

On the Low Algebraic Order Explicit Methods with Vanished Phase-Lag and its First and Second Derivative

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Abstract: In this paper we will study a low algebraic order four-step method requiring this specific method to have vanished the phase-lag and its first and second derivatives. For this specific method we will give the constant value of the parameters in the right hand side part of the method. We will investigate the influence of the elimination of the phase-lag and its first and second derivatives on the efficiency of this method. More specifically we will study the local truncation error of the new method and we will compare it with other methods in the literature (comparative local truncation error analysis). We will also investigate the stability (interval of periodicity) of this method using scalar test equation with frequency different than the frequency of the scalar test equation used for phase-lag analysis (stability analysis). Finally, the new produced method will be applied on the resonance problem of the Schrödinger equation in order to examine its efficiency. We will prove that this kind of methods are effective for the approximate solution of the Schrödinger equation and related periodic initial-value or boundary-value problems.

Keywords: Phase-lag, derivative of the phase-lag, initial value problems, oscillating solution, symmetric, multistep, Schrödinger equation

1. Introduction

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

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

with solution of periodical and/or oscillatory behavior is presented in the present paper. The mathematical models of the above presented problems consists from systems of ordinary differential equations of second order in which the first derivative q' does not appear explicitly (see for numerical methods for these problems [3] - [45] and references therein).

2. Phase-lag Analysis For Symmetric $2k$ Finite Difference Methods

The multistep finite difference methods of the form

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

with k steps over the equally spaced intervals $\{x_i\}_{i=-k}^k \in [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 1 - k(1)k - 1$, where h is called stepsize of integration, can be used for the approximate solution of the initial value problem (1).

Remark. If the method is symmetric then $c_{-i} = c_i$ and $b_{-i} = b_i$, $i = 0(1)k$.

Remark. The Multistep Method (2) is associated with the operator

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

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where $u \in C^2$.

Definition 1.[1] 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 the symmetric $2k$ -step method, $(i = -k(1)k)$, to the scalar test equation

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

we have the following difference equation:

$$A_k(v) q_{n+k} + \dots + A_1(v) q_{n+1} + A_0(v) q_n + A_1(v) q_{n-1} + \dots + A_k(v) q_{n-k} = 0 \tag{5}$$

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

The associated with (5) characteristic equation is given by:

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

Definition 2.[16] 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 $\lambda_i, i = 1(1)2k$ of Eq. (6) satisfy:

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

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

Definition 3.[14], [15] 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 $t = O(v^{p+1})$ as $v \rightarrow \infty$, the order of phase-lag is p .

Definition 4.[2] If for a specific method the phase-lag is equal to zero, then this method is called **phase-fitted**

Theorem 1.[14] The symmetric $2k$ -step method with characteristic equation given by (6) has phase-lag order p and phase-lag constant c given by

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

Remark. We can use the above mentioned formula for a direct computation of the the phase-lag of any symmetric $2k$ -step method.

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

$$-cv^{p+2} + O(v^{p+4}) = \frac{T_0}{T_1} \tag{10}$$

$$T_0 = 2A_2(v) \cos(2v) + 2A_1(v) \cos(v) + A_0(v)$$

$$T_1 = 8A_2(v) + 2A_1(v)$$

3. A New Low Algebraic Order Explicit Method with Vanished Phase-Lag and Its First and Second Derivatives

Let us consider the method

$$q_{n+2} + c_1 (q_{n+1} + q_{n-1}) + c_0 q_n + q_{n-2} = h^2 \left[b_1 (f_{n+1} + f_{n-1}) + b_0 f_n \right] \tag{11}$$

where $f_i = q''(x_i, q_i), i = -2(1)2$.

3.1. Development of the Method

Considering (11), we choose:

$$b_1 = \frac{53}{40} \tag{12}$$

We now define the phase-lag and its first and second derivatives:

$$\text{Phase - Lag(PL)} = \frac{T_2}{8 + 2a_1 + \frac{53v^2}{20}} = 0$$

$$\text{First Derivative of PL} = \frac{T_3}{8 + 2a_1 + \frac{53v^2}{20}} - \frac{53v}{10} \frac{T_4}{\left(8 + 2a_1 + \frac{53v^2}{20}\right)^2} = 0$$

