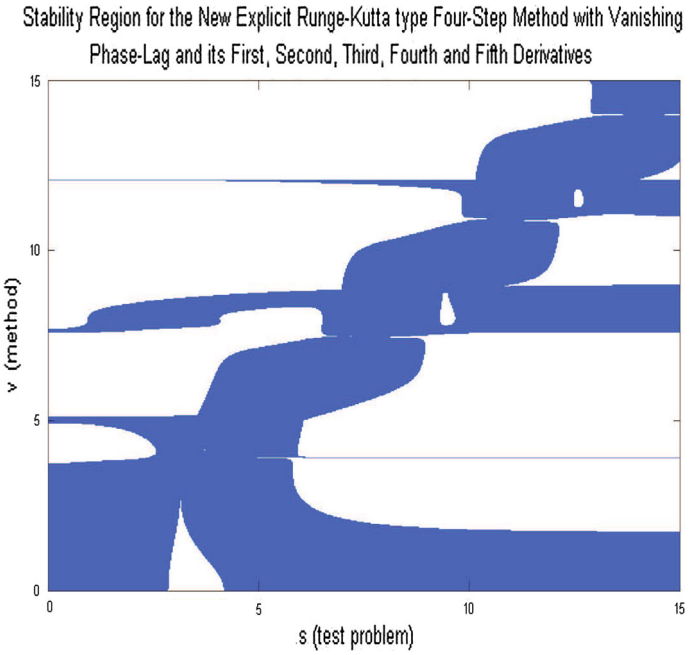

Fig. 7 s–v plane of the new three stage explicit symmetric four-step (10) with the coefficients given by (11) and (19)

Definition 2 (see [21]) If for a method its interval of periodicity is equal to $(0, \infty)$, then this method is called P-stable.

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$.[1]

Remark 12 The properties of P-stability and singularly almost P-stability are existed for the case for which the frequency of the scalar test equation (4) for the phase-lag analysis, w, is equal with the frequency of the scalar test equation (26) for the stability analysis z, i.e. only for the case $w = z$.

The s–v plane of the new three stage explicit symmetric four-step method is given in Fig. 7.

Remark 13 The shadowed area of the the s–v region indicates the stable area, while the white area indicates the unstable area.

Remark 14 In order to study the s–v region we divide the problems into two categories:

– Problems for which the frequency of the scalar test equation for the stability analysis is not equal to the frequency of the scalar test equation for the phase-lag analysis (i.e. $z \neq w$)

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

– Problems for which the frequency of the scalar test equation for the stability analysis is equal to the frequency of the scalar test equation for the phase-lag analysis (i.e. $z = w$)

We note that the Schrödinger equation and its related problems belong into the second category of problems described above.

1. For the first category of problems and in order to define the stability of a proposed method we have to develop and investigate the s–v plane (for our obtained new three stage explicit symmetric four-step method the s–v plane is shown in Fig. 7).
2. For the second category of problems it is sufficient to observe *the surroundings of the first diagonal of the s–v plane*.

The study of the second category of problems, i.e. the study of the case $z = w$ or $s = v$ i.e. the study of the surroundings of the first diagonal of the s–v plane, leads to the result that for the new three stage explicit symmetric four-step method developed in Sect. 5 the interval of periodicity is equal to: $(0, 9.9)$.

The analysis presented above leads to the following theorem:

Theorem 3 *The method produced in Sect. 5:*

– *is of multistage (three stage) type method,*
– *is of tenth algebraic order,*
– *has the phase-lag equal to zero,*
– *has phase-lag's first, second, third, fourth and fifth derivatives equal to zero,*
– *has an interval of periodicity equals to:* $(0, 9.9)$ *in the case where* $z = w$ *or* $s = v$.

8 Numerical results

The study of the efficiency of the new obtained method, will be done examining the approximate solution of the radial time-independent Schrödinger equation.

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

$$q''(r) = [l(l+1)/r^2 + V(r) - k^2]\, q(r), \tag{31}$$

where:

– The function $P(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. For the effective potential, we have the following relation: $P(r) \to 0$ as $r \to \infty$.
– k^2 is a real number which denotes *the energy*,
– l is defined by user integer which denotes the *angular momentum*,
– V is defined by user function denotes the *potential*.

Since we have a boundary boundary value problem it is necessary to define the boundary conditions. the initial condition is given by the definition of the problem:

$$y(0) = 0 \tag{32}$$

while the end condition (second boundary condition), for large values of r, is determined by the model of the problem.

