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

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Abstract A hybrid explicit sixth algebraic order four-step method with phase-lag and its first, second and third derivatives vanished is obtained in this paper. We present the development of the new method, its comparative error analysis and its stability analysis. The resonance problem of the Schrödinger equation, is used in order to study the efficiency of the new developed method. After the presentation of the theoretical and the computational results it is easy to see that the new constructed method is more efficient than other well known methods for the approximate solution of the Schrödinger equation and related initial-value or boundary-value problems with periodic and/or oscillating solutions.

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

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1 Introduction

In the present paper we investigate the efficient numerical solution of special second-order initial-value or boundary-value problems of the form

$$p''(x) = f(x, p), \quad p(x_0) = y_0 \ and \ p'(x_0) = y_0'$$ (1)
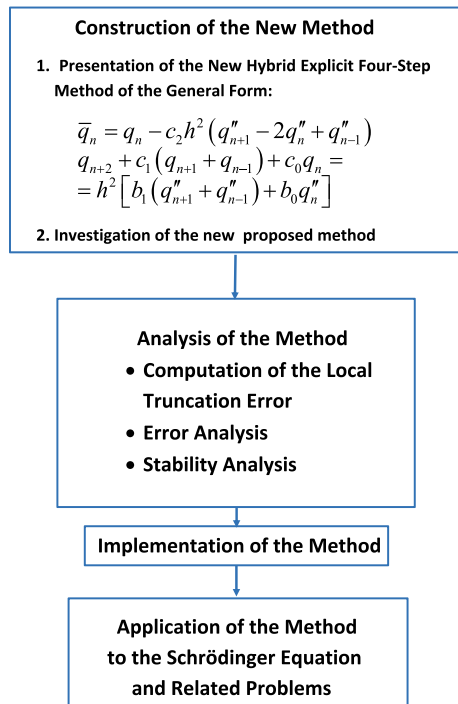
with a periodical and/or oscillatory solutions.

The main feature of this category of problems is that the system of ordinary differential equations which describe the above mathematical models are of second order in which the first derivative p' does not appear explicitly (see for more details [1–120] and references therein).

In Fig. 1, we present the structure of the present paper which is based on the following sections:

In Sect. 2, we present some bibliography on the subject of the research of this paper. Some points of the phase-lag analysis of the symmetric multistep methods are presented in Sect. 3. In Sect. 4 we present the development of the new hybrid explicit four-step method. The comparative error analysis is studied in Sect. 5. In Sect. 6 the stability analysis is described. Finally, in Sect. 7 we present the numerical results produced by the application of the new obtained methods to the resonance problem of the one-dimensional Schrödinger equation. In the same section we comment the

Fig. 1 Flowchart of the formulation of the present paper

Construction of the New Method

1. **Presentation of the New Hybrid Explicit Four-Step Method of the General Form:**

$$\bar{q}_n = q_n - c_2 h^2 \left(q''_{n+1} - 2q''_n + q''_{n-1} \right)$$
$$q_{n+2} + c_1 \left(q_{n+1} + q_{n-1} \right) + c_0 q_n =$$
$$= h^2 \left[b_1 \left(q''_{n+1} + q''_{n-1} \right) + b_0 q''_n \right]$$

2. **Investigation of the new proposed method**

Analysis of the Method
- Computation of the Local Truncation Error
- Error Analysis
- Stability Analysis

Implementation of the Method

Application of the Method to the Schrödinger Equation and Related Problems

comparative application of the new produced method with other well know methods in the literature.

2 Bibliography relevant on the subject of the paper

The approximate solution of the radial time independent Schrödinger equation and the numerical solution of related problems was the subject of extended research the last decades.

The main directions of this research are presented in Fig. 2. The aim and scope of this research was the construction of efficient, fast and reliable algorithms (see for example [1–113]).

Below we give some bibliography on this research:

– Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta–Nyström type have been obtained in [1–7].
– In [8–13] exponentially and trigonometrically fitted Runge–Kutta and Runge–Kutta–Nyström methods are constructed.
– Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [26–54].
– Symplectic integrators are investigated in [55–83].
– Exponentially and trigonometrically multistep methods have been produced in [86–106].
– Nonlinear methods have been studied in [107] and [108]
– Review papers have been presented in [109–113]
– Special issues and Symposia in International Conferences have been developed on this subject (see [32,33])
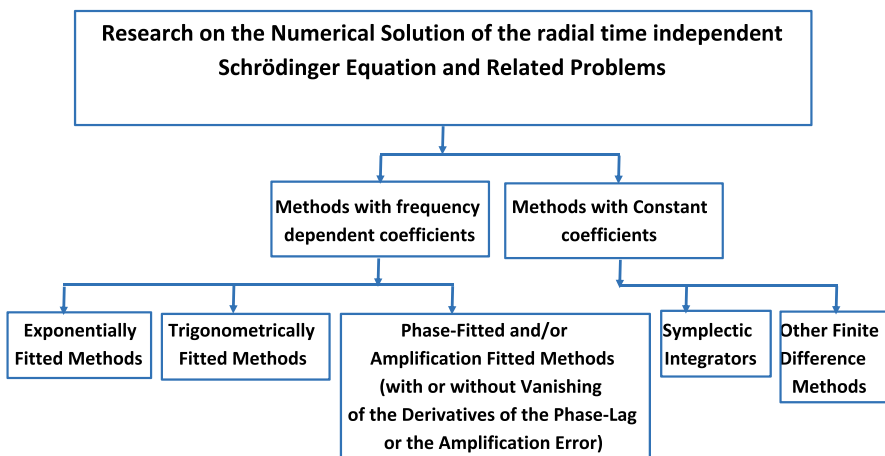
Fig. 2 The main categories of the methods developed the last decades

3 Phase-lag analysis for symmetric multistep finite difference methods

Multistep finite difference methods which can be written in the form

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

are used for the approximate solution of the initial value problems of the form (1).