$$\text{Second Derivative of PL} = \frac{T_5}{8 + 2a_1 + \frac{53v^2}{20}} - \frac{53v}{5} \frac{T_6}{\left(8 + 2a_1 + \frac{53v^2}{20}\right)^2} + \frac{2809v^2}{50} \frac{T_7}{\left(8 + 2a_1 + \frac{53v^2}{20}\right)^3} - \frac{53}{10} \frac{T_8}{\left(8 + 2a_1 + \frac{53v^2}{20}\right)^2} = 0 \tag{13}$$

where

$$\begin{aligned}
 T_2 &= 2 \cos(2v) + 2 \left(a_1 + \frac{53v^2}{40} \right) \cos(v) + v^2 b_0 + a_0 \\
 T_3 &= -4 \sin(2v) + \frac{53v \cos(v)}{10} - 2 \left(a_1 + \frac{53v^2}{40} \right) \sin(v) + 2v b_0 \\
 T_4 &= 2 \cos(2v) + 2 \left(a_1 + \frac{53v^2}{40} \right) \cos(v) + v^2 b_0 + a_0 \\
 T_5 &= -8 \cos(2v) + \frac{53 \cos(v)}{10} - \frac{53v \sin(v)}{5} - 2 \left(a_1 + \frac{53v^2}{40} \right) \cos(v) + 2b_0 \\
 T_6 &= -4 \sin(2v) + \frac{53v \cos(v)}{10} - 2 \left(a_1 + \frac{53v^2}{40} \right) \sin(v) + 2v b_0 \\
 T_7 &= 2 \cos(2v) + 2 \left(a_1 + \frac{53v^2}{40} \right) \cos(v) + v^2 b_0 + a_0 \\
 T_8 &= 2 \cos(2v) + 2 \left(a_1 + \frac{53v^2}{40} \right) \cos(v) + v^2 b_0 + a_0
 \end{aligned}$$

Requesting the above method (11) with coefficient b_1 given by (12) to have the phase-lag and its first and second derivatives vanished, the system of equations (13) must be satisfied.

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

$$\begin{aligned}
 a_0 &= \frac{T_9}{40v \cos(v) - 40 \sin(v)} \\
 a_1 &= \frac{T_{10}}{40v \cos(v) - 40 \sin(v)} \\
 b_0 &= \frac{T_{11}}{40v \cos(v) - 40 \sin(v)}
 \end{aligned} \tag{14}$$

where

$$\begin{aligned}
 T_9 &= -53v^3 \cos(2v) + 40v^2 \sin(3v) + 159 \sin(2v)v^2 - 120 \sin(v)v^2 + 159v^3 + 120v \cos(3v) + 120v \cos(v) - 40 \sin(3v) - 120 \sin(v) \\
 T_{10} &= -53 \cos(v)v^3 - 160 \cos(2v)v - 159 \sin(v)v^2 + 80 \sin(2v) \\
 T_{11} &= 53 \cos(2v)v - 40 \sin(3v) + 53 \sin(2v) + 120 \sin(v) - 159v
 \end{aligned}$$

If the above formulae given by (14) are subject to heavy cancellations for some values of $|v|$ then the following Taylor series expansions should be used :

$$\begin{aligned}
 a_0 &= -\frac{9}{5} - \frac{483v^2}{100} + \frac{713v^4}{875} + \frac{58157v^6}{1260000} - \frac{38340257v^8}{1940400000} + \frac{58336141v^{10}}{38808000000} - \frac{31292125589v^{12}}{47675628000000} \\
 &+ \frac{575150010613v^{14}}{324194270400000000} - \frac{737733960450869v^{16}}{1897184870380800000000} + \frac{360065021805613v^{18}}{788061407696640000000000} + \dots \\
 a_1 &= -\frac{1}{10} + \frac{483v^2}{200} - \frac{713v^4}{1750} + \frac{412v^6}{39375} - \frac{34649v^8}{121275000} - \frac{1669v^{10}}{1212750000} - \frac{11902021v^{12}}{59594535000000} \\
 &- \frac{90449467v^{14}}{10131070950000000} - \frac{40786059791v^{16}}{91210811076000000000} - \frac{7083046376821v^{18}}{320149946876760000000000} + \dots \\
 b_0 &= \frac{5}{4} + \frac{483v^2}{200} - \frac{17043v^4}{28000} + \frac{7493v^6}{120000} - \frac{8825077v^8}{258720000} + \frac{9523639v^{10}}{77616000000} - \frac{3837207833v^{12}}{1271350080000000} \\
 &+ \frac{12780519559v^{14}}{216129513600000000} - \frac{2055406068451v^{16}}{281064425241600000000} + \frac{98198488890517v^{18}}{682986553337088000000000} + (15)
 \end{aligned}$$

