

*Research Article*

# Optimizing a Hybrid Two-Step Method for the Numerical Solution of the Schrödinger Equation and Related Problems with Respect to Phase-Lag

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We use a methodology of optimization of the efficiency of a hybrid two-step method for the numerical solution of the radial Schrödinger equation and related problems with periodic or oscillating solutions. More specifically, we study how the vanishing of the phase-lag and its derivatives optimizes the efficiency of the hybrid two-step method.

## 1. Introduction

In this paper, we investigate the numerical solution of systems of second order differential equations of the form

$$y''(x) = f(x, y), \quad (1.1)$$

while the following initial conditions hold:

$$\begin{aligned} y(x_0) &= y_0, \\ y'(x_0) &= y'_0, \end{aligned} \quad (1.2)$$

where  $f$  is independent of  $y'(x)$ .

Problems for which their models are expressed with the above system of equations can be found in different fields of applied sciences such as astronomy, astrophysics, quantum mechanics, quantum chemistry, celestial mechanics, electronics physical chemistry, and chemical physics (see [1–22]).

The optimization of the efficiency of a numerical method for the numerical solution of the radial Schrödinger equation and related problems with periodic or oscillating solutions is the subject of this paper. More specifically, in this paper, we will investigate how the procedure of vanishing of the phase-lag and its first derivative optimizes, the efficiency of a numerical method. As a result the produced methods via the above procedure, they are very efficient on any problem with periodic or oscillating solutions or on any problem with solution which contains the functions  $\cos$  and  $\sin$  or any combination of them.

The purpose of this paper is the computation of the coefficients of the proposed hybrid two-step method in order:

- (1) to have the highest algebraic order,
- (2) to have the phase-lag vanished,
- (3) and finally, to have the first derivative of the phase-lag vanished as well.

The procedure of vanishing of the phase lag and its first derivative is based on the direct formula for the determination of the phase-lag for  $2m$ -method (see [3, 23]).

We will investigate the efficiency of the new methodology based on the error analysis and stability analysis of the new proposed method. We will also apply the studied methods to the numerical solution of the radial Schrödinger equation and to related problems.

We will consider a hybrid two-step method of sixth algebraic order. Based on this method, we will develop the new optimized method which is of sixth algebraic order and it has phase-lag and its first derivative equal to zero. We will investigate the stability and the error of the produced method. We will apply the obtained method to the resonance problem of the radial Schrödinger equation. This is one of the most difficult problems arising from the radial Schrödinger equation. The construction of the paper is given below.

- (i) In Section 2, the phase-lag analysis of symmetric multistep methods is presented.
- (ii) The development of the new optimized method is presented in Section 3.
- (iii) The error analysis is presented in Section 4.
- (iv) The stability analysis of the new produced method is presented in Section 5.
- (v) The numerical results are presented in Section 6.
- (vi) Finally, in Section 7, we present some remarks and conclusions.

## 2. Phase-Lag Analysis of Symmetric Multistep Methods

For the numerical solution of the initial value problem:

$$u'' = f(x, u), \quad (2.1)$$

consider a multistep method with  $m$  steps which can be used over the equally spaced intervals  $\{x_i\}_{i=0}^m \in [a, b]$  and  $h = |x_{i+1} - x_i|$ ,  $i = 0(1)m - 1$ .

If the method is symmetric, then  $a_i = a_{m-i}$  and  $b_i = b_{m-i}$ ,  $i = 0(1)(m/2)$ .

When a symmetric  $2m$ -step method, that is, for  $i = -m(1)m$ , is applied to the scalar test equation:

$$u'' = -\omega^2 u, \quad (2.2)$$

a difference equation of the form:

$$A_m(H)u_{n+m} + \cdots + A_1(H)u_{n+1} + A_0(H)u_n + A_1(H)u_{n-1} + \cdots + A_m(H)u_{n-m} = 0 \quad (2.3)$$

is obtained, where  $H = \omega h$ ,  $h$  is the step length, and  $A_0(H), A_1(H), \dots, A_m(H)$  are polynomials of  $H = \omega h$ .

The characteristic equation associated with (2.3) is given by:

$$A_m(H)\lambda^m + \cdots + A_1(H)\lambda + A_0(H) + A_1(H)\lambda^{-1} + \cdots + A_m(H)\lambda^{-m} = 0 \quad (2.4)$$

**Theorem 2.1** (see [3, 23]). *The symmetric  $2m$ -step method with characteristic equation given by (2.4) has phase-lag order  $q$  and phase-lag constant  $c$  given by*

$$-cH^{q+2} + O(H^{q+4}) = \frac{2A_m(H) \cos(mH) + \cdots + 2A_j(H) \cos(jH) + \cdots + A_0(H)}{2m^2 A_m(H) + \cdots + 2j^2 A_j(H) + \cdots + 2A_1(H)}. \quad (2.5)$$

The formula mentioned in the above theorem is a direct method for the computation of the phase-lag of any symmetric  $2m$ -step method.