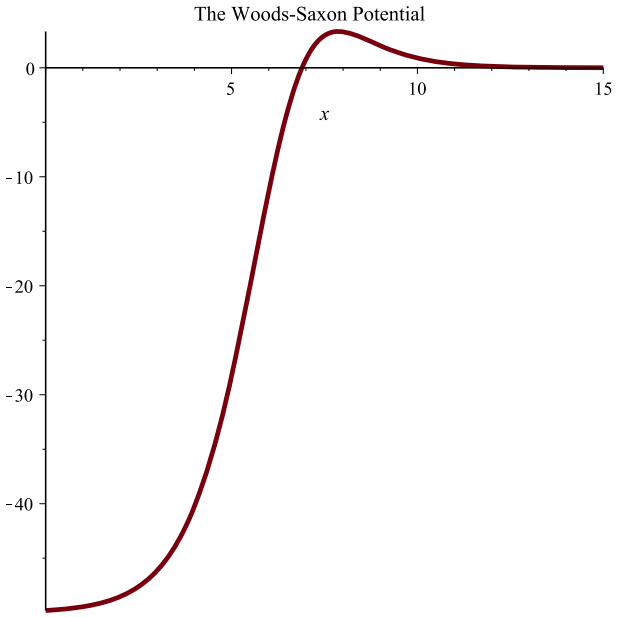

Fig. 8 The Woods–Saxon potential

Our new developed three stage explicit symmetric four-step method belongs to the frequency dependent methods and therefore it is necessary the definition of the value of the parameter w (frequency) in order the method to be applied for the approximate solution of the radial Schrödinger equation. From the model of the radial Schrödinger equation given by (31), the necessary to be defined parameter w is given by (for the case $l = 0$):

$$w = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{33}$$

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

8.1 Woods–Saxon potential

In order to solve the time-independent one-dimensional Schrödinger equation (31) the model of the the potential is necessary. This function is defined by the user. For our numerical experiments we use the known Woods–Saxon potential which is given by

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{34}$$

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

in Fig. 8 we present the scheme of the Woods–Saxon potential.

Based on the analysis presented in [118] we define the frequency w using the values of the potential on some critical points. Investigating some specific potentials

it is possible some critical points to be defined. The methodology of determination of the of the frequency w based on critical points of the potential, is one of several methodologies for the definition of the frequency w (see [28] and references therein).

Remark 15 The above mentioned methodology can be applied to some potentials. One of the type of the potential in which we can apply this methodology is the Woods–Saxon potential.

For our numerical experiments we use the following values of w based on the specific critical points (see for details [1] and [92]):

$$w = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{35}$$

For example, in the point of the integration area $r = 6.5-h$, the value of w is given by: $\sqrt{-37.5+E}$. So, $v = w\,h = \sqrt{-37.5+E}\,h$. In the point of the integration area $r = 6.5-3\,h$, the value of w is given by: $\sqrt{-50+E}$, etc.

8.2 The radial Schrödinger equation and the resonance problem

The problem which we will solve for our numerical experiments is the numerical solution of the radial time independent Schrödinger equation (31) using the mentioned above Woods–Saxon potential (34). Since this problem belongs to the boundary value problems with infinite interval of integration, it is necessary for its approximate solution the infinite integration interval to be approximated by a finite one. For our numerical tests we approximate the infinite interval of integration by the finite interval of integration $r \in [0, 15]$ and we will use a large domain of energies, i.e., $E \in [1, 1000]$.

Remark 16 The potential decays faster than the term $\frac{l(l+1)}{r^2}$ in the case of positive energies, $E = k^2$.

Using the above remark, the Schrödinger equation reduces to:

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{36}$$

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. Consequently, the solution of Eq. (31) (when $r \to \infty$), has the asymptotic form

$$q(r) \approx Akrj_l(kr) - Bkrn_l(kr)$$

$$\approx AC\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan d_l\cos\left(kr-\frac{l\pi}{2}\right)\right] \tag{37}$$

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

$$\tan\delta_l=\frac{y\,(r_2)\,S\,(r_1)-y\,(r_1)\,S\,(r_2)}{y\,(r_1)\,C\,(r_1)-y\,(r_2)\,C\,(r_2)} \tag{38}$$

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 $C\,(r)=-krn_l\,(kr)$. For the initial-value problems (in our numerical experiments the radial Schrödinger equation is treated as an initial-value problem) we need $q_j,\ j=0(1)3$ in order a four-step method to be started. The initial condition defines the first value of q i.e. q_0. Using high order Runge–Kutta–Nyström methods(see [124] and [125]) we determine the values $q_i,\ i=1(1)3$. Now we have all the necessary initial values and we can compute at r_2 of the asymptotic region the phase shift δ_l.

