

A new two-step hybrid method for the numerical solution of the Schrödinger equation

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Abstract With this paper, a new algorithm is developed for the numerical solution of the one-dimensional Schrödinger equation. The new method uses the minimum order of the phase-lag and its derivatives. Error analysis and the numerical results illustrate the efficiency of the new algorithm.

Keywords Multistep methods · Explicit methods · Hybrid methods · Phase-lag · Phase-fitted · Schrödinger equation

Abbreviation

LTE Local truncation error

1 Introduction

The one-dimensional Schrödinger equation can be written as:

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

Many problems in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc. can be express via the above boundary value problem (see for example [1–4]).

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Here are the definitions of some terms in (1):

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

The boundary conditions are:

$$y(0) = 0 \quad (2)$$

and for large values of x , a second boundary condition according to physical considerations.

Recently, a lot of research has been done on the solution of the Shrödinger equation and relevant problems using numerical algorithms. This research aims on the development of fast and dependable methods (see for example [5–18], [19–150]).

The approximate solution of the Shrödinger equation and similar problems can be divided into two main groups:

1. Constant coefficient methods
2. Problem frequency coefficients methods.¹

Efficient numerical new methods, for the solution of the Shrödinger equation and relevant problems, are introduced in the present paper. The above methods are based on the condition of vanishing phase-lag and its derivatives. The study of the efficiency of the new methodology will be effected through error analysis and the application of the new method to the approximate solution of the one-dimensional Shrödinger equation. In especial, a hybrid Numerov-type methods of fourth algebraic order will be developed, based on the requirement mentioned above. The stability and the error of the new method will be examined and the method obtained will be applied to the resonance problem, which is one of the most radial Shrödinger equation difficult problems. This paper is made up of 7 sections concerning the new developed method: Finally, we will apply the new obtained method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. In Sect. 2 the theory is presented. In Sect. 3 the development of the new method is presented. Section 4 includes the error analysis. Section 5 includes the study of the stability of the new methods. Section 6 incorporates the numerical results Sect. 7 contains the final results and the conclusions.

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$y'' = f(x, y) \quad (3)$$

¹ When using a functional fitting algorithm for the solution of the radial Schrödinger equation, the fitted frequency is equal to: $\sqrt{|l(l + 1)/x^2 + V(x) - k^2|}$.

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 $b_i = b_{m-i}$, $i = 0(1)\lfloor \frac{m}{2} \rfloor$.

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

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

a difference equation of the form

$$A_k(H) y_{n+k} + \dots + A_1(H) y_{n+1} + A_0(H) y_n + A_1(H) y_{n-1} + \dots + A_k(H) y_{n-k} = 0 \tag{5}$$

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

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

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

Theorem 1 [121] The symmetric $2k$ -step method with characteristic equation given by (6) has phase-lag order q and phase-lag constant c given by

$$-c H^{q+2} + O(H^{q+4}) = \frac{D_1}{D_2} \tag{7}$$

where

$$D_1 = 2A_k(H) \cos(kH) + \dots + 2A_j(H) \cos(jH) + \dots + A_0(H) \tag{8}$$

$$D_2 = 2k^2 A_k(H) + \dots + 2j^2 A_j(H) + \dots + 2A_1(H) \tag{9}$$

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

3 The new numerov-type hybrid method—construction of the new method

$$\begin{aligned} \bar{y}_{n+1} &= 2y_n - y_{n-1} + h^2 y''_n \\ y_{n+1} + c_1 y_n + y_{n-1} &= h^2 [b_0 (\bar{y}''_{n+1} + y''_{n-1}) + b_1 y''_n] \end{aligned} \tag{10}$$

Application of the above method to the scalar test Eq. (4) gives the following difference equation:

$$A_1(H) y_{n+1} + A_0(H) y_n + A_1(H) y_{n-1} = 0 \tag{11}$$

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

The characteristic equation associated with (11) is given by:

$$A_1(H) \lambda + A_0(H) + A_1(H) \lambda^{-1} = 0 \quad (12)$$

where,

$$\begin{aligned} A_1(H) &= 1 \\ A_0(H) &= c_1 + 2b_0 H^2 - H^4 b_0 + H^2 b_1 \end{aligned}$$