### 3. The Family of Hybrid Methods

#### 3.1. The General Family of Methods

Consider the following family of hybrid two-step methods (see [24]):

$$\begin{aligned} \hat{u}_{n+1} &= 2u_n - u_{n-1} + h^2 f_n, \\ \tilde{u}_{n+1} &= 2u_n - u_{n-1} + \frac{h^2}{12} (\hat{f}_{n+1} + 10f_n + f_{n-1}), \\ \bar{u}_{n-(1/2)} &= \frac{1}{52} (3\tilde{u}_{n+1} + 20u_n + 29u_{n-1}) + \frac{h^2}{4992} (41\hat{f}_{n+1} - 682f_n - 271f_{n-1}), \\ \bar{u}_{n+(1/2)} &= \frac{1}{104} (5\tilde{u}_{n+1} + 146u_n - 47u_{n-1}) + \frac{h^2}{4992} (-59\hat{f}_{n+1} + 1438f_n + 253f_{n-1}), \\ u_{n+1} - 2u_n + u_{n-1} &= h^2 [b_0 (\tilde{f}_{n+1} + f_{n-1}) + b_1 (\bar{f}_{n+(1/2)} + \bar{f}_{n-(1/2)}) + (1 - 2b_0 - 2b_1) f_n]. \end{aligned} \quad (3.1)$$

The above-mentioned method belongs to the families of hybrid (Runge-Kutta type) symmetric two-step methods for the numerical solution of problems of the form  $u'' = f(x, u)$ . In the above general form, the coefficient  $b_0$  and  $b_1$  are free parameters. In the above method,  $h$

is the step size of the integration and  $n$  is the number of steps, that is,  $y_n$  is the approximation of the solution on the point  $x_n$ ,  $x_n = x_0 + nh$ , and  $x_0$  is the initial value point.

### 3.2. The Optimized Hybrid Method of the Family with Vanished Phase-Lag and Its First Derivative

Consider the method (3.1).

If we apply the method (3.1) to the scalar test equation (2.2), we obtain the difference equation (2.3) with  $m = 1$  and  $A_j(H)$ ,  $j = 0, 1$  given by

$$A_0(H) = -2 - b_0H^4 + \frac{1}{12}H^6b_0 - \frac{1}{4}b_1H^4 + \frac{1}{192}H^6b_1 + H^2, \quad A_1(H) = 1. \quad (3.2)$$

Requiring the above method to have its phase-lag vanished and by using the formulae (2.5) (for  $k = 1$ ) and (3.2), we have the following equation:

$$PL = \cos(H) - 1 - \frac{1}{2}b_0H^4 + \frac{1}{24}H^6b_0 - \frac{1}{8}b_1H^4 + \frac{1}{384}H^6b_1 + \frac{1}{2}H^2 = 0. \quad (3.3)$$

Demanding the method to have the first derivative of the phase-lag vanished as well, we have the equation:

$$DPL = -\sin(H) - 2b_0H^3 + \frac{1}{4}H^5b_0 - \frac{1}{2}b_1H^3 + \frac{1}{64}H^5b_1 + H = 0, \quad (3.4)$$

where DPL is the first derivative of the phase-lag.

Requiring now the coefficients of the new proposed method to satisfy the equations (3.3)-(3.4), we obtain the following coefficients of the new developed method:

$$b_0 = \frac{1}{3} \frac{192 \cos(H) - 6 \cos(H)H^2 - 192 + 54H^2 - 2H^4 + 48H \sin(H) - H^3 \sin(H)}{H^6}, \quad (3.5)$$

$$b_1 = \frac{1}{3} \frac{32H^4 + 16H^3 \sin(H) - 288H^2 + 96 \cos(H)H^2 - 192H \sin(H) + 768 - 768 \cos(H)}{H^6}.$$

For some values of  $|\omega|$ , the formulae given by (3.5) are subject to heavy cancellations. In this case, the following Taylor series expansions should be used:

$$b_0 = \frac{1}{60} - \frac{1}{630}H^2 + \frac{13}{302400}H^4 - \frac{19}{29937600}H^6 + \frac{131}{21794572800}H^8$$

$$- \frac{1}{25147584000}H^{10} + \frac{311}{1600593426432000}H^{12} - \frac{37}{50685458503680000}H^{14}$$

$$+ \frac{47}{21615398611107840000}H^{16} - \frac{1}{190088358374154240000}H^{18} + \dots,$$

$$\begin{aligned}
b_1 = & \frac{4}{15} + \frac{2}{315}H^2 - \frac{1}{2700}H^4 + \frac{13}{1871100}H^6 - \frac{101}{1362160800}H^8 \\
& + \frac{43}{81729648000}H^{10} - \frac{269}{100037089152000}H^{12} + \frac{1}{95995186560000}H^{14} \\
& - \frac{557}{17562511371525120000}H^{16} + \frac{1}{12823421001431040000}H^{18} + \dots
\end{aligned} \tag{3.6}$$

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

The local truncation error of the new proposed method (mentioned as NM) is given by

$$\text{LTE}_{\text{NM}} = -\frac{h^8}{20160} \left( u_n^8 + 2\omega^2 u_n^6 + \omega^4 u_n^4 \right) + O(h^{10}). \tag{3.7}$$

#### 4. Error Analysis

We will study the following methods.