The known as resonance problem is being solved for positive energies. This specific problem consists either

- of finding the phase-shift δ_l or
- of finding those E, for $E\in[1,1000]$, at which $\delta_l=\frac{\pi}{2}$.

We solved the latter problem, known as **the resonance problem**.

The boundary conditions for this problem are:

$$q(0)=0,\ \ y(r)=\cos\left(\sqrt{E}r\right)\ \text{for large } r. \tag{39}$$

We calculate the positive eigenenergies in the case of the Woods–Saxon potential resonance problem using:

- The eighth order multi-step method developed by Quinlan and Tremaine [22], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [22], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [22], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [27], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [93], which is indicated as **Method RA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [26], 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 [48], which is indicated as **Method NMPF1**

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

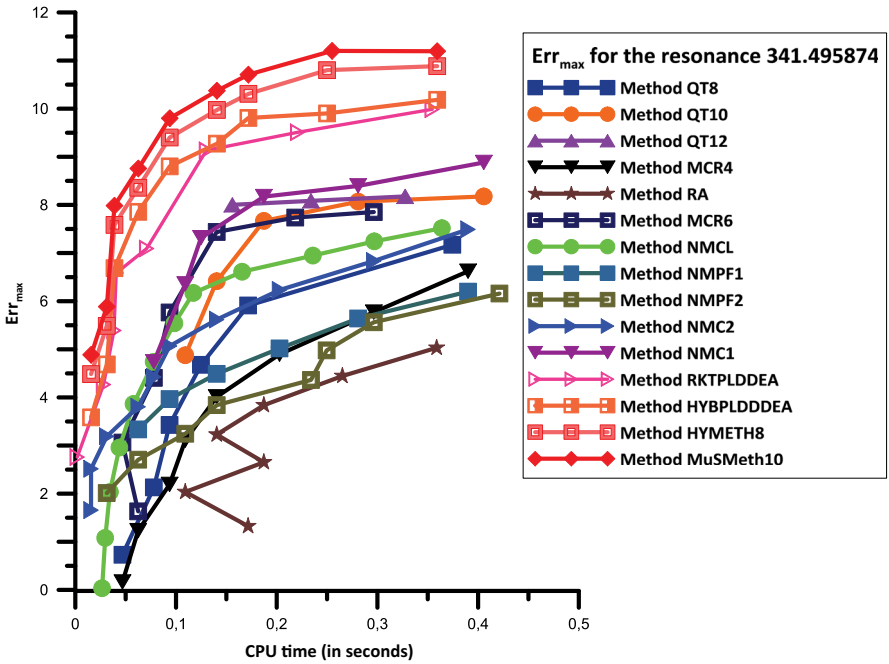

Fig. 9 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

- The Phase-Fitted Method (Case 2) developed in [48], which is indicated as **Method NMPF2**
- The Method developed in [52] (Case 2), which is indicated as **Method NMC2**
- The Method developed in [52] (Case 1), which is indicated as **Method NMC1**
- The Method developed in [45], which is indicated as **Method RKTPLDDEA**
- The Method developed in [58], which is indicated as **Method HYBPLDDDEA**
- The Hybrid Low Computational Computational Cost Four-Step Method developed in [46], which is indicated as **Method HYMETH8**
- The New Obtained Three Stages Explicit Symmetric Four-Step Method which is developed in Sect. 5, which is indicated as **Method MuSMeth10**

The reference values of the eigenenergies which are computed, computed using the well known two-step method of Chawla and Rao [26] with small step size for the integration, are compared with those computed via the above mentioned methods. In Figs. 9 and 10, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{40}$$

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.