We mention that in the formula (2),

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

In the case of symmetric multistep finite difference method we have $c_i = c_{m-i}$ and $b_i = b_{m-i}, \; i = 0(1)\lfloor \frac{m}{2} \rfloor$.

It is known from the literature (see for details [14]) that the multistep finite difference methods of the form (2) are associated with the operator

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

where $p \in C^2$.

Definition 1 [21] The multistep finite difference method (2) is called algebraic of order q if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, \, x, \, x^2, \, \ldots, \, x^{q+1}$.

Now we consider the symmetric $2\,k$-step finite difference method, that is for $i = -k(1)k$. If we apply this method to the scalar test equation

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

the following difference equation is obtained:

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

where

1. $v = \omega \, h$,
2. h is the step length and
3. $A_j(v) \; j = 0(1)k$ are polynomials of v.

Remark 1 The characteristic equation:

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

is associated with (5).

Lambert and Watson [14] introduced the following definition:

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

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

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

Definition 3 [24,25] For any finite difference method corresponding to the characteristic Eq. (6) the phase-lag is defined as the leading term in the expansion of

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

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

Definition 4 [22] **Phase-fitted** is called a method for which the phase-lag vanishes.

Theorem 1 [24] *The symmetric* $2\,k$-step finite difference method with characteristic equation given by (6) has phase-lag order r and phase-lag constant c given by

$$- cv^{r+2} + O(v^{r+4}) = \frac{2\,A_k(v)\,\cos(k\,v) + \cdots + 2\,A_j(v)\,\cos(j\,v) + \cdots + A_0(v)}{2\,k^2\,A_k(v) + \cdots + 2\,j^2\,A_j(v) + \cdots + 2\,A_1(v)} \tag{9}$$

The above theorem gives us a direct formula for the computation of the phase-lag of any symmetric $2\,k$-step finite difference method.

Remark 2 If we have a symmetric four-step finite difference method (i.e. for $k = 2$), and based on the above theorem, we have the direct formula for the computation of the phase-lag for this class of methods. Based on the above theorem, in the case of four-step symmetric finite difference methods, the phase-lag order r and phase-lag constant c can be computed by the direct formula:

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

4 The family of hybrid explicit four-step methods with vanished phase-lag and its first, second and third derivatives

Consider the following explicit symmetric $2\,m$-step finite difference method:

$$p_{n+m} + \sum_{i=0}^{m-1} c_i\,(p_{n+i} + p_{n-i}) + p_{n-m} = h^2 \sum_{i=1}^{m-1} b_i\,\big[\,f(x_{n+i}, p_{n+i}) + f(x_{n-i}, p_{n-i})\big]$$
$$+ b_0\,f(x_n, p_n) \tag{11}$$

Now we can produce from the above form (11) the specific case of $m = 2$. Then, we have the following form of the explicit symmetric four-step finite difference methods [21]:

$$p_{n+2} + c_1 \left(p_{n+1} + p_{n-1}\right) + c_0 \, p_n + q_{n-2} = h^2 \left[b_1 \left(f_{n+1} + f_{n-1}\right) + b_0 \, f_n\right]$$

(12)

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

We introduce now the new proposed hybrid (nonlinear) explicit symmetric four-step finite difference method:

$$\bar{p}_n = p_n - c_2 \, h^2 \left(f_{n+1} - 2 \, f_n + f_{n-1}\right)$$

$$p_{n+2} + c_1 \left(p_{n+1} + p_{n-1}\right) + c_0 \, p_n + q_{n-2} = h^2 \left[b_1 \left(f_{n+1} + f_{n-1}\right) + b_0 \, \bar{f}_n\right]$$

(13)

Choosing (13), we consider:

$$c_1 = -\frac{1}{10}$$

(14)

Remark 3 The above mentioned value for the free parameter c_1 is based on the paper [21] where it has been proved that the above value of c_1 gives for the method (12) the highest accuracy.

Demanding the above hybrid explicit method to have the phase-lag and its first, second and third derivatives vanished, the following system of equations is produced:

$$\text{Phase-Lag (PL)} = \frac{T_1}{\frac{39}{5} + 2 \, v^2 \left(v^2 \, b_0 \, c_2 + b_1\right)} = 0$$

$$\text{First Derivative of PL} = -\frac{T_2}{\left(10 \, v^4 \, b_0 \, c_2 + 10 \, v^2 \, b_1 + 39\right)^2} = 0$$

$$\text{Second Derivative of PL} = -\frac{T_3}{\left(10 \, v^4 \, b_0 \, c_2 + 10 \, v^2 \, b_1 + 39\right)^3} = 0$$

$$\text{Third Derivative of PL} = \frac{T_4}{\left(10 \, v^4 \, b_0 \, c_2 + 10 \, v^2 \, b_1 + 39\right)^4} = 0 \qquad (15)$$

where $T_i, \, i = 1(1)4$ are given in the Appendix A.

We solve the above system of equations and we obtain the coefficients of the new proposed method:

$$b_0 = \frac{T_5}{T_6}, \; b_1 = \frac{T_7}{T_8}$$
$$c_0 = \frac{T_9}{T_{10}}, \; c_2 = \frac{T_{11}}{T_{12}} \tag{16}$$

where T_i, $i = 5(1)10$ are given in the Appendix B.