##### 4.1. Standard Method (i.e., the Method (3.1) with Constant Coefficients)

It holds that

$$\text{LTE}_{\text{CL}} = -\frac{h^8}{20160} u_n^{(8)} + O(h^{10}). \tag{4.1}$$

##### 4.2. New Method with Vanished Phase-Lag and Its First Derivative (Developed in Section 3.2)

It holds that

$$\text{LTE}_{\text{NM}} = -\frac{h^8}{20160} \left( u_n^8 + 2\omega^2 u_n^6 + \omega^4 u_n^4 \right) + O(h^{10}). \tag{4.2}$$

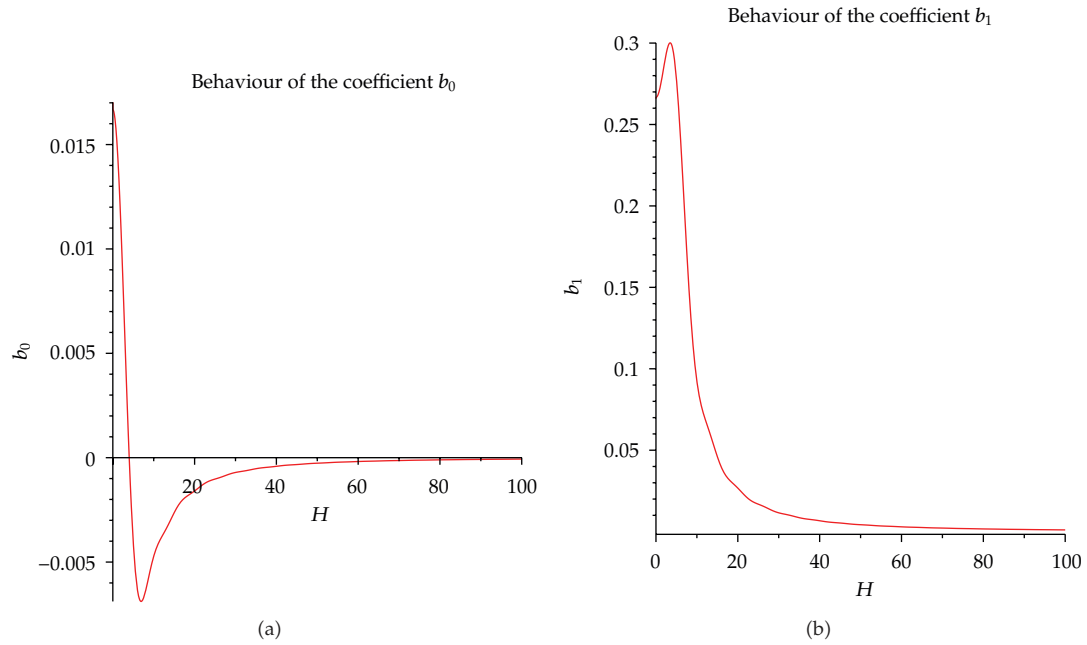
The error analysis is based on the following steps.

- (i) The radial time independent Schrödinger equation is of the form:

$$u''(x) = f(x)u(x). \tag{4.3}$$

- (ii) Based on the paper of Ixaru and Rizea [2], the function  $f(x)$  can be written in the form:

$$f(x) = g(x) + G, \tag{4.4}$$



**Figure 1:** Behaviour of the coefficients of the new proposed method given by (3.5) for several values of  $H = \omega h$ .

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

- (iii) We express the derivatives  $u_n^{(i)}$ ,  $i = 2, 3, 4, \dots$ , which are terms of the local truncation error formulae, in terms of (4.4). The expressions are presented as polynomials of  $G$ .
- (iv) Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae.

We use the procedure mentioned above and the formulae:

$$\begin{aligned}
 u_n^{(2)} &= (V(x) - V_c + G)u(x) \\
 u_n^{(4)} &= \left( \frac{d^2}{dx^2} V(x) \right) u(x) + 2 \left( \frac{d}{dx} V(x) \right) \left( \frac{d}{dx} u(x) \right) \\
 &\quad + (V(x) - V_c + G) \left( \frac{d^2}{dx^2} u(x) \right).
 \end{aligned}$$

$$\begin{aligned}
u_n^{(6)} = & \left( \frac{d^4}{dx^4} V(x) \right) u(x) + 4 \left( \frac{d^3}{dx^3} V(x) \right) \left( \frac{d}{dx} u(x) \right) \\
& + 3 \left( \frac{d^2}{dx^2} V(x) \right) \left( \frac{d^2}{dx^2} u(x) \right) + 4 \left( \frac{d}{dx} V(x) \right)^2 u(x) \\
& + 6(V(x) - V_c + G) \left( \frac{d}{dx} V(x) \right) \left( \frac{d}{dx} u(x) \right) \\
& + 4(V(x) - V_c + G) u(x) \left( \frac{d^2}{dx^2} V(x) \right) \\
& + (V(x) - V_c + G)^2 \left( \frac{d^2}{dx^2} u(x) \right) \\
& \dots
\end{aligned} \tag{4.5}$$

We consider two cases in terms of the value of  $E$ .

- (1) The energy is close to the potential, that is,  $G = V_c - E \approx 0$ . 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 standard method and of the trigonometrically fitted methods.
- (2)  $G \gg 0$  or  $G \ll 0$ . Then  $|G|$  is a large number.

Hence, we have the following asymptotic expansions of the Local Truncation Errors.

