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ORIGINAL PAPER

A Runge–Kutta type four-step method with vanished phase-lag and its first and second derivatives for each level for the numerical integration of the Schrödinger equation

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Abstract The investigation of the impact of the vanishing of the phase-lag and its first and second derivatives on the efficiency of a four-step Runge–Kutta type method of sixth algebraic order is presented in this paper. Based on the above mentioned investigation, a Runge–Kutta type of two level four-step method of sixth algebraic order is produced. The error and the stability of the new obtained method are also studied in the present paper. The obtained new method is applied to the resonance problem of the Schrödinger equation the efficiency of the method to be examined.

Keywords Schrödinger equation · Multistep methods · Hybrid methods · Runge–Kutta type methods · Interval of periodicity · P-stability · Phase-lag · Phase-fitted · Derivatives of the phase-lag

Mathematics Subject Classfication 65L05

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1 Introduction

In this paper, we investigate the numerical solution of the boundary value problem which represents the one dimensional time independent Schrödinger equation that has the form:

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

where the function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential* and 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*, and V is a given function denotes the *potential*.

The boundary conditions of this problem is given by

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

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

The above mentioned problem belongs to the category of the special second-order initial or boundary value problems of the form:

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

with a periodical and/or oscillatory. The main characteristic of this general category of problems is that the system of ordinary differential equations of the form (3) are of second order in which the first derivative q' does not appear explicitly.

In applied sciences (i.e., astronomy, astrophysics, quantum mechanics, quantum chemistry, celestial mechanics, electronics, physical chemistry, chemical physics, …, etc), many problems have their mathematical models of the form of Eq. (1) (see for example [1–4]).

In this paper, we investigate a new methodology for the development of efficient four-step Runge–Kutta type methods. We develop the numerical Runge–Kutta type methods (i.e. methods with more than one stage) with vanished phase-lag and its derivatives on each level of the Runge–Kutta type method, and study how the vanishing of the phase-lag and its derivatives on each level of the method affects the efficiency of the obtained numerical scheme and finally we investigate if the method is more efficient than other methods where the vanishing of the phase-lag and its derivatives is for the whole of the method and not on each stage.

The methods produced are very effective on any problem with periodic or oscillating solutions or solution which contains the functions cos and sin or a combination of them.

In this paper, we will obtain the coefficients of the proposed Runge–Kutta type two-stage four-step method in order to have the highest possible algebraic order, the phase-lag vanished on each stage of the method, the first and second derivatives of the phase-lag vanished on each stage of the method as well.

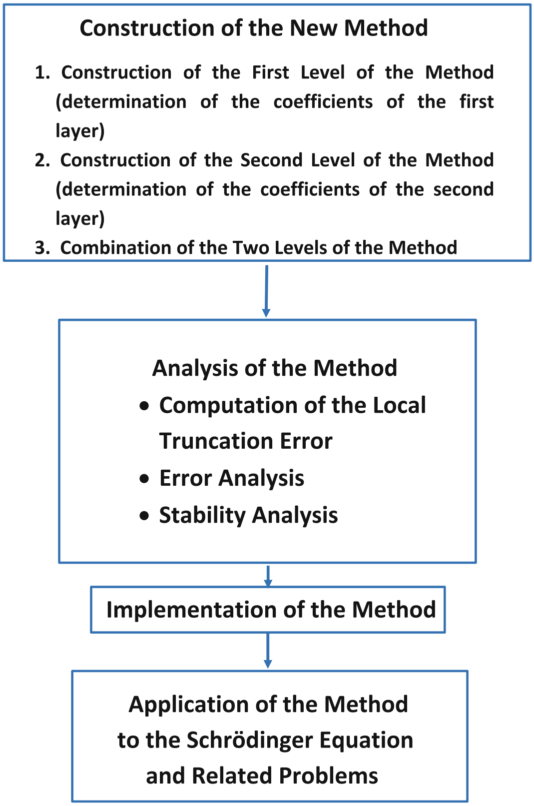


Fig. 1 Flowchart of the presentation of the analysis of the new proposed Runge–Kutta type method

In order to determine the phase-lag and its first and second derivatives, we will use the direct formula for the computation of the phase-lag for a $2m$-method as in [25,28].

In Fig. 1, we present the flowchart of the presentation of the analysis of the new proposed Runge–Kutta type method.

In order to prove the efficiency of the new scheme, we will compare the local truncation error of the new produced method with other methods of the same form (comparative error analysis), and study the stability analysis of the new obtained method and finally we study the results obtained by the application of the new produced method to the resonance problem of the one-dimensional time independent Schrödinger equation. This is one of the most difficult problems arising from the one-dimensional Schrödinger equation.

The paper has the following form:

In Sect. 2, we present some bibliography on the subject. In Sect. 3, we present the phase-lag analysis of symmetric $2k$-methods. Then we develop the new hybrid two-stage four-step method in Sect. 4. In Sect. 5, we develop the comparative error analysis, and study the stability properties of the new obtained method in Sect. 6. In Sect. 7, the numerical results are presented. Finally, we give remarks and conclusions in Sect. 8.

2 Bibliography relevant on the subject of the paper

For the numerical solution of the one-dimensional Schrödinger equation and related problems much research has been don the last decades. The aim and scope of this research was the construction of efficient, fast and reliable algorithms (see for example [5–106]). 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 [22–49].
- Symplectic integrators are investigated in [50–78].
- Exponentially and trigonometrically multistep methods have been produced in [79–99].
- Nonlinear methods have been studied in [100,101]
- Review papers have been presented in [102–106]
- Special issues and Symposia in International Conferences have been developed on this subject (see [107–110]).

3 Phase-lag analysis of symmetric 2 *n*-step methods

If we consider the initial value problem

$$q'' = f(x, q), \tag{4}$$

then we can obtain the numerical solution by considering a multistep method with p steps which can be applied over the equally spaced intervals $\{x_i\}_{i=0}^{p} \subset [a, b]$ and $h = |x_{i+1} - x_i|, i = 0(1)p - 1$.

We choose the case in which the method is symmetric, i.e.,

$$a_i = a_{p-i},\ b_i = b_{p-i},\ i = 0(1)\frac{p}{2}. \tag{5}$$

If we apply a symmetric 2 p-step method, that is for $i = -p(1)p$, to the scalar test equation

$$q'' = -w^2\, q, \tag{6}$$

we obtain a difference equation of the form

$$A_p(v)q_{n+p} + \cdots + A_1(v)q_{n+1} + A_0(v)q_n + A_1(v)q_{n-1} + \cdots + A_p(v)q_{n-p} = 0, \tag{7}$$

where $v = w\, h$, h is the step length and $A_0(v), A_1(v), \ldots, A_p(v)$ are polynomials.

The characteristic equation (which is associated with (7)) is given by:

$$A_p(v)\,\lambda^p + \cdots + A_1(v)\,\lambda + A_0(v) + A_1(v)\,\lambda^{-1} + \cdots + A_p(v)\,\lambda^{-p} = 0 \tag{8}$$

Theorem 1 *[25,28] The symmetric 2m-step method with characteristic equation given by (8) has phase-lag order q and phase-lag constant c given by:*

$$-c\,v^{q+2}+O\left(v^{q+4}\right)=\frac{2A_p(v)\cos(pv)+\cdots+2A_j(v)\cos(jv)+\cdots+A_0(v)}{2p^2A_p(v)+\cdots+2j^2A_j(v)+\cdots+2A_1(v)} \tag{9}$$

Remark 1 The formula (9) is a direct method for the calculation of the phase-lag of any symmetric 2 p-step method.

4 Development of the method

Let us consider the family of hybrid type symmetric four-step methods for the numerical solution of problems of the form $q''=f(x,q)$:

$$\begin{aligned}\hat{q}_{n+2}&=-a_0\,q_{n+1}-2\,q_n-a_0\,q_{n-1}-q_{n-2}+h^2\Big(b_0\,q''_{n+1}+b_1\,q''_n+b_0\,q''_{n-1}\Big)\\ q_{n+2}&-2\,q_{n+1}+2\,q_n-2\,q_{n-1}+q_{n-2}\\ &=h^2\Big[b_4\,\left(\hat{q}''_{n+2}+q''_{n-2}\right)+b_3\,\left(q''_{n+1}+q''_{n-1}\right)+b_2\,q''_n\Big],\end{aligned} \tag{10}$$

where the coefficient $b_i, i=0(1)4$ are free parameters, h is the step size of the integration , n is the number of steps, q_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.