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

The local truncation error of the new produced method (11) (mentioned as *ExplFourStep*) with the coefficients given by (14) - (15) is given by:

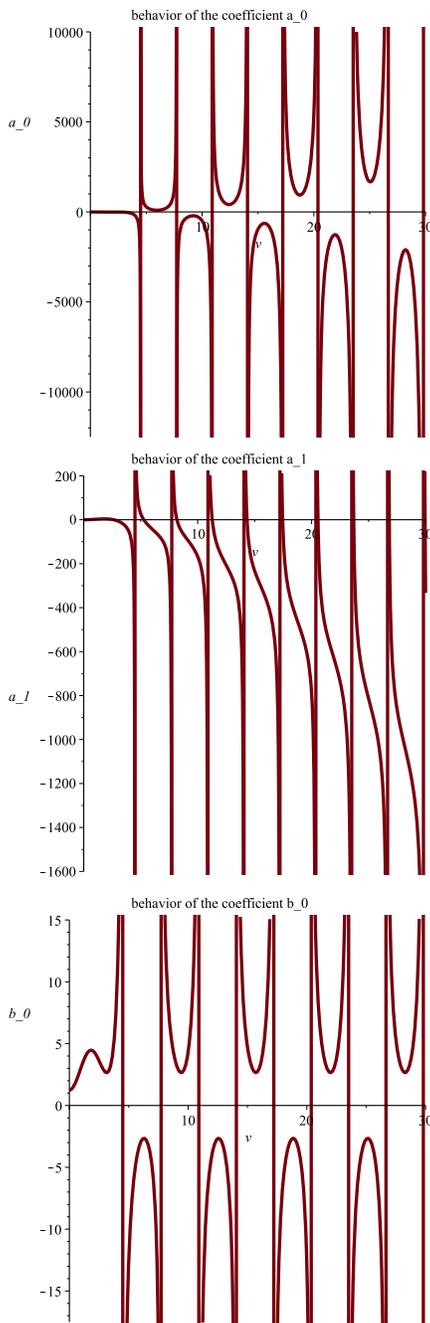


Figure 1: Behavior of the coefficients of the new proposed method given by (14) for several values of $\nu = \phi h$.

$$\begin{aligned}
 LTE_{ExplFourStep} = & \frac{161 h^6}{2400} \left(q_n^{(6)} + 3 \phi^2 q_n^{(4)} \right. \\
 & \left. + 3 \phi^4 q_n^{(2)} + \phi^6 q_n \right) + O(h^8) \quad (16)
 \end{aligned}$$

4. Comparative Error Analysis

The methods mentioned below are investigated :

4.1. Classical Method(i.e. the method (11) with constant coefficients of the Case I)

$$LTE_{CL} = \frac{161 h^6}{2400} q_n^{(6)} + O(h^8) \quad (17)$$

4.2. The Method with Vanished Phase-Lag Produced in [1]

$$LTE_{MethAnasSim} = \frac{161 h^6}{2400} \left(q_n^{(6)} + \phi^2 q_n^{(4)} \right) + O(h^8) \quad (18)$$

4.3. The New Proposed Method with Vanished Phase-Lag and its First Derivative Produced in [44]

$$\begin{aligned}
 LTE_{FourStep} = & \frac{161 h^6}{2400} \left(q_n^{(6)} + 2 \phi^2 q_n^{(4)} \right. \\
 & \left. + \phi^4 q_n^{(2)} \right) + O(h^8) \quad (19)
 \end{aligned}$$

4.4. The New Proposed Method with Vanished Phase-Lag and its First and Second Derivatives Produced in Section 3

$$\begin{aligned}
 LTE_{ExplFourStep} = & \frac{161 h^6}{2400} \left(q_n^{(6)} + 3 \phi^2 q_n^{(4)} \right. \\
 & \left. + 3 \phi^4 q_n^{(2)} + \phi^6 q_n \right) + O(h^8) \quad (20)
 \end{aligned}$$

The procedure contains the following stages

- Computation of the derivatives which are appeared in the formulae of the Local Truncation Errors. We present some formulae of these derivatives in Appendix
- Using the formulae of the derivatives produced in the previous stage, we substitute them in the expressions of the Local Truncation Error. The resulting formulae of the local truncation errors are dependent from the energy E.