### 4.3. Standard Method

It holds that

$$\text{LTE}_{\text{CL}} = h^8 \left( -\frac{1}{20160} w(x) G^4 + \dots \right) + O(h^{10}). \tag{4.6}$$

### 4.4. New Method with Vanished Phase-Lag and Its First Derivative (Developed in Section 3.2)

It holds that

$$\begin{aligned}
\text{LTE}_{\text{NM}} = & h^8 \left[ \left( \frac{1}{2240} \left( \frac{d^2}{dx^2} g(x) \right) u(x) + \frac{1}{10080} \left( \frac{d}{dx} g(x) \right) \frac{d}{dx} u(x) \right. \right. \\
& \left. \left. + \frac{1}{20160} g(x)^2 u(x) \right) G^2 + \dots \right] + O(h^{10}).
\end{aligned} \tag{4.7}$$

From the above equations, we have the following theorem.

**Theorem 4.1.** For the standard hybrid two-step method, the error increases as the fourth power of  $G$ . For the new method with vanished phase-lag and its first derivative (developed in Section 3.2), the error increases as the second power of  $G$ . So, for the numerical solution of the time independent radial Schrödinger equation, the new method with vanished phase-Lag and its first derivative is much more efficient, especially for large values of  $|G| = |V_c - E|$ .

## 5. Stability Analysis

Applying the new method to the scalar test equation:

$$w'' = -z^2 w, \quad (5.1)$$

we obtain the following difference equation:

$$A_1(v, H)(w_{n+1} + w_{n-1}) + A_0(v, H)w_n = 0, \quad (5.2)$$

where

$$A_0(v, H) = \frac{T_0}{H^6}, \quad A_1(v, H) = 1, \quad (5.3)$$

where  $T_0 = -2H^6 - 4v^6 - 6 \cos(H)H^2v^4 + v^6H \sin(H) - H^3 \sin(H)v^4 + 4v^6 \cos(H) + 6H^2v^4 + v^6H^2 - 2H^4v^4 + v^2H^6$  and  $H = \omega h$ ,  $v = zh$ .

The corresponding characteristic equation is given by.

$$A_1(v, H)(\lambda^2 + 1) + A_0(v, H)\lambda = 0. \quad (5.4)$$

*Definition 5.1* (see [25]). A symmetric  $2m$ -step method with the characteristic equation given by (2.4) is said to have an *interval of periodicity*  $(0, v_0^2)$  if, for all  $v \in (0, v_0^2)$ , the roots  $z_i$ ,  $i = 1, 2$  satisfy

$$z_{1,2} = e^{\pm i\zeta(v)}, \quad |z_i| \leq 1, \quad i = 3, 4, \quad (5.5)$$

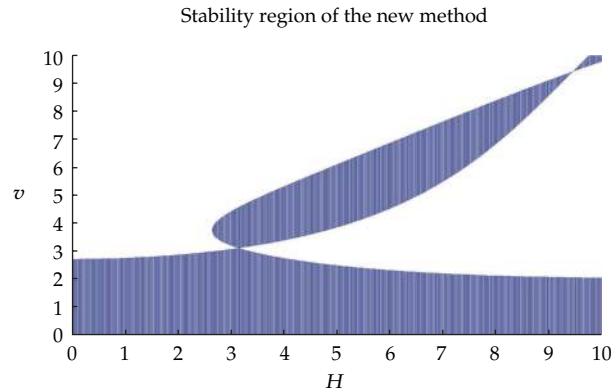
where  $\zeta(v)$  is a real function of  $zh$  and  $v = zh$ .

*Definition 5.2* (see [25]). A method is called P-stable if its interval of periodicity is equal to  $(0, \infty)$ .

*Definition 5.3.* A method is called singularly almost P-stable if its interval of periodicity is equal to  $(0, \infty) - S$  (where  $S$  is a set of distinct points) only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, that is,  $v = H$ .

In Figure 2, we present the  $H$ - $v$  plane for the method developed in this paper. A shadowed area denotes the  $H$ - $v$  region where the method is stable, while a white area denotes the region where the method is unstable.





**Figure 2:**  $v$ - $H$  plane of the new developed method.

**Table 1:** Comparative stability analysis for the methods mentioned in Section 5.

Method	Interval of Periodicity
CL	(0, 7.571916416)
NM (see Section 3.2)	(0, 39.47841760)

*Remark 5.4.* For the solution of the Schrödinger equation, the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to observe the surroundings of the first diagonal of the  $H$ - $v$  plane.

In the case that the frequency of the scalar test equation is equal with the frequency of phase fitting, that is, in the case that  $v = H$  (i.e., see the surroundings of the first diagonal of the  $H$ - $v$  plane), it is easy to see that the interval of periodicity of the new method developed in Section 3.2 is equal to (0, 39.47841760).

From the above analysis, we have the following theorem.

**Theorem 5.5.** *The method developed in Section 3.2 is of eighth algebraic order, has the phase-lag and its first derivative equal to zero, and has an interval of periodicity equals to (0, 39.47841760).*

Based on the analysis presented above, we studied the interval of periodicity of some well-known methods mentioned in the previous paragraph. The results presented in the Table 1.

## 6. Numerical Results

In order to study the efficiency of the new developed method, we apply it

- (i) to the radial time-independent Schrödinger equation, and
- (ii) to a nonlinear orbital problem.

### 6.1. The Radial Schrödinger Equation

The radial Schrödinger equation can be presented as

$$q''(r) = \left[ \frac{l(l+1)}{r^2} + V(r) - k^2 \right] q(r). \quad (6.1)$$

The above equation presents the model for a particle in a central potential field where  $r$  is the radial variable (see [26, 27]).

