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ORIGINAL PAPER

A new high order two-step method with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation

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Abstract In this paper we develop a new hybrid method of high order with phase-lag and its first, second and third derivatives equal to zero. For the produced method we study its error and stability. We apply the newly obtained method to the Schrödinger equation. The application shows the efficiency of the new produced method.

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

Mathematics Subject Classification 65L05

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1 Introduction

The radial time independent Schrödinger equation can be expressed with the boundary value problem:

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

There are many scientific areas of applied sciences in which the mathematical models of their problems are expressed with the above mentioned boundary value problem. Astronomy, astrophysics, quantum mechanics, quantum chemistry, celestial mechanics, electronics physical chemistry and chemical physics are some of them (see for example [1–4]).

For the above model (1), we give the following definitions: (1) The function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(x) \to 0$ as $x \to \infty$, (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 boundary conditions are:

$$q(0) = 0, \tag{2}$$

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

The subject of this paper is to maximize the efficiency of a numerical algorithm for the numerical solution of the Schrödinger equation and related problems with periodic or oscillating solutions. More specifically, the effect of the vanishing of the phase-lag and its first, second and third derivatives on the efficiency of the produced numerical methods will be studied in this paper.

We note here that the obtained methods via the above procedure, are very effective on any problem with periodic or oscillating solutions or on any problem with solution which contains the functions cos and sin or on any problem with solution that is a combination of them.

More specifically, the aim of this paper is the calculation of the coefficients of the introduced hybrid two-step method in order:

1. to have the the highest possible algebraic order
2. to have the phase-lag vanished
3. to have the first derivative of the phase-lag vanished as well
4. to have the second derivative of the phase-lag vanished as well
5. and finally, to have the third derivative of the phase-lag vanished as well

The calculation of the phase-lag and therefore the procedure of vanishing of the phase lag and its first, second and third derivatives is based on the direct formula for the determination of the phase-lag for $2m$-method (see [29] and [26]).

The study of the effectiveness of the new proposed procedure will be based on the investigation of the local truncation error and of the stability analysis of the new proposed method. We will also apply the obtained methods to the resonance problem

of the radial time independent Schrödinger equation. This is one of the most difficult problems arising from the radial Schrödinger equation.

The format of the paper is given below:

- A bibliography relevant on the subject of the paper is presented in Sect. 2.
- In Sect. 3, the phase-lag analysis of symmetric $2k$-methods is developed.
- The new hybrid method is constructed in Sect. 4.
- In Sect. 5, the error analysis is presented.
- The stability properties of the new obtained method are presented in Sect. 6.
- The numerical results are presented in Sect. 7.
- Finally, remarks and conclusions are presented in Sect. 8.

2 Bibliography relevant on the subject of the paper

The last decades much research has been done on the construction of efficient, fast and reliable algorithms for the approximate solution of the radial Schrödinger equation and related problems (see for example [5–102]). 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 obtained in [5–11].
- In [12–17] exponentially and trigonometrically fitted Runge–Kutta and Runge–Kutta Nyström methods are constructed.
- Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [23–49].
- Symplectic integrators are investigated in [50–74].
- Exponentially and trigonometrically multistep methods have been produced in [75–95].
- Nonlinear methods have been studied in [96] and [97]
- Review papers have been presented in [98–102]
- Special issues and Symposia in International Conferences have been developed on this subject (see [103–109])

3 Basic theory on the phase-lag analysis of symmetric multistep methods

Let consider a multistep method with k steps which can be used over the equally spaced intervals $\{x_i\}_{i=0}^{k} \in [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)k-1$, for the numerical solution of the initial value problem

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

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

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

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

a difference equation of the form

$$A_k(H)\, p_{n+k} + \cdots + A_1(H)\, p_{n+1} + A_0(H)\, p_n + A_1(H)\, p_{n-1} + \cdots + A_k(H)\, p_{n-k} = 0 \tag{5}$$

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

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

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

Theorem 1 [26] *and* [29] *The symmetric* $2k$*-step method with characteristic equation given by* (6) *has phase-lag order* q *and phase-lag constant* c *given by:*

