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ORIGINAL PAPER

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

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

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Abstract Based on an optimized explicit four-step method, a new hybrid high algebraic order four-step method is introduced in this paper. For this new hybrid method, we investigate the procedure of vanishing of the phase-lag and its first, second, third and fourth derivatives. More specifically, we investigate: (1) the construction of the new method, i.e. the computation of the coefficients of the method in order its phase-lag and first, second, third and fourth derivatives of the phase-lag to be eliminated, (2) the definition of the local truncation error, (3) the analysis of the local truncation error, (4) the stability (interval of periodicity) analysis (using scalar test equation with frequency different than the frequency of the scalar test equation for the phase-lag analysis). Finally, we investigate computationally the new obtained method by applying it to the numerical solution of the resonance problem of the radial Schrödinger equation. The efficiency of the new developed method is tested comparing this method with well known methods of the literature but also using very recently developed methods.

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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

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Mathematics Subject Classification 65L05

1 Introduction

In this paper, a new hybrid explicit four-step method of eighth algebraic order is proposed. This method is based on an optimal explicit four-step method. The new insights of the proposed method are:

- The new method is an explicit method which can be simply applied to any problem (linear or non-linear)
- The new method has low computational cost, i.e. only two stages
- The high algebraic order of the new obtained method
- The new method is based on an optimal explicit four-step method
- The new produced method has vanished the phase-lag and its first, second, third and fourth derivatives

Our investigation is concerned with the development of special methods for problems with mathematical models of the form:

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

with periodical and/or oscillating solutions.

Remark 1 Based on (1) it is easy to see that the characteristic of the mathematical model of the above mentioned problems is that their models consist of a system of second order ordinary differential equations from which the first derivative y' does not appear explicitly. Applied Sciences which have problems with the above described type of models are: 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 Our investigate has as aim and scope the development of an efficient algorithm for the above described problems. The meaning of the term efficient is an algorithm which is effective , fast and reliable for the approximate solution of the above mentioned problems. An extensive research has been done on this research subject (see for example [5–117]).

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.

A recent bibliography on the subject of this paper is presented in the present section:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta–Nyström type have been obtained in [5–14].

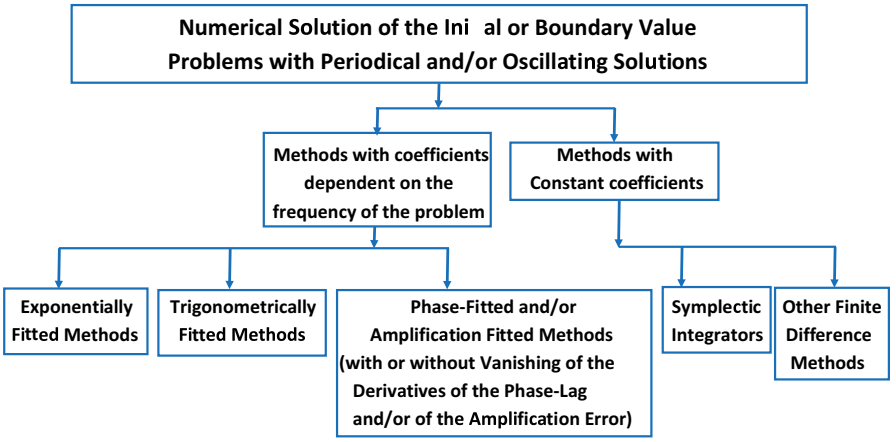

Fig. 1 Main classes of the finite difference methods developed in the last decades

- 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 [25–59].
- Symplectic integrators are investigated in [60–89].
- Exponentially and trigonometrically multistep methods have been produced in [90–110].
- Nonlinear methods have been studied in [111,112].
- Review papers have been presented in [113–117].
- Special issues and Symposia in International Conferences have been developed on this subject (see [118–120]).

In this paper, we will investigate a low computational cost hybrid method which has only two stages. The idea is the vanishing of the phase-lag and its derivatives in the whole method (i.e. when both of stages are applied to the scalar test equation). Our investigation will examine how this elimination of the phase-lag and its derivatives affects the effectiveness of the final proposed method. We will also compare the developed method with other well known methods of the literature in order to investigate its efficiency.

Remark 3 Methods produced using the above mentioned methodology can be applied effectively to (1) problems with periodic solution and/or, (2) problems with oscillating solution, (3) problems with solutions containing functions cos and sin, (4) problems with solutions containing combination of the functions cos and sin.

A short description of the investigation for this paper is presented in Sect. 2. In Sect. 3, we present the phase-lag analysis of symmetric $2m$ methods. The development of the new proposed low cost explicit hybrid four-step method is presented in Sect. 4. A comparative local truncation error (LTE) analysis with other similar methods is presented in Sect. 5. In Sect. 6, we describe the stability analysis of the new produced method. We use scalar test equation with frequency different than the frequency of the