In (6.1), we have the following terms.

- (i) The function  $W(r) = l(l+1)/r^2 + V(r)$  is called *the effective potential*. This satisfies  $W(r) \rightarrow 0$  as  $r \rightarrow \infty$ .
- (ii) The quantity  $k^2$  is a real number denoting *the energy*.
- (iii) The quantity  $l$  is a given integer representing the *angular momentum*.
- (iv)  $V$  is a given function which denotes the *potential*.

We note here that the models which are given via the radial Schrödinger equation are boundary-value problems. In these cases, the boundary conditions are

$$q(0) = 0 \quad (6.2)$$

and a second boundary condition, for large values of  $r$ , determined by physical considerations.

In order to apply the new obtained method to the radial Schrödinger equation, the value of parameter  $\omega$  is needed. In (6.1), the parameter  $\omega$  is given by

$$\omega = \sqrt{|q(r)|} = \sqrt{|V(r) - E|}, \quad (6.3)$$

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

#### 6.1.1. Woods-Saxon Potential

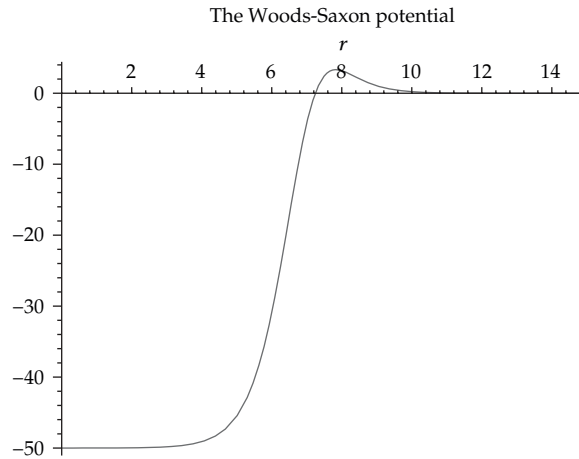
We use as a potential the well-known Woods-Saxon potential which can be written as

$$V(r) = \frac{u_0}{1+y} - \frac{u_0 y}{a(1+y)^2} \quad (6.4)$$

with  $y = \exp[(r - R_0)/a]$ ,  $u_0 = -50$ ,  $a = 0.6$ , and  $X_0 = 7.0$ .

The behaviour of Woods-Saxon potential is shown in Figure 3.

It is well known that for some potentials, such as the Woods-Saxon potential, the definition of parameter  $\omega$  is given not as a function of  $r$  but as based on some critical points which have been defined from the investigation of the appropriate potential (see for details [28]).



**Figure 3:** The Woods-Saxon potential.

For the purpose of obtaining our numerical results, it is appropriate to choose  $v$  as follows (see for details [2, 26]):

$$\omega = \begin{cases} \sqrt{-50 + E}, & \text{for } r \in [0, 6.5 - 2h], \\ \sqrt{-37.5 + E}, & \text{for } r = 6.5 - h \\ \sqrt{-25 + E}, & \text{for } r = 6.5 \\ \sqrt{-12.5 + E}, & \text{for } r = 6.5 + h \\ \sqrt{E}, & \text{for } r \in [6.5 + 2h, 15]. \end{cases} \quad (6.5)$$

For example, in the point of the integration region  $r = 6.5$ , the value of  $\omega$  is equal to  $\sqrt{-25 + E}$ . So,  $H = \omega h = \sqrt{-25 + E}h$ . In the point of the integration region  $r = 6.5 - 3h$ , the value of  $\omega$  is equal to  $\sqrt{-50 + E}$ , and so forth.

### 6.1.2. Radial Schrödinger Equation—The Resonance Problem

We consider the numerical solution of the radial Schrödinger equation (6.1) in the well-known case of the Woods-Saxon potential (6.4). In order to solve this problem numerically, we must approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration, we take the domain of integration as  $r \in [0, 15]$ . We consider equation (6.1) in a rather large domain of energies, that is,  $E \in [1, 1000]$ .

In the case of positive energies,  $E = k^2$ , the potential decays faster than the term  $l(l + 1)/x^2$  and the Schrödinger equation effectively reduces to

$$q''(r) + \left( k^2 - \frac{l(l+1)}{r^2} \right) q(r) = 0, \quad (6.6)$$

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 equation (6.1) (when  $r \rightarrow \infty$ ) has the asymptotic form:

$$\begin{aligned} q(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC \left[ \sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right) \right], \end{aligned} \quad (6.7)$$

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

$$\tan \delta_l = \frac{q(r_2)S(r_1) - q(r_1)S(r_2)}{q(r_1)C(r_1) - q(r_2)C(r_2)}, \quad (6.8)$$

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  $q_j$ ,  $j = 0, 1$  before starting a two-step method. From the initial condition, we obtain  $q_0$ . The value  $q_1$  is obtained by using high-order Runge-Kutta-Nyström methods (see [29–31]). With these starting values, we evaluate at  $r_2$  of the asymptotic region the phase shift  $\delta_l$ .