4.1 First level of the hybrid method

Consider the first level of the above mentioned method:

$$q_{n+2}+a_n\,q_{n+1}+2\,q_n+a_0\,q_{n-1}+q_{n-2}=h^2\Big(b_0\,q''_{n+1}+b_1\,q''_n+b_0\,q''_{n-1}\Big) \tag{11}$$

When we apply this to the scalar test Eq. (6), we get the difference Eq. (7) with $p=2$ and $A_j(v)\,,\ j=0,\ 1,\ 2$ given by:

$$A_2(v)=1,\ A_1(v)\ =\ a_0+v^2\,b_0A_0(v)=2+v^2\,b_1 \tag{12}$$

Requiring the above method to have the phase-lag and its first and second derivatives to vanish, we obtain the following system of equations [using the formulae (9) (for $p=2$) and (12)]:

$$\text{Phase-Lag} = \frac{1}{2}\,\frac{4\ (\cos(v))^2 + 2a_0\ \cos(v) + 2\ \cos(v)\ v^2 b_0 + v^2 b_1}{4 + a_0 + v^2 b_0} = 0 \tag{13}$$

$$\text{First Derivative of the Phase-Lag} = -\frac{F_1}{\left(4 + a_0 + v^2 b_0\right)^2} = 0 \tag{14}$$

where

$$\begin{aligned}
F_1 =\ & 16\ \cos(v)\sin(v) + 4\ \cos(v)\sin(v)\,a_0 + 4\ \cos(v)\sin(v)\ v^2 b_0 + 4\ \sin(v)\,a_0\\
& + \sin(v)\,a_0{}^2 + 2\ \sin(v)\,a_0 v^2 b_0 + 4\ \sin(v)\,v^2 b_0 + \sin(v)\,v^4 b_0{}^2\\
& - 8\ \cos(v)\,v\,b_0 - 4\,v\,b_1 - v\,b_1 a_0 + 4\,v\,b_0\,(\cos(v))^2
\end{aligned}$$

$$\text{Second Derivative of the Phase-Lag} = -\frac{F_2}{\left(4 + a_0 + v^2 b_0\right)^3} = 0 \tag{15}$$

where

$$\begin{aligned}
F_2 =\ & -64 - 16\,v^3 b_0{}^2 \cos(v)\sin(v) + 16\ (\cos(v))^2\,a_0 v^2 b_0 + 16\ \cos(v)\,a_0 v^2 b_0\\
& + 3\ \cos(v)\,a_0{}^2 v^2 b_0 + 3\ \cos(v)\,a_0 v^4 b_0{}^2 + 16\ \sin(v)\ v b_0 a_0\\
& + 3\,b_1 a_0 v^2 b_0 - 8\,a_0 v^2 b_0 - 32\,a_0 - 16\,b_1 - 8\,a_0 b_1 - 4\,v^4 b_0{}^2\\
& - 4\,a_0{}^2 - b_1 a_0{}^2 + 16\,b_0\,(\cos(v))^2 - 16\,v b_0 \cos(v)\sin(v)\,a_0 + 16\ \cos(v)\,a_0\\
& + 64\ (\cos(v))^2\,a_0 + 8\ (\cos(v))^2\,a_0{}^2 + 8\ \cos(v)\,a_0{}^2 + \cos(v)\,a_0{}^3 - 32\,v^2 b_0\\
& + 64\ (\cos(v))^2\ v^2 b_0 + 8\cos(v)\ v^4 b_0{}^2 + 8\,(\cos(v))^2\ v^4 b_0{}^2 + 4\,b_0\,(\cos(v))^2\,a_0\\
& + \cos(v)\ v^6 b_0{}^3 + 16\ \sin(v)\ v^3 b_0{}^2 - 8\ \cos(v)\,b_0 a_0 + 12\,b_1 v^2 b_0\\
& + 24\ \cos(v)\,b_0{}^2 v^2 - 12\,v^2 b_0{}^2\,(\cos(v))^2 + 64\ \sin(v)\ v b_0 - 32\ \cos(v)\,b_0\\
& + 128\ (\cos(v))^2 + 16\ \cos(v)\ v^2 b_0 - 64\,v b_0 \cos(v)\sin(v)
\end{aligned}$$

The coefficients of the first level of the proposed hybrid four-step methods are defined by the solution of the above system of Eqs. (13)–(15):

$$\begin{aligned}
a_0 &= \frac{-v^2 \sin(3\,v) + 3\,v^2 \sin(v) + 7\ \cos(v)\ v - 3\,v\cos(3\,v) + 3\ \sin(v) + 3\ \sin(3\,v)}{-3\,v + v\cos(2\,v) - 3\ \sin(2\,v)}\\
b_0 &= \frac{\cos(v)\ v + 3\,v\cos(3\,v) + v^2 \sin(3\,v) - 3\,v^2 \sin(v) - \sin(v) - \sin(3\,v)}{-3\,v^3 + v^3 \cos(2\,v) - 3\,v^2 \sin(2\,v)}\\
b_1 &= \frac{2\ \sin(2\,v) + \sin(4\,v) - 3\,v - v\cos(4\,v) - 4\,v\cos(2\,v)}{-3\,v^3 + v^3 \cos(2\,v) - 3\,v^2 \sin(2\,v)}
\end{aligned} \tag{16}$$

The formulae given by (16) are subject to heavy cancellations for some values of $|w|$. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
a_0 = & -2+\frac{3}{80}v^6-\frac{47}{10080}v^8+\frac{47}{80640}v^{10}-\frac{547}{7603200}v^{12}+\frac{503207}{96864768000}v^{14}\\
&-\frac{870781}{871782912000}v^{16}+\frac{194612701}{355687428096000}v^{18}-\frac{5286219803}{51607012294656000 0}v^{20}\\
&+\frac{444499768241}{41629656584355840000 0}v^{22}-\frac{3306991067063}{689387113036932710400 00}v^{24}\\
&+\frac{357983689303064647}{16938241367317436694528000000}v^{26}\\
&+\frac{816598959203681}{615936049720634061619200000 0}v^{28}+\cdots\\
b_0 = & \frac{7}{6}-\frac{9}{40}v^2-\frac{1}{10080}v^4+\frac{3259}{1814400}v^6-\frac{9197}{79833600}v^8+\frac{14763719}{435891456000}v^{10}\\
&-\frac{5295347}{5230697472000}v^{12}+\frac{37189991}{108883906560000}v^{14}-\frac{266119714361}{851515702861824000 0}v^{16}\\
&+\frac{3176521552291}{562000363888803840000 0}v^{18}-\frac{137264450201}{17217460365557760000 0}v^{20}\\
&-\frac{86602787462431411}{282304022788623944908800000 0}v^{22}\\
&-\frac{88184994365249323}{871109556033468172861440000 0}v^{24}\\
&+\frac{412024065777428151 1}{35367047974958807818174464000000}v^{26}+\cdots\\
b_1 = & -\frac{1}{3}+\frac{9}{20}v^2-\frac{1133}{5040}v^4+\frac{47651}{907200}v^6-\frac{280939}{39916800}v^8+\frac{192066541}{217945728000}v^{10}\\
&-\frac{4516411}{47551795200}v^{12}+\frac{2077986997}{205204285440000}v^{14}-\frac{1007668088177}{851515702861824000}v^{16}\\
&+\frac{312947531382179}{281000181944401920000 0}v^{18}-\frac{245257668582937}{17234677825923317760000}v^{20}\\
&+\frac{188374982059936416 1}{141115201139431197245440000 00}v^{22}\\
&-\frac{23116629052873612297}{152444172305856930250752000000}v^{24}\\
&+\frac{29442050268474159397}{16075930897708549008261120000 00}v^{26}\cdots
\end{aligned} \tag{17}
$$

Figure 2 shows the behavior of the coefficients a_0, b_0 and b_1.