Applying the formula (7) with $k = 1$ we have that the phase-lag is equal to:

$$PL = \cos(H) + \frac{1}{2} c_1 + b_0 H^2 - \frac{1}{2} H^4 b_0 + \frac{1}{2} H^2 b_1 \quad (13)$$

The first and second derivatives of the phase-lag are the following:

$$\dot{P}L = -\sin(H) + 2b_0 H - 2H^3 b_0 + H b_1 \quad (14)$$

$$\ddot{P}L = -\cos(H) + 2b_0 - 6b_0 H^2 + b_1 \quad (15)$$

Requiring the phase-lag and its first and second derivatives to be equal to zero we find out the coefficients given in “Appendix A”.

The Taylor series expansions of the above coefficients are given also in “Appendix B”.

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

The local truncation error of the new method is presented.

$$LTE = \frac{h^6}{360} \left(y_n^{(6)} + 2\omega^2 y_n^{(4)} + 2\omega^4 y_n^{(2)} + \omega^6 y_n \right) \quad (16)$$

4 Error analysis

We will study the following methods:

- The Numerov’s Method (mentioned as $PL0$)
- The New Developed Method (mentioned as $PL1$)

The error analysis is based on the following steps:

- The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x) y(x) \quad (17)$$

- Based on the paper of Ixaru and Rizea [20], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \quad (18)$$

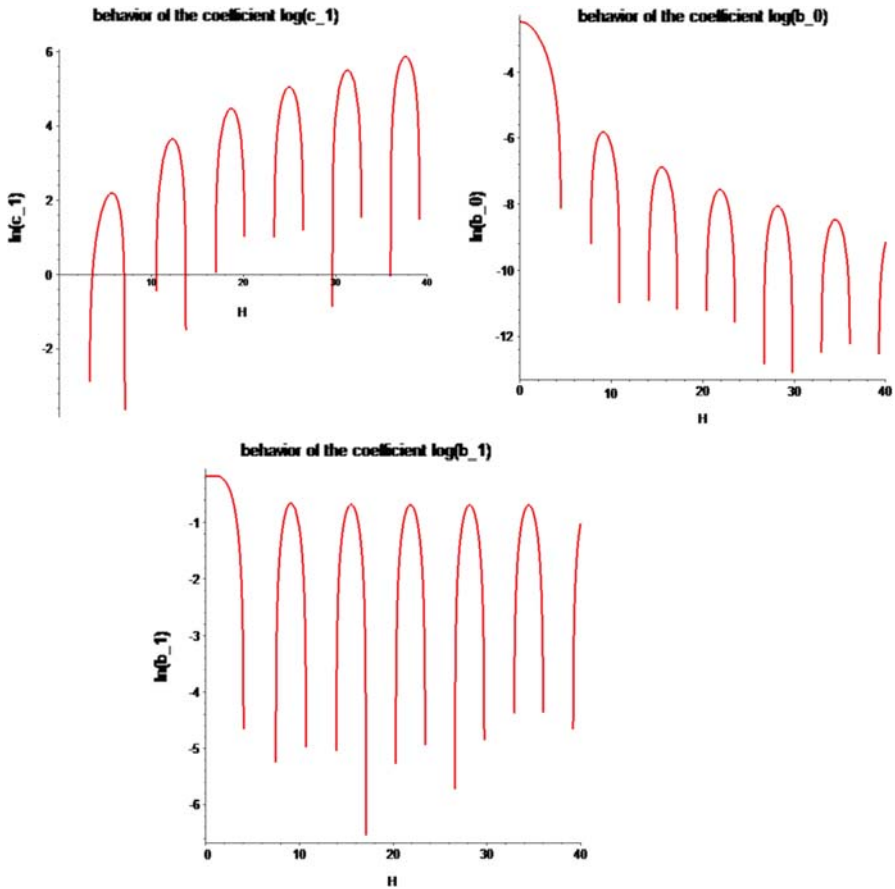


Fig. 1 Behavior of the coefficients of the new method given by (38, 39, 40) for several values of H

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

- We express the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \dots$, which are terms of the local truncation error formulae, in terms of the Eq.(17). The expressions are presented as polynomials of G
- Finally, we substitute the derivatives, which are produced, into the local truncation error formulae

Based on the procedure mentioned above and on the formulae:

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

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

we obtain the expressions of the local truncation error mentioned in “Appendix C”. We consider two cases in terms of the value of E :

- The Energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in G are considered. 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 new developed methods.
- $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number. So, we have the following asymptotic expansions of the Eqs. (44) and (45).

