

## An explicit four-step method with vanished phase-lag and its first and second derivatives

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**Abstract** In this paper we will develop an explicit fourth algebraic order four-step method with phase-lag and its first and second derivatives vanished. The comparative error and the stability analysis of the above mentioned paper is also presented. The new obtained method is applied on the resonance problem of the Schrödinger equation in order to examine its efficiency. The theoretical and the computational results shown that the new obtained method is more efficient than other well known methods for the numerical solution of the Schrödinger equation and related initial-value or boundary-value problems with periodic and/or oscillating solutions.

**Keywords** Phase-lag · Initial value problems · Oscillating solution · Symmetric · Multistep · Schrödinger equation

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## 1 Introduction

In the present paper the approximate solution of special second-order initial-value problems of the form (see [1] for details)

$$q''(x) = f(x, q), \quad q(x_0) = y_0 \quad \text{and} \quad q'(x_0) = y'_0 \quad (1)$$

with a periodical and/or oscillatory solutions is studied. For this kind of problems, the main characteristic of the mathematical models is that the system of ordinary differential equations which describe the above models are of second order in which the first derivative  $y'$  does not appear explicitly (see [2–119] and references therein).

## 2 Analysis of the phase-lag for symmetric multistep methods

Multistep methods of the form

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

can be used for the numerical solution of the above mentioned initial value problem (1). In the formula (2),  $m$  means the number of steps over the equally spaced intervals  $\{x_i\}_{i=0}^m \in [a, b]$  and  $h = |x_{i+1} - x_i|$ ,  $i = 0(1)m - 1$ , where  $h$  is called stepsize of integration.

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

The Multistep Method (2) is associated with the operator

$$L(x) = \sum_{i=0}^m c_i u(x + ih) - h^2 \sum_{i=0}^m b_i u''(x + ih) \quad (3)$$

where  $u \in C^2$  (see for details [15]).

**Definition 1** [22] The multistep method (2) is called algebraic of order  $p$  if the associated linear operator  $L$  vanishes for any linear combination of the linearly independent functions  $1, x, x^2, \dots, x^{p+1}$ .

If we apply  $s$  symmetric  $2k$ -step method, that is for  $i = -k(1)k$ , to the scalar test equation

$$y'' = -\omega^2 y \quad (4)$$

the following difference equation is obtained:

$$\begin{aligned} A_k(v) y_{n+k} + \dots + A_1(v) y_{n+1} + A_0(v) y_n \\ + A_1(v) y_{n-1} + \dots + A_k(v) y_{n-k} = 0 \end{aligned} \quad (5)$$

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

The characteristic equation :

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

is associated with (5).

Lambert and Watson [15] introduced the following definition:

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

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

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

**Definition 3** [25, 26] For any method corresponding to the characteristic equation (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  $v \rightarrow \infty$ , the order of phase-lag is  $r$ .

**Definition 4** [23] Phase-fitted is called a method for which the phase-lag vanishes

**Theorem 1** [25] The symmetric  $2k$ -step method with characteristic equation given by (6) has phase-lag order  $r$  and phase-lag constant  $c$  given by

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

The formula proposed from the above theorem gives us a direct method to calculate the phase-lag of any symmetric  $2k$ -step method.

*Remark 1* For the specific case of the symmetric four-step method (i.e. for  $k = 2$ ), and based on the above theorem, we conclude that a symmetric four-step method has phase-lag order  $p$  and phase-lag constant  $c$  given which can be computed by the direct formula:

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

### 3 The family of explicit four-step methods with vanished phase-lag and its first and second derivatives

We write the explicit symmetric  $2m$ -step method as :

$$\begin{aligned} q_{n+m} + \sum_{i=0}^{m-1} c_i (q_{n+i} + q_{n-i}) + q_{n-m} \\ = h^2 \sum_{i=1}^{m-1} b_i [f(x_{n+i}, q_{n+i}) + f(x_{n-i}, q_{n-i})] + b_0 f(x_n, q_n) \end{aligned} \quad (11)$$

From the form (11) with  $m = 2$  we get the following form of the explicit symmetric four-step methods [22]:

$$q_{n+2} + c_1 (q_{n+1} + q_{n-1}) + c_0 q_n + q_{n-2} = h^2 [b_1 (f_{n+1} + f_{n-1}) + b_0 f_n] \quad (12)$$

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

Considering (12), we choose:

$$c_1 = -\frac{1}{10} \quad (13)$$

*Remark 2* The above choice for the free parameter  $c_1$  is based on the paper [22]. In this study it has been proved that the above value of  $c_1$  gives for the method (12) the higher accuracy.