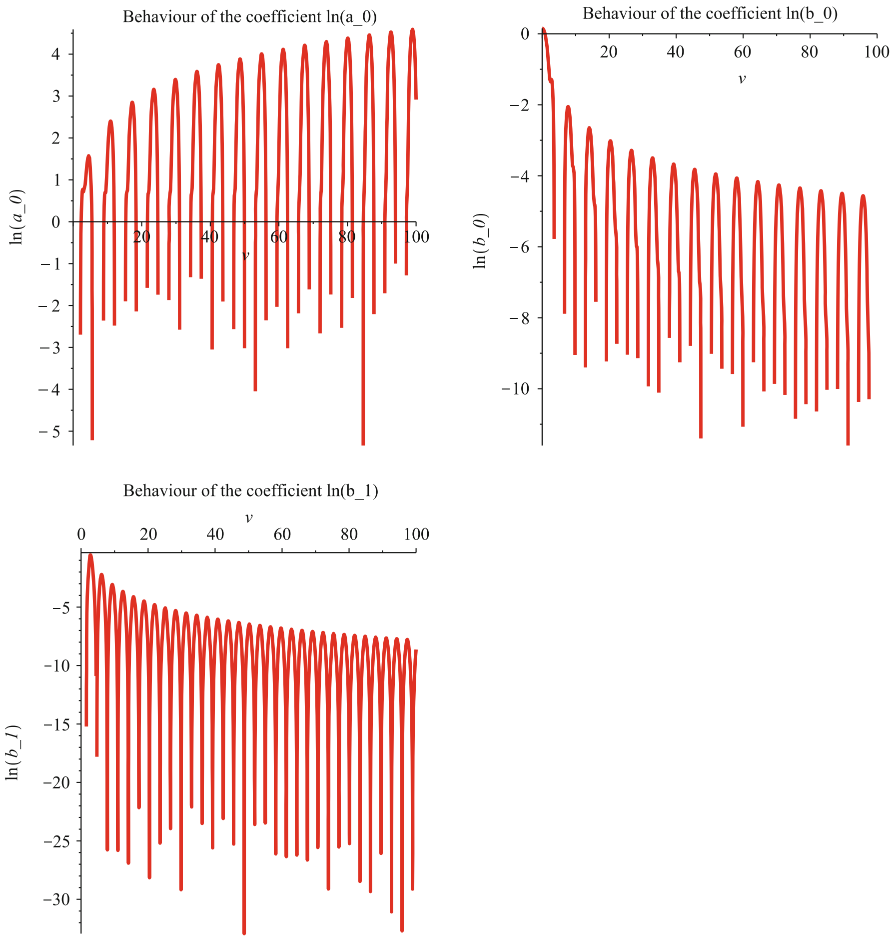


Fig. 2 Behavior of the coefficients of the method given by (16) for several values of $v = w\,h$

4.2 Second Level of the Method

We consider now the second level of the method (10):

$$q_{n+2} - 2\,q_{n+1} + 2\,q_n - 2\,q_{n-1} + q_{n-2} \\ = h^2 \left(b_4\, q''_{n+2} + b_3\, q''_{n+1} + b_2\, q''_n + b_3\, q''_{n-1} + b_4\, q''_{n-2} \right) \tag{18}$$

If we apply the second level (18) to the scalar test Eq. (6), the difference Eq. (7) with $p = 2$ and $A_j(v)$, $j = 0,\ 1,\ 2$ given by:

$$A_2\,(v) = 1 + v^2\, b_4,\ A_1\,(v) \ = \ -2 + v^2\, b_3 A_0\,(v) = 2 + \ v^2\, b_2 \tag{19}$$

is produced.

If now we require the above second level of the method (10) to have the phase-lag and its first and second derivatives to vanish, the following system of equations is obtained [using the formulae (9) (for $p = 2$) and (19)]:

$$\text{Phase-Lag} = \frac{2\left(\cos(v)\right)^2 v^2 b_4 + 2\left(\cos(v)\right)^2 + \cos(v)\, v^2 b_3 - 2\cos(v) - 2\, v^2 b_4 + v^2 b_2}{2 + 4\, v^2 b_4 + v^2 b_3} = 0 \tag{20}$$

$$\text{First Derivative of the Phase-Lag} = -\frac{F_3}{\left(2 + 4\, v^2 b_4 + v^2 b_3\right)^2} = 0 \tag{21}$$

where

$$\begin{aligned} F_3 = {} & 24\cos(v)\, v^2 b_4 \sin(v) + 16\cos(v)\, v^4 {b_4}^2 \sin(v) + 4\cos(v)\sin(v)\, v^2 b_3 \\ & + 4\sin(v)\, v^4 b_3 b_4 + 8\left(\cos(v)\right)^2 v\, b_4 - 8\cos(v)\, v\, b_3 + \sin(v)\, v^4 {b_3}^2 \\ & - 8\sin(v)\, v^2 b_4 + 4\, v\left(\cos(v)\right)^2 b_3 - 16\, v\cos(v)\, b_4 + 8\cos(v)\sin(v) + 4\, v\, b_4 \\ & - 2\, v\, b_2 + 4\cos(v)\, v^4 b_4 \sin(v)\, b_3 - 4\sin(v) \end{aligned}$$

$$\text{Second Derivative of the Phase-Lag} = \frac{F_4}{\left(2 + 4\, v^2 b_4 + v^2 b_3\right)^3} = 0 \tag{22}$$

where

$$\begin{aligned} F_4 = {} & 16 + 80\, v^2 b_4 + 16\, v^2 b_3 + 32\cos(v)\, v^4 {b_4}^2 + 32\cos(v)\, v^2 b_4 \\ & + 16\cos(v)\, b_3 - 16\left(\cos(v)\right)^2 b_4 + 64\, v^6 {b_4}^3 - 8\, b_4 + 4\, b_2 - 24\, v^2 b_2 b_4 \\ & - 6\, v^2 b_2 b_3 + 12\, v^2 b_4 b_3 + 48\, v^4 b_3 b_4 - 32\sin(v)\, v b_3 \\ & - 192\, v^2\cos(v)\, {b_4}^2 - 64 v\sin(v)\, b_4 + 12\, v^2\left(\cos(v)\right)^2 {b_3}^2 - 128\sin(v)\, {b_4}^2 v^3 \\ & + 96\left(\cos(v)\right)^2 v^2 {b_4}^2 - 24\cos(v)\, v^2 {b_3}^2 - \cos(v)\, v^6 {b_3}^3 - 16\sin(v)\, v^3 {b_3}^2 \\ & - 256\left(\cos(v)\right)^2 v^4 {b_4}^2 - 128\left(\cos(v)\right)^2 v^6 {b_4}^3 - 2\cos(v)\, v^4 {b_3}^2 \\ & - 32\left(\cos(v)\right)^2 v^2 b_3 - 8\left(\cos(v)\right)^2 v^4 {b_3}^2 - 32\left(\cos(v)\right)^2 \\ & + 64\cos(v)\, v b_4 \sin(v) + 96\cos(v)\, v^3 b_4 \sin(v)\, b_3 + 4\, v^6 b_4 {b_3}^2 \\ & + 32\, v^6 {b_4}^2 b_3 - 96\sin(v)\, v^3 b_3 b_4 - 8\cos(v)\, v^6 {b_3}^2 b_4 - 16\cos(v)\, v^6 b_3 {b_4}^2 \\ & - 8\left(\cos(v)\right)^2 v^6 b_4 {b_3}^2 - 64\left(\cos(v)\right)^2 v^6 {b_4}^2 b_3 \\ & - 96\left(\cos(v)\right)^2 v^4 b_4 b_3 + 16\cos(v)\sin(v)\, {b_3}^2 v^3 + 128\cos(v)\, v^3 {b_4}^2 \sin(v) \\ & + 32\, v\cos(v)\sin(v)\, b_3 - 144\cos(v)\, v^2 b_3 b_4 + 72\left(\cos(v)\right)^2 v^2 b_4 b_3 \\ & - 8\left(\cos(v)\right)^2 b_3 + 32\cos(v)\, b_4 + 48\, v^2 {b_4}^2 + 4\, v^4 {b_3}^2 + 128\, v^4 {b_4}^2 \\ & + 8\cos(v) + 4\cos(v)\, v^2 b_3 - 160\left(\cos(v)\right)^2 v^2 b_4 \end{aligned}$$

The coefficients of the second level of the proposed hybrid four-step methods are defined by the solution of the above system of Eqs. (20)–(22):

$$\begin{aligned} b_2 &= \frac{F_5}{v^4 \sin(3\, v) - 3\, v^4 \sin(v)} \quad b_3 = \frac{F_6}{v^4 \sin(3\, v) - 3\, v^4 \sin(v)} \\ b_4 &= \frac{F_7}{v^4 \sin(3\, v) - 3\, v^4 \sin(v)} \end{aligned} \tag{23}$$

where

$$F_5 = -18\,v - 2\,v^2 \sin(3\,v) + 6\,v^2 \sin(v) - 4\,v\cos(2\,v) + 15\,\sin(3\,v) + 12\,\sin(v) + 28\,\cos(v)\,v - 3\,v\cos(3\,v) - v\cos(5\,v) - 2\,v\cos(4\,v) - 6\,\sin(4\,v) - 24\,\sin(2\,v) + 3\,\sin(5\,v)$$

$$F_6 = 16\,\cos(v)\,v - 12\,\sin(2\,v) - 6\,\sin(4\,v) + 2\,v^2\sin(3\,v) - 6\,v^2\sin(v) - 12\,v + 4\,v\cos(4\,v) - 8\,v\cos(2\,v) + 12\,\sin(3\,v) + 12\,\sin(v)$$

$$F_7 = -v^2\sin(3\,v) + 3\,v^2\sin(v) + 7\,\cos(v)\,v - 6\,v + 2\,v\cos(2\,v) - 3\,v\cos(3\,v) + 3\,\sin(v) + 3\,\sin(3\,v) - 6\,\sin(2\,v)$$