The Numerov’s Method

$$\text{LTE}_{\text{PL0}} = \frac{1}{240} y(x) G^3 + \dots \quad (19)$$

The New Developed Method

$$\text{LTE}_{\text{PL1}} = \frac{1}{90} \left(\frac{d^2}{dx^2} g(x) \right) y(x) G + \dots \quad (20)$$

From the above equations we have the following theorem:

Theorem 2 For the Numerov’s Method the error increases as the third power of G . For the New Method the error increases as the first power of G . So, for the numerical solution of the time independent radial Schrödinger equation the new obtained Method is the most accurate one, especially for large values of $|G| = |V_c - E|$.

5 Stability analysis

The scalar test equation is given below

$$y''(x) = -v^2 y(x), \quad v \neq \omega \quad (21)$$

where the new presented method is applied. The obtained difference equation is:

$$A_1(H, s) y_{n+1} + A_0(H, s) y_n + A_1(H, s) y_{n-1} = 0 \tag{22}$$

where $s = vh$, h is the step length and $A_0(H, s)$ and $A_1(H, s)$ are polynomials of s .

The characteristic equation associated with (22) is given by:

$$A_1(H, s) s + A_0(H, s) + A_1(H, s) s^{-1} = 0 \tag{23}$$

where

$$\begin{aligned} A_1(H, s) &= 1 \\ A_0(H, s) &= c_1 + s^2 (2b_0 + b_1) - s^4 b_0 \end{aligned} \tag{24}$$

Definition 1 (see [146]) A symmetric four-step method with the characteristic equation given by (23) is said to have an *interval of periodicity* $(0, \omega_0^2)$ if, for all $\omega \in (0, \omega_0^2)$, the roots z_i , $i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i \phi(vh)}, |z_i| \leq 1, i = 3, 4 \tag{25}$$

where $\phi(vh)$ is a real function of vh and $s = vh$.

Definition 2 (see [146]) A method is called *P-stable* if its interval of periodicity is equal to $(0, \infty)$.

Theorem 3 (see [147]) A symmetric two-step method with the characteristic equation given by (23) is said to have a nonzero *interval of periodicity* $(0, s_0^2)$ if, for all $s \in (0, s_0^2)$ the following relations are hold

$$P_1(H, s) P_2(H, s) < 0, \tag{26}$$

where $H = \omega h$, $s = t h$ and:

$$\begin{aligned} P_1(H, s) &= A_0(H, s) + 2 A_1(H, s), \\ P_2(H, s) &= A_0(H, s) - 2 A_1(H, s) \end{aligned} \tag{27}$$

Definition 3 A method is called singularly almost *P-stable* if its interval of periodicity is equal to $(0, \infty) - S$ ² only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $H = s$

Based on (24) the stability polynomials (27) for the new developed methods take the form:

$$\begin{aligned} P_1(H, s) &= 2 + c_1 + s^2 (2b_0 + b_1) - s^4 b_0, \\ P_2(H, s) &= -2 + c_1 + s^2 (2b_0 + b_1) - s^4 b_0 \end{aligned} \tag{28}$$

² where S is a set of distinct points.

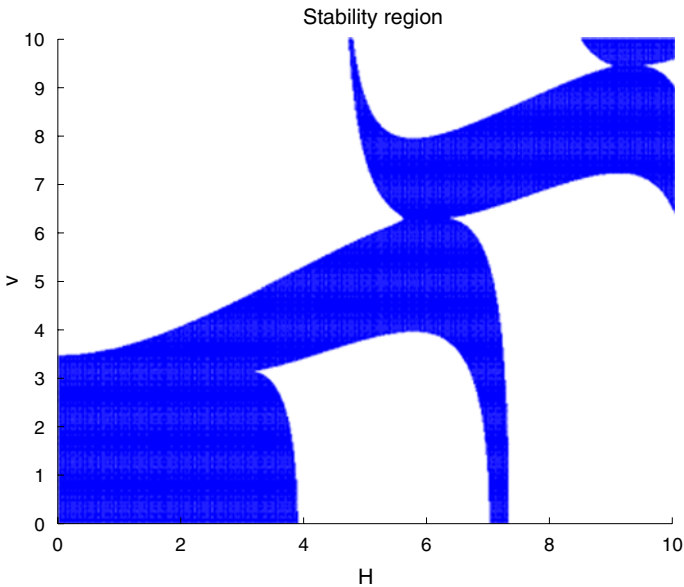


Fig. 2 s - H plane of the new method of the family of method developed in this paper

In the Fig. 2 we present the $s - H$ plane for the new method of the new family of method developed in this paper (Sect. 3).