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

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

4 Development of the new method

Let us consider the following family of hybrid (Runge–Kutta type) symmetric two-step methods for the numerical solution of problems of the form $p'' = f\,(x, p)$ (see [100]):

$$\begin{aligned}
\hat{p}_{n+1} &= 2\, p_n - p_{n-1} + h^2\, f_n \\
\tilde{p}_{n+1} &= 2\, p_n - p_{n-1} + \frac{h^2}{12}\left(\hat{f}_{n+1} + 10\, f_n + f_{n-1}\right) \\
\bar{p}_{n-\frac{1}{2}} &= \frac{1}{52}\,(3\, \tilde{p}_{n+1} + 20\, p_n + 29\, p_{n-1}) \\
&\quad + \frac{h^2}{4992}\left(41\, \hat{f}_{n+1} - 682\, f_n - 271\, f_{n-1}\right) \\
\bar{p}_{n+\frac{1}{2}} &= \frac{1}{104}\,(5\, \tilde{p}_{n+1} + 146\, p_n - 47\, p_{n-1}) \\
&\quad + \frac{h^2}{4992}\left(-59\, \hat{f}_{n+1} + 1438\, f_n + 253\, f_{n-1}\right) \\
p_{n+1} + a_0\, p_n + p_{n-1} &= h^2\left[b_0\left(\tilde{f}_{n+1} + f_{n-1}\right) + b_1\left(\bar{f}_{n+\frac{1}{2}} + \bar{f}_{n-\frac{1}{2}}\right) + b_2\, f_n\right]
\end{aligned} \tag{8}$$

In the above general form:

– the coefficient b_0, b_1, b_2 and a_0 are free parameters,
– h is the step size of the integration,
– n is the number of steps,
– p_n is the approximation of the solution on the point x_n
– $x_n = x_0 + n\,h$ and
– x_0 is the initial value point.

Application of the method (8) to the scalar test equation (4) leads to the difference equation (5) with $k = 1$ and $A_j\,(H),\ \ j = 0, 1$ given by:

$$A_0\,(H) = a_0 + 2\,b_0\,H^2 - b_0\,H^4 + \frac{1}{12}\,H^6\,b_0 + 2\,b_1\,H^2 - \frac{1}{4}\,b_1\,H^4 + \frac{1}{192}\,H^6\,b_1 + H^2\,b_2,\quad A_1\,(H) = 1 \tag{9}$$

We demand the above mentioned method to have its phase-lag vanished. Using the formulae (7) (for $k = 1$) and (9), the following equation is obtained:

$$\text{Phase-Lag} = \cos\,(H) + \frac{1}{2}\,a_0 + b_0\,H^2 - \frac{1}{1}2\,b_0\,H^4 + \frac{1}{1}24\,H^6\,b_0 + b_1\,H^2 - \frac{1}{1}8\,b_1\,H^4 + \frac{1}{384}\,H^6\,b_1 + \frac{1}{2}\,H^2 b_2 = 0 \tag{10}$$

Requiring now the method to have the first derivative of the phase-lag vanished as well, the following equation is obtained:

$$\text{First Derivative of the Phase-Lag} = -\sin\,(H) + 2\,b_0\,H - 2\,b_0\,H^3 + \frac{1}{4}\,H^5\,b_0 + 2\,b_1\,H - \frac{1}{2}\,b_1\,H^3 + \frac{1}{64}\,H^5\,b_1 + H\,b_2 = 0 \tag{11}$$

Demanding for the new obtained method the second derivative of the phase-lag to be vanished as well, the following equation is obtained:

$$\text{Second Derivative of the Phase-Lag} = -\cos\,(H) + 2\,b_0 - 6\,b_0\,H^2 + \frac{5}{4}\,b_0\,H^4 + 2\,b_1 - \frac{3}{2}\,b_1\,H^2 + \frac{5}{64}\,b_1\,H^4 + b_2 = 0 \tag{12}$$

Finally, we require for the new produced method the third derivative of the phase-lag to be vanished as well. Therefore, the following equation is obtained:

$$\text{Third Derivative of the Phase-Lag} = \sin\,(H) - 12\,b_0\,H + 5\,b_0\,H^3 - 3\,b_1\,H + \frac{5}{16}\,b_1\,H^3 = 0 \tag{13}$$