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

$$\begin{aligned} \text{Phase-Lag(PL)} &= \frac{T_1}{\frac{39}{5} + 2v^2b_1} = 0 \\ \text{First Derivative of PL} &= -\frac{T_2}{(10v^2b_1 + 39)^2} = 0 \\ \text{Second Derivative of PL} &= -\frac{T_3}{(10v^2b_1 + 39)^3} = 0 \end{aligned} \quad (14)$$

where

$$\begin{aligned} T_1 &= 2 \cos(2v) + 2 \left( -\frac{1}{10} + v^2b_1 \right) \cos(v) + v^2b_0 + c_0 \\ T_2 &= 100 \sin(v) v^4 b_1^2 + 400 \sin(v) \cos(v) v^2 b_1 + 400 v b_1 (\cos(v))^2 \\ &\quad + 380 \sin(v) v^2 b_1 - 800 v b_1 \cos(v) + 100 v b_1 c_0 + 1560 \sin(v) \cos(v) \\ &\quad - 390 v b_0 - 200 v b_1 - 39 \sin(v) \end{aligned}$$

$$\begin{aligned}
 T_3 = & 1000 \cos(v) v^6 b_1^3 + 8000 (\cos(v))^2 v^4 b_1^2 - 16000 \sin(v) \cos(v) v^3 b_1^2 \\
 & + 7700 \cos(v) v^4 b_1^2 - 12000 (\cos(v))^2 v^2 b_1^2 + 16000 \sin(v) v^3 b_1^2 \\
 & - 4000 v^4 b_1^2 + 62400 (\cos(v))^2 v^2 b_1 + 24000 \cos(v) v^2 b_1^2 - 3000 v^2 b_1^2 c_0 \\
 & - 62400 \sin(v) \cos(v) v b_1 + 14430 \cos(v) v^2 b_1 + 11700 v^2 b_0 b_1 + 6000 v^2 b_1^2 \\
 & + 15600 (\cos(v))^2 b_1 + 62400 v b_1 \sin(v) - 31200 v^2 b_1 + 121680 (\cos(v))^2 \\
 & - 31200 b_1 \cos(v) + 3900 b_1 c_0 - 1521 \cos(v) - 15210 b_0 - 7800 b_1 - 60840
 \end{aligned}$$

Solving the above system of equations, we obtain the coefficients of the new proposed method:

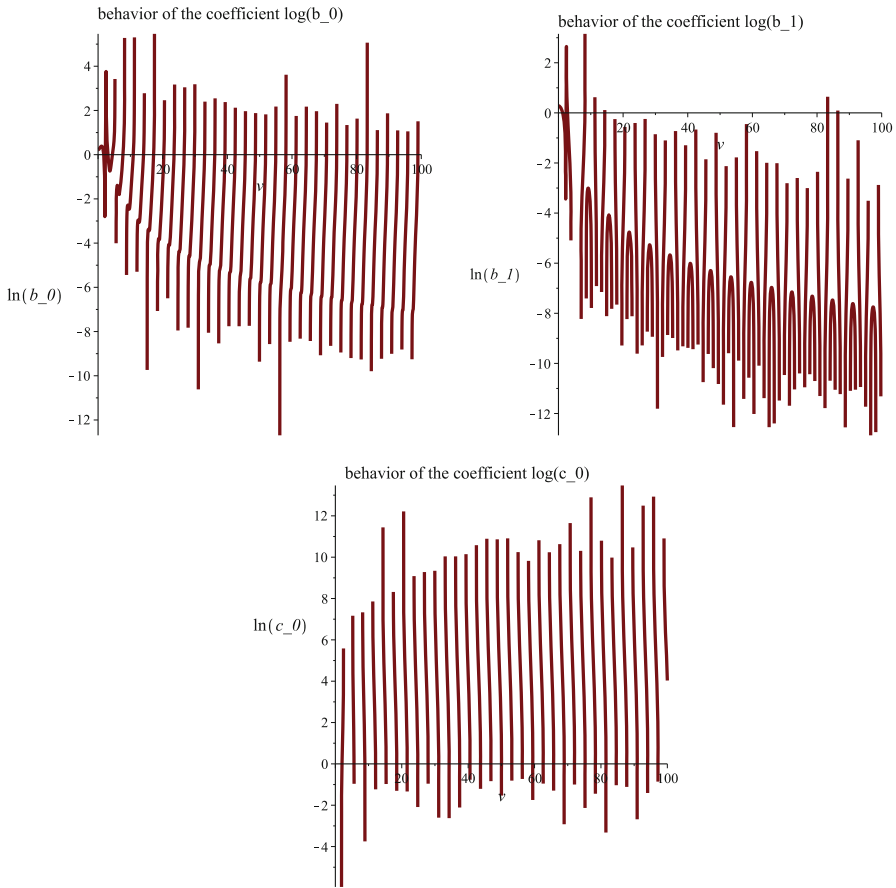
$$\begin{aligned}
 b_0 &= \frac{T_4}{10 \cos(v) v^3 + 30 v^2 \sin(v)}, \quad b_1 = \frac{T_5}{10 \cos(v) v^3 + 30 v^2 \sin(v)} \\
 c_0 &= \frac{T_6}{10 v \cos(v) + 30 \sin(v)} \tag{15}
 \end{aligned}$$