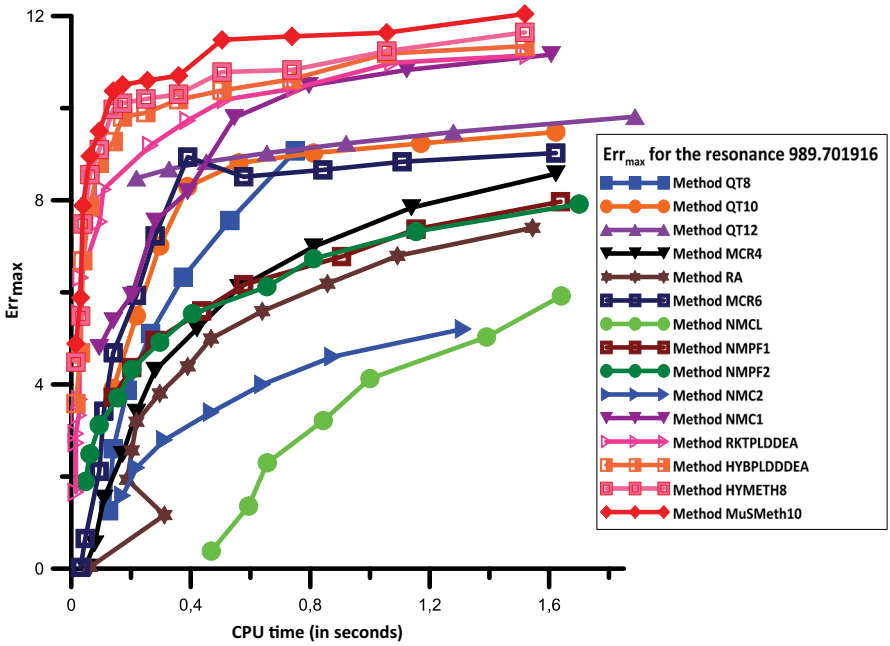

Fig. 10 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

9 Conclusions

A new three stage tenth algebraic order symmetric explicit four-step method was studied in this paper. More specifically, we developed an explicit method with vanished phase-lag and its first, second, third, fourth and fifth derivatives. We studied the new proposed method as one block. We also investigated the effection of the vanishing procedure on the computational effectiveness of the obtained method.

We theoretically studied the the comparative local truncation error analysis and the stability analysis.

The numerical solution of the resonance problem of the radial time independent Schrödinger equation given us the numerical experiments based on which we studied the computational efficiency of the obtained method.

Remark 17 The new developed method is very efficient on any problem with oscillating and/or periodical solutions or problems with solutions contain the functions cos and sin or any combination of them.

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

1. The classical form of the sixth algebraic order 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 [27], which is indicated as **Method MCR4**. Both the above mentioned methods are more

efficient than the exponentially-fitted method of Raptis and Allison [93], which is indicated as **Method RA**. The method **Method NMCL** is more efficient than the eighth algebraic order multistep method developed by Quinlan and Tremaine [22], which is indicated as **Method QT8**, the Phase-Fitted Method (Case 1) developed in [48], which is indicated as **Method NMPF1** and the Phase-Fitted Method (Case 2) developed in [48], which is indicated as **Method NMPF1**.

2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [22], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [27], 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 [22], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the classical form of the sixth algebraic order four-step method developed in Sect. 4, which is indicated as **Method NMCL**.
3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [22], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [22], which is indicated as **Method QT10**
4. The Method developed in [52] (Case 1), which is indicated as **Method NMC1** is more efficient than the twelfth algebraic order multistep method developed by Quinlan and Tremaine [22], which is indicated as **Method QT12**
5. The Method developed in [45], which is indicated as **Method RKTPLDDEA** is more efficient than the method developed in [52] (Case 1), which is indicated as **Method NMC1**.
6. The Method developed in [58], which is indicated as **Method HYBPLDDDEA** is more efficient than method developed in [45], which is indicated as **Method RKTPLDDEA**.
7. The low computational cost hybrid explicit four-step method of eight algebraic order with vanished phase-lag and its first, second, third and fourth derivatives developed in [46], which is indicated as **Method HYMETH8**, is more efficient than the Method developed in [58], which is indicated as **Method HYBPLDDDEA**.
8. Finally, the New Obtained Three Stages Explicit Symmetric Four-Step Method which is developed in Sect. 5, which is indicated as **Method MuSMeth10**, 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).

Complince with Ethical Standards

Conflict of interest The authors declare that they have no conflict of interest.