We demand now the coefficients of the new proposed method to satisfy the Eqs. (10)–(13). Therefore, the following coefficients of the new developed method are obtained:

$$\begin{aligned} a_0 &= 1/24\, H^3 \sin(H) + 3/8 \cos(H) H^2 - \frac{11}{8} H \sin(H) - 2\cos(H) \\ b_0 &= \frac{1}{24}\frac{T_0}{H^5},\ b_1 = \frac{1}{3}\frac{T_1}{H^5},\ b_2 = \frac{1}{8}\frac{T_2}{H^5} \end{aligned} \tag{14}$$

where:

$$\begin{aligned} T_0 &= \sin(H) H^4 + 5\cos(H) H^3 - 21\sin(H) H^2 - 48\cos(H) H + 48\sin(H) \\ T_1 &= -2\sin(H) H^4 - 10\cos(H) H^3 + 18\sin(H) H^2 + 24\cos(H) H - 24\sin(H) \\ T_2 &= -\sin(H) H^6 - 7\cos(H) H^5 + 25\sin(H) H^4 + 50\cos(H) H^3 \\ &\quad -82\sin(H) H^2 - 96\cos(H) H + 96\sin(H) \end{aligned}$$

For some values of $|\omega|$ the formulae given by (14) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} a_0 &= -2 + \frac{1}{20160} H^8 - \frac{1}{453600} H^{10} + \frac{1}{23950080} H^{12} \\ &\quad - \frac{1}{2179457280} H^{14} + \frac{1}{298896998400} H^{16} \\ &\quad - \frac{1}{57164050944000} H^{18} + \cdots \\ b_0 &= \frac{1}{60} - \frac{1}{315} H^2 + \frac{17}{90720} H^4 - \frac{1}{199584} H^6 \\ &\quad + \frac{47}{622702080} H^8 - \frac{17}{23351328000} H^{10} + \frac{31}{6351561216000} H^{12} \\ &\quad - \frac{61}{2534272925184000} H^{14} + \frac{31}{340606281144729600} H^{16} \\ &\quad - \frac{1}{3672161468591616000} H^{18} + \cdots \\ b_1 &= \frac{4}{15} + \frac{4}{315} H^2 - \frac{11}{5670} H^4 + \frac{2}{31185} H^6 \\ &\quad - \frac{41}{38918880} H^8 + \frac{31}{2918916000} H^{10} - \frac{29}{396972576000} H^{12} \\ &\quad + \frac{29}{79196028912000} H^{14} - \frac{149}{106439462857728000} H^{16} \\ &\quad + \frac{31}{7344322937183232000} H^{18} + \cdots \end{aligned} \tag{15}$$

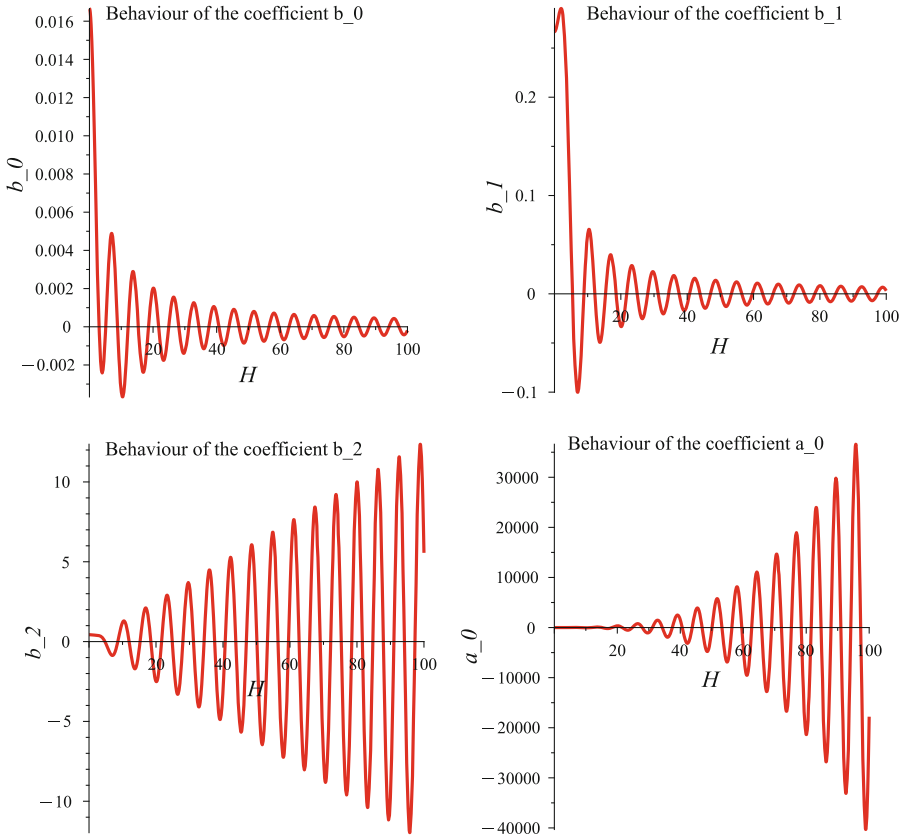

Fig. 1 Behavior of the coefficients of the new proposed method given by (14) for several values of $H = \omega h$

