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ORIGINAL PAPER

A new hybrid two-step method with vanished phase-lag and its first and second derivatives for the numerical solution of the Schrödinger equation and related problems

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Abstract The maximization 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 via the procedure of vanishing of the phase-lag and its derivatives is studied in this paper. More specifically, we investigate the vanishing of the phase-lag and its first and second derivatives and how this disappearance maximizes the efficiency of the hybrid two-step method.

Keywords Numerical solution · Schrödinger equation · Multistep methods · Hybrid methods · Interval of periodicity · P-stability · Phase-lag · Phase-fitted · Derivatives of the phase-lag

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1 Introduction

In theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc., many problems can be expressed via the radial time independent Schrödinger equation (see for example [1–4]), which can be presented with the boundary value problem:

$$y''(x) = \left[l(l+1)/x^2 + V(x) - k^2\right] y(x). \tag{1}$$

For the above model (1) we give the following definitions:

- The function $W(x) = l(l+1)/x^2 + V(x)$ is called *the effective potential*. This satisfies $W(x) \to 0$ as $x \to \infty$
- 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:

$$y(0) = 0 \tag{2}$$

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

On the algorithmic development of efficient, fast and reliable methods for the approximate solution of the radial Schrödinger equation, much research has been done the last decades (see for example [5–87]. In the following we mention some bibliography:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge-Kutta and Runge-Kutta Nyström type have been developed in [5–8].
- In [9–14] exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are obtained.
- Multistep phase-fitted methods and multistep methods with minimal phase-lag are developed in [18–37].
- Symplectic integrators are studied in [38–59].
- Exponentially and trigonometrically multistep methods have been developed in [60–80].
- Nonlinear methods have been studied in [81,82].
- Review papers have been written in [83–87].
- Special issues and Symposia in International Conferences have been created on this subject (see [88–94]).

In this paper we will study the development of efficient numerical methods for the approximate solution of initial-value problems with periodical or oscillating behavior of the solutions. The construction of the new methods is based on the requirement of vanishing the phase-lag and its first and second derivatives.

We will study the efficiency of the new developed methods via:

– the error analysis
– the stability analysis
– the application of the new methods in the numerical solution of the one-dimensional Schrödinger equation with specific potential.

More specifically, we will develop a family of implicit symmetric two-step hybrid methods of sixth algebraic order. The construction of the new family of methods is based on the requirement of vanishing the phase-lag and its first and second derivatives. We will study the stability and the error of the new proposed 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. The paper is organized as follows.

– The theory of the new methodology is presented in Sect. 2.
– The development of the new method is presented in Sect. 3.
– In Sect. 4 we will present the error analysis.
– The stability properties of the new obtained method are presented in Sect. 5.
– The numerical results are presented in Sect. 6.
– Finally, a discussion on remarks and conclusions is presented in Sect. 7.

2 Phase-lag analysis of symmetric multistep methods

For the approximate solution of the initial value problem

$$q'' = f(x, q) \tag{3}$$

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

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

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

a difference equation of the form

$$A_m(H)\, q_{n+m} + \cdots + A_1(H)\, q_{n+1} + A_0(H)\, q_n + A_1(H)\, q_{n-1} + \cdots + A_m(H)\, q_{n-m} = 0 \tag{5}$$

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

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

$$A_m(H)\, \lambda^m + \cdots + A_1(H)\, \lambda + A_0(H) + A_1(H)\, \lambda^{-1} + \cdots + A_m(H)\, \lambda^{-m} = 0 \tag{6}$$

Theorem 1 [21] *and* [24] *The symmetric* $2m$*-step method with characteristic equation given by* (6) *has phase-lag order* q *and phase-lag constant* c *given by:*

$$-c\,H^{p+2}+O\left(H^{p+4}\right) = \frac{2\,A_m(H)\,\cos(m\,H)+\cdots+2\,A_j(H)\,\cos(j\,H)+\cdots+A_0(H)}{2\,m^2\,A_m(H)+\cdots+2\,j^2\,A_j(H)+\cdots+2\,A_1(H)} \tag{7}$$