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

$$b_0 = \frac{5}{4} + \frac{23}{560} v^4 - \frac{1259}{100800} v^6 + + \frac{9967}{53222400} v^8$$
$$- \frac{189179}{3492720000} v^{10} + \frac{7772041}{2615348736000} v^{12}$$
$$+ \frac{434711603}{635156121600000} v^{14} + \frac{11249576581}{118266069841920000} v^{16}$$
$$+ \frac{96270093790883}{14050009097220096000000} v^{18} + \cdots$$

$$b_1 = \frac{53}{40} - \frac{23}{1120} v^4 - \frac{121}{201600} v^6 - \frac{713}{21288960} v^8$$
$$+ \frac{236861}{27941760000} v^{10} + \frac{9724763}{5230697472000} v^{12}$$
$$+ \frac{143249983}{684014284800000} v^{14} + \frac{4303500293}{394220232806400000} v^{16}$$
$$- \frac{2148508540481}{2161539861110784000000} v^{18} + \cdots$$

$$c_0 = -\frac{9}{5} + \frac{23}{6720} v^8 - \frac{109}{1008000} v^{10} + \frac{41}{3193344} v^{12}$$
$$- \frac{10583}{5588352000} v^{14} - \frac{29369}{116237721600} v^{16}$$
$$- \frac{219269}{8420630400000} v^{18} + \cdots$$

$$c_2 = -\frac{161}{3000} + \frac{23}{2100} v^2 + \frac{19493}{12600000} v^4 - \frac{80437069}{87318000000} v^6$$
$$+ \frac{30323213}{498960000000} v^8 + \frac{43592759593}{1059458400000000} v^{10}$$
$$- \frac{35200693505111}{3241942704000000000} v^{12} - \frac{681898980020813647}{1280599787507040000000000} v^{14}$$
$$+ \frac{6652855944464510537}{9313453000051200000000000} v^{16}$$
$$- \frac{13893797143983011464 9523}{148447127367816076800000000000} v^{18} + \cdots \tag{17}$$
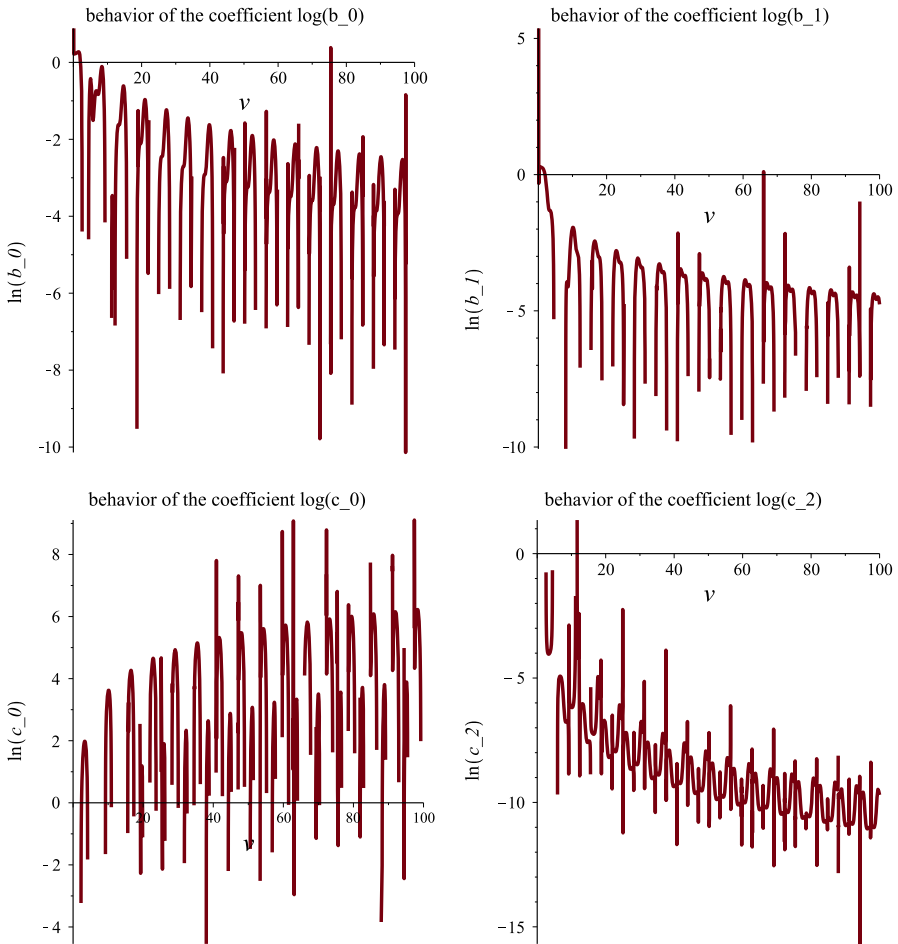
Fig. 3 Behavior of the coefficients of the new proposed method given by (16) for several values of $v = \omega h$

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

The new obtained method (12) (mentioned as *Four Step I*) with the coefficients given by (16) and (17) has a local truncation error which is given by:

$$LTE_{Four\ Step\ New\ Hybrid} = \frac{23\,h^8}{6720} \left(p_n^{(8)} + 4\,\omega^2\,p_n^{(6)} + 6\,\omega^4\,p_n^{(4)} + 4\,\omega^6\,p_n^{(2)} + \omega^8\,p_n \right)$$
$$+ O\left(h^{10}\right) \tag{18}$$

5 Comparative error analysis

We will study two classes of methods:

– Explicit linear four-step methods of algebraic order four and

– The new hybrid (nonlinear) explicit four-step method of algebraic order six

Therefore, we will investigate the following cases:

5.1 The fourth algebraic order classical method (i.e. the method (12) with constant coefficients)

$$LTE_{CL} = \frac{161\,h^6}{2400}\,p_n^{(6)} + O\left(h^8\right) \tag{19}$$

5.2 The fourth algebraic order method with vanished phase-lag produced in [21]

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

5.3 The fourth algebraic order method with vanished phase-lag and its first derivative produced in [49]

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

5.4 The fourth algebraic order method with vanished phase-lag and its first and second derivatives in [53]

$$LTE_{FourStepII} = \frac{161\,h^6}{2400}\left(p_n^{(6)} + 3\,\omega^2\,p_n^{(4)} + 3\,\omega^4\,p_n^{(2)} + \omega^6\,p_n\right) + O\left(h^8\right) \tag{22}$$

5.5 The sixth algebraic order hybrid method with vanished phase-lag and its first, second and third derivatives developed in Sect. 4

$$LTE_{FourStepIII} = \frac{23\,h^8}{6720}\left(p_n^{(8)} + 4\,\omega^2\,p_n^{(6)} + 6\,\omega^4\,p_n^{(4)} + 4\,\omega^6\,p_n^{(2)} + \omega^8\,p_n\right)$$
$$+ O\left(h^{10}\right) \tag{23}$$

The procedure contains the following stages

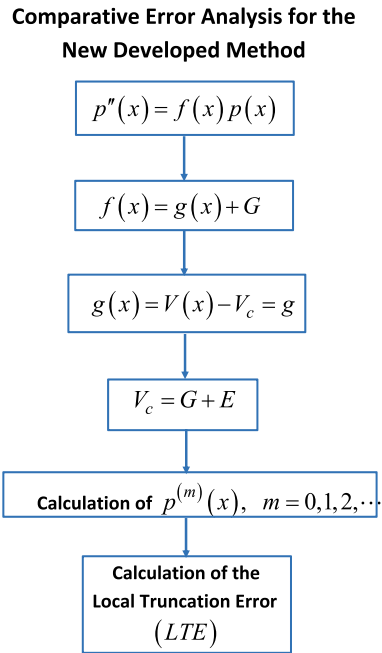– The radial time independent Schrödinger equation is of the form

$$p''(x) = f(x)\,p(x) \tag{24}$$

– Based on the paper of Ixaru and Rizea [86], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \tag{25}$$

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

Fig. 4 Flowchart for the
comparative error analysis

**Comparative Error Analysis for the
New Developed Method**

$$p''(x) = f(x)p(x)$$

$$f(x) = g(x) + G$$

$$g(x) = V(x) - V_c = g$$

$$V_c = G + E$$

Calculation of $p^{(m)}(x),\ \ m = 0,1,2,\cdots$

Calculation of the
Local Truncation Error
(LTE)

– We express the derivatives $p_n^{(i)}$, $i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of the Eq. (25). The expressions are presented as polynomials of G
– Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae

For the error analysis we follow the flowchart mentioned in the Fig. 4.

Based on the Eq. (25), we calculate the derivatives which presented in the formulae of the local truncation errors:

$$p_n^{(2)} = (V(x) - V_c + G)\ p(x)$$

$$p_n^{(3)} = \left(\frac{d}{dx} g(x)\right) p(x) + (g(x) + G) \frac{d}{dx} p(x)$$

$$p_n^{(4)} = \left(\frac{d^2}{dx^2} g(x)\right) p(x) + 2\left(\frac{d}{dx} g(x)\right) \frac{d}{dx} p(x)$$
$$+ (g(x) + G)^2\ p(x)$$

$$p_n^{(5)} = \left(\frac{d^3}{dx^3} g(x)\right) p(x) + 3\left(\frac{d^2}{dx^2} g(x)\right) \frac{d}{dx} p(x)$$
$$+ 4(g(x) + G)\ p(x) \frac{d}{dx} g(x) + (g(x) + G)^2 \frac{d}{dx} p(x)$$

$$p_n^{(6)} = \left(\frac{d^4}{dx^4} g(x)\right) p(x) + 4\left(\frac{d^3}{dx^3} g(x)\right) \frac{d}{dx} p(x)$$

$$+7\,(g\,(x)+G)\,p\,(x)\,\frac{d^2}{dx^2}g\,(x)+4\left(\frac{d}{dx}g\,(x)\right)^2 p\,(x)$$

$$+6\,(g\,(x)+G)\left(\frac{d}{dx}p\,(x)\right)\frac{d}{dx}g\,(x)$$

$$+\,(g\,(x)+G)^3\,p\,(x)$$

$$p_n^{(7)}=\left(\frac{d^5}{dx^5}g\,(x)\right)p\,(x)+5\left(\frac{d^4}{dx^4}g\,(x)\right)\frac{d}{dx}p\,(x)$$

$$+11\,(g\,(x)+G)\,p\,(x)\,\frac{d^3}{dx^3}g\,(x)+15\left(\frac{d}{dx}g\,(x)\right)p\,(x)$$

$$\frac{d^2}{dx^2}g\,(x)+13\,(g\,(x)+G)\left(\frac{d}{dx}p\,(x)\right)\frac{d^2}{dx^2}g\,(x)$$

$$+10\left(\frac{d}{dx}g\,(x)\right)^2\frac{d}{dx}p\,(x)+9\,(g\,(x)+G)^2\,p\,(x)$$

$$\frac{d}{dx}g\,(x)+(g\,(x)+G)^3\,\frac{d}{dx}p\,(x)$$

$$p_n^{(8)}=\left(\frac{d^6}{dx^6}g\,(x)\right)p\,(x)+6\left(\frac{d^5}{dx^5}g\,(x)\right)\frac{d}{dx}p\,(x)$$