$$
\begin{aligned}
b_2 \;=\; & \frac{13}{30} - \frac{2}{105} H^2 + \frac{53}{15120} H^4 - \frac{79}{249480} H^6 \\
& + \frac{1061}{103783680} H^8 - \frac{331}{1945944000} H^{10} + \frac{503}{288707328000} H^{12} \\
& - \frac{151}{12422906496000} H^{14} + \frac{1591}{25803506147328000} H^{16} \\
& - \frac{269}{1129895836489728000} H^{18} + \cdots
\end{aligned}
$$

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:

$$
\mathrm{LTE}_{NM} = -\frac{h^8}{20160} \left(p_n^{(8)} + 4\,\omega^2 p_n^{(6)} + 6\,\omega^4 p_n^{(4)} + 4\,\omega^6 p_n^{(2)} + \omega^8 p_n \right) + O\left(h^{10}\right) \tag{16}
$$

5 Error analysis

We will study the following methods:

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

$$\mathrm{LTE}_{CL} = -\frac{h^8}{20160}\, p_n^{(8)} + O\left(h^{10}\right) \tag{17}$$

5.2. Method with vanished phase-lag and its first derivative (developed in [43])

$$\mathrm{LTE}_{SI} = -\frac{h^8}{20160}\left(p_n^{(8)} + 2\,\omega^2 p_n^{(6)} + \omega^4 p_n^{(4)}\right) + O\left(h^{10}\right) \tag{18}$$

5.3. Method with vanished phase-lag and its first and second derivatives (developed in [48])

$$\mathrm{LTE}_{AS} = -\frac{h^8}{20160}\left(p_n^{(8)} + 3\,\omega^2 p_n^{(6)} + 3\,\omega^4 p_n^{(4)} + \omega^6 p_n^{(2)}\right) + O\left(h^{10}\right) \tag{19}$$

5.4. Method with vanished phase-lag and its first, second and third derivatives (developed in Sect. 4)

$$\mathrm{LTE}_{NM} = -\frac{h^8}{20160}\left(p_n^{(8)} + 4\,\omega^2 p_n^{(6)} + 6\,\omega^4 p_n^{(4)} + 4\,\omega^6 p_n^{(2)} + \omega^8 p_n\right) + O\left(h^{10}\right) \tag{20}$$

The following procedure is applied:

1. The radial time independent Schrödinger equation is of the form

$$p''(x) = f(x)\; p(x) \tag{21}$$

2. Based on the paper of Ixaru and Rizea [75], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \tag{22}$$

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

3. We express the derivatives $p_n^{(i)}$, $i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of the Eq. (22). The expressions are presented as polynomials of G
4. Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae

Using the procedure mentioned above and the formulae:

$$
\begin{aligned}
p_n^{(2)} &= (V(x) - V_c + G)\, q(x) \\
p_n^{(4)} &= \left(\frac{d^2}{dx^2} V(x)\right) q(x) + 2 \left(\frac{d}{dx} V(x)\right) \left(\frac{d}{dx} q(x)\right) \\
&\quad + (V(x) - V_c + G) \left(\frac{d^2}{dx^2} q(x)\right) \\
p_n^{(6)} &= \left(\frac{d^4}{dx^4} V(x)\right) q(x) + 4 \left(\frac{d^3}{dx^3} V(x)\right) \left(\frac{d}{dx} q(x)\right) \\
&\quad + 3 \left(\frac{d^2}{dx^2} V(x)\right) \left(\frac{d^2}{dx^2} q(x)\right) + 4 \left(\frac{d}{dx} V(x)\right)^2 q(x) \\
&\quad + 6\, (V(x) - V_c + G) \left(\frac{d}{dx} V(x)\right) \left(\frac{d}{dx} q(x)\right) \\
&\quad + 4\, (V(x) - V_c + G)\, q(x) \left(\frac{d^2}{dx^2} V(x)\right) \\
&\quad + (V(x) - V_c + G)^2 \left(\frac{d^2}{dx^2} q(x)\right) \\
&\quad \cdots
\end{aligned}
\tag{23}
$$

we obtain the expressions of the local truncation errors. For the classical method (i.e. the method (8) with constant coefficients) the expression can be found in [48]. For the method with vanished phase-lag and its First Derivative the expression can be found in [43]. For the method with vanished phase-lag and its first and second derivatives the expression can be found in [48]. Finally, for the new developed method the expression can be found in the Appendix.