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 [36]):

$$\begin{aligned}
\hat{q}_{n+1} &= 2\,q_n - q_{n-1} + h^2\,f_n\\
\tilde{q}_{n+1} &= 2\,q_n - q_{n-1} + \frac{h^2}{12}\left(\hat{f}_{n+1} + 10\,f_n + f_{n-1}\right)\\
\bar{q}_{n-\frac{1}{2}} &= \frac{1}{52}\,(3\,\tilde{q}_{n+1} + 20\,q_n + 29\,q_{n-1})\\
&\quad + \frac{h^2}{4992}\left(41\,\hat{f}_{n+1} - 682\,f_n - 271\,f_{n-1}\right)\\
\bar{q}_{n+\frac{1}{2}} &= \frac{1}{104}\,(5\,\tilde{q}_{n+1} + 146\,q_n - 47\,q_{n-1})\\
&\quad + \frac{h^2}{4992}\left(-59\,\hat{f}_{n+1} + 1438\,f_n + 253\,f_{n-1}\right)\\
q_{n+1} - 2\,q_n + q_{n-1} &= h^2\left[b_0\left(\tilde{f}_{n+1} + f_{n-1}\right) + b_1\left(\bar{f}_{n+\frac{1}{2}} + \bar{f}_{n-\frac{1}{2}}\right) + b_2\,f_n\right]
\end{aligned} \tag{8}$$

In the above family:

- the coefficients b_0, b_1 and b_2 are free parameters,
- h is the step size of the integration,
- n is the number of steps, i.e. q_n is the approximation of the solution on the point x_n and $x_n = x_0 + n\,h$ and
- x_0 is the initial value point.

3.2 The new hybrid method of the family with vanished phase-lag and its first and second derivatives

Let us consider the method (8)

If we apply the method (8) to the scalar test equation (4) we obtain the difference equation (5) with $m = 1$ and $A_j(H)$, $j = 0, 1$ given by:

$$A_0(H) = -2 + 2b_0H^2 - b_0H^4 + \frac{1}{12}H^6b_0 + 2b_1H^2 - \frac{1}{4}b_1H^4 + \frac{1}{192}H^6b_1 + H^2b_2,\ A_1(H) = 1 \tag{9}$$

We require the above hybrid method to have its phase-lag vanished. Using the formulae (7) (for $m = 1$) and (9), we have the following equation:

$$PL = \cos(H) - 1 + b_0H^2 - \frac{1}{2}b_0H^4 + \frac{1}{24}H^6b_0 + b_1H^2 - \frac{1}{8}b_1H^4 + \frac{1}{384}H^6b_1 + \frac{1}{2}H^2b_2 = 0 \tag{10}$$

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

$$DPL = -\sin(H) + 2b_0H - 2b_0H^3 + \frac{1}{4}H^5b_0 + 2b_1H - \frac{1}{2}b_1H^3 + \frac{1}{64}H^5b_1 + Hb_2 = 0 \tag{11}$$

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

Finally, demanding the method to have the second derivative of the phase-lag vanished as well, we have the equation

$$DDPL = -\cos(H) + 2b_0 - 6b_0H^2 + \frac{5}{4}b_0H^4 + 2b_1 - \frac{3}{2}b_1H^2 + \frac{5}{64}b_1H^4 + b_2 = 0 \tag{12}$$

where *DDPL* is the second derivative of the phase-lag.

Demanding now the coefficients of the new proposed hybrid method to satisfy the Eqs. (10)–(12), we obtain the following coefficients of the new developed method:

$$\begin{aligned} b_0 &= \frac{1}{6}\frac{T_0}{H^6} \\ b_1 &= \frac{1}{3}\frac{T_1}{H^6} \\ b_2 &= \frac{1}{4}\frac{T_2}{H^6} \end{aligned} \tag{13}$$

where

$$
\begin{aligned}
T_0 &= 192 - 12\,H^2 - 120\,H\,\sin(H) + 36\,H^2\,\cos(H)\\
&\quad +7\,H^3\,\sin(H) - H^4\,\cos(H) - 192\,\cos(H)\\
T_1 &= 8\,H^4\,\cos(H) - 56\,H^3\,\sin(H) - 144\,H^2\,\cos(H)\\
&\quad +96\,H^2 + 240\,H\,\sin(H) - 384 + 384\,\cos(H)\\
T_2 &= 768 - 768\,\cos(H) + 24\,H^4 - 240\,H^2 + 336\,H^2\,\cos(H) - 480\,H\,\sin(H)\\
&\quad +140\,H^3\,\sin(H) - 44\,H^4\,\cos(H) - 9\,H^5\,\sin(H) + H^6\,\cos(H)
\end{aligned}
$$