where

$$\begin{aligned}
 T_4 &= 30 v^2 \sin(v) - 10 v^2 \sin(3v) + v \cos(2v) \\
 &\quad + 80 v \cos(v) - 20 \sin(v) + \sin(2v) - 20 \sin(3v) - 3v \\
 T_5 &= -40 v \cos(2v) + v \cos(v) + 20 \sin(2v) - \sin(v) \\
 T_6 &= -30 v^2 \sin(v) + 10 v^2 \sin(3v) - v \cos(2v) \\
 &\quad - 50 v \cos(v) + 30 v \cos(3v) + 30 \sin(v) \\
 &\quad + 3 \sin(2v) - 30 \sin(3v) + 3v
 \end{aligned}$$

The following Taylor series expansions should be used in the cases that the formulae given by (15) are subject to heavy cancellations for some values of  $|v|$ :

$$\begin{aligned}
 b_0 &= \frac{5}{4} + \frac{161}{400} v^2 - \frac{1403}{6720} v^4 + \frac{140143}{6048000} v^6 \\
 &\quad - \frac{55771}{29568000} v^8 + \frac{1918751}{111767040000} v^{10} - \frac{166408997}{17435658240000} v^{12} \\
 &\quad - \frac{22339736197}{17784371404800000} v^{14} - \frac{1218700512811}{5676771352412160000} v^{16} \\
 &\quad - \frac{665139026325233}{18733345462960128000000} v^{18} + \dots \\
 b_1 &= \frac{53}{40} - \frac{161}{800} v^2 + \frac{253}{67200} v^4 - \frac{8353}{12096000} v^6 - \frac{1767}{19712000} v^8 \\
 &\quad - \frac{307801}{20321280000} v^{10} - \frac{87506899}{34871316480000} v^{12} \\
 &\quad - \frac{2114562269}{5081248972800000} v^{14} - \frac{3917589452563}{56767713524121600000} v^{16} \\
 &\quad - \frac{428777309305897}{37466690925920256000000} v^{18} + \dots
 \end{aligned}$$



**Fig. 1** Behavior of the coefficients of the new proposed method given by (15) for several values of  $v = \omega h$

$$\begin{aligned}
 c_0 = & -\frac{9}{5} + \frac{161}{2400} v^6 - \frac{23}{2240} v^8 + \frac{269}{268800} v^{10} \\
 & - \frac{23789}{1596672000} v^{12} + \frac{1126793}{223534080000} v^{14} + \frac{16463}{26417664000} v^{16} \\
 & + \frac{11494958767}{106706228428800000} v^{18} + \dots
 \end{aligned}
 \tag{16}$$

The behavior of the coefficients is given in the following Fig. 1.