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

- The energy is close to the potential, i.e., $G = V_c - E \approx 0$. 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.
- $G >> 0$ or $G << 0$. Then $|G|$ is a large number.

Therefore, we have the following asymptotic expansions of the local truncation errors.

5.5. Classical method (for details see in [48])

$$
\mathrm{LTE}_{CL} = h^8 \left(-\frac{1}{20160}\, p\,(x)\; G^4 + \cdots\right) + O\left(h^{10}\right) \tag{24}
$$

5.6. New method with vanished phase-lag and its first derivative (developed in [43])

$$\mathrm{LTE}_{SI} = h^8 \left[\left(\frac{1}{2240} \left(\frac{d^2}{dx^2} g(x) \right) p(x) + \frac{1}{10080} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} p(x) + \frac{1}{20160} g(x)^2 p(x) \right) G^2 + \cdots \right] + O\left(h^{10}\right) \tag{25}$$

5.7. New method with vanished phase-lag and its first and second derivatives (developed in [48])

$$\mathrm{LTE}_{AS} = h^8 \left[\left(\frac{1}{5040} \left(\frac{d^2}{dx^2} g(x) \right) p(x) \right) G^2 + \cdots \right] + O\left(h^{10}\right) \tag{26}$$

5.8. Method with vanished phase-lag and its first, second and third derivatives (developed in Sect. 4)

$$\mathrm{LTE}_{NM} = h^8 \left[\left(\frac{1}{1680} \left(\frac{d^4}{dx^4} g(x) \right) p(x) + \frac{1}{2520} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} p(x) + \frac{1}{1260} g(x)\, p(x) \frac{d^2}{dx^2} g(x) + \frac{1}{1680} \left(\frac{d}{dx} g(x) \right)^2 p(x) \right) G + \cdots \right] + O\left(h^{10}\right) \tag{27}$$

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 method with vanished phase-lag and its First Derivative (developed in* [43]*), the error increases as the second power of G. For the Method with vanished phase-lag and its first and second derivatives (developed in* [48]*), the error increases as the second power of G. For the method with vanished phase-lag and its first, second and third derivatives (developed in Sect. 4), the error increases as the first 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, second and third derivatives is much more efficient, especially for large values of* $|G| = |V_c - E|$.

6 Stability analysis

Let us apply the new obtained method to the scalar test equation:

$$q'' = -z^2 q, \tag{28}$$

We note that $z \neq \omega$. Thus, we obtain the following difference equation:

$$A_1(\mathrm{v}, H)\,(q_{n+1} + q_{n-1}) + A_0(\mathrm{v}, H)\, q_n = 0 \tag{29}$$

where

$$A_0(\mathrm{v}, H) = \frac{1}{24}\frac{T_3}{H^5}, \quad A_1(\mathrm{v}, H) = 1 \tag{30}$$

where $T_3 = H^8 \sin(H) + 9\cos(H) H^7 - 33\sin(H) H^6 - 48\cos(H) H^5 + 3\sin(H) H^4\mathrm{v}^4 + 15\cos(H) H^3\mathrm{v}^4 - 15\sin(H) H^2\mathrm{v}^4 - \mathrm{v}^6\sin(H) H^2 - 3\,\mathrm{v}^6\cos(H) H + 45\sin(H) H^4\mathrm{v}^2 - 3\,\mathrm{v}^2\sin(H) H^6 - 21\,\mathrm{v}^2\cos(H) H^5 + 3\,\mathrm{v}^6\sin(H)$ and $\mathrm{v} = z\,h$.

The corresponding characteristic equation is given by:

$$A_1(\mathrm{v}, H)\left(\lambda^2 + 1\right) + A_0(\mathrm{v}, H)\,\lambda = 0 \tag{31}$$

Definition 1 (*see* [18]) A symmetric $2k$-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 z_i, $i = 1, 2$ satisfy

$$\lambda_{1,2} = e^{\pm i\,\zeta(\mathrm{v})},\ |\lambda_i| \leq 1,\ i = 3, 4, \ldots \tag{32}$$

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

Definition 2 (*see* [18]) 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 $(0, \infty) - S$[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. A shadowed area denotes the $H - \mathrm{v}$ region where the method is stable, while a white area denotes the region where the method is unstable.