References

1. L.G. Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
2. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)

3. I. Prigogine, S. Rice (eds.), *Advances in Chemical Physics Vol. 30: New Methods in Computational Quantum Mechanics* (Wiley, London, 1997)
4. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
5. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. J. Math. Chem. **30**(1), 121–131 (2001)
6. K. Tselios, T.E. Simos, Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**(1), 173–181 (2005)
7. Z.A. Anastassi, T.E. Simos, An optimized Runge–Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**(1), 1–9 (2005)
8. D.F. Papadopoulos, T.E. Simos, A new methodology for the construction of optimized Runge–Kutta–Nyström methods. Int. J. Mod. Phys. C **22**(6), 623–634 (2011)
9. D.F. Papadopoulos, T.E. Simos, A modified Runge–Kutta–Nyström method by using phase lag properties for the numerical solution of orbital problems. Appl. Math. Inf. Sci. **7**(2), 433–437 (2013)
10. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic Runge–Kutta–Nyström methods. Appl. Math. Inf. Sci. **7**(1), 81–85 (2013)
11. A.A. Kosti, Z.A. Anastassi, T.E. Simos, Construction of an optimized explicit Runge–Kutta–Nyström method for the numerical solution of oscillatory initial value problems. Comput. Math. Appl. **61**(11), 3381–3390 (2011)
12. Z. Kalogiratou, T. Monovasilis, G. Psihoyios, T.E. Simos, Runge–Kutta type methods with special properties for the numerical integration of ordinary differential equations. Phys. Rep. Rev. Sect. Phys. Lett. **536**(3), 75–146 (2014)
13. Z. Kalogiratou, T. Monovasilis, T.E. Simos, A fourth order modified trigonometrically fitted symplectic Runge–Kutta–Nyström method. Comput. Phys. Commun. **185**(12), 3151–3155 (2014)
14. A.A. Kosti, Z.A. Anastassi, T.E. Simos, An optimized explicit Runge–Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems. J. Math. Chem. **47**(1), 315–330 (2010)
15. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nyström methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. J. Math. Chem. **31**(2), 211–232 (2002)
16. T.E. Simos, A fourth algebraic order exponentially-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation. IMA J. Numer. Anal. **21**(4), 919–931 (2001)
17. T.E. Simos, Exponentially-fitted Runge–Kutta–Nyström method for the numerical solution of initial-value problems with oscillating solutions. Appl. Math. Lett. **15**(2), 217–225 (2002)
18. C. Tsitouras, T.E. Simos, Optimized Runge–Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
19. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge–Kutta methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 281–293 (2005)
20. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge–Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. J. Math. Chem. **41**(1), 79–100 (2007)
21. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
22. G.D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits. Astron. J. **100**, 1694–1700 (1990)
23. C. Tsitouras, I.T. Famelis, T.E. Simos, On modified Runge–Kutta trees and methods. Comput. Math. Appl. **62**(4), 2101–2111 (2011)
24. http://burtleburtle.net/bob/math/multistep.html
25. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. J. Math. Chem. **29**(4), 281–291 (2001)
26. M.M. Chawla, P.S. Rao, An explicit sixth-order method with phase-lag of order eight for $y'' = f(t, y)$. J. Comput. Appl. Math. **17**, 363–368 (1987)
27. M.M. Chawla, P.S. Rao, An Noumerov-typ method with minimal phase-lag for the integration of second order periodic initial-value problems II Explicit Method. J. Comput. Appl. Math. **15**, 329–337 (1986)
28. T.E. Simos, P.S. Williams, A finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**, 189–205 (1997)

29. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. J. Math. Chem. **29**(4), 293–305 (2001)
30. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. J. Math. Chem. **31**(2), 135–144 (2002)
31. A. Konguetsof, T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 93–106 (2003)
32. T.E. Simos, I.T. Famelis, C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions. Numer. Algorithms **34**(1), 27–40 (2003)
33. D.P. Sakas, T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation. J. Comput. Appl. Math. **175**(1), 161–172 (2005)
34. T.E. Simos, Optimizing a class of linear multi-step methods for the approximate solution of the radial Schrödinger equation and related problems with respect to phase-lag. Cent. Eur. J. Phys. **9**(6), 1518–1535 (2011)
35. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 317–331 (2005)
36. H. Van de Vyver, Phase-fitted and amplification-fitted two-step hybrid methods for $y'' = f(x, y)$. J. Comput. Appl. Math. **209**(1), 33–53 (2007)
37. H. Van de Vyver, An explicit Numerov-type method for second-order differential equations with oscillating solutions. Comput. Math. Appl. **53**, 1339–1348 (2007)
38. T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation. J. Math. Chem. **46**(3), 981–1007 (2009)
39. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A new symmetric eight-step predictor-corrector method for the numerical solution of the radial Schrödinger equation and related orbital problems. Int. J. Mod. Phys. C **22**(2), 133–153 (2011)
40. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A symmetric eight-step predictor-corrector method for the numerical solution of the radial Schrödinger equation and related IVPs with oscillating solutions. Comput. Phys. Commun. **182**(8), 1626–1637 (2011)
41. T.E. Simos, Optimizing a hybrid two-step method for the numerical solution of the Schrödinger equation and related problems with respect to phase-lag. J. Appl. Math. Article ID 420387 (2012)
42. T.E. Simos, A two-step method with vanished phase-lag and its first two derivatives for the numerical solution of the Schrödinger equation. J. Math. Chem. **49**(10), 2486–2518 (2011)
43. I. Alolyan, T.E. Simos, A family of high-order multistep methods with vanished phase-lag and its derivatives for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **62**(10), 3756–3774 (2011)
44. I. Alolyan, T.E. Simos, A new four-step hybrid type method with vanished phase-lag and its first derivatives for each level for the approximate integration of the Schrödinger equation. J. Math. Chem. **51**, 2542–2571 (2013)
45. I. Alolyan, T.E. Simos, A Runge–Kutta type four-step method with vanished phase-lag and its first and second derivatives for each level for the numerical integration of the Schrödinger equation. J. Math. Chem. **52**, 917–947 (2014)
46. I. Alolyan, T.E. Simos, Efficient low computational cost hybrid explicit four-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical integration of the Schrödinger equation. J. Math. Chem. (2015). doi:10.1007/s10910-015-0522-6
47. I. Alolyan, Z.A. Anastassi, T.E. Simos, A new family of symmetric linear four-step methods for the efficient integration of the Schrödinger equation and related oscillatory problems. Appl. Math. Comput. **218**(9), 5370–5382 (2012)
48. Z.A. Anastassi, T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems. J. Comput. Appl. Math. **236**(16), 3880–3889 (2012)
49. G.A. Panopoulos, T.E. Simos, An optimized symmetric 8-step semi-embedded predictor–corrector method for IVPs with oscillating solutions. Appl. Math. Inf. Sci. **7**(1), 73–80 (2013)
50. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A new eight-step symmetric embedded predictor–corrector method (EPCM) for orbital problems and related IVPs with oscillatory solutions. Astron. J. **145**(3) Article Number: 75. doi:10.1088/0004-6256/145/3/75 (2013)
51. T.E. Simos, New high order multiderivative explicit four-step methods with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation. Construction and theoretical analysis. J. Math. Chem. **51**(1), 194–226 (2013)