For some values of $|\omega|$ the formulae given by (13) are subject to heavy cancellations. In this case, the following Taylor series expansions should be used:

$$
\begin{aligned}
b_0 &= \frac{1}{60} - \frac{1}{420}H^2 + \frac{31}{302400}H^4 - \frac{1}{467775}H^6 + \frac{23}{871782912}H^8\\
&\quad -\frac{47}{217945728000}H^{10} + \frac{41}{32665171968000}H^{12} - \frac{1}{182760066720000}H^{14}\\
&\quad +\frac{193}{10407414146088960000}H^{16} - \frac{1}{19886166722219212800}H^{18} + \cdots\\
b_1 &= \frac{4}{15} + \frac{1}{105}H^2 - \frac{19}{18900}H^4 + \frac{7}{267300}H^6 - \frac{97}{272432160}H^8\\
&\quad +\frac{167}{54486432000}H^{10} - \frac{263}{14291012736000}H^{12} + \frac{389}{4751761734720000}H^{14}\\
&\quad -\frac{61}{216821128043520000}H^{16} + \frac{83}{107716736412020736000}H^{18} + \cdots\\
b_2 &= \frac{13}{30} - \frac{1}{70}H^2 + \frac{13}{7200}H^4 - \frac{13}{133056}H^6 + \frac{8401}{3632428800}H^8\\
&\quad -\frac{1117}{36324288000}H^{10} + \frac{70349}{266765571072000}H^{12} - \frac{80419}{50685458503680000}H^{14}\\
&\quad +\frac{22123}{3122224243826688000}H^{16} - \frac{1613}{65949022293073920000}H^{18} + \cdots
\end{aligned}
\tag{14}
$$

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

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

$$
LTE_{NM} = -\frac{h^8}{20160}\left(q_n^8 + 3\,\omega^2 q_n^6 + 3\,\omega^4 q_n^4 + \omega^2 q_n^6\right) + O\left(h^{10}\right). \tag{15}
$$

4 Error analysis

We will study the following methods:

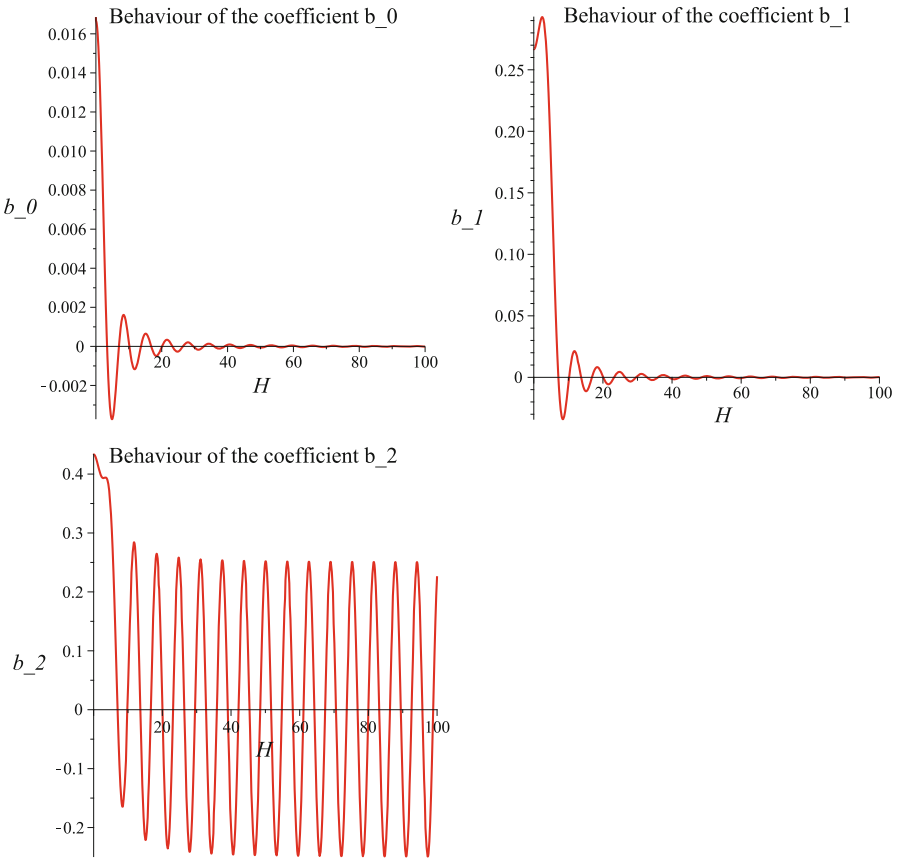

Fig. 1 Behavior of the coefficients of the new proposed method given by (13) for several values of $H = \omega h$