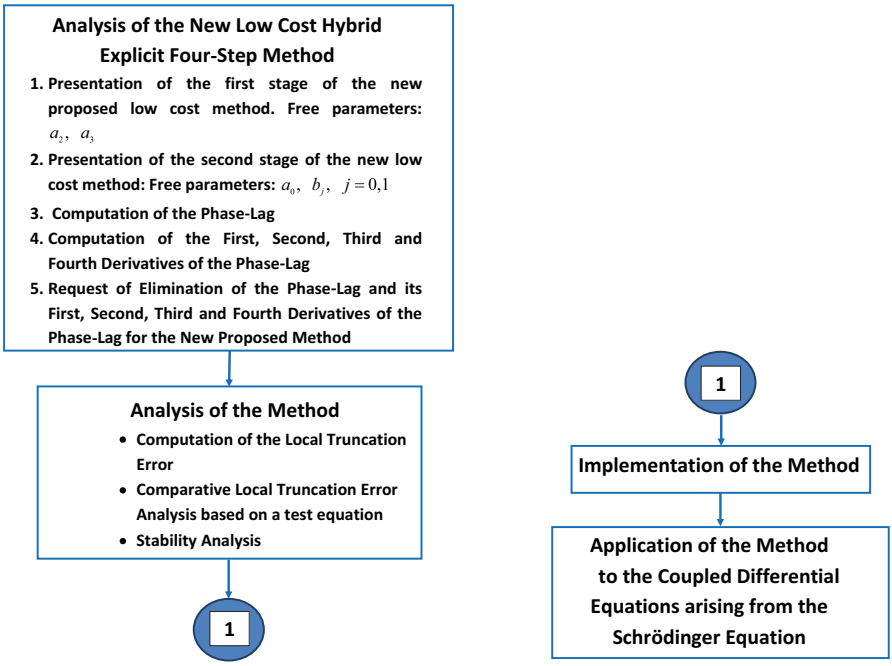

Fig. 2 Flowchart of the presentation of the analysis of the new proposed predictor–corrector high algebraic order method

scalar test equation for the phase-lag analysis. Numerical results on the approximate solution of the resonance problem of the radial Schrödinger type are presented in Sect. 7. Some remarks and conclusions are finally presented in Sect. 8.

2 Analysis of the new low computational cost hybrid four-step method

In Fig. 2, we present the flowchart of the analysis for the new low cost four-step method.

The subjects of our research in the present paper are:

- The calculation of the coefficients of the new low cost hybrid method in order to have
  1. the highest algebraic accuracy ,
  2. eliminated phase-lag ,
  3. eliminated first derivative of the phase-lag ,
  4. eliminated second derivative of the phase-lag ,
  5. eliminated third derivative of the phase-lag ,
  6. eliminated fourth derivative of the phase-lag ,
- The study of the produced LTE. We will compare the LTE analysis of the new low cost four-step hybrid method with other methods of the same form.
- The study of the stability of the new low cost method. For the specific study, we will use a scalar test equation with frequency different than the frequency of the scalar test equation for the phase-lag analysis.

– The study of the efficiency/effectiveness of the new obtained low cost four-step method using the approximate solution of the resonance problem of the radial Schrödinger equation.

Remark 4 For the computation of the phase-lag and its derivatives, we will use the direct formula for any $2m$ symmetric multistep method developed by Simos and his coworkers in [28,31].

3 Phase-lag analysis of symmetric $2m$-step methods

In the present paper, we investigate the numerical solution of the initial or boundary value problem of the form (1). More specifically, we will study the case of using a multistep method with $2m$ steps for the numerical solution of the problem (1):

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

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 5 If $b_m \neq 0$, the method is implicit and if $b_m = 0$ it is explicit.

Remark 6 The method (2) is symmetric if

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

If we apply the method (2) with coefficients (3) (i.e. a symmetric $2m$-step method) to the scalar test equation

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

the following difference equation is obtained

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

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

The associated characteristic equation of the difference equation (5) is given by:

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

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

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

Remark 7 A direct method for the computation of the phase-lag of any symmetric $2m$-step method is given by the formula (7).

Remark 8 For the method which will be studied in this paper—for the low cost hybrid symmetric four-step method—the number $m = 2$ and the direct formula for the computation of the phase-lag is given by:

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

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

4 The new low computational cost proposed method

We consider the family of hybrid explicit symmetric four-step methods for the numerical solution of initial or boundary value problems of the form $y'' = f(x, y)$:

$$\begin{aligned} \bar{y}_n &= y_n - a_2\,h^2\left(y''_{n+1}-2\,y''_n+y''_{n-1}\right)-2\,a_3\,h^2\,y''_n \\ &\quad y_{n+2}+a_1\,y_{n+1}+a_0\,y_n+a_1\,y_{n-1}+y_{n-2} \\ &= h^2\left[b_1\,\left(y''_{n+1}+y''_{n-1}\right)+b_0\,\bar{y}''_n\right], \end{aligned} \tag{9}$$

where

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

and the coefficient $a_i,\ i = 0,\ 2,\ 3$ and $b_j,\ j = 0,\ 1$ are free parameters, h is the step size of the integration , n is the number of steps, y_n is the approximation of the solution on the point x_n, x_n, $x_n = x_0 + n\,h$ and x_0 is the initial value point.

The construction of the new hybrid low cost method is presented in the flowchart of the Fig. 3.

Our study for the new hybrid method (9) is based on the above flowchart. Therefore, we apply the new method (9) to the scalar test equation (4). The result of this application is the difference equation (5) with $m = 2$ and $A_j(v)$, $j = 0,\ 1,\ 2$ given by:

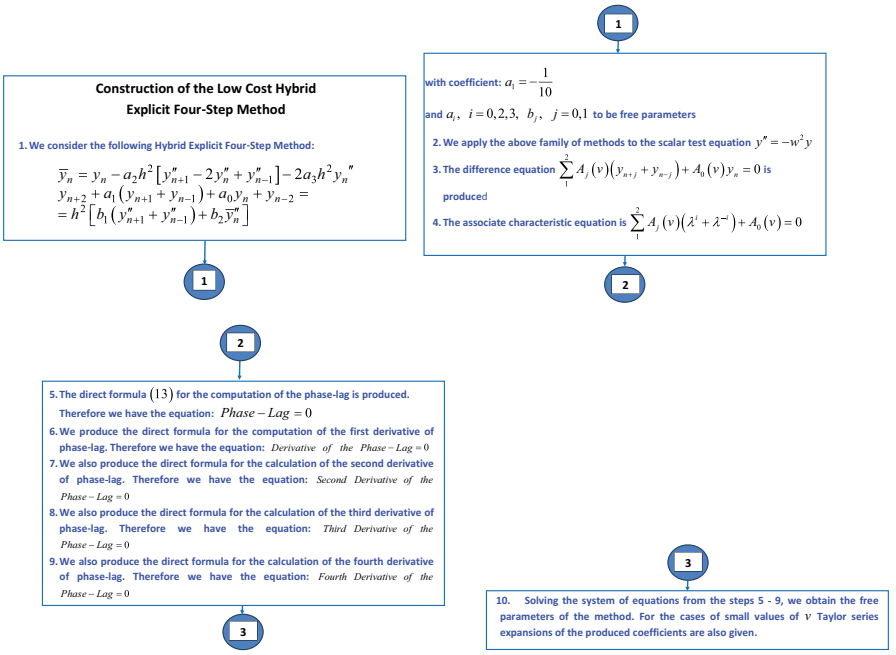

Fig. 3 Flowchart of the construction of any method of the family

$$A_2(v) = 1,\ A_1(v) = -\frac{1}{10} + v^2\left(v^2\,a_2\,b_0 + b_1\right)$$
$$A_0(v) = a_0 + v^2\,b_0\left(-2\,a_2\,v^2 + 2\,a_3\,v^2 + 1\right) \tag{11}$$

Using the formulae (8) and (11) and since our method (9) requests vanishing of the phase-lag and its first, second, third and fourth derivatives, the following system of equations is obtained:

$$\text{Phase-Lag} = \frac{T_0}{T_{denom}} = 0 \tag{12}$$
$$\text{First Derivative of the Phase-Lag} = \frac{T_1}{T_{denom}^2} = 0 \tag{13}$$
$$\text{Second Derivative of the Phase-Lag} = \frac{T_2}{T_{denom}^3} = 0 \tag{14}$$
$$\text{Third Derivative of the Phase-Lag} = \frac{T_3}{T_{denom}^4} = 0 \tag{15}$$
$$\text{Fourth Derivative of the Phase-Lag} = \frac{T_4}{T_{denom}^5} = 0 \tag{16}$$

where $T_j,\ j = 0(1)4$ and T_{denom} are given in Supplement Material A.

The solution of the above mentioned system of equations (12)–(16) gives the coefficients of the new low cost hybrid explicit four-step method:

$$a_3 = \frac{1}{4}\frac{T_5}{T_6}, \quad a_2 = \frac{1}{4}\frac{T_7}{T_8}, \quad a_0 = -\frac{1}{5}\frac{T_9}{T_{10}}$$
$$b_1 = -\frac{1}{5}\frac{T_{11}}{v^2\,T_{10}}, \quad b_0 = \frac{2}{5}\frac{T_{12}}{v^2\,T_{10}} \tag{17}$$

where T_i, $i = 5(1)12$ are given in Supplement Material B.

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

$$\begin{aligned}
a_3 = &-\frac{23}{162} + \frac{13789\,v^2}{944784} + \frac{1353383\,v^4}{151524457920} + \frac{257030521337\,v^6}{3866146543828800} \\
&- \frac{196786440533006381\,v^8}{4606104900051667584000} + \frac{323195010132376530919\,v^{10}}{39958420618438221457958400} \\
&+ \frac{74290704402157849162252614 91\,v^{12}}{17046693786768424406756799390720000} \\
&+ \frac{60206654185492044894693775573\,v^{14}}{97086248207454542129107084029960000 0} \\
&- \frac{17890543478220411720210383352400611281\,v^{16}}{14021683361930409503723496047076202782720000 00} \\
&- \frac{50507895841319749072828019947999278182291\,v^{18}}{35776325097965439848750500164114931400110080000000} + \cdots \\
a_2 = &-\frac{253}{5400} - \frac{13789\,v^2}{19683000} + \frac{24860200613\,v^4}{44194633560000} + \frac{5603512683427\,v^6}{80544719663100000} \\
&- \frac{18793107478018265309\,v^8}{13434472625150697120000 00} - \frac{11978480323108721237476 93\,v^{10}}{58272696735222406292856000 0000} \\
&+ \frac{45880103997455953119952972 1657\,v^{12}}{35513945389100884180743320640000 0000} \\
&+ \frac{45038508304217300916628869155441\,v^{14}}{80905206839545451774255903358300 0000000} \\
&- \frac{18396036644350200310686810152021988829997\,v^{16}}{34762090001452473561314500616709752732160000000000} \\
&- \frac{67195781981382165124246827942245305967683 87\,v^{18}}{55090355676214898317822328151263934221184000000000000} + \cdots \\
a_0 = &-\frac{9}{5} + \frac{13789\,v^{10}}{84672000} - \frac{70241\,v^{12}}{4694215680} + \frac{43110959\,v^{14}}{59147117568000} \\
&- \frac{44855753\,v^{16}}{1761508701388800} + \frac{3432896953273\,v^{18}}{11413783706083799040000} + \cdots
\end{aligned}$$