In the case that the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $H = s$, we have the Fig. 3 for the stability polynomials of the new developed methods. A method is P -stable if the $s - H$ plane is completely shadowed. From the above diagrams it is easy for one to see that the interval of periodicity of all the new methods is equal to: $(0, \pi^2)$.

Remark 1 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 $w - H$ plane.

6 Numerical results—conclusion

The radial time independent Schrödinger equation is used to check the efficiency of the new method obtained in paragraphs 3.1–3.4.

We need the value of parameter v , in order to apply the new methods to the radial Schrödinger equation. For every problem of the one-dimensional Schrödinger equation given by (1) the parameter v is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \quad (29)$$

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

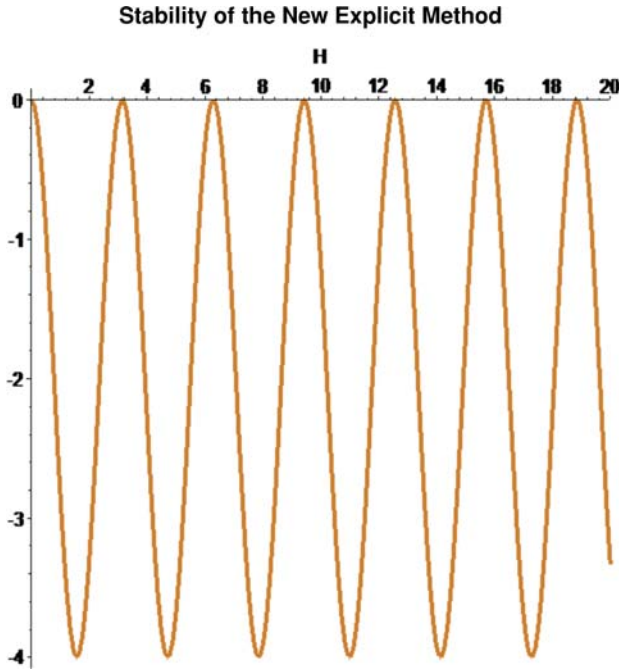


Fig. 3 Stability polynomial of the new developed method in the case that $H = s$

6.1 Woods–Saxon potential

We use as potential the well known Woods–Saxon potential given by

$$V(x) = \frac{u_0}{1 + z} - \frac{u_0 z}{a(1 + z)^2} \tag{30}$$

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

The behavior of Woods–Saxon potential is shown in the Fig. 4.

It is well known that for some potentials, such as the Woods–Saxon potential, the definition of parameter v is not given as a function of x but based on some critical points which have been defined from the investigation of the appropriate potential (see for details [13]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [13]):

$$v = \begin{cases} \sqrt{-50 + E}, & \text{for } x \in [0, 6.5 - 2h], \\ \sqrt{-37.5 + E}, & \text{for } x = 6.5 - h \\ \sqrt{-25 + E}, & \text{for } x = 6.5 \\ \sqrt{-12.5 + E}, & \text{for } x = 6.5 + h \\ \sqrt{E}, & \text{for } x \in [6.5 + 2h, 15] \end{cases} \tag{31}$$