The formulae given by (23) are subject to heavy cancellations for some values of $|w|$. In this case the following Taylor series expansions should be used:

$$b_2 = \frac{7}{60} + \frac{19}{336}v^2 - \frac{1093}{100800}v^4 + \frac{17749}{9979200}v^6 + \frac{698293}{12108096000}v^8 + \frac{3165689}{174356582400}v^{10} + \frac{2072867219}{889218570240000}v^{12} + \frac{5662897453}{17739910476288000}v^{14} + \frac{2772391899877}{66904805224857600000}v^{16} + \frac{12311866905617}{2350183339898634240000}v^{18} + \frac{30464861505489379}{47050670464770657484800000}v^{20} + \frac{13095830186993}{166649364101903155200000}v^{22}\ldots$$

$$b_3 = \frac{13}{15} - \frac{19}{504}v^2 + \frac{103}{25200}v^4 + \frac{4891}{9979200}v^6 + \frac{2221963}{27243216000}v^8 + \frac{1044143}{87178291200}v^{10} + \frac{52839173}{31757806080000}v^{12} + \frac{47149992299}{212878925715456000}v^{14} + \frac{477390285503}{16726201306214400000}v^{16} + \frac{46337692108619}{12926008369442488320000}v^{18} + \frac{15562903075200133}{35288002848577993113600000}v^{20} + \frac{215105978014253}{4032914611266056355840000}v^{22} + \frac{35139511603773340037}{552610124608731372158976000000 0}v^{24} + \cdots$$

$$b_4 = \frac{3}{40} + \frac{19}{2016}v^2 + \frac{269}{201600}v^4 + \frac{1273}{6652800}v^6 + \frac{5849539}{217945728000}v^8 + \frac{1273619}{348713164800}v^{10} + \frac{22006867}{45600952320000}v^{12} + \frac{3306233257}{53219731428864000}v^{14} + \frac{1046327020939}{133809610449715200000}v^{16} + \frac{5546864378273}{5744892608641105920000}v^{18} + \frac{33108571855055119}{282304022788623944908800000}v^{20} + \frac{80923485190841}{5761306587522937651200000}v^{22} + \cdots \quad (24)$$

Figure 3 shows the behavior of the coefficients b_2, b_3 and b_4.

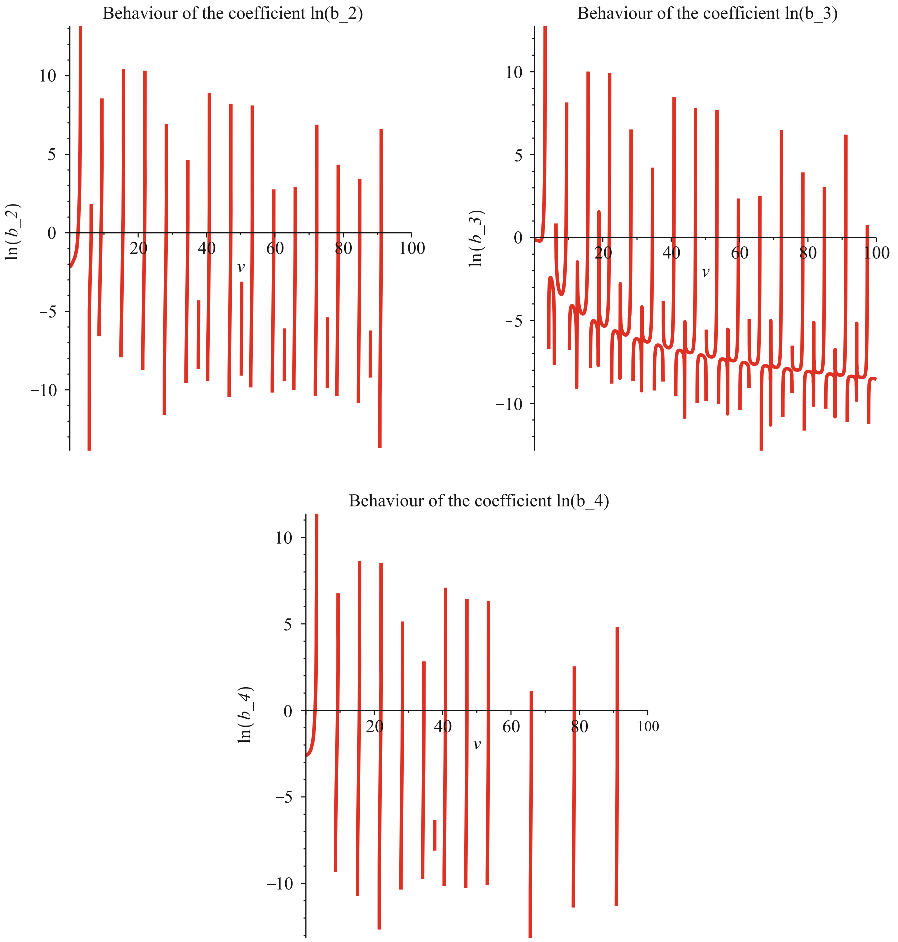


Fig. 3 Behavior of the coefficients of the new proposed method given by (23) for several values of $v = w\,h$

Figure 4 shows the flowchart of the construction of the new proposed method.

The combination of the above two mentioned levels leads to the proposed method (10) with the coefficients given by (16), (17), (23) and (24).

The local truncation error of this new proposed method (mentioned as $HybMethI$) is given by:

$$LTE_{HybMeth} = \frac{751\,h^8}{302400}\left(q_n^{(8)} + 3\,w^2\,q_n^{(6)} + 3w^4\,q_n^{(4)} + w^6\,q_n^{(2)}\right) + O\left(h^{10}\right) \qquad (25)$$

where $q_n^{(j)}$ is the jth derivative of q_n.

5 Comparative error analysis

We will study the following methods:

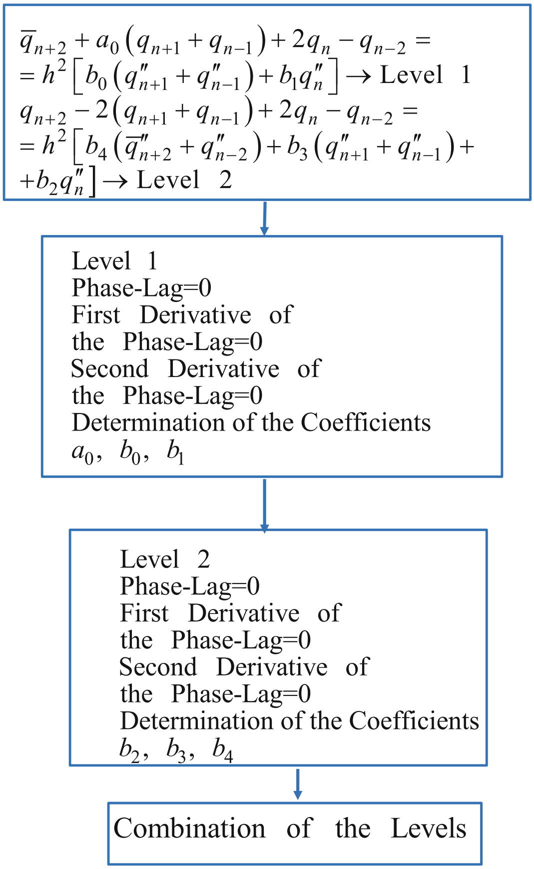


Fig. 4 Flowchart of the development of the new proposed method

5.1 Classical method (i.e. the method (10) with constant coefficients)

$$LTE_{CL} = -\frac{751\, h^8}{302400}\, p_n^{(8)} + O\left(h^{10}\right) \tag{26}$$

5.2 The hybrid method with vanished phase-lag and its first derivative in each level developed in [42]

$$LTE_{Meth\ I} = \frac{751\, h^8}{302400} \left(q_n^{(8)} + 2 w^2 q_n^{(6)} + w^4 q_n^{(4)} \right) + O\left(h^{10}\right) \tag{27}$$

5.3 The new proposed Runge–Kutta type method with vanished phase-lag and its first and second derivatives in each level developed in section 3

$$LTE_{Meth\ II} = -\frac{751 h^8}{302400} \left(q_n^{(8)} + 3 w^2 q_n^{(6)} + 3 w^4 q_n^{(4)} + w^6 q_n^{(2)} \right) + O\left(h^{10}\right) \tag{28}$$

For the Error Analysis we follow the Flowchart mentioned in the Fig. 5.