The new obtained method (12) (mentioned as *FourStepI*) with the coefficients given by (15)–(16) has a local truncation error which is given by:

$$LTE_{Four\ Step\ New} = \frac{161 h^6}{2400} \left( q_n^{(6)} + 3 \omega^2 q_n^{(4)} + 3 \omega^4 q_n^{(2)} + \omega^6 q_n \right) + O(h^8) \tag{17}$$

### 4 Comparative error analysis

We will investigate the following cases:

4.1 Classical method (i.e. the method (12) with constant coefficients)

$$LTE_{CL} = \frac{161 h^6}{2400} q_n^{(6)} + O(h^8) \tag{18}$$

4.2 The method with vanished phase-lag produced in [22]

$$LTE_{MethAnasSim} = \frac{161 h^6}{2400} \left( q_n^{(6)} + \omega^2 q_n^{(4)} \right) + O(h^8) \tag{19}$$

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

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

4.4 The method with vanished phase-lag and its first and second derivatives developed in Sect. 3

$$LTE_{FourStepII} = \frac{161 h^6}{2400} \left( q_n^{(6)} + 3 \omega^2 q_n^{(4)} + 3 \omega^4 q_n^{(2)} + \omega^6 q_n \right) + O(h^8) \tag{21}$$

The procedure contains the following stages

- The radial time independent Schrödinger equation is of the form

$$q''(x) = f(x) q(x) \tag{22}$$

- Based on the paper of Ixaru and Rizea [84], the function  $f(x)$  can be written in the form:

$$f(x) = g(x) + G \tag{23}$$

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

- We express the derivatives  $q_n^{(i)}$ ,  $i = 2, 3, 4, \dots$ , which are terms of the local truncation error formulae, in terms of the Eq. (23). 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

We present the derivatives which presented in the formulae of the Local Truncation Errors:

$$\begin{aligned}
 q_n^{(2)} &= (V(x) - V_c + G) q(x) \\
 q_n^{(3)} &= \left( \frac{d}{dx} g(x) \right) q(x) + (g(x) + G) \frac{d}{dx} q(x) \\
 q_n^{(4)} &= \left( \frac{d^2}{dx^2} g(x) \right) q(x) + 2 \left( \frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + (g(x) + G)^2 q(x) \\
 q_n^{(5)} &= \left( \frac{d^3}{dx^3} g(x) \right) q(x) + 3 \left( \frac{d^2}{dx^2} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + 4 (g(x) + G) q(x) \frac{d}{dx} g(x) + (g(x) + G)^2 \frac{d}{dx} q(x) \\
 q_n^{(6)} &= \left( \frac{d^4}{dx^4} g(x) \right) q(x) + 4 \left( \frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + 7 (g(x) + G) q(x) \frac{d^2}{dx^2} g(x) + 4 \left( \frac{d}{dx} g(x) \right)^2 q(x) \\
 &\quad + 6 (g(x) + G) \left( \frac{d}{dx} q(x) \right) \frac{d}{dx} g(x) \\
 &\quad + (g(x) + G)^3 q(x) \\
 q_n^{(7)} &= \left( \frac{d^5}{dx^5} g(x) \right) q(x) + 5 \left( \frac{d^4}{dx^4} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + 11 (g(x) + G) q(x) \frac{d^3}{dx^3} g(x) + 15 \left( \frac{d}{dx} g(x) \right) q(x) \\
 &\quad \frac{d^2}{dx^2} g(x) + 13 (g(x) + G) \left( \frac{d}{dx} q(x) \right) \frac{d^2}{dx^2} g(x) \\
 &\quad + 10 \left( \frac{d}{dx} g(x) \right)^2 \frac{d}{dx} q(x) + 9 (g(x) + G)^2 q(x) \\
 &\quad \times \frac{d}{dx} g(x) + (g(x) + G)^3 \frac{d}{dx} q(x) \\
 q_n^{(8)} &= \left( \frac{d^6}{dx^6} g(x) \right) q(x) + 6 \left( \frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} q(x) \\
 &\quad + 16 (g(x) + G) q(x) \frac{d^4}{dx^4} g(x) + 26 \left( \frac{d}{dx} g(x) \right) q(x) \\
 &\quad \times \frac{d^3}{dx^3} g(x) + 24 (g(x) + G) \left( \frac{d}{dx} q(x) \right) \frac{d^3}{dx^3} g(x)
 \end{aligned}$$



$$\begin{aligned}
 &+ 15 \left( \frac{d^2}{dx^2} g(x) \right)^2 q(x) + 48 \left( \frac{d}{dx} g(x) \right) \\
 &\left( \frac{d}{dx} q(x) \right) \frac{d^2}{dx^2} g(x) + 22 (g(x) + G)^2 q(x) \\
 &\times \frac{d^2}{dx^2} g(x) + 28 (g(x) + G) q(x) \left( \frac{d}{dx} g(x) \right)^2 \\
 &+ 12 (g(x) + G)^2 \left( \frac{d}{dx} q(x) \right) \frac{d}{dx} g(x) \\
 &+ (g(x) + G)^4 q(x) \dots
 \end{aligned}$$