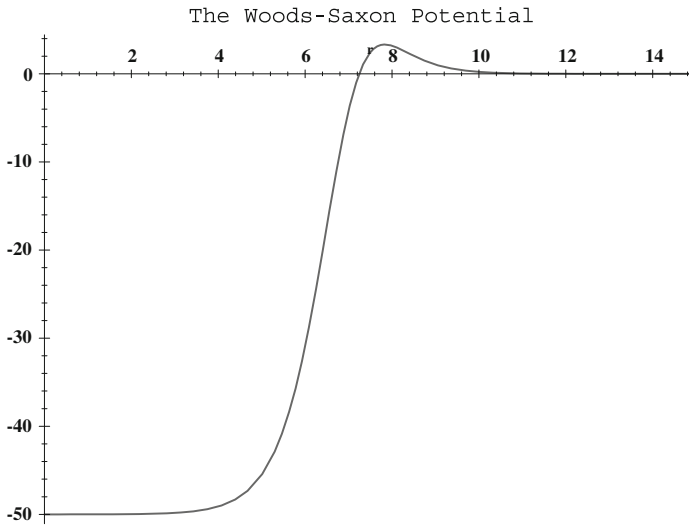


Fig. 4 The Woods–Saxon potential

6.2 Radial Schrödinger equation—the resonance problem

Consider the numerical solution of the radial time independent Schrödinger Equation (1) in the well-known case of the Woods–Saxon potential (30). In order to solve this problem numerically we need to 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 $x \in [0, 15]$. We consider Eq. (1) in a rather large domain of energies, i.e. $E \in [1, 1000]$.

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

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2} \right) y(x) = 0 \quad (32)$$

for x greater than some value X .

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$ where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of Eq. (1) has (when $x \rightarrow \infty$) the asymptotic form

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC \left[\sin \left(kx - \frac{l\pi}{2} \right) + \tan\delta_l \cos \left(kx - \frac{l\pi}{2} \right) \right] \end{aligned} \quad (33)$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \quad (34)$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need y_0 before starting a one-step method. From the initial condition we obtain y_0 . With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l .

For positive energies we have the so-called resonance problem. This problem consists either of finding the phase-shift δ_l or finding those E , for $E \in [1, 1, 000]$, at which $\delta_l = \pi/2$. We actually solve the latter problem, known as *the resonance problem* when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

$$y(0) = 0, y(x) = \cos(\sqrt{E}x) \text{ for large } x. \tag{35}$$

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

- the Numerov’s method which is indicated as *Method I*
- The two-step method developed by Raptis and Allison (which is indicated as *Method II*) [10]
- The two-step method developed by Ixaru and Rizea (which is indicated as *Method III*) [13]

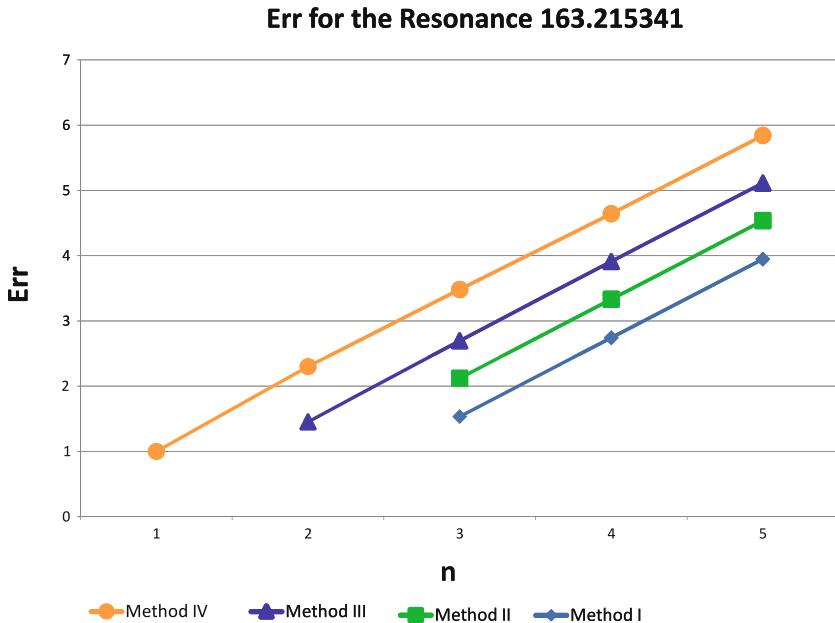


Fig. 5 Error Errmax for several values of n for the eigenvalue $E_1 = 163.215341$. The nonexistence of a value of Errmax indicates that for this value of n , Errmax is positive