–Our study is based on the investigation of two special cases in terms of the value of E (which is appeared in the Local Truncation Error formulae produced in the above second stage of the algorithm of local truncation error analysis) :

1. The Energy and the potential are closed each other, i.e., $G = V_c - E \approx 0$. Consequently, all the terms in the local truncation error formulae with terms of several power of G are equal approximately equal to zero. Therefore, we consider only the terms of the polynomials with power to G equal to zero i.e. the free from G terms of the polynomials of local truncation error. In this case (free from G terms) the free terms of the polynomials in G are the same for the cases of the classical method (constant coefficients) and of the methods with vanished the phase-lag and its derivatives. Consequently, for these values of G , the methods are of comparable accuracy.

2. $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number.

–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

$$LTE_{CL} = h^6 \left(\frac{161}{2400} q(x) G^3 + \dots \right) + O(h^8) \quad (21)$$

4.6. The Method with Vanished Phase-Lag Produced in [1]

$$LTE_{MethAnasSim} = h^6 \left(\frac{161}{2400} g(x) y(x) G^2 + \dots \right) + O(h^8) \quad (22)$$

4.7. The New Proposed Method with Vanished Phase-Lag and its First Derivative Produced in [44]

$$LTE_{FourStepII} = h^6 \left[\left(\frac{161}{2400} (g(x))^2 q(x) + \frac{161}{1200} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) + \frac{161}{480} \left(\frac{d^2}{dx^2} g(x) \right) q(x) \right) G + \dots \right] + O(h^8) \quad (23)$$

4.8. The New Proposed Method with Vanished Phase-Lag and its First and Second Derivatives Produced in Section 3

$$LTE_{ExplFourStep} = \frac{161 h^6}{600} \left(\left(\frac{d^2}{dx^2} g(x) \right) q(x) G + \dots \right) + O(h^8) \quad (24)$$

From the above equations we have the following theorem:

Theorem 2. –Classical Low Algebraic Order Four-Step Explicit Method: For this method the error increases as the third power of G .

–Low Algebraic Order Four-Step Explicit Phase-Fitted Method developed in [1]: For this method the error increases as the second power of G .

–Low Algebraic Order Four-Step Explicit Method with Vanished Phase-lag and its First Derivative developed in [44]: For this method the error increases as the first power of G .

–Low Algebraic Order Four-Step Explicit Method with Vanished Phase-lag and its First and Second Derivatives developed in Section 3: For this method the error increases as the first power of G but with coefficient lower than the coefficient of the first power of G of the method developed in [44].

So, for the approximate integration of the time independent radial Schrödinger equation the New Obtained Low Algebraic Order Method with Vanished Phase-Lag and its First and Second Derivatives is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

5. Stability Analysis

In this section we will study the stability of the new developed method. For this reason we apply the new obtained method to the scalar test equation:

$$q'' = -\omega^2 q. \tag{25}$$

where $\omega \neq \phi$ and where ϕ is the frequency in the scalar test equation (4) where was based the phase-lag analysis investigated above.

The above application to the scalar test equation (25) leads to the following difference equation:

$$A_2(s, v) (q_{n+2} + q_{n-2}) + A_1(s, v) (q_{n+1} + q_{n-1}) + A_0(s, v) q_n = 0 \tag{26}$$

where

$$A_2(s, v) = 1, A_1(s, v) = -\frac{1}{40} \frac{T_{12}}{v \cos(v) - \sin(v)}$$

$$A_0(s, v) = \frac{1}{20} \frac{T_{13}}{v \cos(v) - \sin(v)} \tag{27}$$

where

$$T_{12} = -53 \cos(v) s^2 v + 53 \cos(v) v^3 + 320 v (\cos(v))^2 + 53 \sin(v) s^2 + 159 \sin(v) v^2 - 160 \sin(v) \cos(v) - 160 v$$

$$T_{13} = -80 (\cos(v))^2 \sin(v) s^2 + 80 (\cos(v))^2 \sin(v) v^2 + 53 (\cos(v))^2 s^2 v - 53 (\cos(v))^2 v^3 + 240 v (\cos(v))^3 + 53 \sin(v) \cos(v) s^2 + 159 \sin(v) \cos(v) v^2 - 80 \sin(v) (\cos(v))^2 + 80 \sin(v) s^2 - 80 \sin(v) v^2 - 106 s^2 v + 106 v^3 - 120 v \cos(v) - 40 \sin(v)$$

and $s = \omega h$.