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)  $G \gg 0$  or  $G \ll 0$ . Then  $|G|$  is a large number.
2. Finally we compute the asymptotic expansions of the Local Truncation Errors

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

#### 4.5 Classical method

$$LTE_{CL} = h^6 \left( \frac{161}{2400} q(x) G^3 + \dots \right) + O(h^8) \tag{24}$$

#### 4.6 The method with vanished phase-lag produced in [22]

$$LTE_{MethAnasSim} = h^6 \left( \frac{161}{2400} g(x) q(x) G^2 + \dots \right) + O(h^8) \tag{25}$$

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

$$\begin{aligned}
 LTE_{FourStep1} = h^6 &\left[ \left( \frac{161}{2400} (g(x))^2 q(x) + \frac{161}{1200} \left( \frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) \right. \right. \\
 &\left. \left. + \frac{161}{480} \left( \frac{d^2}{dx^2} g(x) \right) q(x) \right) G + \dots \right] + O(h^8) \tag{26}
 \end{aligned}$$

4.8 The method with vanished phase-lag and its first and second derivatives developed in Sect. 3

$$LTE_{FourStep11} = h^6 \left( \frac{161}{600} \left( \frac{d^2}{dx^2} g(x) \right) q(x) G + \dots \right) + O(h^8) \quad (27)$$

From the above equations we have the following theorem:

**Theorem 2** *For the Classical Four-Step Explicit Method, the error increases as the third power of  $G$ . For the Four-Step Explicit Phase-Fitted Method developed in [22], 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 [50], the error increases as the first power of  $G$ . Finally, for the Four-Step Explicit Method with Vanished Phase-lag and its First and Second Derivatives produced in Sect. 3, the error increases as the first power of  $G$  but it has lower coefficients than the method developed in [50]. So, for the numerical solution of the time independent radial Schrödinger equation the the Methods developed in [50] and the New Proposed Method with Vanished Phase-Lag and its First and Second Derivatives are the most efficient from theoretical point of view, especially for large values of  $|G| = |V_c - E|$ .*

## 5 Stability analysis

In order to investigate the stability of the new developed methods, we apply them to the scalar test equation:

$$y'' = -\phi^2 y. \quad (28)$$

This leads to the following difference equation:

$$A_2(s, v) (y_{n+2} + y_{n-2}) + A_1(s, v) (y_{n+1} + y_{n-1}) + A_0(s, v) y_n = 0 \quad (29)$$

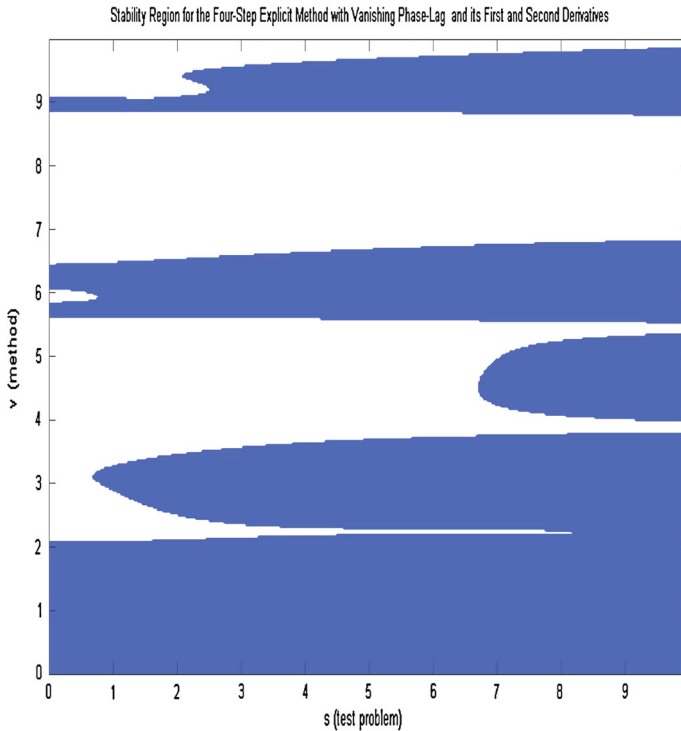
where

$$\begin{aligned} A_2(s, v) &= 1, \quad A_1(s, v) = -\frac{1}{10} + \frac{T_7}{10 \cos(v) v^3 + 30 v^2 \sin(v)} \\ A_0(s, v) &= \frac{T_8}{10 v \cos(v) + 30 \sin(v)} \end{aligned} \quad (30)$$