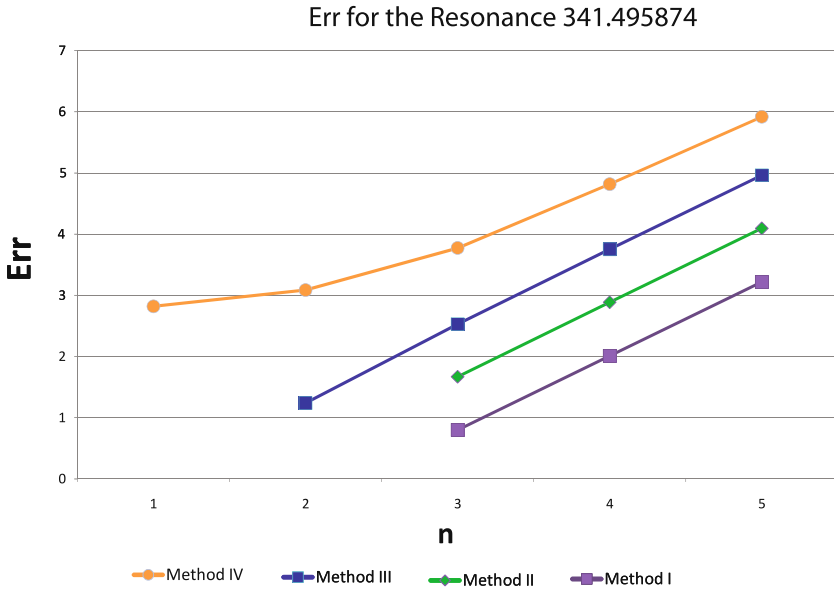


Fig. 6 Error Errmax for several values of n for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Errmax indicates that for this value of n , Errmax is positive

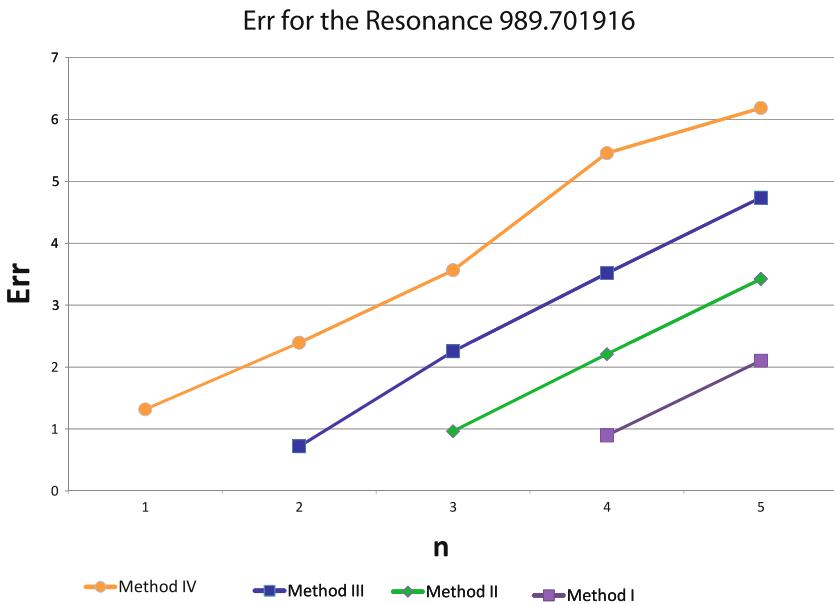


Fig. 7 Error Errmax for several values of n for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Errmax indicates that for this value of n , Errmax is positive

- the new Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero obtained in Sect. 3 which is indicated as *Method IV*. for several step sizes $h = 3/101/2^n$.

The computed eigenenergies are compared with exact ones. In Fig. 5 we present the maximum absolute error $\log_{10}(\text{Err})$ where

$$\text{Err} = |E_{\text{calculated}} - E_{\text{accurate}}| \tag{36}$$

of the eigenenergy E_1 , for several values of NFE = number of Function Evaluations. In Figs. 6 and 7 we present the maximum absolute error $\log_{10}(\text{Err})$ where

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

of the eigenenergies E_2 and E_3 , for several values of n .

7 Conclusions

In the present paper we have developed a hybrid two-step method of fourth algebraic order for the numerical solution of the radial Schrödinger equation.

More specifically we have developed a hybrid two-step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero.

We have applied the new method to the resonance problem of the radial Schrödinger equation.