Remark. The frequency of the scalar test equation (25), ω , which is used for the stability analysis is not equal with the frequency of the scalar test equation (4), ϕ , which is used for the phase-lag analysis, i.e. $\omega \neq \phi$.

Based on the analysis presented in Section 2, we have the following definitions:

Definition 5. (see [16]) *P-stable methods* is called the method with interval of periodicity equal to $(0, \infty)$.

Definition 6. *Singularly almost P-stable* is called the method with interval of periodicity equal to $(0, \infty) - S$ ¹. The term *singularly almost P-stable method* is used only in the cases when the frequency of the scalar test equation for the phase-lag analysis is equal with the frequency of the scalar test equation for the stability analysis, i.e. $\omega = \phi$.

The $s - v$ plane for the method obtained in this paper is shown in Figure 2.

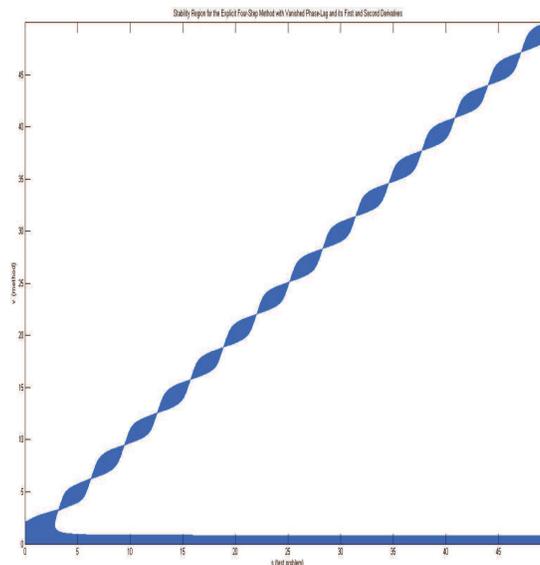


Figure 2: $s - v$ plane of the new produced method with vanished phase-lag and its first and second derivatives

Remark. In order one to read the the $s - v$ region, the following must be taken into account:

- The shadowed area denotes where the method is stable,
- The white area denotes the region where the method is unstable.

Remark. There are problems for which their mathematical models require the observation of **the surroundings of the first diagonal of the $s - v$ plane**. These are the cases of the mathematical models where the frequency of the scalar test equation used for the phase-lag analysis is equal with the frequency of the scalar test equation used for the stability analysis. In this category belong many problems in sciences and engineering (for example the time independent Schrödinger equation).

¹ where S is a set of distinct points

Based on the above remark, we investigate the case where the frequency of the scalar test equation used for the phase-lag analysis is equal with the frequency of the scalar test equation used for the stability analysis, 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 extract the results that the interval of periodicity of the new developed method is equal to: $(0, 256)$.

The above study leads to the following theorem:

Theorem 3. *The method obtained in section 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: $(0, 256)$ when the frequency of the scalar test equation used for the phase-lag analysis is equal with the frequency of the scalar test equation used for the stability analysis

6. Numerical results

In this section we will study the effectiveness of the new developed low algebraic order explicit four-step method. The study will take place via the numerical solution of the one-dimensional time-independent Schrödinger equation.

The radial time independent Schrödinger equation has a mathematics model of the form :

$$q''(r) = [l(l+1)/r^2 + V(r) - k^2]q(r). \tag{28}$$

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

$$y(0) = 0 \tag{29}$$

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

The mathematical model of the radial time independent Schrödinger equation (28) consists from functions, quantities and parameters. Here we give the definitions of these functions, quantities and parameters :

- 1.The function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(x) \rightarrow 0$ 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 method proposed in this paper belongs to the category of the frequency dependent methods. Therefore in order to apply these methods to any problem, the frequency must be determined , i.e. we have to define the parameter ϕ (see for example the notation after (4) and the formulae in section 3) must be defined. For the category of problems

of the radial Schrödinger equation, the parameter ϕ (for $l = 0$) is given by :

$$\phi = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{30}$$

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

6.1. Woods-Saxon potential

The well known Woods-Saxon potential is use for our numerical experiments. The model of the Woods-Saxon potential is given by :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0 q}{a(1+q)^2} \tag{31}$$

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 Figure 5.