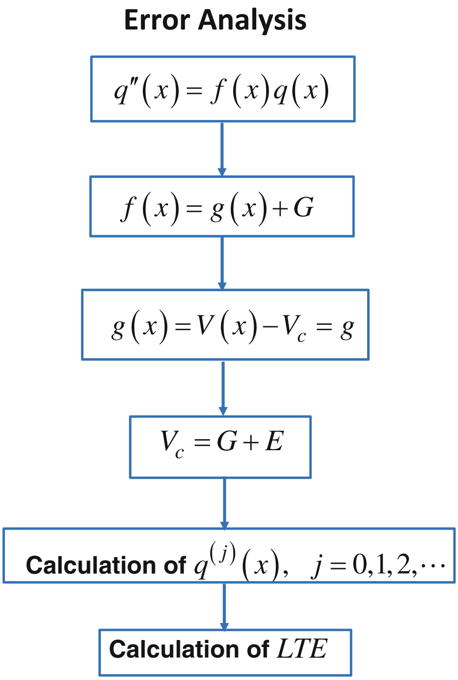


Fig. 5 Flowchart for the comparative error analysis

We use the algorithm described on the flowchart together with the formulae:

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

$$q_n^{(7)} = \left(\frac{d^5}{dx^5} g(x)\right) q(x) + 5 \left(\frac{d^4}{dx^4} g(x)\right) \frac{d}{dx} q(x)$$
$$+ 11 \, (g(x) + G)\, q(x) \frac{d^3}{dx^3} g(x) + 15 \left(\frac{d}{dx} g(x)\right) q(x) \frac{d^2}{dx^2} g(x)$$
$$+ 13 \, (g(x) + G) \left(\frac{d}{dx} q(x)\right) \frac{d^2}{dx^2} g(x) + 10 \left(\frac{d}{dx} g(x)\right)^2 \frac{d}{dx} q(x)$$
$$+ 9 \, (g(x) + G)^2 q(x) \frac{d}{dx} g(x) + (g(x) + G)^3 \frac{d}{dx} q(x)$$
$$q_n^{(8)} = \left(\frac{d^6}{dx^6} g(x)\right) q(x) + 6 \left(\frac{d^5}{dx^5} g(x)\right) \frac{d}{dx} q(x)$$
$$+ 16 \, (g(x) + G)\, q(x) \frac{d^4}{dx^4} g(x) + 26 \left(\frac{d}{dx} g(x)\right) q(x) \frac{d^3}{dx^3} g(x)$$
$$+ 24 \, (g(x) + G) \left(\frac{d}{dx} q(x)\right) \frac{d^3}{dx^3} g(x) + 15 \left(\frac{d^2}{dx^2} g(x)\right)^2 q(x)$$
$$+ 48 \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} q(x)\right) \frac{d^2}{dx^2} g(x) + 22 \, (g(x) + G)^2 q(x) \frac{d^2}{dx^2} g(x)$$
$$+ 28 \, (g(x) + G)\, q(x) \left(\frac{d}{dx} g(x)\right)^2$$
$$+ 12 \, (g(x) + G)^2 \left(\frac{d}{dx} q(x)\right) \frac{d}{dx} g(x) + (g(x) + G)^4 q(x) \cdots$$

Based on the above we produce the expressions of the Local Truncation Errors.

Two cases in terms of the value of E are studied during the investigation of the Local Truncation Errors:

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

Based on the analysis presented above, we have the following asymptotic expansions of the Local Truncation Errors:

5.4 Classical method

$$LTE_{CL} = h^8 \left(\frac{751}{302400} q(x)\; G^4 + \cdots\right) + O\left(h^{10}\right) \tag{29}$$

5.5 The hybrid method with vanished phase-lag and its first derivative in each level developed in [42]

$$LTE_{Meth\ I} = h^8 \Big[\Big(\frac{751}{33600} \left(\frac{d^2}{dx^2} g(x) \right) q(x) + \frac{751}{151200} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} q(x) + \frac{751}{302400} (g(x))^2 q(x) \Big) G^2 + \cdots \Big] + O\left(h^{10}\right) \tag{30}$$

5.6 The new proposed Runge–Kutta type method with vanished phase-lag and its first and second derivatives in each level developed in section 3

$$LTE_{Meth\ II} = h^8 \Big[\Big(\frac{751}{75600} \left(\frac{d^2}{dx^2} g(x) \right) q(x) \Big) G^2 + \cdots \Big] + O\left(h^{10}\right) \tag{31}$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Runge–Kutta type Four-Step Method the error increases as the fourth power of* G. *For the method with vanished phase-lag and its first derivative in each level which developed in [42], the error increases as the second power of* G. *Finally, for the the method with vanished phase-lag and its first and second derivatives in each level developed in Sect. 3, the error increases as the second power of* G. *So, for the numerical solution of the time independent radial Schrödinger equation the Method with Vanished Phase-Lag and its First Derivatives in each level and the New Proposed Method with Vanished Phase-Lag and its its First and Second Derivatives in each level are the most efficient and they have the same approximately behavior, from theoretical point of view, especially for large values of* $|G| = |V_c - E|$.

6 Stability analysis

For the Stability analysis is based on the Flowchart mentioned in the Fig. 6.

The analysis mentioned on the flowchart we will applied as follows:

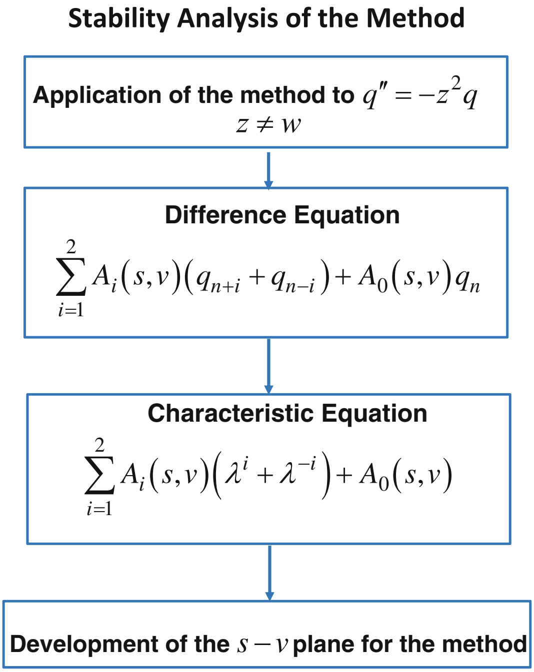
- We will study the stability of the first layer of the new proposed Runge–Kutta type method
- We will study the stability of the second layer of the new proposed Runge–Kutta type method
- We will study the stability of the new proposed Runge–Kutta type two layer method.

6.1 Stability analysis for the first layer of the new proposed Runge–Kutta type method

Let us apply the first layer of the new proposed Runge–Kutta type method (11) with the coefficients given by (16) to the scalar test equation:

$$q'' = -z^2 q. \tag{32}$$

Fig. 6 Flowchart for the stability analysis



This leads to the following difference equation:

$$A_2\,(s,\,v)\ \ (q_{n+2}+q_{n-2})+A_1\,(s,\,v)\ \ (q_{n+1}+q_{n-1})+A_0\,(s,\,v)\ \ q_n=0 \tag{33}$$

where

$$A_2\,(s,\,v)=1,\ A_1\,(s,\,v)=-2\,\frac{F_8}{v^2\left(-\left(\cos\,(v)\right)^2 v+3\ \sin\,(v)\cos\,(v)+2\,v\right)}$$
$$A_0\,(s,\,v)=-2\,\frac{F_9}{v^2\ (v\cos\,(2\,v)-3\ \sin\,(2\,v)-3\,v)} \tag{34}$$

where

$$\begin{aligned}F_8 &= \sin\,(v)\,(\cos\,(v))^2\,s^2v^2-\sin\,(v)\,(\cos\,(v))^2\,v^4+3\ (\cos\,(v))^3\,s^2v\\&\quad-3\ (\cos\,(v))^3\,v^3-\sin\,(v)\,(\cos\,(v))^2\,s^2+3\ \sin\,(v)\,(\cos\,(v))^2\,v^2-\sin\,(v)\,s^2v^2\\&\quad+\sin\,(v)\,v^4-2\ \cos\,(v)\,s^2v+4\ \cos\,(v)\,v^3\\F_9 &= (\cos\,(2\,v))^2\,s^2v-\cos\,(2\,v)\sin\,(2\,v)\,s^2+2\ \cos\,(2\,v)\,s^2v\\&\quad-\cos\,(2\,v)\,v^3-\sin\,(2\,v)\,s^2+3\ \sin\,(2\,v)\,v^2+s^2v+3\,v^3\end{aligned}$$

and $s = z\,h$.

Remark 2 the frequency of the scalar test Eq. (6), w, is not equal with the frequency of the scalar test Eq. (32), z, i.e. $z \neq w$.

The corresponding characteristic equation is given by:

$$A_2\,(s,v)\,\left(\lambda^4+1\right)+A_1\,(s,v)\,\left(\lambda^3+\lambda\right)+A_0\,(s,v)\,\lambda^2\;=\;0 \tag{35}$$

Definition 1 (see [18]) A symmetric $2\,k$-step method with the characteristic equation given by (8) is said to have an *interval of periodicity* $\left(0, \mathrm{v}_0^2\right)$ if, for all $s \in \left(0, s_0^2\right)$, the roots $\lambda_i,\ i = 1(1)4$ satisfy

$$\lambda_{1,2} = e^{\pm i\,\zeta(s)},\ |\lambda_i| \le 1,\ i = 3, 4, \cdots \tag{36}$$

where $\zeta(s)$ is a real function of $z\,h$ and $s = z\,h$.