Based on the results presented above we have the following conclusions:

- The two-step method developed by Raptis and Allison [10] (Method II) is more efficient than Numerov’s Method (Method I) but less efficient than the other two methods.
- The two-step method developed by Ixaru and Rizea [13] (Method III) is more efficient than Numerov’s Method (Method I) and method developed by Raptis and Allison (Method II) but less efficient than the new obtained method.
- Finally the new developed two-step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero (Method IV) is the most efficient than all the other methods.

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

Appendix A

$$c_1 = -2 \cos(H) + \frac{1}{4} H^2 \cos(H) - \frac{5}{4} H \sin(H) \tag{38}$$

$$b_0 = -\frac{1}{4} \frac{-\sin(H) + H \cos(H)}{H^3} \tag{39}$$

$$b_1 = -\frac{1}{2} \frac{\sin(H) - H \cos(H) - 3 H^2 \sin(H) + \cos(H) H^3}{H^3} \tag{40}$$

Appendix B

$$\begin{aligned}
 c_1 = & -2 + \frac{1}{360} H^6 - \frac{1}{6720} H^8 + \frac{1}{302400} H^{10} - \frac{1}{23950080} H^{12} \\
 & + \frac{1}{2905943040} H^{14} - \frac{1}{498161664000} H^{16} \\
 & + \frac{1}{114328101888000} H^{18} - \dots \quad (41)
 \end{aligned}$$

$$\begin{aligned}
 b_0 = & \frac{1}{12} - \frac{1}{120} H^2 + \frac{1}{3360} H^4 - \frac{1}{181440} H^6 + \frac{1}{15966720} H^8 \\
 & - \frac{1}{2075673600} H^{10} + \frac{1}{373621248000} H^{12} - \frac{1}{88921857024000} H^{14} \\
 & + \frac{1}{27032244535296000} H^{16} - \frac{1}{10218188434341888000} H^{18} + \dots \quad (42)
 \end{aligned}$$

$$\begin{aligned}
 b_1 = & \frac{5}{6} + \frac{1}{60} H^2 - \frac{1}{112} H^4 + \frac{37}{90720} H^6 \\
 & - \frac{67}{7983360} H^8 + \frac{1}{9884160} H^{10} - \frac{151}{186810624000} H^{12} \\
 & + \frac{41}{8892185702400} H^{14} - \frac{89}{4505374089216000} H^{16} \\
 & + \frac{337}{5109094217170944000} H^{18} + \dots \quad (43)
 \end{aligned}$$

Appendix C

The classical method of the family

$$\begin{aligned}
 LTE_{PLO} = & \frac{1}{240} y(x) G^3 + \frac{1}{80} g(x) y(x) G^2 \\
 & + \left[\frac{1}{40} \frac{dg(x)}{dx} \frac{dy(x)}{dx} + \frac{7}{240} y(x) \frac{d^2g(x)}{dx^2} + \frac{1}{80} g^2(x) y(x) \right] G \\
 & + \frac{1}{240} y(x) \frac{d^4g(x)}{dx^4} + \frac{1}{60} \frac{d^3g(x)}{dx^3} \frac{dy(x)}{dx} \\
 & + \frac{7}{240} y(x) g(x) \frac{d^2g(x)}{dx^2} + \frac{1}{240} y(x) g^3(x) \\
 & + \frac{1}{60} y(x) \left(\frac{dg(x)}{dx} \right)^2 + \frac{1}{40} g(x) \frac{dg(x)}{dx} \frac{dy(x)}{dx} \quad (44)
 \end{aligned}$$

The new developed method of the family

$$\begin{aligned}
 LTE_{PLI} = & \frac{1}{90} y(x) \frac{d^2 g(x)}{dx^2} G + \frac{7}{360} g(x) y(x) \frac{d^2 g(x)}{dx^2} + \frac{1}{360} y(x) g^3(x) \\
 & + \frac{1}{360} y(x) \frac{d^4 g(x)}{dx^4} + \frac{1}{90} \frac{d^3 g(x)}{dx^3} \frac{dy(x)}{dx} \\
 & + \frac{1}{90} y(x) \left(\frac{dg(x)}{dx} \right)^2 + \frac{1}{60} g(x) \frac{dg(x)}{dx} \frac{dy(x)}{dx} \quad (45)
 \end{aligned}$$

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