4.1 Classical method (i.e. the method (8) with constant coefficients)

$$LTE_{CL} = -\frac{h^8}{20160} q_n^{(8)} + O\left(h^{10}\right) \tag{16}$$

4.2 New method with vanished phase-lag and its first and second derivatives (developed in Sect. 3.2)

$$LTE_{NM} = -\frac{h^8}{20160}\left(q_n^8 + 3\,\omega^2 q_n^6 + 3\,\omega^4 q_n^4 + \omega^2 q_n^6\right) + O\left(h^{10}\right) \tag{17}$$

In order to study the error of the above mentioned methods, we follow the procedure mentioned below:

– The radial time independent Schrödinger equation is of the form

$$q''(x) = f(x)\, q(x) \tag{18}$$

– Based on the paper of Ixaru and Rizea [60], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \tag{19}$$

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 $q_n^{(i)}$, $i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of the Eq. (19). 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 use the procedure mentioned above and the formulae:

$$\begin{aligned}
q_n^{(2)} &= (V(x) - V_c + G)\, q(x) \\
q_n^{(4)} &= \left(\frac{d^2}{dx^2} V(x)\right) q(x) + 2 \left(\frac{d}{dx} V(x)\right) \left(\frac{d}{dx} q(x)\right) \\
&\quad + (V(x) - V_c + G) \left(\frac{d^2}{dx^2} q(x)\right) \\
q_n^{(6)} &= \left(\frac{d^4}{dx^4} V(x)\right) q(x) + 4 \left(\frac{d^3}{dx^3} V(x)\right) \left(\frac{d}{dx} q(x)\right) \\
&\quad + 3 \left(\frac{d^2}{dx^2} V(x)\right) \left(\frac{d^2}{dx^2} q(x)\right) + 4 \left(\frac{d}{dx} V(x)\right)^2 q(x) \\
&\quad + 6\, (V(x) - V_c + G) \left(\frac{d}{dx} V(x)\right) \left(\frac{d}{dx} q(x)\right) \\
&\quad + 4\, (V(x) - V_c + G)\, q(x) \left(\frac{d^2}{dx^2} V(x)\right) \\
&\quad + (V(x) - V_c + G)^2 \left(\frac{d^2}{dx^2} q(x)\right) \ldots
\end{aligned} \tag{20}$$

we obtain the expressions mentioned in the Appendix.

We consider two cases in terms of the value of E:

1. 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.
2. $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number.

Therefore, we have the following asymptotic expansions of the Local Truncation Errors:

4.3 Classical method

$$LTE_{CL} = h^8 \left(-\frac{1}{20160} q(x) G^4 + \cdots \right) + O\left(h^{10}\right) \tag{21}$$

4.4 New method with vanished phase-lag and its first derivative (developed in Sect. 3.2)

$$LTE_{NM} = h^8 \left[\left(\frac{1}{5040} \left(\frac{d^2}{dx^2} g(x) \right) q(x) \right) G^2 + \cdots \right] + O\left(h^{10}\right) \tag{22}$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Hybrid Two-Step Method the error increases as the fourth power of G. For the new method with vanished phase-lag and its first and second derivatives (developed in Sect. 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 and second derivatives 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:

$$u'' = -z^2 u, \tag{23}$$

we obtain the following difference equation:

$$A_1(\mathrm{v}, H)\ (u_{n+1} + u_{n-1}) + A_0(\mathrm{v}, H)\ u_n = 0 \tag{24}$$

where

$$A_0(\mathrm{v}, H) = \frac{1}{4} \frac{T_3}{H^6}, \quad A_1(\mathrm{v}, H) = 1 \tag{25}$$

where $T_3 = -8H^6 + 24\mathrm{v}^2H^4 + 8\mathrm{v}^6 - 5\mathrm{v}^6H\sin(H) + 24H^2\cos(H)\mathrm{v}^4 + \mathrm{v}^6H^2\cos(H) + 14H^3\sin(H)\mathrm{v}^4 - 2H^4\cos(H)\mathrm{v}^4 - 24H^4\cos(H)\mathrm{v}^2 - 9\mathrm{v}^2H^5\sin(H) + \mathrm{v}^2H^6\cos(H) - 24H^2\mathrm{v}^4 - 8\mathrm{v}^6\cos(H)$ and $H = \omega h$, $\mathrm{v} = z\,h$.