$$
\begin{aligned}
b_0 = {} & \frac{81}{28} - \frac{13789\,v^2}{35280} + \frac{514081\,v^4}{9779616} - \frac{161722807\,v^6}{123223161600} \\
& - \frac{63428323157\,v^8}{80735815480320} + \frac{381354897348343\,v^{10}}{5944679013585312000} \\
& - \frac{1318361709125692223\,v^{12}}{455409969872743581696000} + \frac{10600930992096878467\,v^{14}}{1147633124079313825873920000} \\
& - \frac{20597760327850294781060 3\,v^{16}}{2377976167411023799178573414400000} \\
& + \frac{46298716134741086398304563\,v^{18}}{599249994187577997393000500428800000} + \cdots \\
b_1 = {} & \frac{141}{280} + \frac{13789\,v^2}{70560} - \frac{514081\,v^4}{19559232} + \frac{161722807\,v^6}{246446323200} \\
& - \frac{11558001461\,v^8}{807358154803200} + \frac{5370545390141\,v^{10}}{19022972843472998400} \\
& + \frac{20838432004969571\,v^{12}}{9108199397454871633920000} + \frac{87686104037081959\,v^{14}}{4590532496317255303495 6800} \\
& + \frac{53929663347835927866899\,v^{16}}{475595233482204759835714682880000} \\
& + \frac{59657355983835853478909 27\,v^{18}}{11984999883751559947860010008576000 00} + \cdots
\end{aligned} \tag{18}
$$

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

The new obtained method is the low cost hybrid four-step method (9) with the coefficients given by (17)–(18).

The LTE of this new proposed method (mentioned as $HyMeth8$) is given by:

$$
\begin{aligned}
LTE_{HyMeth8} = {} & \frac{13789\,h^{10}}{84672000}\Big(y_n^{(10)} + 5\,w^2\,y_n^{(8)} + 10\,w^4\,y_n^{(6)} \\
& + 10\,w^6\,y_n^{(4)} + 5w^8\,y_n^{(2)} + w^{10}\,y_n\Big) + O(h^{12})
\end{aligned} \tag{19}
$$

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

5 Comparative error analysis

We will study the following similar methods:

5.1 Classical predictor–corrector explicit four-step method, i.e. the method (9) with constant coefficients

$$
LTE_{CL} = \frac{13789\,h^{10}}{84672000}\,y_n^{(10)} + O(h^{12}) \tag{20}
$$

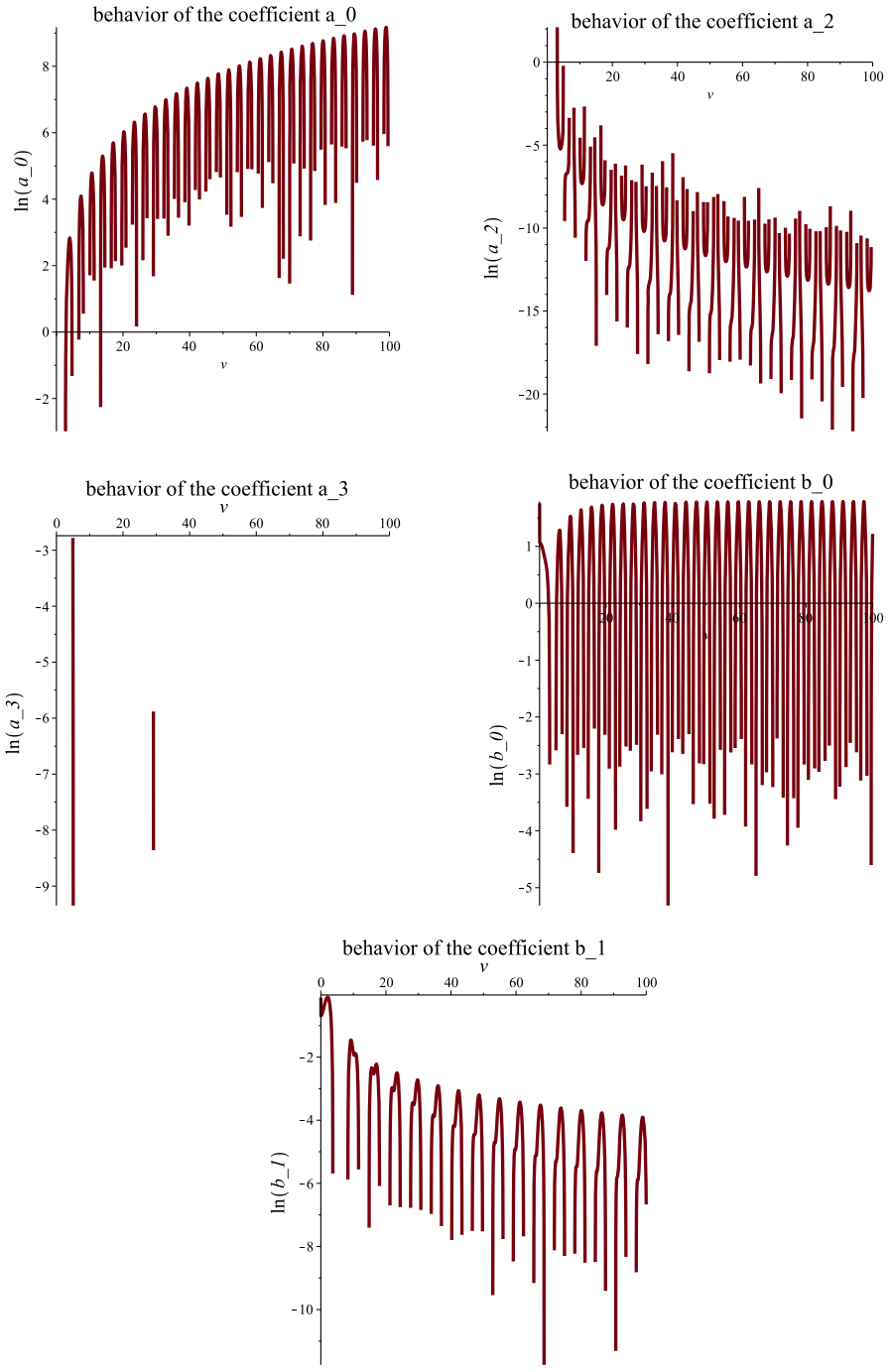

Fig. 4 Behavior of the coefficients of the new proposed method given by (17) for several values of $v = w\,h$