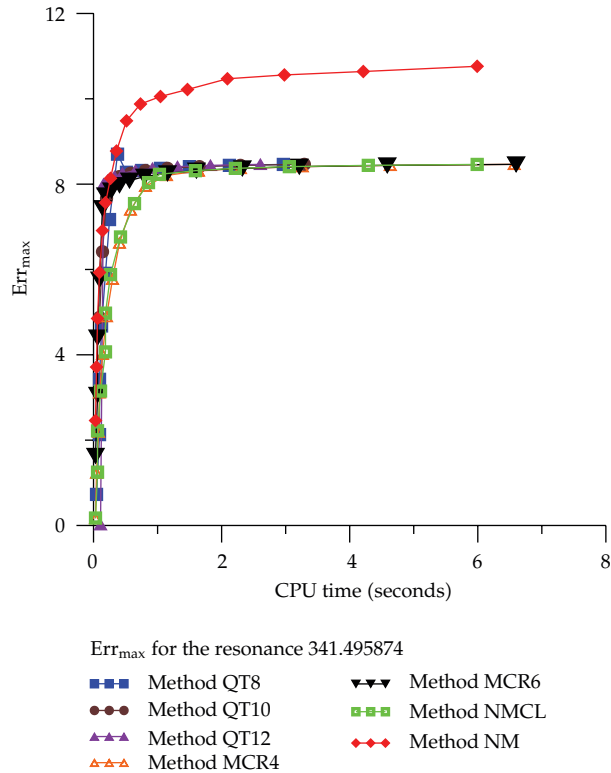
For positive energies, we have the so-called resonance problem. This problem consists either of finding the phase-shift  $\delta_l$  or finding those  $E$ , for  $E \in [1, 1000]$ , at which  $\delta_l = \pi/2$ . We actually solve the latter problem, known as *the resonance problem*.

The boundary conditions for this problem are

$$q(0) = 0, \quad q(r) = \cos(\sqrt{Er}) \text{ for large } r. \quad (6.9)$$

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

- (i) The eighth-order multistep method developed by Quinlan and Tremaine [32], which is indicated as *Method QT8*.
- (ii) The tenth-order multistep method developed by Quinlan and Tremaine [32], which is indicated as *Method QT10*.
- (iii) The twelfth-order multistep method developed by Quinlan and Tremaine [32], which is indicated as *Method QT12*.
- (iv) The fourth-algebraic-order method of Chawla and Rao with minimal phase-lag [33], which is indicated as *Method MCR4*.
- (v) The hybrid sixth-algebraic-order method developed by Chawla and Rao with minimal phase-lag [4], which is indicated as *Method MCR6*.
- (vi) The standard form of the eighth-algebraic-order method developed in Section 3.2, which is indicated as *Method NMCL*. (with the term standard we mean the method of Section 3.2 with constant coefficients.)
- (vii) The new developed hybrid two-step method with vanished phase-lag and its first derivative (obtained in Section 3.2), which is indicated as *Method NM*.



**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.

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

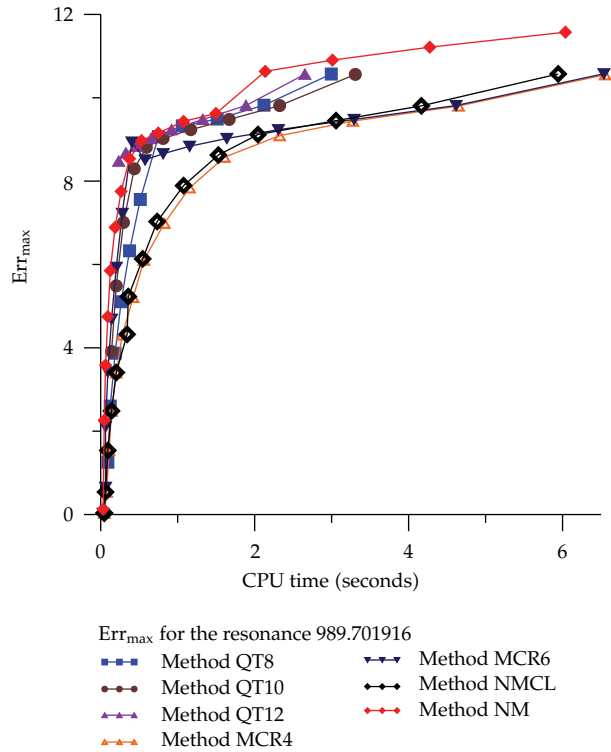
$$Err = |E_{calculated} - E_{accurate}|, \tag{6.10}$$

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.

### 6.2. A Nonlinear Orbital Problem

Consider the nonlinear system of equations:

$$u'' + W^2u = \frac{2uv - \sin(2Wx)}{(u^2 + v^2)^{3/2}}, \quad u(0) = 1, \quad u'(0) = 0,$$



**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.

$$v'' + W^2v = \frac{u^2 - v^2 - \cos(2Wx)}{(u^2 + v^2)^{3/2}}, \quad v(0) = 0, \quad v'(0) = W. \tag{6.11}$$