$$+16\,(g\,(x)+G)\,p\,(x)\,\frac{d^4}{dx^4}g\,(x)+26\left(\frac{d}{dx}g\,(x)\right)p\,(x)$$

$$\frac{d^3}{dx^3}g\,(x)+24\,(g\,(x)+G)\left(\frac{d}{dx}p\,(x)\right)\frac{d^3}{dx^3}g\,(x)$$

$$+15\left(\frac{d^2}{dx^2}g\,(x)\right)^2 p\,(x)+48\left(\frac{d}{dx}g\,(x)\right)$$

$$\left(\frac{d}{dx}p\,(x)\right)\frac{d^2}{dx^2}g\,(x)+22\,(g\,(x)+G)^2\,p\,(x)$$

$$\frac{d^2}{dx^2}g\,(x)+28\,(g\,(x)+G)\,p\,(x)\left(\frac{d}{dx}g\,(x)\right)^2$$

$$+12\,(g\,(x)+G)^2\left(\frac{d}{dx}p\,(x)\right)\frac{d}{dx}g\,(x)$$

$$+\,(g\,(x)+G)^4\,p\,(x)$$

$$\cdots$$

For the completion of the comparative error analysis which is based on the mathematical models expressed via the Eq. (24), we follow the procedure described below:

1. We study two cases in terms of the value of E within the local truncation error analysis:
   a) The energy is close to the potential, i.e. $G = V_c - E \approx 0$. Consequently, the free terms of the polynomials in G are considered only. Thus, for these values

of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G are the same for the cases of the classical method and of the methods with vanished the phase-lag and its derivatives.

b) $G >> 0$ or $G << 0$. Then $|G|$ is a large number.

2. Finally we compute the asymptotic expansions of the local truncation errors

The analysis presented above leads to the following asymptotic expansions of the local truncation errors:

5.6 Classical method

$$LTE_{CL} = h^6 \left(\frac{161}{2400} p(x) G^3 + \cdots \right) + O\left(h^8\right) \qquad (26)$$

5.7 The method with vanished phase-lag produced in [21]

$$LTE_{MethAnasSim} = h^6 \left(\frac{161}{2400} g(x) p(x) G^2 + \cdots \right) + O\left(h^8\right) \qquad (27)$$

5.8 The method with vanished phase-lag and its first derivative produced in [49]

$$LTE_{FourStepI} = h^6 \left[\left(\frac{161}{2400} (g(x))^2 p(x) + \frac{161}{1200} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} p(x) \right.\right.$$
$$\left.\left. + \frac{161}{480} \left(\frac{d^2}{dx^2} g(x) \right) p(x) \right) G + \cdots \right] + O\left(h^8\right) \qquad (28)$$

5.9 The method with vanished phase-lag and its first and second derivatives developed in [53]

$$LTE_{FourStepII} = h^6 \left(\frac{161}{600} \left(\frac{d^2}{dx^2} g(x) \right) p(x) G + \cdots \right) + O\left(h^8\right) \qquad (29)$$

5.10 The sixth algebraic order hybrid method with vanished phase-lag and its first, second and third derivatives developed in Section 4

$$LTE_{FourStepIII} = \frac{23}{6720} h^8 \left[\left[12 \left(\frac{d^4}{dx^4} g(x) \right) p(x) \right.\right.$$
$$+ 8 \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} p(x) + 16 g(x) p(x) \frac{d^2}{dx^2} g(x)$$
$$\left.\left. + 12 \left(\frac{d}{dx} g(x) \right)^2 p(x) \right] G + \cdots \right] + O\left(h^8\right) \qquad (30)$$

From the above equations we have the following theorem:

Theorem 2 – *Fourth algebraic order methods: for the classical four-step explicit method, the error increases as the third power of G. For the four-step explicit phase-fitted method developed in [21], the error increases as the second power of G. For the four-step explicit method with vanished phase-lag and its first derivative obtained in [49], the error increases as the first power of G. For the four-step explicit method with vanished phase-lag and its first and second derivatives produced in [53], the error increases as the first power of G but it has lower coefficients than the method developed in [49].*
  – *Sixth algebraic order methods: for the four-step hybrid explicit method with vanished phase-lag and its first, second and third derivatives produced in Sect. 4, the error increases as the first power of G.*
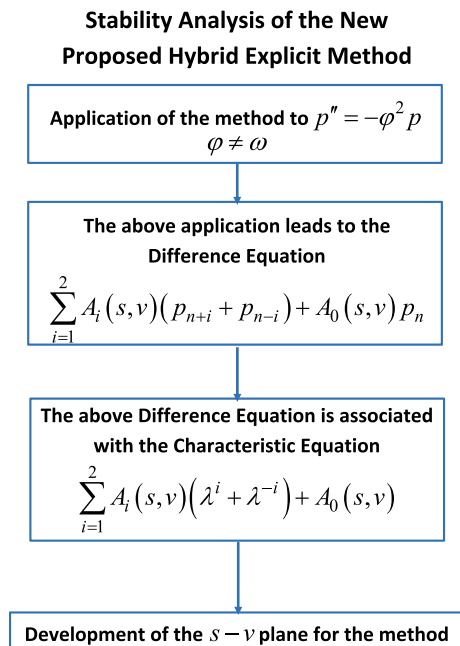
So, for the numerical solution of the time independent radial Schrödinger equation the method developed in Sect. 4 with vanished phase-lag and its first, second and third derivatives is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

6 Stability analysis

The stability analysis of the new hybrid four-step explicit method is based on the Flowchart mentioned in the Fig. 5.