52. T.E. Simos, On the explicit four-step methods with vanished phase-lag and its first derivative. Appl. Math. Inf. Sci. **8**(2), 447–458 (2014)
53. G.A. Panopoulos, T.E. Simos, A new optimized symmetric embedded predictor–corrector method (EPCM) for initial-value problems with oscillatory solutions. Appl. Math. Inf. Sci. **8**(2), 703–713 (2014)
54. T.E. Simos, An explicit four-step method with vanished phase-lag and its first and second derivatives. J. Math. Chem. **52**(3), 833–855 (2014)
55. T.E. Simos, An explicit linear six-step method with vanished phase-lag and its first derivative. J. Math. Chem. **52**(7), 1895–1920 (2014)
56. T.E. Simos, A new explicit hybrid four-step method with vanished phase-lag and its derivatives. J. Math. Chem. **52**(7), 1690–1716 (2014)
57. I. Alolyan, T.E. Simos, A family of explicit linear six-step methods with vanished phase-lag and its first derivative. J. Math. Chem. **52**(8), 2087–2118 (2014)
58. I. Alolyan, T.E. Simos, A hybrid type four-step method with vanished phase-lag and its first, second and third derivatives for each level for the numerical integration of the Schrödinger equation. J. Math. Chem. **52**(9), 2334–2379 (2014)
59. T.E. Simos, A new explicit four-step method with vanished phase-lag and its first and second derivatives. J. Math. Chem. **53**(1), 402–429 (2015)
60. G.A. Panopoulos, T.E. Simos, An eight-step semi-embedded predictor–corrector method for orbital problems and related IVPs with oscillatory solutions for which the frequency is unknown. J. Comput. Appl. Math. **290**, 1–15 (2015)
61. A. Konguetsof, A new two-step hybrid method for the numerical solution of the Schrödinger equation. J. Math. Chem. **47**(2), 871–890 (2010)
62. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation. J. Math. Chem. **34**(1–2), 83–94 (2003)
63. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation. J. Math. Chem. **35**(1), 55–63 (2004)
64. T. Monovasilis, T.E. Simos, New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation. J. Math. Chem. **42**(3), 535–545 (2007)
65. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **37**(3), 263–270 (2005)
66. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **40**(3), 257–267 (2006)
67. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 83–92 (2003)
68. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae of high-order for long-time integration of orbital problems. Appl. Math. Lett. **22**(10), 1616–1621 (2009)
69. Z. Kalogiratou, T.E. Simos, Newton–Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
70. T.E. Simos, High order closed Newton–Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation. Appl. Math. Comput. **209**(1), 137–151 (2009)
71. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for the solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**(3), 787–801 (2008)
72. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation. J. Math. Chem. **44**(2), 483–499 (2008)
73. T.E. Simos, High-order closed Newton–Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. Comput. Phys. Commun. **178**(3), 199–207 (2008)
74. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for numerical integration of the Schrödinger equation. Comput. Lett. **3**(1), 45–57 (2007)
75. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. RevMexAA **42**(2), 167–177 (2006)
76. T.E. Simos, Closed Newton–Cotes trigonometrically-fitted formulae for long-time integration. Int. J. Mod. Phys. C **14**(8), 1061–1074 (2003)
77. T.E. Simos, New closed Newton–Cotes type formulae as multilayer symplectic integrators. J. Chem. Phys. **133**(10), Article Number: 104108 (2010)

78. T.E. Simos, New stable closed Newton–Cotes trigonometrically fitted formulae for long-time integration. Abstr. Appl. Anal. Article Number: 182536. doi:10.1155/2012/182536 (2012)
79. T.E. Simos, High order closed Newton–Cotes exponentially and trigonometrically fitted formulae as multilayer symplectic integrators and their application to the radial Schrödinger equation. J. Math. Chem. **50**(5), 1224–1261 (2012)
80. T.E. Simos, Accurately closed Newton–Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation. Int. J. Mod. Phys. C **24**(3). doi:10.1142/S0129183113500149 (2013)
81. T.E. Simos, New open modified Newton Cotes type formulae as multilayer symplectic integrators. Appl. Math. Model. **37**(4), 1983–1991 (2013)
82. G. Vanden Berghe, M. Van Daele, Exponentially fitted open Newton–Cotes differential methods as multilayer symplectic integrators. J. Chem. Phys. **132**, 204107 (2010)
83. Z. Kalogiratou, T. Monovasilis, T.E. Simos, A fifth-order symplectic trigonometrically fitted partitioned Runge–Kutta method. In: *International Conference on Numerical Analysis and Applied Mathematics, SEP 16-20, 2007 Corfu, GREECE, Numerical Analysis and Applied Mathematics. AIP Conference Proceedings* vol. 936 (2007), pp. 313–317
84. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Families of third and fourth algebraic order trigonometrically fitted symplectic methods for the numerical integration of Hamiltonian systems. Comput. Phys. Commun. **177**(10), 757–763 (2007)
85. T. Monovasilis, T.E. Simos, Symplectic methods for the numerical integration of the Schrödinger equation. Comput. Mater. Sci. **38**(3), 526–532 (2007)
86. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Computation of the eigenvalues of the Schrödinger equation by symplectic and trigonometrically fitted symplectic partitioned Runge–Kutta methods. Phys. Lett. A **372**(5), 569–573 (2008)
87. Z. Kalogiratou, T. Monovasilis, T.E. Simos, New modified Runge–Kutta–Nyström methods for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **60**(6), 1639–1647 (2010)
88. T. Monovasilis, Z. Kalogiratou, T.E. Simos, A family of trigonometrically fitted partitioned Runge–Kutta symplectic methods. Appl. Math. Comput. **209**(1), 91–96 (2009)
89. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Two new phase-fitted symplectic partitioned Runge–Kutta methods. Int. J. Mod. Phys. C **22**(12), 1343–1355 (2011)
90. K. Tselios, T.E. Simos, Optimized fifth order symplectic integrators for orbital problems. Rev. Mex. Astron. Astrofis. **49**(1), 11–24 (2013)
91. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Symplectic partitioned Runge–Kutta methods with minimal phase-lag. Comput. Phys. Commun. **181**(7), 1251–1254 (2010)
92. L.G. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. Comput. Phys. Commun. **19**, 23–27 (1980)
93. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
94. J. Vigo-Aguiar, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **32**(3), 257–270 (2002)
95. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor–corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
96. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor–corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**(1), 137–147 (2005)
97. T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution. Appl. Math. Lett. **17**(5), 601–607 (2004)
98. T.E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation. Acta Appl. Math. **110**(3), 1331–1352 (2010)
99. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **31**(4), 371–404 (2002)
100. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. J. Math. Chem. **34**(1–2), 39–58 (2003)
101. T.E. Simos, Exponentially-fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
102. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. J. Math. Chem. **40**(3), 305–318 (2006)
103. H. Van de Vyver, A trigonometrically fitted explicit hybrid method for the numerical integration of orbital problems. Appl. Math. Comput. **189**(1), 178–185 (2007)