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. $s = v$.

In Fig. 7 we present the $s - v$ plane for the first layer of the Runge–Kutta type method developed in this paper. A shadowed area denotes the $s - v$ region where the method is stable, while a white area denotes the region where the method is unstable.

6.2 Stability analysis for the second layer of the new proposed Runge–Kutta type method

We apply the second layer of the new proposed Runge–Kutta type method (18) with the coefficients given by (23) to the scalar test Eq. (32). This leads to the difference Eq. (33) with:

$$\begin{aligned} A_2\,(s,v) &= -\frac{F_{10}}{\sin(v)\,(\cos(v)+1)\,v^4},\ A_1\,(s,v) = -2\,\frac{F_{11}}{\sin(v)\,(\cos(v)+1)\,v^4} \\ A_0\,(s,v) &= 2\,\frac{F_{12}}{\sin(v)\,(\cos(v)+1)\,v^4} \end{aligned} \tag{37}$$

where

$$\begin{aligned} F_{10} = &\sin(v)\cos(v)\,s^2v^2-\sin(v)\cos(v)\,v^4 \\ &+\ \sin(v)\,s^2v^2-\sin(v)\,v^4+3\,s^2v\,(\cos(v))^2 \\ &-\ 3\,\sin(v)\cos(v)\,s^2+2\,\cos(v)\,s^2v-2\,s^2v \\ F_{11} = &-\sin(v)\cos(v)\,s^2v^2+\sin(v)\cos(v)\,v^4 \\ &-\ 4\,(\cos(v))^3\,s^2v+6\,\sin(v)\,(\cos(v))^2\,s^2 \\ &-\ \sin(v)\,s^2v^2+\sin(v)\,v^4-4\,s^2v\,(\cos(v))^2+2\,\cos(v)\,s^2v \end{aligned}$$

[1] Where S is a set of distinct points

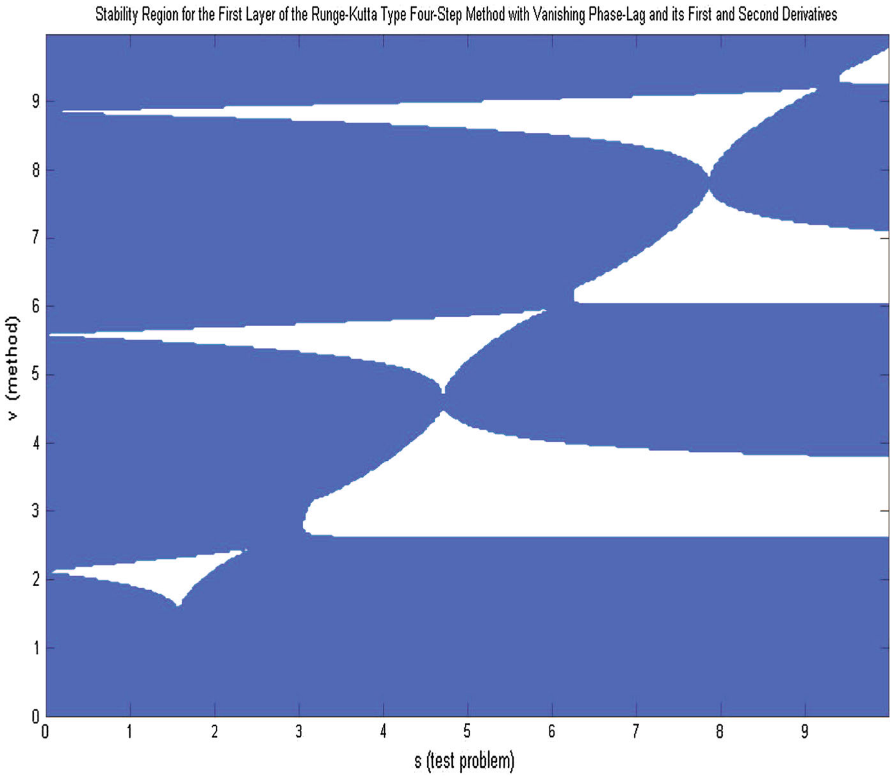


Fig. 7 $s - v$ plane of the first layer of the new Runge–Kutta type obtained method

$$\begin{aligned}F_{12} = & -2\,s^2 v\,(\cos(v))^4 + 6\,\sin(v)\,(\cos(v))^3\,s^2 \\ & - \sin(v)\cos(v)\,s^2 v^2 + \sin(v)\cos(v)\,v^4 - 4\,(\cos(v))^3\,s^2 v \\ & - \sin(v)\,s^2 v^2 + \sin(v)\,v^4 - 3\,s^2 v\,(\cos(v))^2 \\ & + 3\,\sin(v)\cos(v)\,s^2 - 2\,\cos(v)\,s^2 v + 2\,s^2 v\end{aligned}$$

and $s = z\,h$.

In Fig. 8 we present the $s - v$ plane for the second layer of the Runge–Kutta type method developed in this paper. A shadowed area denotes the $s - v$ region where the method is stable, while a white area denotes the region where the method is unstable.

6.3 Stability analysis for the new proposed Runge–Kutta type method

Let us apply the new obtained method (10) with the coefficients given by (16), (17), (23) and (24) to the scalar test Eq. (32). This leads to the difference Eq. (33) with:

$$A_2\,(s, v) = 1,\ A_1\,(s, v) = 2\,\frac{F_{13}}{F_{14}} A_0\,(s, v) = -2\,\frac{F_{15}}{F_{14}} \tag{38}$$

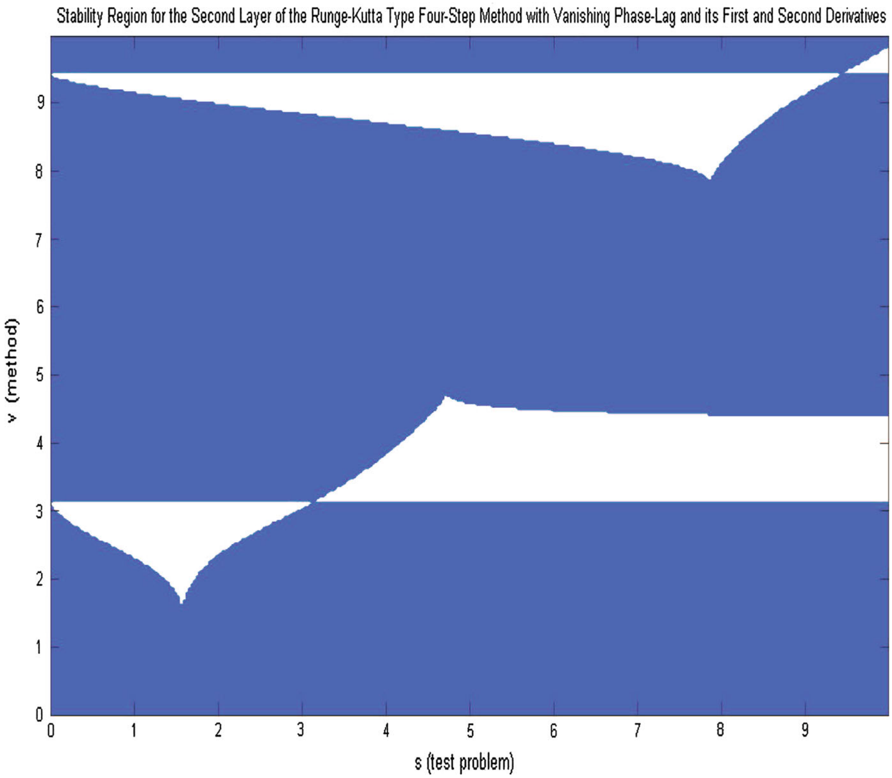


Fig. 8 $s - v$ plane of the second layer of the new Runge–Kutta type obtained method