The corresponding characteristic equation is given by:

$$A_1(\mathrm{v}, H)\left(\lambda^2 + 1\right) + A_0(\mathrm{v}, H)\ \lambda = 0 \tag{26}$$

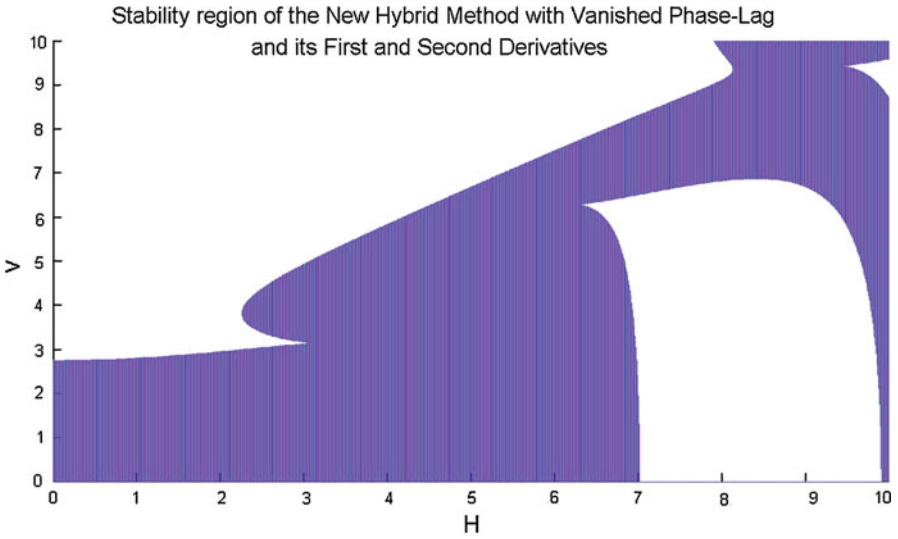

Fig. 2 $v - H$ plane of the the new developed method

Definition 1 (see [15]) A symmetric $2m$-step method with the characteristic equation given by (6) is said to have an *interval of periodicity* $\left(0, \mathrm{v}_0^2\right)$ if, for all $\mathrm{v} \in \left(0, \mathrm{v}_0^2\right)$, the roots λ_i, $i = 1, 2$ satisfy

$$\lambda_{1,2} = e^{\pm i\,\zeta(\mathrm{v})},\ |\lambda_i| \leq 1,\ i = 3, 4 \tag{27}$$

where $\zeta(\mathrm{v})$ is a real function of $z\,h$ and $\mathrm{v} = z\,h$.

Definition 2 (see [15]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - K$[1] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e., $\mathrm{v} = H$.

In Fig. 2 we present the $H - \mathrm{v}$ plane for the method developed in this paper. The shadowed area denotes the $H - \mathrm{v}$ region where the method is stable, while the white area denotes the region where the method is unstable.

Remark 1 For the solution of the Schrödinger type equations the frequency of the phase 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 $H - \mathrm{v}$ plane.

The interval of periodicity of the new method developed in Sect. 3.2 is equal to: $(0, 9.869604404)$ in the case that the frequency of the scalar test equation is equal with

[1] Where K is a set of distinct points.

Table 1 Comparative stability analysis for the methods mentioned in Sect. 5

Method	Interval of periodicity
CL	(0, 7.571916416)
NM(see Sect. 3.2)	(0, 9.869604404)

the frequency of phase fitting, i.e., in the case that $v = H$ (i.e., see the surroundings of the first diagonal of the $H - v$ plane).

From the above analysis we have the following theorem:

Theorem 3 *The method developed in Sect. 3.2 is of sixth algebraic order, has the phase-lag and its first and second derivatives equal to zero and has an interval of periodicity equals to:* $(0, 9.869604404)$.