Remark 1 For the solution of the Schrödinger equation 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.

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 $\mathrm{v} = H$ (i.e. see the surroundings of the first diagonal of the $H - \mathrm{v}$ plane), it is easy to see that the interval of periodicity of the new method developed in Sect. 3 is equal to: $(0, \infty) - S$, where $S = \pi, 2\pi, 3\pi, \ldots$.

From the above analysis we have the following theorem:

Theorem 3 *The method developed in Sect. 4 is of eighth algebraic order, has the phase-lag and its first, second and third derivatives equal to zero and has an interval of periodicity equals to:* $(0, \infty) - S$, *where* $S = \pi, 2\pi, 3\pi, \ldots$.

Based on the analysis presented above, we studied the interval of periodicity of the following methods:

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

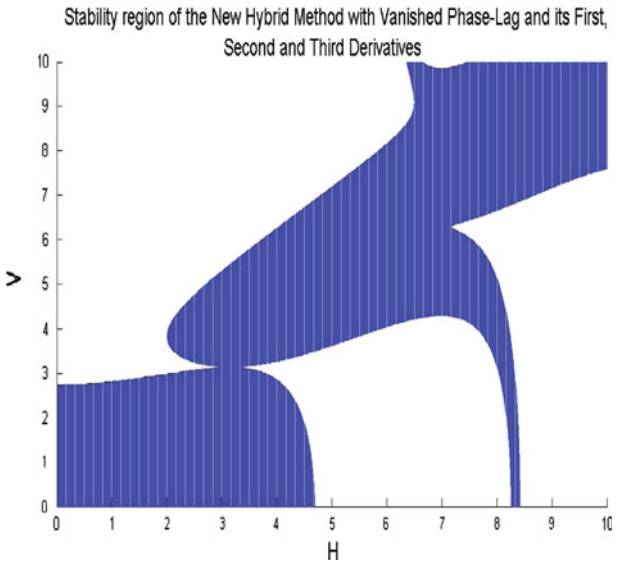

Fig. 2 $v - H$ plane of the the new developed method

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

Method	Interval of periodicity
CL	$(0, 7.571916416)$
SI (see [43])	$(0, 39.47841760)$
AS (see [48])	$(0, 9.869604404)$
NM (see Sect. 4)	$(0, \infty) - S$, where $S = \pi, 2\pi, 3\pi, \ldots$

- The classical method of sixth algebraic order (indicated as **CL**) presented in [43]
- The hybrid sixth algebraic order method with vanished the phase-lag and its first derivative developed in [43] (indicated as **SI**)
- The hybrid sixth algebraic order method with vanished the phase-lag and its first and second derivatives developed in [48] (indicated as **AS**)
- The hybrid eighth algebraic order method with vanished the phase-lag and its first, second and third derivatives developed in Sect. 4 (indicated as **NM**)

The results presented in the Table 1.

7 Numerical results

In this section, we will apply the new developed method to the radial time-independent Schrödinger equation (1).

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

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

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

7.1 Woods-Saxon potential

For the purpose of the present application, we use the well known Woods-Saxon potential which can be written as

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

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

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

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 [101]).

For the purpose of obtaining our numerical results, it is appropriate to choose v as follows (see for details [1] and [75]):

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

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

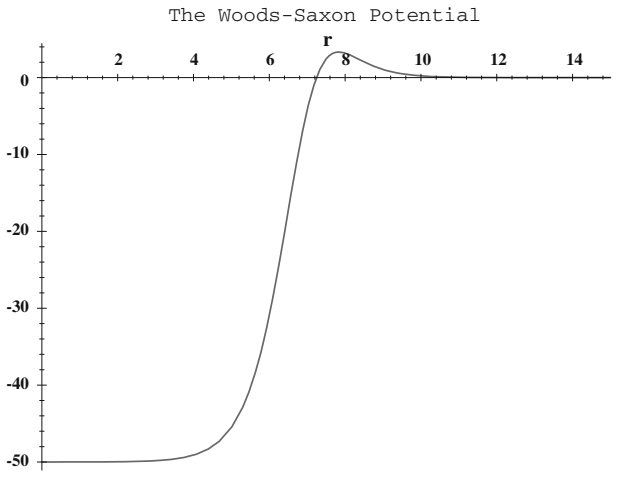

Fig. 3 The Woods–Saxon potential

7.2 Radial Schrödinger equation: the resonance problem

For the purpose of this application, we consider the numerical solution of the one dimensional time independent Schrödinger equation (1) in the well-known case of the Woods-Saxon potential (34). In order to solve this problem numerically, we must approximate the true (infinite) interval of integration by a finite interval. For our numerical illustration, we take the domain of integration as $r \in [0, 15]$. 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 $\frac{l(l+1)}{r^2}$ and the Schrödinger equation effectively reduces to

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

for r greater than some value R.