The analytical solution of the problem is the following:

$$u(x) = \cos(Wx), \quad v(x) = \sin(Wx). \tag{6.12}$$

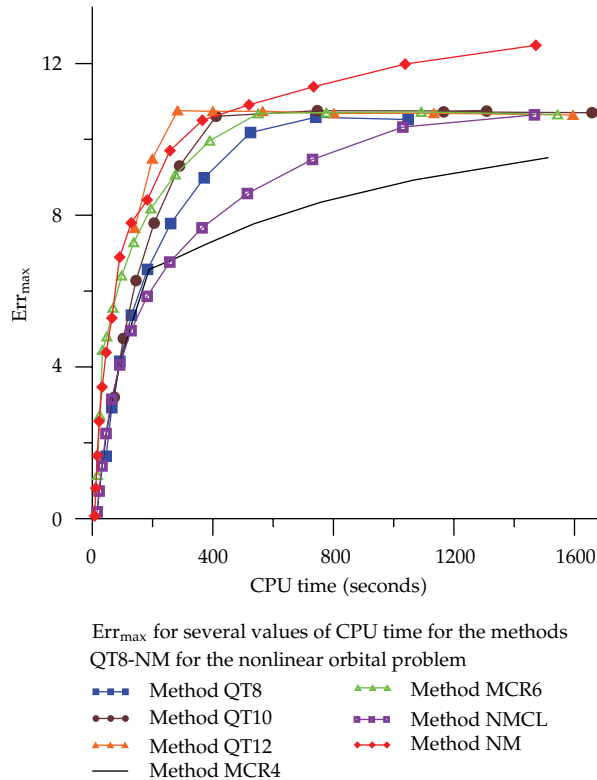
The system of equations (6.11) has been solved for  $0 \leq x \leq 10000$  and  $W = 10$  using the methods mentioned in Section 6.1.

For this problem, we have  $\omega = 10$ . The numerical results obtained for the seven methods mentioned above were compared with the analytical solution. Figure 6 shows the absolute errors  $Err_{max}$  defined by

$$Err_{max} = \left| \log_{10} \left[ \max(\|u(x)_{calculated} - u(x)_{theoretical}\|, \|v(x)_{calculated} - v(x)_{theoretical}\|) \right] \right|, \tag{6.13}$$

$x \in [0, 10000],$

for several values of the CPU time (in seconds).



**Figure 6:** Accuracy (digits) for several values of CPU time (in seconds) for the nonlinear orbital problem. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU time, accuracy (digits) is less than 0.

## 7. Conclusions

The purpose of this paper was the optimization of the efficiency of a hybrid two-step method for the approximate solution of the radial Schrödinger equation and related problems. We have described how the methodology of vanishing of the phase-lag and its first derivative optimize the behaviour of the specific numerical method. The results of the application of this methodology was a hybrid two-step method that is very efficient on any problem with oscillating solutions or problems with solutions contain the functions  $\cos$  and  $\sin$  or any combination of them.

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

- (1) The standard form of the eighth-algebraic-order method developed in Section 3.2, which is indicated as *Method NMCL*, is more efficient than the fourth-algebraic-order method of Chawla and Rao with minimal phase-lag [33], which is indicated as *Method MCR4*.
- (2) The tenth-order multistep method developed by Quinlan and Tremaine [32], which is indicated as *Method QT10*, is more efficient than the fourth-algebraic-order method of Chawla and Rao with minimal phase-lag [33], which is indicated as *Method MCR4*. *Method QT10* is also more efficient than the eighth-order multistep method developed by Quinlan and Tremaine [32], which is indicated as *Method*

QT8. Finally, *Method QT10* is also more efficient than the hybrid sixth-algebraic-order method developed by Chawla and Rao with minimal phase-lag [4], which is indicated as *Method MCR6*.

- (3) The twelfth-order multistep method developed by Quinlan and Tremaine [32], which is indicated as *Method QT12*, is more efficient than the tenth-order, multistep method developed by Quinlan and Tremaine [32], which is indicated as *Method QT10*.
- (4) Finally, the new developed hybrid two-step method with vanished phase-lag and its first derivative (obtained in Section 3.2), which is indicated as *Method NM*, is the most efficient one.

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

## Acknowledgment

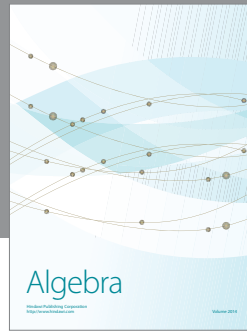
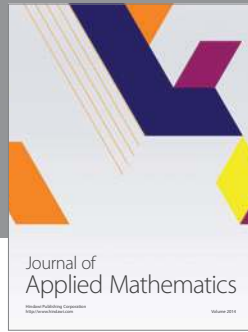
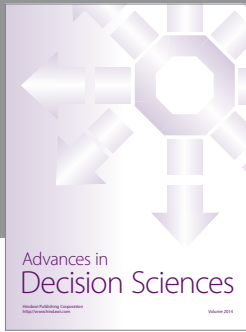
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## References