Based on the analysis presented above, we studied the interval of periodicity of the classical method and the method developed in this paper. The results are presented in the Table 1.

6 Numerical results

The efficiency of the new developed method is studied via its application to the one-dimensional time-independent Schrödinger equation (1).

In order to apply the new developed method to the radial Schrödinger equation, the value of parameter ω is needed. In (1), the parameter ω is given by (for the case $l = 0$):

$$\omega = \sqrt{|V(x) - k^2|} = \sqrt{|V(x) - E|} \tag{28}$$

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

6.1 Woods-Saxon potential

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

$$V(x) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{29}$$

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

The behavior of Woods-Saxon potential is shown in Fig. 3.

It is well known that for some potentials, such as the Woods-Saxon potential, the definition of parameter ω is given not as a function of x but as based on some critical points which have been defined from the investigation of the appropriate potential (see for details [86]).

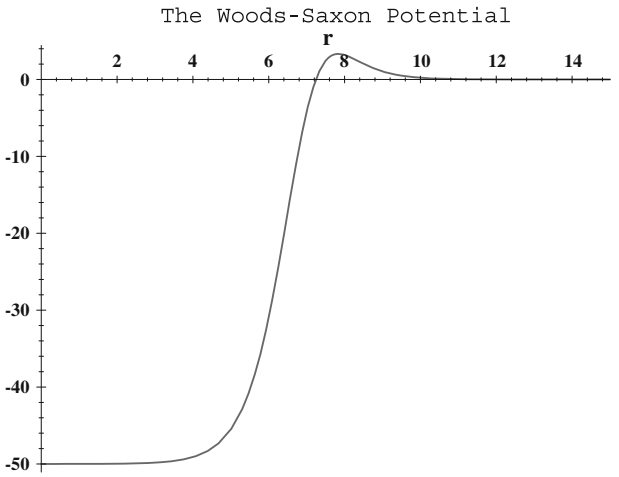

Fig. 3 The Woods-Saxon potential

For the purpose of obtaining our numerical results, it is appropriate to choose v as follows (see for details [1] and [60]):

$$\omega = \begin{cases} \sqrt{-50+E}, & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } x = 6.5-h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5+h \\ \sqrt{E}, & \text{for } x \in [6.5+2h, 15] \end{cases} \tag{30}$$

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

6.2 Radial Schrödinger equation: the resonance problem

We consider the numerical solution of the radial Schrödinger equation (1) in the well-known case of the Woods-Saxon potential (29). 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 $x \in [0, 15]$. 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 decays faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{31}$$

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) (when $x \to \infty$), has the asymptotic form

$$\begin{aligned} y(x) &\approx Akxj_l(kx) - Bkxn_l(kx) \\ &\approx AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{32}$$

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

$$\tan\delta_l = \frac{y(x_2)\,S(x_1) - y(x_1)\,S(x_2)}{y(x_1)\,C(x_1) - y(x_2)\,C(x_2)} \tag{33}$$

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 $y_j,\ j = 0,\ 1$ before starting a two-step method. From the initial condition, we obtain y_0. The value y_1 is obtained by using high order Runge-Kutta-Nyström methods(see [95] and [96]). With these starting values, we evaluate at x_2 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 $E \in [1, 1000]$, 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:

$$y(0) = 0,\ \ y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{34}$$

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 [20], which is indicated as Method MCR4.
- The exponentially-fitted method of Raptis and Allison [61], which is indicated as Method MRA.
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [19], which is indicated as Method MCR6.