The above equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions, respectively. Thus, the solution of Eq. (1) (when $r \to \infty$), has the asymptotic form

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

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

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

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need $q_j,\ j = 0,\ 1$ 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 [110] and [111]). With these starting values, we evaluate at r_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:

$$q(0) = 0,\ q(r) = \cos\left(\sqrt{E}r\right) \quad \text{for large } r. \tag{39}$$

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

- The eighth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [76], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [24], which is indicated as **Method MCR6**
- The classical form of the sixth algebraic order method developed in Sect. 4, which is indicated as **Method NMCL**.[2]
- The hybrid two-step method of sixth algebraic order with vanished phase-lag and its first derivative, which was developed in [43] and is indicated as **Method MSI**
- The hybrid two-step method of sixth algebraic order with vanished phase-lag and its first and second derivatives, which was indicated in [48] and is indicated as **Method MAS**
- The hybrid two-step method of sixth algebraic order with vanished phase-lag and its first, second and third derivatives (obtained in Sect. 4), which is indicated as **Method NM3**

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

$$Err = |E_{calculated} - E_{accurate}| \tag{40}$$

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

8 Conclusions

In this paper we have studied the vanishing procedure for the phase-lag and its first, second and third derivatives and how this procedure affects the efficiency of the produced method for the approximate solution of the radial Schrödinger equation and related problems. 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:

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

[3] The reference values are computed using the well known two-step method of Chawla and Rao [24] with small step size for the integration.

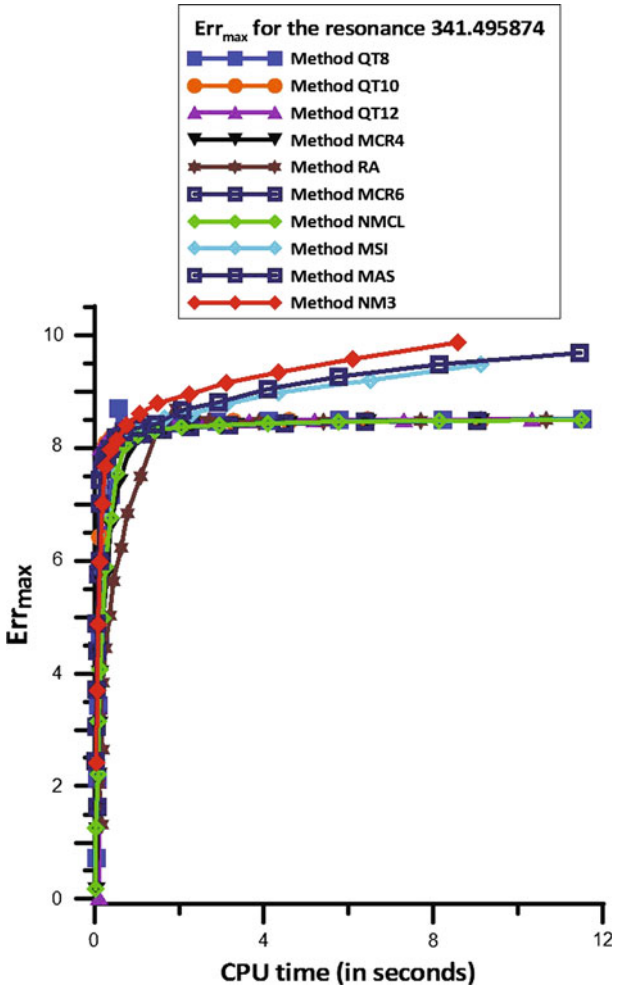

Fig. 4 Accuracy (digits) for several values of *CPU* time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (*digits*) indicates that for this value of CPU, accuracy (digits) is less than 0

1. The classical form of the sixth algebraic order method developed in Sect. 4, 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 [25], which is indicated as **Method MCR4**. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [76], which is indicated as **Method MRA**.
2. The tenth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the