104. T.E. Simos, A family of four-step trigonometrically-fitted methods and its application to the Schrodinger equation. J. Math. Chem. **44**(2), 447–466 (2009)
105. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. **45**(4), 1102–1129 (2009)
106. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation. J. Math. Chem **37**(3), 295–316 (2005)
107. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order predictor–corrector methods. J. Math. Chem. **40**(3), 269–293 (2006)
108. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**(3), 162–174 (2005)
109. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. J. Math. Chem. **27**(4), 343–356 (2000)
110. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. **45**(4), 1102–1129 (2009)
111. C. Tang, W. Wang, H. Yan, Z. Chen, High-order predictorcorrector of exponential fitting for the N-body problems. J. Comput. Phys. **214**(2), 505–520 (2006)
112. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions. J. Math. Chem. **46**(2), 604–620 (2009)
113. S. Stavroyiannis, T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs. Appl. Numer. Math. **59**(10), 2467–2474 (2009)
114. S. Stavroyiannis, T.E. Simos, A nonlinear explicit two-step fourth algebraic order method of order infinity for linear periodic initial value problems. Comput. Phys. Commun. **181**(8), 1362–1368 (2010)
115. Z.A. Anastassi, T.E. Simos, Numerical multistep methods for the efficient solution of quantum mechanics and related problems. Phys. Rep. **482**, 1–240 (2009)
116. R. Vujasin, M. Sencanski, J. Radic-Peric, M. Peric, A comparison of various variational approaches for solving the one-dimensional vibrational Schrödinger equation. MATCH Commun. Math. Comput. Chem. **63**(2), 363–378 (2010)
117. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)
118. L.G. Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **38**(3), 329–337 (1985)
119. J. Vigo-Aguiar, T.E. Simos, Review of multistep methods for the numerical solution of the radial Schrödinger equation. Int. J. Quantum Chem. **103**(3), 278–290 (2005)
120. T.E. Simos, G. Psihoyios, Special issue: The international conference on computational methods in sciences and engineering 2004–preface. J. Comput. Appl. Math. **191**(2), 165–165 (2006)
121. T.E. Simos, G. Psihoyios, Special issue: Selected papers of the international conference on computational methods in sciences and engineering (ICCMSE 2003) Kastoria, Greece, 12–16 September 2003—preface. J. Comput. Appl. Math. **175**(1), IX–IX (2005)
122. T.E. Simos, J. Vigo-Aguiar, Special Issue: Selected papers from the conference on computational and mathematical methods for science and engineering (CMMSE-2002) - Alicante University, Spain, 20–25 September 2002—preface. J. Comput. Appl. Math. **158**(1), IX–IX (2003)
123. T.E. Simos, I. Gutman, Papers presented on the international conference on computational methods in sciences and engineering (Castoria, Greece, September 12–16, 2003). MATCH Commun. Math. Comput. Chem **53**(2), A3–A4 (2005)
124. J.R. Dormand, M.E.A. El-Mikkawy, P.J. Prince, Families of Runge–Kutta–Nyström formulae. IMA J. Numer. Anal. **7**, 235–250 (1987)
125. J.R. Dormand, P.J. Prince, A family of embedded Runge–Kutta formulae. J. Comput. Appl. Math. **6**, 19–26 (1980)