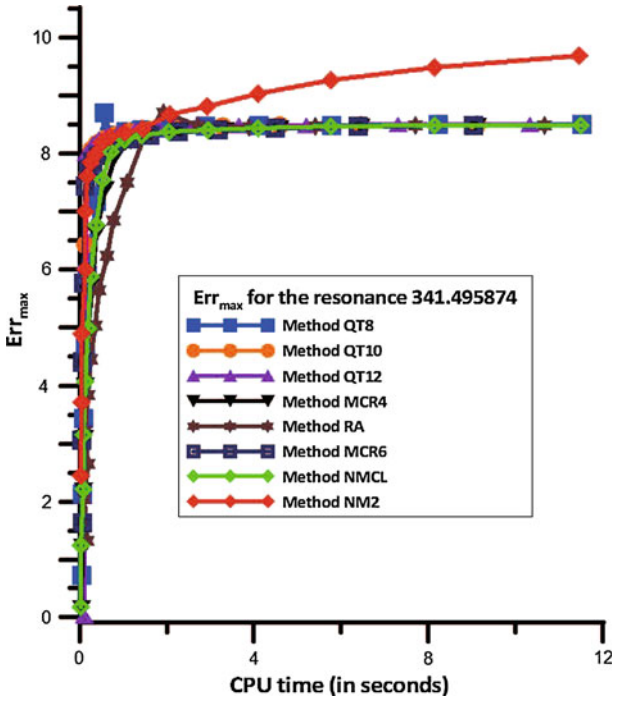

Fig. 4 Accuracy (Digits) for several values of CPU Time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

- The classical form of the sixth algebraic order method developed in Sect. 3.2, which is indicated as Method NMCL.[2]
- The new developed hybrid two-step method with vanished phase-lag and its first and second derivatives (obtained in Sect. 3.2), which is indicated as Method NM.

The computed eigenenergies are compared with reference values. [3] In Figs. 4 and 5, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{35}$$

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.

[2] With the term classical we mean the method of Sect. 3.2 with constant coefficients.

[3] The reference values are computed using the well known two-step method of Chawla and Rao [19] with small step size for the integration.

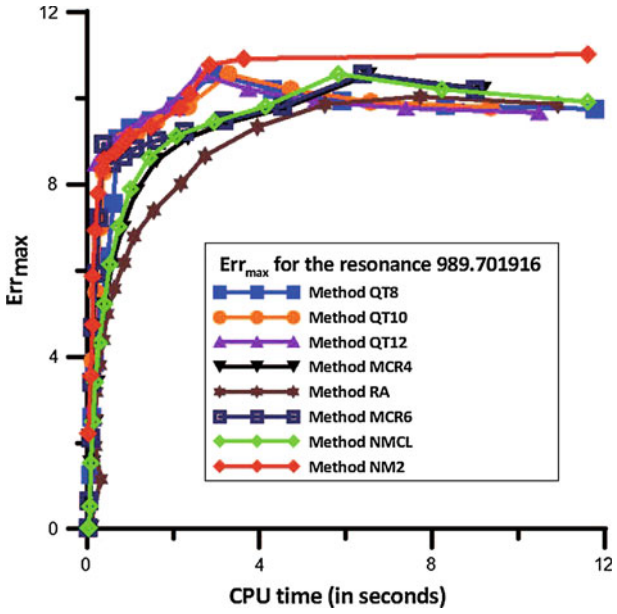

Fig. 5 Accuracy (Digits) for several values of CPU Time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

7 Conclusions

The purpose of this paper was the maximization of the efficiency of a hybrid two-step method for the approximate solution of the one-dimensional Schrödinger equation and related problems. We have presented the procedure with which the methodology of vanishing of the phase-lag and its first and second derivatives maximizes the efficiency of the new obtained numerical method. As a result of the application of the above mentioned procedure, we have produced 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 classical form of the sixth algebraic order method developed in Sect. 3.2, which is indicated as Method NMCL is of the same efficiency with the fourth algebraic order method of Chawla and Rao with minimal phase-lag [20], which is indicated as Method MCR4. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [61], which is indicated as Method MRA.
2. The tenth order multi-step 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 [20], 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 also more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [19], which is indicated as Method MCR6.

3. The twelfth order multi-step method developed by Quinlan and Tremaine [16], which is indicated as Method QT12 is more efficient than the tenth order multi-step method developed by Quinlan and Tremaine [16], which is indicated as Method QT10.
4. Finally, the New developed hybrid two-step method with vanished phase-lag and its first and second derivatives (obtained in Sect. 3.2), which is indicated as Method NM 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