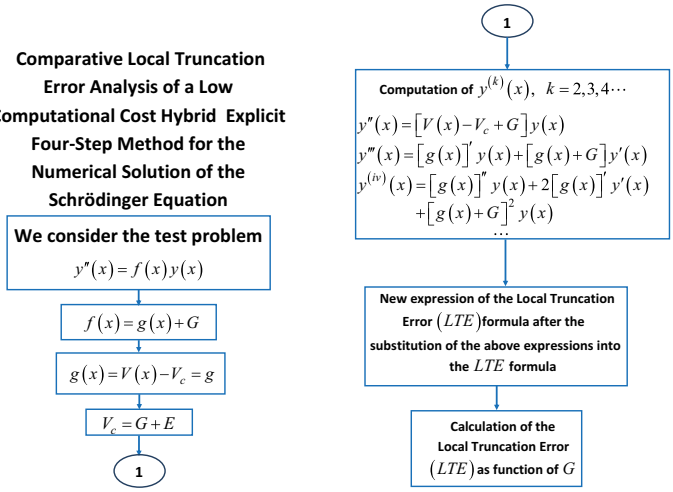

Fig. 5 Flowchart of the algorithm for the computations on the comparative error analysis

5.2 The low computational cost hybrid explicit four-step method with vanished phase-lag and its first, second, third and fourth derivatives developed in Sect. 4

$$LTE_{HyMeth8} = \frac{13789\,h^{10}}{84672000}\left(y_n^{(10)} + 5\,w^2\,y_n^{(8)} + 10\,w^4\,y_n^{(6)} + 10\,w^6\,y_n^{(4)} + 5w^8\,y_n^{(2)} + w^{10}\,y_n\right) + O(h^{12}) \tag{21}$$

The flowchart based on which we will investigate our comparative LTE analysis is presented in the Fig. 5.

Based on the above flowchart, we have to calculate the derivatives included in the formulae of the LTE (based on the test equation which we use for the comparative LTE analysis). These formulae of the derivatives are given by:

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

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

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

– **The Energy** (E) **is closed to the potential**, i.e., $G = V_c - E \approx 0$. Therefore, all the terms of the formulae of the LTE which include non zero powers of G (i.e. $G^j,\ j \neq 0$) are equal to zero (since $G \approx 0$). Consequently, only the free of G terms of the formulae of the LTE exist.

Remark 9 Same multistep methods with different coefficients have the same free of G terms in the formulae of the LTE.

Based on the above mentioned remark in the specific case the formulae of the LTE for both cases of methods (i.e. classical methods (methods with constant coefficients) and methods with vanished the phase-lag and its derivatives) are the same. Therefore, the error for the 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.

– **The Energy** (E) **is far from the potential i.e. for the quantity** G **we have:** $G \gg 0$ **or** $G \ll 0$. Then $|G|$ is a large number. In this case the formulae of the LTE are different for the numerical methods of the same family (classical methods (methods with constant coefficients) and (2) methods with vanished the phase-lag and its derivatives).

The asymptotic expressions of the LTEs (based on the methodology presented above) are given by:

5.3 Classical method

$$LTE_{CL} = h^{10}\left(\frac{13789\, y\,(x)}{84672000}\right) G^5 + \cdots + O(h^{12}) \tag{22}$$

5.4 The predictor–corrector explicit four-step method with vanished phase-lag and its first, second, third and fourth derivatives developed in Sect. 4

$$LTE_{HyMeth8} = h^{10}\left(\frac{13789\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4} g\,(x)\right) y\,(x)}{5292000}\right) G^2 + \cdots + O(h^{12}) \tag{23}$$

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

Theorem 2 *The Analysis presented above gives us the following conclusions:*

– *For the Classical Hybrid Explicit Four-Step Method the error increases as the fifth power of* G.
– *For the Hybrid Explicit Four-Step Method with Vanished Phase-Lag and its First, Second, Third and Fourth Derivatives developed in Sect. 4, the error increases as the second power of* G.

So, for the numerical solution of the Schrödinger equation the New Proposed Low Computational Cost Hybrid Explicit Four-Step Method with Vanished Phase-Lag and its First, Second, Third and Fourth Derivatives developed in Sect. 4 is the most efficient, from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

6 Stability analysis

Our stability analysis for the new low cost hybrid explicit four-step method (9) with the coefficients given by (10) and (17) is based on the flowchart presented Fig. 6.