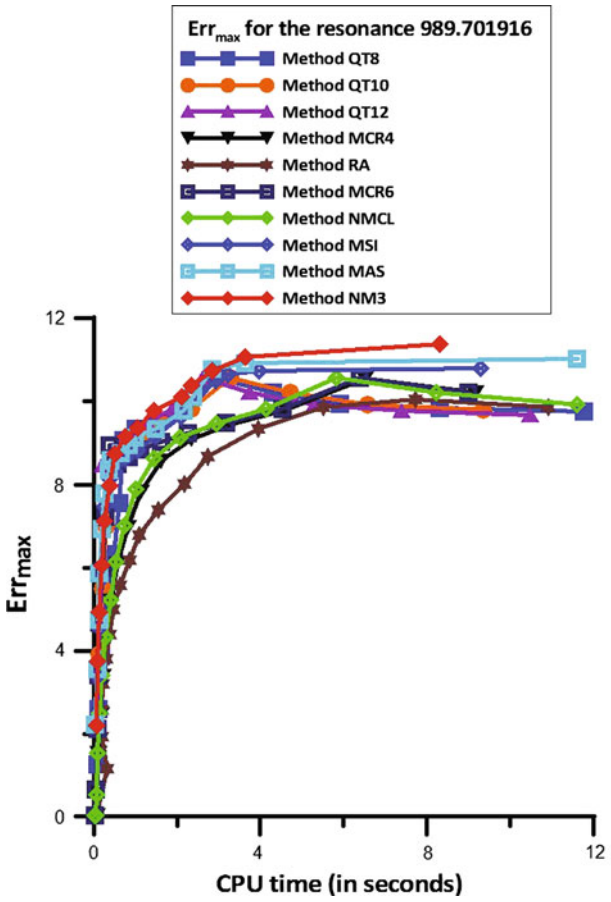

Fig. 5 Accuracy (digits) for several values of *CPU* time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (*digits*) indicates that for this value of CPU, accuracy (digits) is less than 0

eighth order multi-step method developed by Quinlan and Tremaine [19], 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 [24], which is indicated as **Method MCR6**.

3. The twelfth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT12** is more efficient than the tenth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10**
4. The hybrid two-step method with vanished phase-lag and its first derivative (obtained in [43]), which is indicated as **Method MSI** is more efficient than the twelfth order multi-step method developed by Quinlan and Tremaine [19].
5. The hybrid two-step method with vanished phase-lag and its first and second derivatives (obtained in [48]), which is indicated as **Method MAS** is more efficient

than the hybrid two-step method with vanished phase-lag and its first derivative (obtained in [43]).

6. Finally, the New developed hybrid two-step method with vanished phase-lag and its first, second and third derivatives (obtained in Sect. 4), which is indicated as **Method NM3** 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

New method with vanished phase-lag and its first, second and third derivative (developed in Sect. 4)

$$\begin{aligned}
\mathrm{LTE}_{NM} = h^8 \Bigg[& \left(\frac{1}{1680} \left(\frac{d^4}{dx^4} g(x) \right) p(x) + \frac{1}{2520} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} p(x) \right. \\
& \left. + \frac{1}{1260} g(x) p(x) \frac{d^2}{dx^2} g(x) + \frac{1}{1680} \left(\frac{d}{dx} g(x) \right)^2 p(x) \right) G \\
& + \frac{1}{20160} \left(\frac{d^6}{dx^6} g(x) \right) p(x) + \frac{1}{3360} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} p(x) \\
& + \frac{1}{1260} g(x) p(x) \frac{d^4}{dx^4} g(x) + \frac{1}{1344} \left(\frac{d^2}{dx^2} g(x) \right)^2 p(x) \\
& + \frac{13}{10080} \left(\frac{d}{dx} g(x) \right) p(x) \frac{d^3}{dx^3} g(x) + \frac{1}{840} g(x) \left(\frac{d}{dx} p(x) \right) \frac{d^3}{dx^3} g(x) \\
& + \frac{1}{1680} (g(x))^2 \left(\frac{d}{dx} p(x) \right) \frac{d}{dx} g(x) + \frac{1}{20160} (g(x))^4 p(x) \\
& + \frac{1}{420} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} p(x) \right) \frac{d^2}{dx^2} g(x) \\
& + \frac{11}{10080} (g(x))^2 p(x) \frac{d^2}{dx^2} g(x) + \frac{1}{720} g(x) p(x) \left(\frac{d}{dx} g(x) \right)^2 \Bigg] \qquad (41)
\end{aligned}$$

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