Classical method

$$
\begin{aligned}
LTE_{\mathrm{CL}} = h^8\Bigg[& \left(\frac{1}{20160}\,q\,(x)\right) G^4 + \left(\frac{1}{5040}\,g\,(x)\,q\,(x)\right) G^3 \\
& + \left(\frac{11}{10080}\left(\frac{d^2}{dx^2}\,g\,(x)\right) q\,(x) + \frac{1}{1680}\left(\frac{d}{dx}\,g\,(x)\right)\frac{d}{dx}q\,(x)\right. \\
& \left. + \frac{1}{3360}\,(g\,(x))^2\,q\,(x)\right) G^2 + \left(\frac{1}{1260}\left(\frac{d^4}{dx^4}g\,(x)\right) q\,(x)\right. \\
& + \frac{1}{840}\left(\frac{d^3}{dx^3}g\,(x)\right)\frac{d}{dx}q\,(x) + \frac{1}{840}\,g\,(x)\left(\frac{d}{dx}q\,(x)\right)\frac{d}{dx}g\,(x) \\
& + \frac{11}{5040}\,g\,(x)\,q\,(x)\,\frac{d^2}{dx^2}g\,(x) + \frac{1}{720}\left(\frac{d}{dx}g\,(x)\right)^2 q\,(x) \\
& \left. + \frac{1}{5040}\,(g\,(x))^3\,q\,(x)\right) G + \frac{1}{20160}\left(\frac{d^6}{dx^6}g\,(x)\right) q\,(x) \\
& + \frac{1}{3360}\left(\frac{d^5}{dx^5}g\,(x)\right)\frac{d}{dx}q\,(x) + \frac{1}{1260}\,g\,(x)\,q\,(x)\,\frac{d^4}{dx^4}g\,(x) \\
& + \frac{1}{1344}\left(\frac{d^2}{dx^2}g\,(x)\right)^2 q\,(x) + \frac{13}{10080}\left(\frac{d}{dx}g\,(x)\right) q\,(x)\,\frac{d^3}{dx^3}g\,(x) \\
& + \frac{1}{840}\,g\,(x)\left(\frac{d}{dx}q\,(x)\right)\frac{d^3}{dx^3}g\,(x) + \frac{1}{1680}\,(g\,(x))^2\left(\frac{d}{dx}q\,(x)\right)\frac{d}{dx}g\,(x) \\
& + \frac{1}{420}\left(\frac{d}{dx}g\,(x)\right)\left(\frac{d}{dx}q\,(x)\right)\frac{d^2}{dx^2}g\,(x)
\end{aligned}
$$

$$+\frac{11}{10080}\,(g(x))^2\,q(x)\,\frac{d^2}{dx^2}g(x)+\frac{1}{720}\,g(x)\,q(x)\left(\frac{d}{dx}g(x)\right)^2$$
$$+\frac{1}{20160}\,(g(x))^4\,q(x)\Bigg] \tag{36}$$

New method with vanished phase-lag and its first derivative (developed in Sect. 3.2)

$$\begin{aligned}LTE_{\mathrm{NM}} = h^8\Bigg[&\left(\frac{1}{5040}\left(\frac{d^2}{dx^2}g(x)\right)q(x)\right)G^2+\left(\frac{13}{20160}\left(\frac{d^4}{dx^4}g(x)\right)q(x)\right.\\
&+\frac{1}{1680}\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}q(x)+\frac{1}{3360}\,g(x)\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}g(x)\\
&+\frac{23}{20160}\,g(x)\,q(x)\,\frac{d^2}{dx^2}g(x)+\frac{1}{1260}\left(\frac{d}{dx}g(x)\right)^2q(x)\\
&\left.+\frac{1}{20160}\,(g(x))^3\,q(x)\right)G+\frac{1}{20160}\left(\frac{d^6}{dx^6}g(x)\right)q(x)\\
&+\frac{1}{3360}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}q(x)+\frac{1}{1260}\,g(x)\,q(x)\,\frac{d^4}{dx^4}g(x)\\
&+\frac{1}{1344}\left(\frac{d^2}{dx^2}g(x)\right)^2q(x)+\frac{13}{10080}\left(\frac{d}{dx}g(x)\right)q(x)\,\frac{d^3}{dx^3}g(x)\\
&+\frac{1}{840}\,g(x)\left(\frac{d}{dx}q(x)\right)\frac{d^3}{dx^3}g(x)\\
&+\frac{1}{1680}\,(g(x))^2\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}\\
&+\frac{1}{420}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}q(x)\right)\frac{d^2}{dx^2}g(x)+\frac{11}{10080}\,(g(x))^2\,q(x)\,\frac{d^2}{dx^2}\\
&\times g(x)+\frac{1}{720}\,g(x)\,q(x)\left(\frac{d}{dx}g(x)\right)^2+\frac{1}{20160}\,(g(x))^4\,q(x)\Bigg]\end{aligned} \tag{37}$$

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