where

$$\begin{aligned} T_7 &= s^2 (-40 v \cos(2v) + v \cos(v) + 20 \sin(2v) - \sin(v)) \\ T_8 &= -30 v^2 \sin(v) + 10 v^2 \sin(3v) - v \cos(2v) - 50 v \cos(v) \\ &\quad + 30 v \cos(3v) + 30 \sin(v) + 3 \sin(2v) - 30 \sin(3v) + 3 v \end{aligned}$$

and  $s = \phi h$ .



**Fig. 2**  $s$ - $v$  plane of the the new obtained method with vanished phase-lag and its first and second derivatives

*Remark 3* The frequency of the scalar test Eq. (4),  $\omega$ , is not equal with The frequency of the scalar test Eq. (28),  $\phi$ , i.e.  $\omega \neq \phi$ .

We have the following definitions:

**Definition 5** (see [15]) 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. 2 we present the  $s$ - $w$  plane for the method developed in this paper.

*Remark 4* 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 5* There are mathematical models where it is appropriate to observe the surroundings of the first diagonal of the  $s$ - $v$  plane. One category consists mathematical models where 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. Many problems in

<sup>1</sup> Where  $S$  is a set of distinct points

sciences and engineering belong to this category of mathematical models (for example the time independent Schrödinger equation).

Based on the above mentioned remark, the category of mathematical models where the frequency of the scalar test equation is equal with the frequency of phase fitting is now investigated, i.e. we study the case where  $s = v$  (i.e. see the surroundings of the first diagonal of the  $s$ - $v$  plane). Based on this investigation we produce the result that the interval of periodicity of the new method obtained in Sect. 3 are equal to:  $(0, 4.1)$ .

The above investigation leads to the following theorem:

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

- *is of fourth algebraic order,*
- *has the phase-lag and its first and second derivatives equal to zero*
- *has an interval of periodicity equals to:  $(0, 4.1)$  when the frequency of the scalar test equation is equal with the frequency of phase fitting*

## 6 Numerical results

We will study the efficiency of the new obtained explicit four-step method applying it on the numerical solution the radial time-independent Schrödinger equation (see [120–122]).

The radial time independent Schrödinger equation has a mathematics model given by :

$$y''(r) = [l(l + 1)/r^2 + V(r) - k^2]y(r). \quad (31)$$

is a boundary value problem which has the following boundary conditions :

$$y(0) = 0 \quad (32)$$

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 (31) :

1. The function  $W(r) = l(l + 1)/r^2 + V(r)$  is called *the effective potential*. This satisfies  $W(x) \rightarrow 0$  as  $x \rightarrow \infty$ ,
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 value of parameter (frequency)  $\omega$  must be determined for the new obtained method since it is frequency dependent method, in order to be applied to any problem (see for example the notation after (4) and the formulae in Sect. 3). The parameter  $\omega$  for the case of the one-dimensional Schrödinger equation is given by (for  $l = 0$ ) :

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

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

### 6.1 Woods–Saxon potential

The well known Woods–Saxon potential is used for the purpose of our numerical tests. We can write it with the form:

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

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. 3.

Studying some potentials, such as the Woods–Saxon potential, one can finds some basic points in their form and can uses these basic points for discrete approximation of the the parameter  $\omega$  (see for details [110]).

Based on the investigations mentioned above and for the purpose of our tests, we choose  $\omega$  as follows (see for details [123] and [84]):