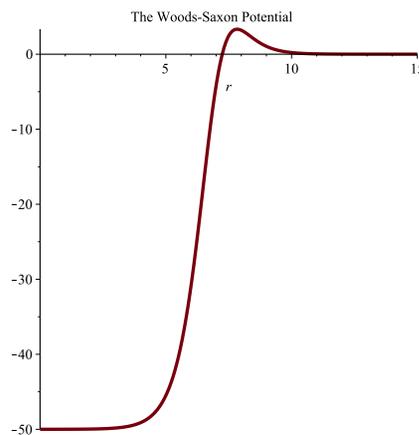


Figure 3: The Woods-Saxon potential.

Some critical points on the description of the potential can be defined for some potentials, such as the Woods-Saxon potential. These critical points then are used in order to determine the value of the parameter ϕ (see for details [45]).

Using the methodology presented in [46] and [47] and for the purpose of our tests, we choose ϕ as follows :

$$\phi = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5 - 2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5 - h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5 + h \\ \sqrt{E}, & \text{for } r \in [6.5 + 2h, 15] \end{cases} \tag{32}$$

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.

6.2. Radial Schrödinger Equation - The Resonance Problem

In this section the effectiveness of the new obtained method is investigated using the numerical solution of the radial time independent Schrödinger equation (28) with the Woods-Saxon potential (31). Initially it is necessary to approximate the true interval of integration, which is equal to $r \in (0, \infty)$, by a finite one. For our numerical purposes we consider the integration interval $r \in [0, 15]$. We will solve the above mentioned problem described by equation (28) in a rather large domain of energies, i.e., $E \in [1, 1000]$.

The Schrödinger equation effectively reduces to

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{33}$$

for r greater than some value R for the case of positive energies, $E = k^2$. This is because the potential decays faster than the term $\frac{l(l+1)}{r^2}$.

In the above mathematical model, the differential 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 equation (28) (when $r \rightarrow \infty$), has the asymptotic form

$$q(r) \approx Akrj_l(kr) - Bkrn_l(kr) \approx AC \left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kr - \frac{l\pi}{2}\right) \right] \tag{34}$$

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

$$\tan \delta_l = \frac{y(r_2)S(r_1) - y(r_1)S(r_2)}{y(r_1)C(r_1) - y(r_2)C(r_2)} \tag{35}$$

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 [48] and [49]). With these starting values, we evaluate at r_2 of the asymptotic region the phase shift δ_l .

The known as resonance problem is hold for the case of positive energies. 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:

$$q(0) = 0, q(r) = \cos(\sqrt{E}r) \text{ for large } r. \tag{36}$$

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

- The eighth order multi-step method developed by Quinlan and Tremaine [50], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [50], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [50], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [52], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [51], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [53], which is indicated as **Method MCR6**
- The classical form of the fourth algebraic order four-step method developed in Section 3, which is indicated as **Method NMCL²**.
- The Phase-Fitted Method (Case 1) developed in [1], which is indicated as **Method NMPF1**
- The Phase-Fitted Method (Case 2) developed in [1], which is indicated as **Method NMPF2**
- The Method developed in [44] (Case 2), which is indicated as **Method NMC2**
- The Method developed in [44] (Case 1), which is indicated as **Method NMC1**
- The New Obtained Method developed in Section 3, which is indicated as **Method NMPLD2V**

Table 1: Characteristics of the Methods of the same algebraic order compared in our numerical experiments. PL: Phase-Lag, DPL: First Derivative of the Phase-Lag, DDPL: Second Derivative of the Phase-Lag

Method	Algebraic Order	PL	DPL	DDPL
NMPF1	4	0	$-\frac{161}{9360} v^5$	$-\frac{161}{1040} v^4$
NMPF2	4	0	$-\frac{329}{17040} v^5$	$-\frac{987}{5680} v^4$
NMC1	4	0	0	$-\frac{161}{2340} v^4$
NMC2	4	0	0	$-\frac{329}{4260} v^4$
NMPLD2V	4	0	0	0

We defined some reference values using the well known two-step method of Chawla and Rao [53] with small step size for the integration. We then compared the numerically calculated eigenenergies with these reference values. In Figures 4 and 5, we present the maximum absolute error $Err_{max} = |\log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{37}$$

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of CPU time (in seconds).