Based on the above flowchart, and in order to study the stability of the new developed hybrid method, we apply it to the scalar test equation:

Fig. 5 Flowchart for the stability analysis of the new proposed method

Stability Analysis of the New Proposed Hybrid Explicit Method

Application of the method to $p'' = -\varphi^2 p$
$\varphi \neq \omega$

The above application leads to the Difference Equation

$$\sum_{i=1}^{2} A_i(s,v)(p_{n+i} + p_{n-i}) + A_0(s,v) p_n$$

The above Difference Equation is associated with the Characteristic Equation

$$\sum_{i=1}^{2} A_i(s,v)(\lambda^i + \lambda^{-i}) + A_0(s,v)$$

Development of the $s - v$ plane for the method

$$p'' = -\phi^2 \, p. \tag{31}$$

This leads to the following difference equation:

$$A_2\,(s,\,v)\,(p_{n+2} + p_{n-2}) + A_1\,(s,\,v)\,(p_{n+1} + p_{n-1}) + A_0\,(s,\,v)\,p_n = 0 \tag{32}$$

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

$$A_2\,(s,\,v) \;=\; 1, \quad A_1\,(s,\,v) \;=\; c_1 + s^2\left(b_0\,c_2\,s^2 + b_1\right)$$
$$A_0\,(s,\,v) \;=\; c_0 + s^2\,b_0\left(-2\,c_2\,s^2 + 1\right) \tag{33}$$

where c_i, $i = 0(1)2\,b_j$, $j = 0,\,1$ are given in (16) and (17).

Remark 4 We mention that the frequency of the scalar test Eq. (4), ω, is not equal with the frequency of the scalar test Eq. (31), ϕ, i.e. $\omega \neq \phi$.

We give the following definitions:

Definition 5 (see [14]) A method is called P-stable if its interval of periodicity is equal to $(0,\,\infty)$.

Definition 6 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0,\,\infty) - S^1$ only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $s = v$.

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

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

Remark 6 From the $s - v$ area one can chose several parts depending on mathematical model of the specific problem. The time independent Schrödinger equation belongs to a category of mathematical models where it is appropriate to observe **the surroundings of the first diagonal of the** $s - v$ **plane**. In these categories of mathematical models in order to apply the new obtained methods, the frequency of the phase fitting must be equal to the frequency of the scalar test equation.

For the time independent Schrödinger equation and due to the above mentioned remark, the frequency of the scalar test equation is equal with the frequency of phase fitting. Therefore, we investigate the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s - v$ plane). Based on this study we obtain that the interval of periodicity of the new method produced in Sect. 4 are equal to: $(0, 4.2)$.

The above investigation leads to the following theorem:

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[1] Where S is a set of distinct points

Stability Region for the New Hybric Explicit Four-Step Method
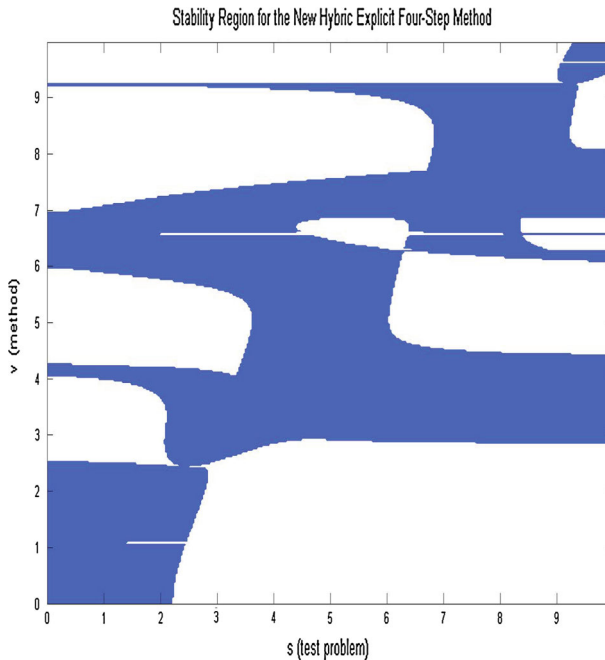
Fig. 6 $s - v$ plane of the the new obtained method with vanished phase-lag and its first and second derivatives

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

- *is of sixth algebraic order,*
- *has the phase-lag and its first, second and third derivatives equal to zero*
- *has an interval of periodicity equals to:* $(0, 4.2)$ *when the frequency of the scalar test equation is equal with the frequency of phase fitting*

7 Numerical results

In this section we will apply the new developed sixth algebraic order explicit hybrid four-step method on the approximate solution the one-dimensional time-independent Schrödinger equation. The main purpose of this application is the examination of the efficiency of the new constructed method.

The mathematical model of the one-dimensional time independent Schrödinger equation can be written as (see [122–125]):

$$p''(r) = [l(l+1)/r^2 + V(r) - k^2]p(r). \tag{34}$$

The above mathematical model is a boundary value problem which has the following boundary conditions:

$$p(0) = 0 \tag{35}$$

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

Below we give some definitions of the functions, quantities and parameters for the above mathematical model (34):

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

The new produced method, since it belongs to the category of methods with frequency dependent coefficients, has a parameter ω, which is called frequency, which must be determined. The determination of this parameter ω is necessary in order the new obtained method to be applied to any problem (see for example the notation after (4) and the formulae in Sect. 4). This parameter ω for the case of the radial time independent Schrödinger equation is given by (for $l = 0$):

$$\omega = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{36}$$

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

7.1 Woods–Saxon potential

In order to apply the new developed method to the radial time independent Schrödinger equation, we need to define a potential. For the purpose of the numerical applications of this paper, we will use the well known Woods–Saxon potential, which can be written as:

$$V(r) = \frac{u_0}{1 + q} - \frac{u_0 q}{a(1 + q)^2} \tag{37}$$

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

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

There are studies in the literature where critical points of some potentials are presented. These points are used in order one to use for for discrete approximations. Based on analogous studies (see for details [112]) we use such critical points for the Woods–Saxon potential for the discrete approximation of the parameter ω.