Applying the above described method to the scalar test equation:

$$y'' = -z^2\, y \tag{24}$$

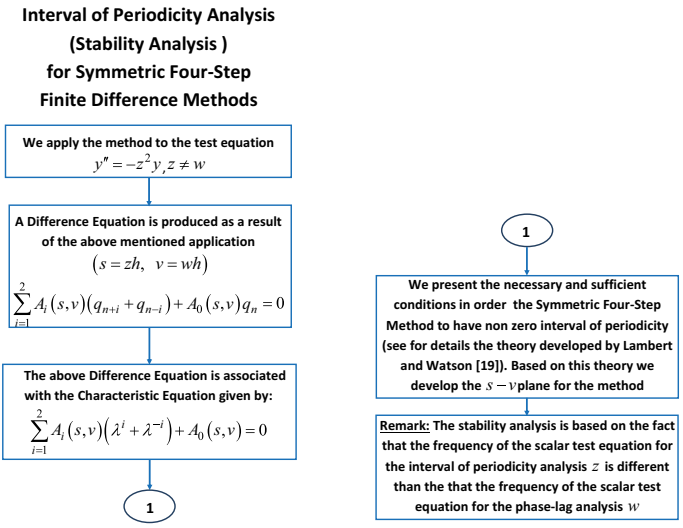

Fig. 6 Flowchart for the stability analysis of the new low cost hybrid explicit four-step method

we have the following difference equation:

$$A_2(s, v)\ (y_{n+2} + y_{n-2}) + A_1(s, v)\ (y_{n+1} + y_{n-1}) + A_0(s, v)\ y_n = 0 \quad (25)$$

where

$$A_2(s, v) = 1, \quad A_1(s, v) = \frac{1}{10}\frac{T_{13}}{T_{14}}, \quad A_0(s, v) = \frac{1}{5}\frac{T_{15}}{T_{14}} \quad (26)$$

where $s = z\,h$ and $T_j,\ j = 13(1)15$ are given in Supplement Material C.

Remark 10 The frequency of the scalar test equation (4) for the phase-lag analysis, w, is different than the frequency of the scalar test equation (24) for the stability analysis, z i.e. $z \neq w$.

The characteristic equation which is associated to the difference equation (25) is given by:

$$A_2(s, v)\ (\lambda^4 + 1) + A_1(s, v)\ (\lambda^3 + \lambda) + A_0(s, v)\ \lambda^2 = 0 \quad (27)$$

Definition 1 (see [21]) A symmetric $2\,m$-step method with the characteristic equation given by (27) 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

$$\lambda_{1,2} = e^{\pm i\,\zeta(s)}, \quad |\lambda_i| \leq 1, \quad i = 3, 4, \ldots \quad (28)$$

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

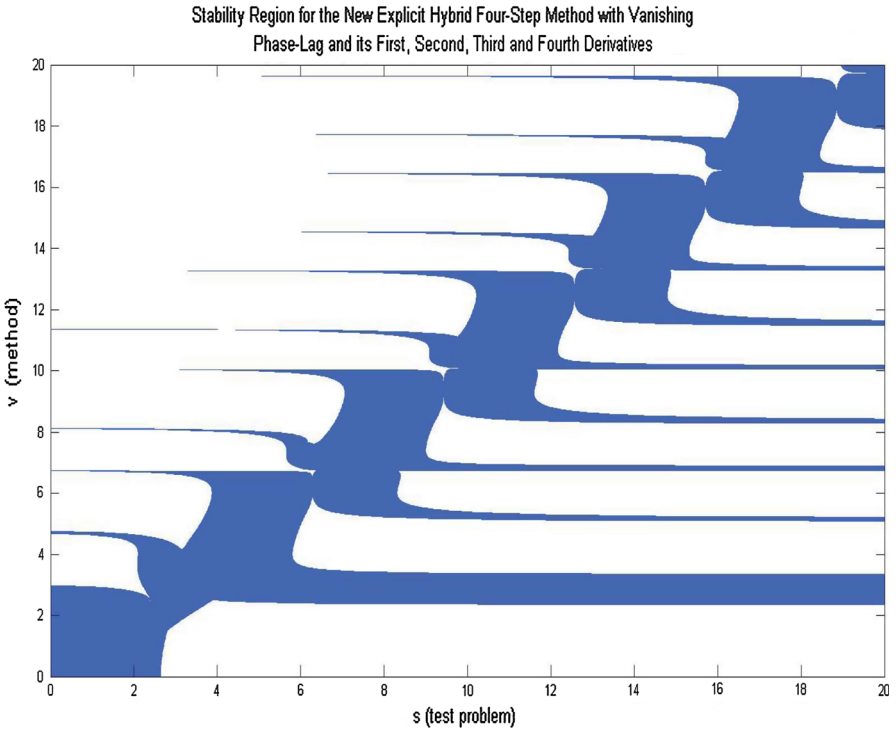

Fig. 7 s–v plane of the predictor–corrector symmetric explicit four-step method (9) with the coefficients given by (10) and (17)

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 11 A method can be characterized as singularly almost P-stable only in 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 (24) for the stability analysis z, i.e. only when $w = z$.

In Fig. 7, we present the s–v plane of the new proposed low cost hybrid four-step method. The shadowed area of the s–v region is the stable area, while the white area is the unstable area.

Remark 12 The investigation of the stability of the above mentioned family of methods leads to two categories of problems for which these methods can be applied:

– Problems where 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 where 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. $z = w$)

The Schrödinger equation and related problems are belonged into the second category of problems described above.

For the first category of problems we have to develop the s–v plane in order to investigate the stability of the proposed method (see Fig. 7 for our new obtained hybrid low computational cost symmetric four-step method).

For the second category of problems we have to observe **the surroundings of the first diagonal of the s–v plane**.

Investigating the second category of problems, i.e. investigating the case where $z = w$ or $s = v$ (i.e. seeing the surroundings of the first diagonal of the s–v plane), we extract the result that the interval of periodicity of the new produced four-step method developed in Sect. 4 is equal to: $(0, 16)$.

From the above analysis, we have the following theorem:

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

– *is of hybrid type method*
– *is of a low computational cost since it has only two stages*
– *is of eighth algebraic order,*
– *has the phase-lag equals to zero*
– *has phase-lag's first, second, third and fourth derivatives equal to zero*
– *has an interval of periodicity equals to:* $(0, 16)$ *in 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*

7 Numerical results

7.1 Radial Schrödinger equation

In order to examine the efficiency of the new developed method, the numerical solution of the radial time-independent Schrödinger equation will be examined.