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

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

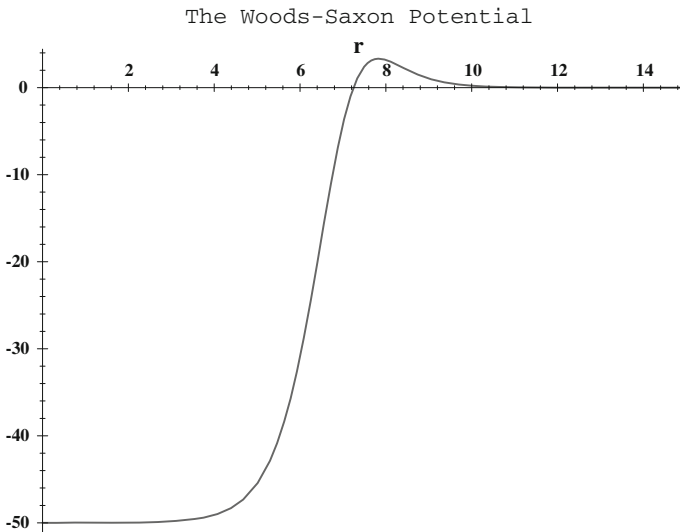


Fig. 3 The Woods–Saxon potential

## 6.2 Radial Schrödinger equation: the resonance problem

For the study of the efficiency of the new obtained method, we will study the approximate solution of the one-dimensional time independent Schrödinger equation (31) using as potential the Woods–Saxon potential (34). The strategy for the approximate solution of this problem consists the conversion of the infinite interval of integration (which is the true interval of integration) to a finite one. For the purposes of our numerical experiments we choose the integration interval  $r \in [0, 15]$ . We consider Eq. (31) 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 Schrödinger equation effectively reduces to

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

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

$$\begin{aligned} y(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC \left[ \sin \left( kr - \frac{l\pi}{2} \right) + \tan \delta_l \cos \left( kr - \frac{l\pi}{2} \right) \right] \end{aligned} \quad (37)$$

where  $\delta_l$  is the phase shift that may be calculated from the formula

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

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  $C(r) = -krn_l(kr)$ . 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 [117] and [118]). With these starting values, we evaluate at  $r_2$  of the asymptotic region the phase shift  $\delta_l$ .

For positive energies, we have the so-called resonance problem. This problem consists either of finding the phase-shift  $\delta_l$  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:

$$y(0) = 0, \quad y(r) = \cos(\sqrt{Er}) \quad \text{for large } r. \quad (39)$$

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

- The eighth order multi-step method developed by Quinlan and Tremaine [16], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [16], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [16], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [29], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [85], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [28], 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<sup>2</sup>**.
- The Phase-Fitted Method (Case 1) developed in [22], which is indicated as **Method NMPF1**
- The Phase-Fitted Method (Case 2) developed in [22], which is indicated as **Method NMPF2**
- The Four-Step Method with vanished phase-lag and its first derivative (Case 2) developed in [50], which is indicated as **Method NMC2**
- The Four-Step Method with vanished phase-lag and its first derivative (Case 1) developed in [50], which is indicated as **Method NMC1**
- The New Obtained Method developed in Sect. 3, which is indicated as **Method NMPFD12**

The numerically calculated eigenenergies are compared with reference values<sup>3</sup>. In Figs. 4 and 5, we present the maximum absolute error  $Err_{max} = |\log_{10}(Err)|$  where

$$Err = |E_{calculated} - E_{accurate}| \quad (40)$$

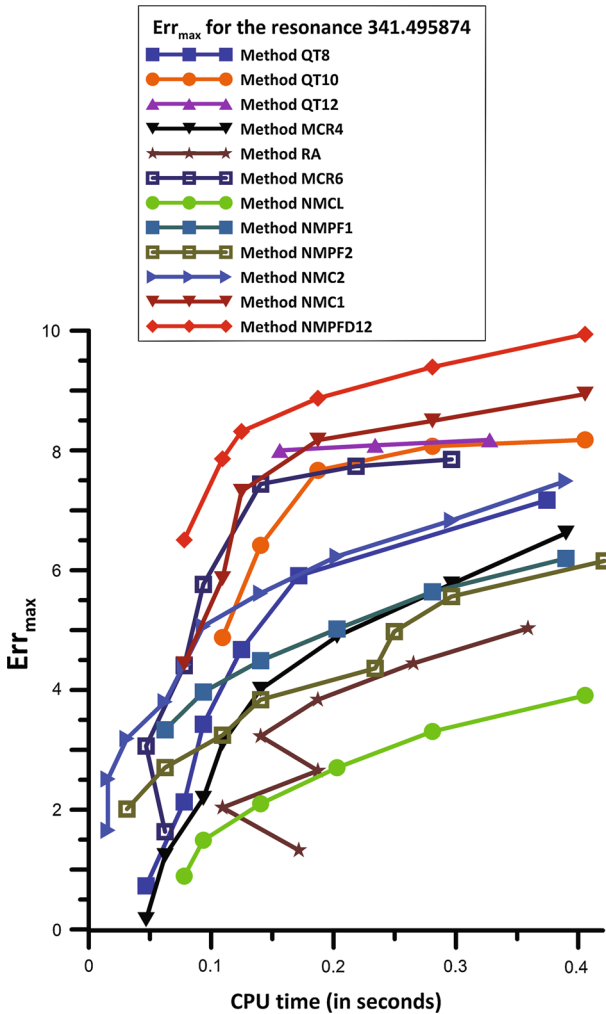
of the eigenenergies  $E_2 = 341.495874$  and  $E_3 = 989.701916$  respectively, for several values of CPU time (in seconds). We note that the CPU time (in seconds) counts the computational cost for each method.