Based on the investigations mentioned above and for the purpose of our tests, we choose ω as follows (see for details [121] and [86]):

$$\phi = \begin{cases} \sqrt{-50 + E}, & \text{for } r \in [0, 6.5 - 2h], \\ \sqrt{-37.5 + E}, & \text{for } r = 6.5 - h \\ \sqrt{-25 + E}, & \text{for } r = 6.5 \\ \sqrt{-12.5 + E}, & \text{for } r = 6.5 + h \\ \sqrt{E}, & \text{for } r \in [6.5 + 2h, 15] \end{cases} \tag{38}$$
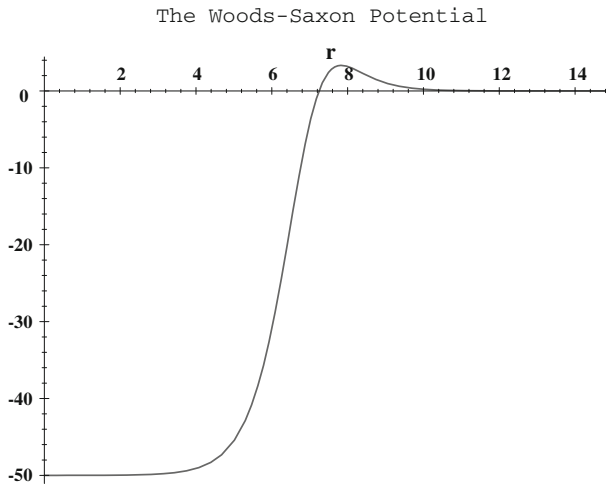
Fig. 7 The Woods–Saxon potential

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

7.2 Radial Schrödinger equation: the resonance problem

In order to investigate the efficiency of the new produced method, the numerical solution of the radial time independent Schrödinger Eq. (34),with the Woods–Saxon potential (37), is studied.

7.3 Strategy of the numerical solution

The conversion of the infinite interval of integration (which is the true interval of integration) to a finite one is a basic part of the strategy for the numerical solution of the above mentioned problem.

For our computational example we choose the integration interval $r \in [0, 15]$.

We will investigate the case of Eq. (34) in a rather large domain of energies, i.e. $E \in [1, 1000]$.

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

$$y''(r) + \left(k^2 - \frac{l(l+1)}{r^2} \right) y(r) = 0 \tag{39}$$

for r greater than some value R.

The above equation has linearly independent solutions $kr j_l(kr)$ and $kr n_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus, the solution of Eq. (34) (when $r \to \infty$), has the asymptotic form

$$y(r) \approx Akrj_l(kr) - Bkrn_l(kr)$$
$$\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \tag{40}$$

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

$$\tan\delta_l = \frac{y(r_2)S(r_1) - y(r_1)S(r_2)}{y(r_1)C(r_1) - y(r_2)C(r_2)} \tag{41}$$

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need y_j, $j = 0,(1)3$ before starting a four-step method. From the initial condition, we obtain y_0. The values y_i, $i = 1(1)3$ are obtained by using high order Runge–Kutta–Nyström methods (see [118] and [119]). With these starting values, we evaluate at r_2 of the asymptotic region the phase shift δ_l.

In the case of positive energies, we have the so-called resonance problem. This problem consists either of finding the phase-shift δ_l or finding those E, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$. We actually solve the latter problem, known as **the resonance problem**.

The boundary conditions for this problem are:

$$y(0) = 0, \quad y(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{42}$$

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

- The eighth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [28], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [87], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [27], which is indicated as **Method MCR6**
- The classical form of the fourth algebraic order four-step method developed in Sect. 3, which is indicated as **Method NMCL**[2].
- The phase-fitted method (Case 1) developed in [21], which is indicated as **Method NMPF1**
- The phase-fitted method (Case 2) developed in [21], which is indicated as **Method NMPF2**

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[2] With the term classical we mean the method of Sect. 3 with constant coefficients
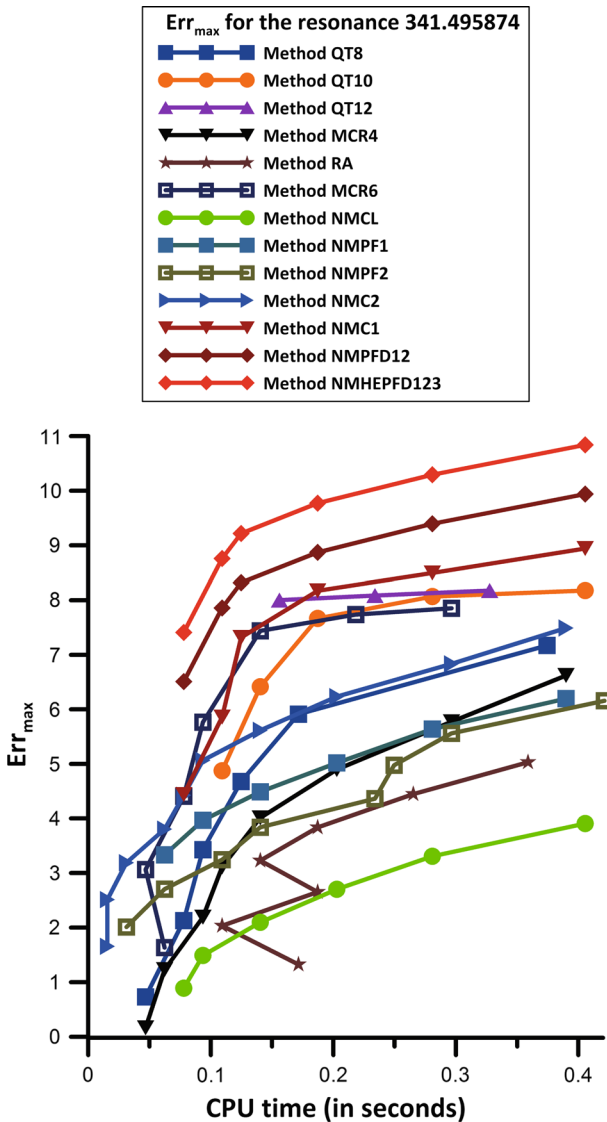
Fig. 8 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