where

$$\begin{aligned} F_{13} = & -2\ (\cos(v))^3\, s^2 v^6 - 9\ (\cos(v))^5\, s^2 v^2 + \cos(v)\, s^2 v^6 \\ & - 4\ \sin(v)\, s^2 v^5 - 5\ (\cos(v))^2\, s^4 v^2 - 2\ (\cos(v))^2\, s^2 v^6 \\ & - \cos(v)\, s^4 v^4 + 7\ \cos(v)\, s^4 v^2 + (\cos(v))^4\, s^2 v^6 + (\cos(v))^5\, s^2 v^6 \\ & - \sin(v)\, (\cos(v))^2\, v^7 + 13\ (\cos(v))^5\, s^4 v^2 - 19\ (\cos(v))^3\, s^4 v^2 \\ & - 10\ \cos(v)\, s^2 v^4 + 2\ (\cos(v))^2\, s^4 v^4 - (\cos(v))^4\, s^4 v^4 \\ & - \sin(v)\, (\cos(v))^3\, v^7 + 9\ (\cos(v))^3\, s^2 v^2 \\ & - 11\ (\cos(v))^5\, s^2 v^4 + 2\ \sin(v)\, s^4 v^3 - 2\ (\cos(v))^4\, s^2 v^4 \\ & + 20\ (\cos(v))^3\, s^2 v^4 + 2\ (\cos(v))^3\, s^4 v^4 + 7\ (\cos(v))^4\, s^4 v^2 \\ & - (\cos(v))^5\, s^4 v^4 + 2\ \sin(v)\cos(v)\, v^7 + 6\ \sin(v)\, (\cos(v))^4\, s^4 v^3 \\ & - 6\ \sin(v)\, (\cos(v))^4\, s^2 v^5 + 5\ \sin(v)\, (\cos(v))^3\, s^4 v^3 \\ & - 4\ \sin(v)\, (\cos(v))^3\, s^2 v^5 - 12\ \sin(v)\, (\cos(v))^4\, s^4 v \\ & - 7\ \sin(v)\, (\cos(v))^2\, s^4 v^3 + 10\ \sin(v)\, (\cos(v))^2\, s^2 v^5 \\ & - 2\ \sin(v)\, (\cos(v))^3\, s^4 v - 6\ \sin(v)\, (\cos(v))^3\, s^2 v^3 \\ & + 8\ \sin(v)\, (\cos(v))^2\, s^4 v - 4\ \sin(v)\cos(v)\, s^4 v^3 \end{aligned}$$

$$
\begin{aligned}
&+ 4\,\sin(v)\cos(v)\,s^2v^5 - 3\,(\cos(v))^3\,v^6 + 3\,(\cos(v))^2\,v^6 \\
&+ 3\,(\cos(v))^3\,s^4 - 3\,(\cos(v))^4\,v^6 - 3\,(\cos(v))^5\,s^4 \\
&+ 3\,v^6\cos(v) - s^4v^4 + s^2v^6 + 2\,\sin(v)\,v^7
\end{aligned}
$$

$$
\begin{aligned}
F_{14} = &\Big(\sin(v)\,(\cos(v))^3\,v + 3\,(\cos(v))^4 \\
&+ \sin(v)\,(\cos(v))^2\,v + 3\,(\cos(v))^3 - 2\,\sin(v)\cos(v)\,v \\
&- 3\,(\cos(v))^2 - 2\,\sin(v)\,v - 3\,\cos(v)\Big)v^6
\end{aligned}
$$

$$
\begin{aligned}
F_{15} = &\,2\,(\cos(v))^6\,s^2v^4 - \sin(v)\,(\cos(v))^2\,v^7 + 6\,(\cos(v))^5\,s^4v^2 \\
&- 2\,(\cos(v))^3\,s^4v^2 - \sin(v)\,(\cos(v))^3\,v^7 + 4\,(\cos(v))^5\,s^2v^4 \\
&- 4\,(\cos(v))^4\,s^2v^4 - 8\,(\cos(v))^3\,s^2v^4 - 6\,(\cos(v))^4\,s^4v^2 \\
&+ 2\,\sin(v)\cos(v)\,v^7 - 6\,(\cos(v))^6\,s^4 + 6\,(\cos(v))^4\,s^4 \\
&+ 2\,\sin(v)\,(\cos(v))^4\,s^4v^3 - 4\,\sin(v)\,(\cos(v))^4\,s^4v \\
&+ 4\,\sin(v)\,(\cos(v))^3\,s^4v + 12\,\sin(v)\,(\cos(v))^3\,s^2v^3 \\
&- 3\,(\cos(v))^3\,v^6 + 3\,(\cos(v))^2\,v^6 - 3\,(\cos(v))^4\,v^6 \\
&+ 3\,v^6\cos(v) + 2\,\sin(v)\,(\cos(v))^5\,s^4v^3 - 12\,\sin(v)\,(\cos(v))^5\,s^4v \\
&- 12\,\sin(v)\,(\cos(v))^5\,s^2v^3 - 12\,\sin(v)\,(\cos(v))^4\,s^2v^3 \\
&+ 18\,(\cos(v))^4\,s^2v^2 - 18\,(\cos(v))^6\,s^2v^2 \\
&+ 8\,(\cos(v))^6\,s^4v^2 + 2\,\sin(v)\,v^7
\end{aligned}
$$

and $s = z\,h$.

In Fig. 9 we present the $s - v$ plane for the Runge–Kutta type method developed in this paper. A shadowed area denotes the $s - v$ region where the method is stable, while a white area denotes the region where the method is unstable.

Remark 3 For the solution of the Schrödinger equation the frequency of the phase fitting is equal to the frequency of the scalar test equation. So, for this case of problems it is necessary to observe **the surroundings of the first diagonal of the $s - v$ plane**.

We study now the case where the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $s = v$ (i.e. see the surroundings of the first diagonal of the $s - v$ plane). Based on this study we extract the result that the interval of periodicity of the new method developed in Sect. 3 is equal to: (0, 6.05).

From the above analysis we have the following theorem:

Theorem 3 *The method developed in Sect. 3:*

- *is of sixth algebraic order,*
- *has the phase-lag and its first and second derivatives equal to zero on the first level of the hybrid method*
- *has the phase-lag and its first and second derivatives equal to zero on the second level of the hybrid method*
- *has an interval of periodicity equals to:* (0, 6.05) *in the case where the frequency of the scalar test equation is equal with the frequency of phase fitting.*

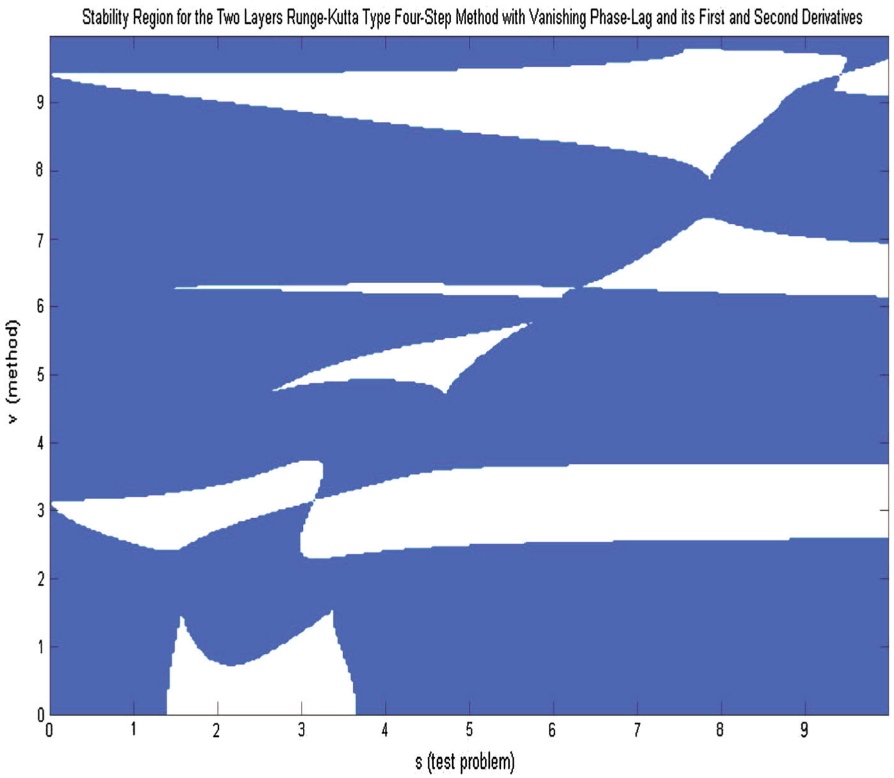


Fig. 9 $s - v$ plane of the new Runge–Kutta type obtained method

7 Numerical results

In order to study the effectiveness of the new obtained method, the numerical solution of the the radial time-independent Schrödinger equation (1) is used

Since the new proposed method is a frequency dependent method, it is necessary the value of parameter w to be defined. This definition is necessary in order the application of the new obtained method to the radial Schrödinger equation to be possible. Based on (1), the parameter w is given by (for the case $l = 0$):

$$w = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{39}$$

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

7.1 Woods–Saxon potential

In order to use the numerical solution of the time-independent Schrödinger equation (1), a definition of the potential is needed. For the present numerical tests we will use

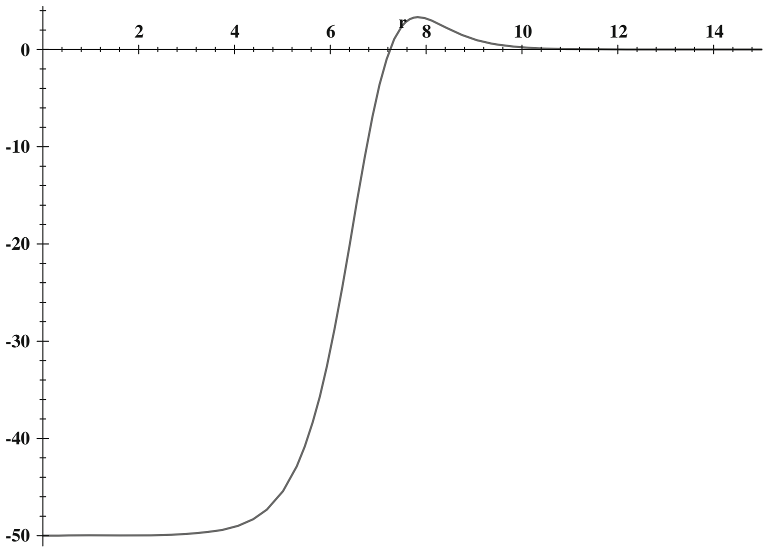


Fig. 10 The Woods–Saxon potential

the well known Woods–Saxon potential. We can write this potential as

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{40}$$

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. 10.