The radial time-independent Schrödinger equation has the form:

$$y''(r) = [l(l+1)/r^2 + V(r) - k^2]\, y(r), \tag{29}$$

where:

– The function $Q(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. For the effective potential, we have the following relation: $Q(r) \to 0$ 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*.

The above described problem is a boundary value problem. Therefore, we need two boundary conditions. The first is given by the definition of the problem:

$$y(0) = 0 \tag{30}$$

while the second boundary condition, for large values of r, is determined by physical considerations.

Since the new obtained hybrid low computational cost symmetric explicit four-step method is a frequency dependent methods, the determination of the value of the parameter w (frequency) in order to be possible the application of the method to the numerical solution of the radial Schrödinger equation. Based on the mathematical model given by (29), the parameter w is given by (for the case $l = 0$):

$$w = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{31}$$

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

7.1.1 Woods–Saxon potential

The model of the time-independent radial Schrödinger equation (29) consists of the function of the potential (which is defined by the user). The known Woods–Saxon potential is used for our numerical tests. The Woods–Saxon potential is given by

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{32}$$

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

The behavior of Woods–Saxon potential is shown in Fig. 8.

In order to determine the frequency w , some values of the potential on critical points are defined (see for details [116]). The critical point are defined studying the specific potential. The above described methodology for the definition of the frequency w is one of several methodologies for the determination of the frequency for these type of methods (see [28] and references therein).

Remark 13 The above described methodology is known applied to some potentials, such as the Woods–Saxon potential.

Here is the methodology for the choice of w for our numerical tests (see for details [1,90]):

$$w = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{33}$$

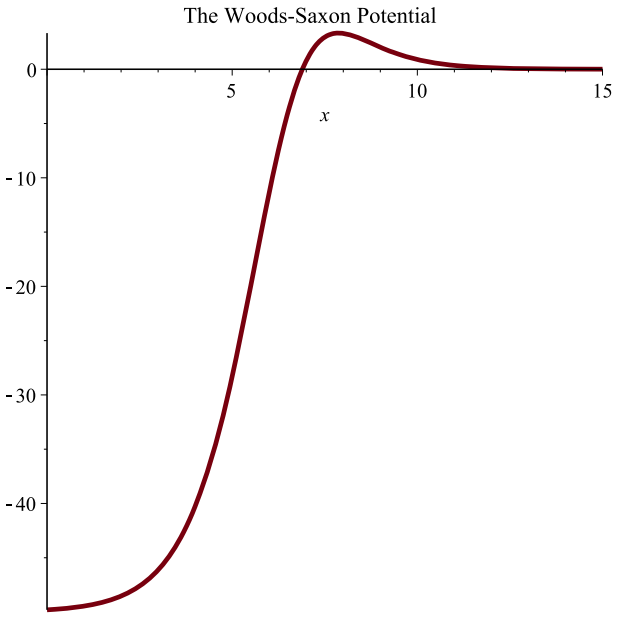

Fig. 8 The Woods–Saxon potential

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

7.1.2 The radial Schrödinger equation and the resonance problem

We will use for our numerical tests the approximate solution of the radial time independent Schrödinger equation (29) with Woods–Saxon potential (32). This problem belongs to the boundary value problems which has an infinite interval of integration. For the purpose of the numerical solution of the above mentioned problem we have to approximate the infinite interval of integration by a finite one. For our numerical experiments we consider the interval of integration $r \in [0, 15]$ and a large domain of energies, i.e., $E \in [1, 1000]$.

Remark 14 In the case of positive energies, $E = k^2$ the potential decays faster than the term $\frac{l(l+1)}{r^2}$.

Based on the above remark, the Schrödinger equation reduces to:

$$y''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) y(r) = 0 \tag{34}$$

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 equation (29) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} y(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{35}$$

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

$$\tan \delta_l = \frac{y(r_2)\, S(r_1) - y(r_1)\, S(r_2)}{y(r_1)\, C(r_1) - y(r_2)\, C(r_2)} \tag{36}$$

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 (the radial Schrödinger equation is treated as an initial-value problem) we need y_j, $j = 0(1)3$ before starting a four-step method. The initial condition defines the first value of y i.e. y_0. Using high order Runge–Kutta–Nyström methods(see [121,122]) we determine the values y_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.

For positive energies, we have the so-called resonance problem. This 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:

$$y(0) = 0, \;\; y(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{37}$$

The positive eigenenergies of the Woods–Saxon potential resonance problem are computed 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 [27] with minimal phase-lag, which is indicated as **Method MCR4**.
- The exponentially-fitted method of Raptis and Allison [91], which is indicated as **Method RA**.
- The hybrid sixth algebraic order method developed by Chawla and Rao [26] with minimal phase-lag, which is indicated as **Method MCR6**.