– The four-step method with vanished phase-lag and its first derivative (Case 2) developed in [49], which is indicated as **Method NMC2**
– The four-step method with vanished phase-lag and its first derivative (Case 1) developed in [49], which is indicated as **Method NMC1**
– The four-step method with vanished phase-lag and its first and second derivatives developed in [53], which is indicated as **Method NMPFD12**
– The new hybrid sixth algebraic order four-step explicit method developed in Sect. 4, which is indicated as **Method NMHEPFD123**
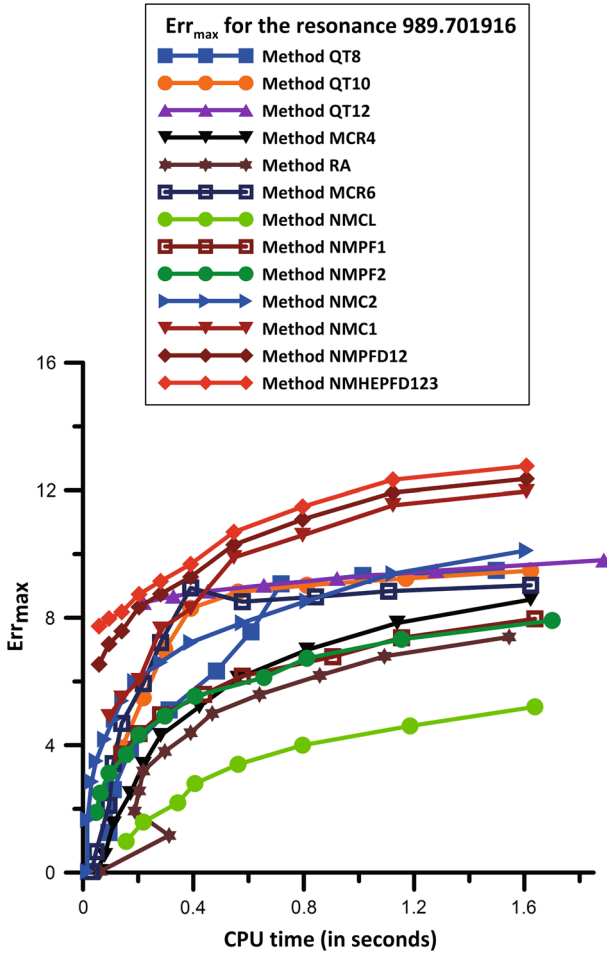
Fig. 9 Accuracy (digits) for several values of CPU time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

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

$$Err = |E_{calculated} - E_{accurate}| \qquad (43)$$

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.

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

8 Conclusions

In the present paper we produced a hybrid explicit sixth algebraic order four-step method which was based on the family of methods studied by Anastassi and Simos [21]. The aim and scope of the present paper was the study of the vanishing of the phase-lag and its first, second and third derivative of the obtained method. For the new developed method we presented a comparative error and stability analysis. The examination of the behavior of the vanishing of the phase-lag and its first, second and third derivatives on the efficiency of the new produced method we have applied it to the approximate solution of the radial time independent Schrödinger equation and related problems.

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

1. The classical form of the tenth algebraic order four-step multiderivative method developed in Sect. 3, which is indicated as **Method NMCL** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [28], which is indicated as **Method MCR4**. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [87], which is indicated as **Method MRA**.

2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [15], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [28], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [15], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [27], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.

3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [15], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [15], which is indicated as **Method QT10**

4. The phase-fitted method (Case 1) developed in [21], which is indicated as **Method NMPF1** is more efficient than the classical form of the fourth algebraic order four-step method developed in Sect. 3, which is indicated as **Method NMCL**, the exponentially-fitted method of Raptis and Allison [87] and the phase-fitted method (Case 2) developed in [21], which is indicated as **Method NMPF2**

5. The four-step method with vanished phase-lag and its first derivative (Case 2) developed in [49], which is indicated as **Method NMC2** is more efficient than the classical form of the fourth algebraic order four-step method developed in Sect. 3, which is indicated as **Method NMCL**, the exponentially-fitted method of Raptis and Allison [87] and the phase-fitted method (Case 2) developed in [21], which is indicated as **Method NMPF2** and the phase-fitted method (Case 1) developed in [21], which is indicated as **Method NMPF1**

6. The four-step method with vanished phase-lag and its first derivative (Case 1) developed in [49], which is indicated as **Method NMC2**, is the more efficient than all the above mentioned methods.

7. The four-step method with vanished phase-lag and its first and second derivatives developed in developed in [53], which is indicated as **Method NMPFD12** is more efficient than all the above mentioned methods

8. The new obtained hybrid explicit sixth algebraic order dour-step method with vanished phase-lag and its first, second and third derivatives developed in developed in Sect. 4, which is indicated as **Method NMHEPFD123** is the most efficient one

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

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