There are several methodologies in order to define the frequency w. One well known (see for details [105]), which is applied to some potentials, such as the Woods–Saxon potential, consists from the determination of some critical points, which are defined from the investigation of the appropriate potential.

For the purpose of obtaining our numerical results, it is appropriate to choose v as follows (see for details [1,79]):

$$w = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{41}$$

For example, in the point of the integration region $r = 6.5 - h$, the value of w is equal to: $\sqrt{-37.5+E}$. So, $v = w\,h = \sqrt{-37.5+E}\,h$. In the point of the integration region $r = 6.5 - 3\,h$, the value of w is equal to: $\sqrt{-50+E}$, etc.

7.2 Radial Schrödinger equation: the resonance problem

For the purpose of this application, let consider the numerical solution of the radial time independent Schrödinger equation (1) using as potential the known case of the Woods–Saxon potential (40). This is a problem with infinite interval of integration. This has to approximated by a finite one. We take the integration interval $r \in [0, 15]$ for the purposes of our numerical experiments. 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

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{42}$$

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

$$\begin{aligned} q(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{43}$$

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

$$\tan \delta_l = \frac{q(r_2)\, S(r_1) - q(r_1)\, S(r_2)}{q(r_1)\, C(r_1) - q(r_2)\, C(r_2)} \tag{44}$$

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, $j = 0, (1)3$ before starting a four-step method. From the initial condition, we obtain q_0. The values q_i, $i = 1(1)3$ are obtained by using high order Runge–Kutta–Nyström methods (see [111,112]). 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:

$$q(0) = 0, \; q(r) = \cos\left(\sqrt{E} r\right) \text{ for large } r. \tag{45}$$

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 [24] with minimal phase-lag, which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [80], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao [23] with minimal phase-lag, which is indicated as **Method MCR6**
- The classical form of the sixth algebraic order four-step method developed in Sect. 4, which is indicated as **Method NMCL**.[2]
- The four-step method of sixth algebraic order with vanished phase-lag and its first derivative in each level (obtained in [42]), which is indicated as **Method HYB-PLDEA**
- The four-step method of sixth algebraic order with vanished phase-lag and its first and second derivatives in each level (obtained in Sect. 4), which is indicated as **Method RKTPLDDEA**.

The numerically calculated eigenenergies are compared with reference values.[3] In Figs. 11 and 12, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{46}$$

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 presented a new methodology for the development of four-step hybrid type methods of sixth algebraic order with vanished phase-lag and its derivatives. This new methodology is based on the vanishing of the phase-lag and its derivatives in each level of the hybrid method. We have also investigated the influencing of the vanishing of the phase-lag and its first derivative on the efficiency of the above mentioned methods for the numerical solution of the radial Schrödinger equation and related problems. Based on the the above, a two-stage four-step sixth algebraic order methods with vanished phase-lag and its first derivative in each level was obtained. This new method 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 Sect. 4 with constant coefficients

[3] The reference values are computed using the well known two-step method of Chawla and Rao [23] with small step size for the integration

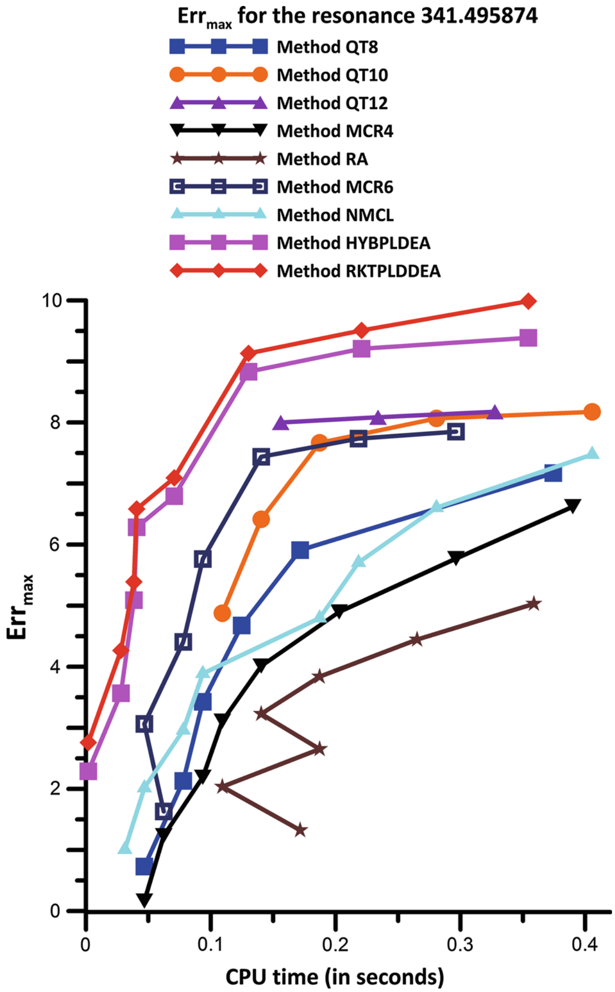


Fig. 11 Accuracy (digits) for several values of CPU Time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

1. The classical form of the sixth algebraic order four-step method developed in Sect. 4, which is indicated as **Method NMCL** is more efficient than the fourth algebraic order method of Chawla and Rao [24] with minimal phase-lag, which is indicated as **Method MCR4**. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [80], which is indicated as **Method MRA**.
2. The tenth algebraic order multistep 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 [24] with minimal phase-lag, 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 [19], which is indicated as

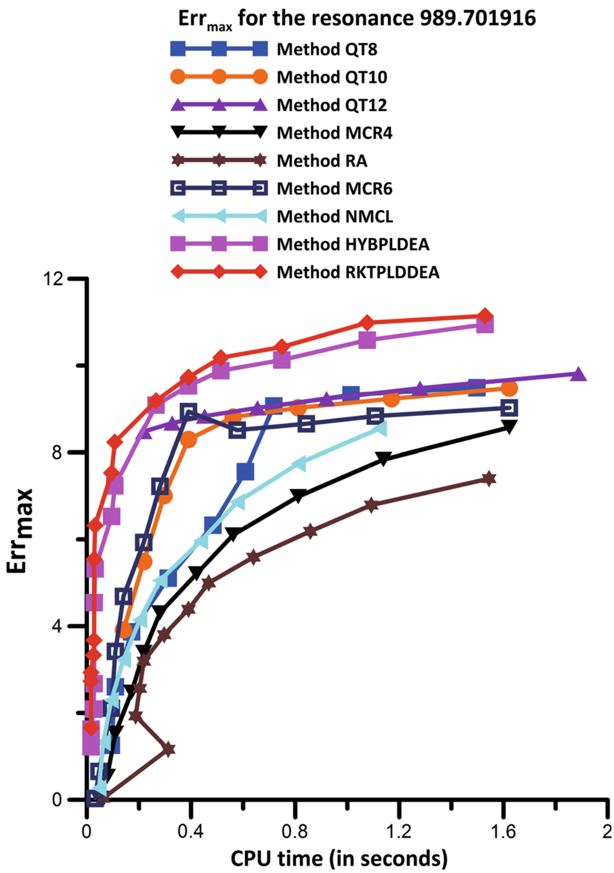


Fig. 12 Accuracy (digits) for several values of CPU Time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of accuracy (digits) indicates that for this value of CPU, accuracy (digits) is <0

Method QT8. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao [23] with minimal phase-lag, which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.

3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10**
4. The hybrid four-step two-stage sixth algebraic order method with vanished phase-lag and its first derivative in each level of the method (obtained in [42]), which is indicated as **Method HYBPLDEA** is the more efficient than all the above mentioned methods.
5. The four-step method of sixth algebraic order with vanished phase-lag and its first and second derivatives in each level (obtained in Sect. 4), which is indicated as **Method RKTPLDDEA**, 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).

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