## 7 Conclusions

In the present paper we developed an explicit four-step method. This method was based on the family of methods studied by Anastassi and Simos [22]. The investigation of the vanishing of the phase-lag and its first and second derivative of a method of the above mentioned family of the methods was the aim and scope of this paper. For the new obtained method we presented a comparative error and stability analysis. In order to examine the behavior of the vanishing of the phase-lag and its first and

<sup>2</sup> With the term classical we mean the method of Sect. 3 with constant coefficients

<sup>3</sup> The reference values are computed using the well known two-step method of Chawla and Rao [28] with small step size for the integration



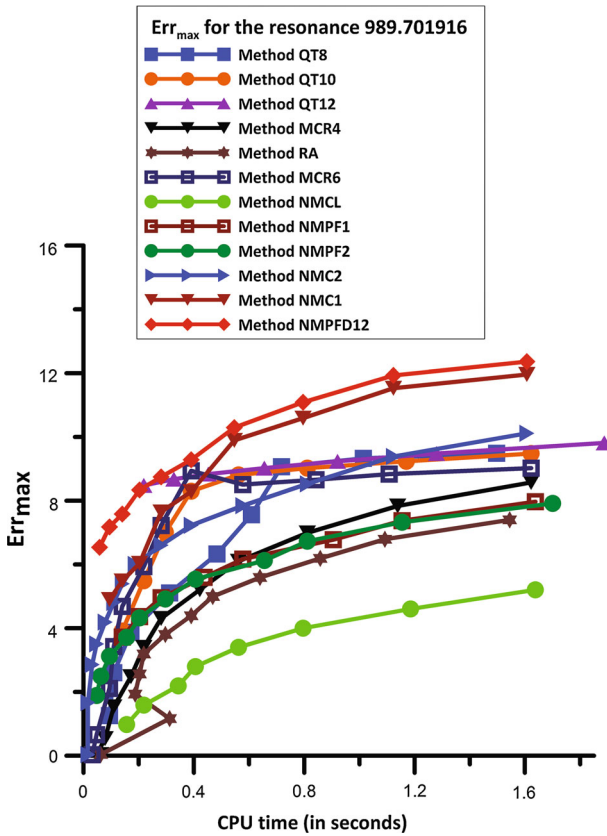
**Fig. 4** Accuracy (digits) for several values of *CPU* Time (in seconds) for the eigenvalue  $E_2 = 341.495874$ . The nonexistence of a value of accuracy (Digits) indicates that for this value of *CPU*, accuracy (digits) is less than 0

second derivative on the efficiency of the new produced method we have applied it to the numerical solution of the one-dimensional 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 [29], which is indicated as **Method MCR4**. Both the above mentioned methods are more





**Fig. 5** 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

efficient than the exponentially-fitted method of Raptis and Allison [85], which is indicated as **Method MRA**.

2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [16], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [29], 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 [16], 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 [28], 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 [16], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [16], which is indicated as **Method QT10**

4. The Phase-Fitted Method (Case 1) developed in [22], 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 [85] and the Phase-Fitted Method (Case 2) developed in [22], which is indicated as **Method NMPF2**
5. The Four-Step Method with vanished phase-lag and its first derivative (Case 2) developed in [50], 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 [85] and the Phase-Fitted Method (Case 2) developed in [22], which is indicated as **Method NMPF2** and the Phase-Fitted Method (Case 1) developed in [22], which is indicated as **Method NMPF1**
6. The Four-Step Method with vanished phase-lag and its first derivative (Case 1) developed in [50], which is indicated as **Method NMC2**, is the most efficient one than all the above mentioned methods.
7. The New Obtained Method developed in Sect. 3, which is indicated as **Method NMPFD12** 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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