- [1] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Series in Computational Mathematics, 2nd edition, 2006.
- [2] L. Gr. Ixaru and M. Rizea, "A numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies," *Computer Physics Communications*, vol. 19, no. 1, pp. 23–27, 1980.
- [3] A. Konguetsof and T. E. Simos, "A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 93–106, 2003.
- [4] M. M. Chawla and P. S. Rao, "An explicit sixth-order method with phase-lag of order eight for  $y' = f(t, y)$ ," *Journal of Computational and Applied Mathematics*, vol. 17, no. 3, pp. 365–368, 1987.
- [5] J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problems*, vol. 7, Chapman & Hall, London, UK, 1994.
- [6] W. Zhu, X. Zhao, and Y. Tang, "Numerical methods with a high order of accuracy applied in the quantum system," *Journal of Chemical Physics*, vol. 104, no. 6, pp. 2275–2286, 1996.
- [7] J. C. Chiou and S. D. Wu, "Open Newton-Cotes differential methods as multilayer symplectic integrators," *Journal of Chemical Physics*, vol. 107, no. 17, pp. 6894–6898, 1997.
- [8] T. E. Simos, "A fourth algebraic order exponentially-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation," *IMA Journal of Numerical Analysis*, vol. 21, no. 4, pp. 919–931, 2001.
- [9] T. E. Simos, "Exponentially-fitted Runge-Kutta-Nyström method for the numerical solution of initial-value problems with oscillating solutions," *Applied Mathematics Letters*, vol. 15, no. 2, pp. 217–225, 2002.
- [10] Ch. Tsitouras and T. E. Simos, "Optimized Runge-Kutta pairs for problems with oscillating solutions," *Journal of Computational and Applied Mathematics*, vol. 147, no. 2, pp. 397–409, 2002.
- [11] Z. Kalogiratou, Th. Monovasilis, and T. E. Simos, "Symplectic integrators for the numerical solution of the Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 83–92, 2003.
- [12] Z. Kalogiratou and T. E. Simos, "Newton-Cotes formulae for long-time integration," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 75–82, 2003.



- [13] G. Psihoyios and T. E. Simos, "Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions," *Journal of Computational and Applied Mathematics*, vol. 158, no. 1, pp. 135–144, 2003.
- [14] T. E. Simos, I. T. Famelis, and C. Tsitouras, "Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions," *Numerical Algorithms*, vol. 34, no. 1, pp. 27–40, 2003.
- [15] T. E. Simos, "Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution," *Applied Mathematics Letters*, vol. 17, no. 5, pp. 601–607, 2004.
- [16] K. Tselios and T. E. Simos, "Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics," *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 173–181, 2005.
- [17] D. P. Sakas and T. E. Simos, "Multiderivative methods of eighth algebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 161–172, 2005.
- [18] G. Psihoyios and T. E. Simos, "A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions," *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 137–147, 2005.
- [19] Z. A. Anastassi and T. E. Simos, "An optimized Runge-Kutta method for the solution of orbital problems," *Journal of Computational and Applied Mathematics*, vol. 175, no. 1, pp. 1–9, 2005.
- [20] T. E. Simos, "Closed Newton-Cotes trigonometrically-fitted formulae of high order for long-time integration of orbital problems," *Applied Mathematics Letters*, vol. 22, no. 10, pp. 1616–1621, 2009.
- [21] S. Stavroyiannis and T. E. Simos, "Optimization as a function of the phase-lag order of nonlinear explicit two-step  $P$ -stable method for linear periodic IVPs," *Applied Numerical Mathematics*, vol. 59, no. 10, pp. 2467–2474, 2009.
- [22] T. E. Simos, "Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation," *Acta Applicandae Mathematicae*, vol. 110, no. 3, pp. 1331–1352, 2010.
- [23] T. E. Simos and P. S. Williams, "A finite-difference method for the numerical solution of the Schrödinger equation," *Journal of Computational and Applied Mathematics*, vol. 79, no. 2, pp. 189–205, 1997.
- [24] T. E. Simos and P. S. Williams, "On finite difference methods for the solution of the Schrödinger equation," *Computers and Chemistry*, vol. 23, no. 6, pp. 513–554, 1999.
- [25] J. D. Lambert and I. A. Watson, "Symmetric multistep methods for periodic initial value problems," *Journal of the Institute of Mathematics and its Applications*, vol. 18, no. 2, pp. 189–202, 1976.
- [26] L.Gr. Ixaru and M. Micu, *Topics in Theoretical Physics*, Central Institute of Physics, Bucharest, Romania, 1978.
- [27] L. D. Landau and F. M. Lifshitz, *Quantum Mechanics*, Pergamon, New York, NY, USA, 1965.
- [28] T. E. Simos and P. S. Williams, "A new Runge-Kutta-Nyström method with phase-lag of order infinity for the numerical solution of the Schrödinger equation," *MATCH Communications in Mathematical and in Computer Chemistry*, no. 45, pp. 123–137, 2002.
- [29] J. R. Dormand and P. J. Prince, "Runge-Kutta-Nyström triples," *Computers & Mathematics with Applications*, vol. 13, no. 12, pp. 937–949, 1987.
- [30] J. R. Dormand, M. E. A. El-Mikkawy, and P. J. Prince, "High-order embedded Runge-Kutta-Nyström formulae," *IMA Journal of Numerical Analysis*, vol. 7, no. 4, pp. 423–430, 1987.
- [31] J. R. Dormand, M. E. A. El-Mikkawy, and P. J. Prince, "Families of Runge-Kutta-Nyström formulae," *IMA Journal of Numerical Analysis*, vol. 7, no. 2, pp. 235–250, 1987.
- [32] G. D. Quinlan and S. Tremaine, "Symmetric multistep methods for the numerical integration of planetary orbits," *Astronomical Journal*, vol. 100, no. 5, pp. 1694–1700, 1990.
- [33] M. M. Chawla and P. S. Rao, "A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial value problems—II. Explicit method," *Journal of Computational and Applied Mathematics*, vol. 15, no. 3, pp. 329–337, 1986.



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