² with the term classical we mean the method of Section 3 with constant coefficients

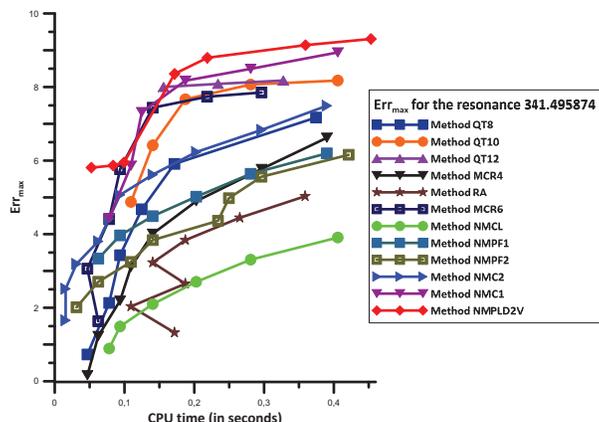


Figure 4: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

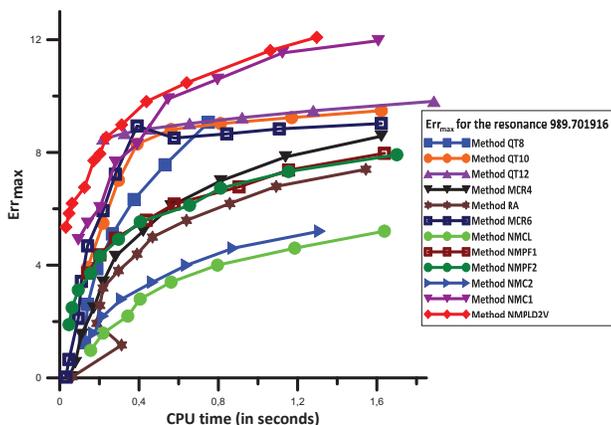


Figure 5: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

We note that the CPU time (in seconds) counts the computational cost for each method.

7. Conclusions

In this paper, we studied a family of low algebraic order explicit four-step methods. The main subjects of this study was:

- the investigation of the vanishing of the phase-lag and its first and second derivatives

- the comparative error analysis
- the stability analysis.
- the computational behavior of the new produced method and its effectiveness on the numerical solution of the radial Schrödinger equation and related problems.

From the numerical experiments mentioned above, we have the following :

- 1.The classical form of the tenth algebraic order four-step multiderivative method developed in Section 3, which is indicated as **Method NMCL** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [52], which is indicated as **Method MCR4**. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [51], which is indicated as **Method MRA**.
- 2.The tenth algebraic order multistep method developed by Quinlan and Tremaine [50], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [52], 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 [50], 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 [53], 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 [50], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [50], which is indicated as **Method QT10**
- 4.The Phase-Fitted Method (Case 1) developed in [1], which is indicated as **Method NMPF1** is more efficient than the classical form of the fourth algebraic order four-step method developed in Section 3, which is indicated as **Method NMCL**, the exponentially-fitted method of Raptis and Allison [51] and the Phase-Fitted Method (Case 2) developed in [1], which is indicated as **Method NMPF2**
- 5.The Method developed in [44] (Case 2), which is indicated as **Method NMC2** is more efficient than the classical form of the fourth algebraic order four-step method developed in Section 3, which is indicated as **Method NMCL**, the exponentially-fitted method of Raptis and Allison [51] and the Phase-Fitted Method (Case 2) developed in [1], which is indicated as **Method NMPF2** and the Phase-Fitted Method (Case 1) developed in [1], which is indicated as **Method NMPF1**
- 6.The Method developed in [44] (Case 1), which is indicated as **Method NMC1**, is the more efficient than all the other methods mentioned above.
- 7.The New Obtained Method developed in Section 3, which is indicated as **Method NMPLD2V**, 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).

Appendix: Formulae of the derivatives of q_n

Formulae of the derivatives which presented in the formulae of the Local Truncation Errors:

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

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

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