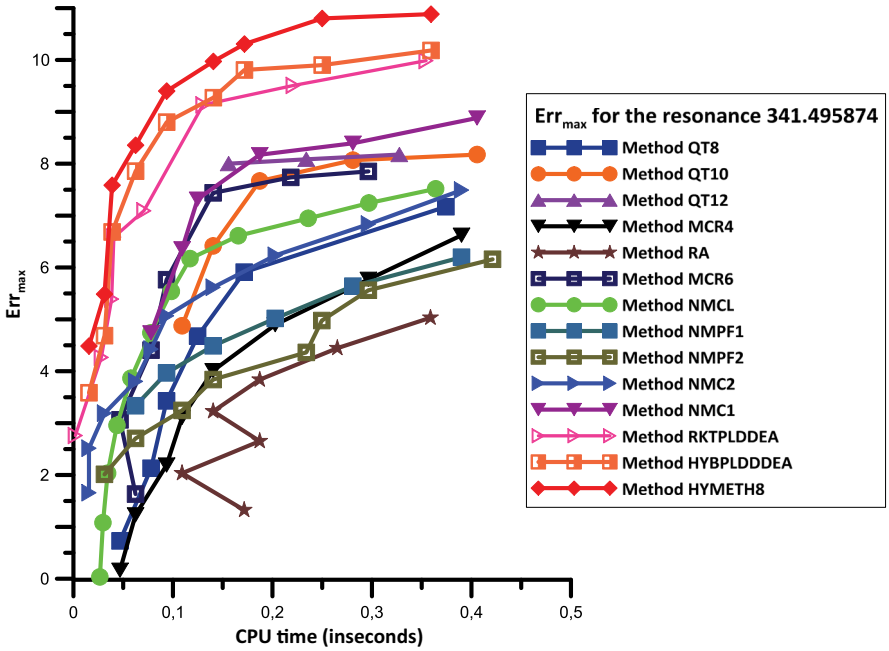

Fig. 9 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

- The 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 [47], which is indicated as **Method NMPF1**.
- The Phase-Fitted Method (Case 2) developed in [47], which is indicated as **Method NMPF2**.
- The Method developed in [51] (Case 2), which is indicated as **Method NMC2**.
- The Method developed in [51] (Case 1), which is indicated as **Method NMC1**.
- The Method developed in [45], which is indicated as **Method RKTPLDDEA**.
- The Method developed in [57], which is indicated as **Method HYBPLDDDEA**.
- The New Obtained Hybrid Low Computational Cost Four-Step Method developed in Sect. 4, which is indicated as **Method HYMETH8**.

We compare the computed eigenenergies via the above mentioned methods with reference values.[3] In Figs. 9 and 10, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{38}$$

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

[3] The reference values are computed using the well known two-step method of Chawla and Rao [26] with small step size for the integration.

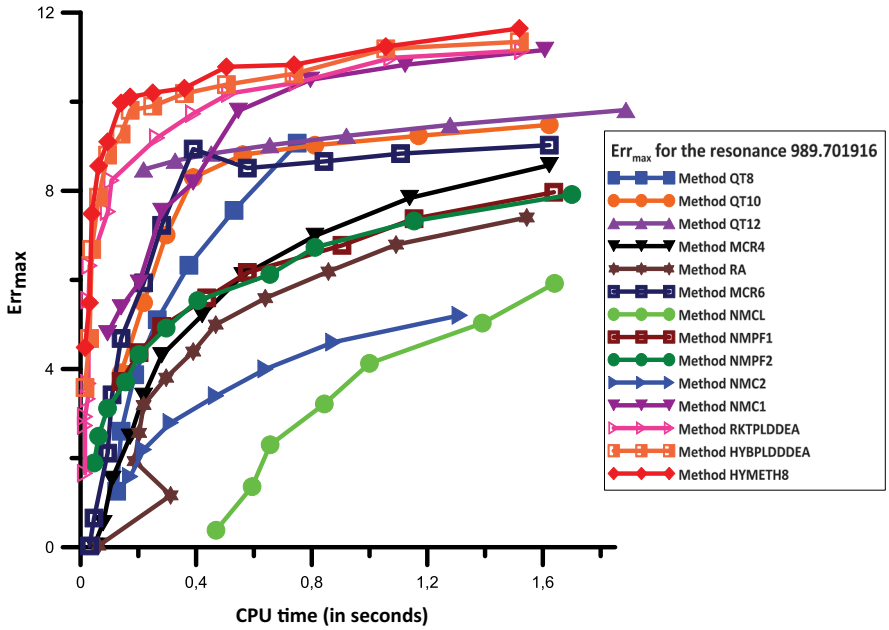

Fig. 10 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is less than 0

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

An efficient low computational cost hybrid explicit four-step method of eight algebraic order was investigated in this paper. More specifically, we constructed a method with vanishing the phase-lag and its first, second, third and fourth derivatives. We investigated the specific method as one block. We also studied how this vanishing procedure effects on the computational efficiency of the proposed method.

The theoretical investigation of the developed method consists of the comparative LTE analysis and the stability analysis (using scalar test equation with frequency different than the frequency of the phase-lag analysis).

We studied also the computational efficiency of the obtained method via numerical tests which was based on the numerical solution of the resonance problem of the radial time independent Schrödinger equation.

The new introduced 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 experiments described 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 [27] with minimal phase-lag, which is indicated as **Method MCR4**. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [91], 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 [47], which is indicated as **Method NMPF1** and the Phase-Fitted Method (Case 2) developed in [47], 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 [27] with minimal phase-lag, 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 [51] (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 [51] (Case 1), which is indicated as **Method NMC1**.
6. The Method developed in [57], which is indicated as **Method HYBPLDDDEA** is more efficient than method developed in [45], which is indicated as **Method RKTPLDDEA**.
7. Finally, low computational cost hybrid explicit four-step method of eight algebraic order with vanished phase-lag and its first, second, third and fourth derivatives (obtained in Sect. 4), which is indicated as **Method HYMETH8**, 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).

Conflict of interest None.

Informed Consent Consent to submit has been received explicitly from all co-authors, as well as from the responsible authorities—tacitly or explicitly—at the institute/organization where the work has been carried out, before the work is submitted.

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