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ORIGINAL PAPER

A new four-step Runge–Kutta type method with vanished phase-lag and its first, second and third derivatives for the numerical solution of the Schrödinger equation

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Abstract The construction of new four-step Runge–Kutta type method of sixth algebraic order with vanished phase-lag and its first, second and third derivatives is presented in this paper. We present a comparative error and stability analysis for the produced new method. In order to test the efficiency of the obtained method, an application to the resonance problem of the Schrödinger equation is described.

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

1 Introduction

An investigation of the approximate solution of the radial time independent Schrödinger equation is presented in this paper.

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The radial time independent Schrödinger equation can written as a boundary value problem with the following form:

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

There are many research areas, within the applied sciences, for which the mathematical models of their problems can be written with the above mentioned boundary value problem. Some research areas are:

1. astronomy,
2. astrophysics,
3. quantum mechanics,
4. quantum chemistry,
5. celestial mechanics,
6. electronics
7. physical chemistry
8. chemical physics etc

(see for example [1–4])

We mention the following definitions for the above model (1) :

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

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

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

The subject of this paper is the investigation of a two-stage four-step Runge–Kutta type (hybrid) sixth algebraic order method. We investigate how the the vanishing of the phase-lag and its first, second and third derivatives affects the efficiency of the obtained numerical scheme.

We mention that the the above procedure produces methods that are very effective on any problem with:

1. periodic or
2. oscillating solutions or
2. solution which contains the functions cos and sin or
4. solution that is a combination of the functions cos and sin.

In more details, in this paper we will define the coefficients of the proposed Runge–Kutta type (hybrid) two-stage four-step method in order to have:

1. the highest possible algebraic order

2. the phase-lag vanished
3. the first derivative of the phase-lag vanished as well
4. the second derivative of the phase-lag vanished as well
5. the third derivative of the phase-lag vanished as well

The computation of the phase-lag and its first, second and third derivatives will be done via the direct formula for the determination of the phase-lag for a $2\,m$-method (see [23] and [26]).

We will also study the effectiveness of the new obtained scheme via

1. the investigation of the local truncation error of the new produced method and other methods of the same form (comparative error analysis),
2. the investigation of the stability analysis of the new produced method and
3. the application of the new obtained 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 format of the paper is given below:

– A bibliography relevant on the subject is presented in Sect. 2.
– The phase-lag analysis of symmetric $2k$-methods is presented in Sect. 3.
– In Sect. 4, we obtain the new hybrid two-stage four-step method.
– The comparative error analysis is presented in Sect. 5.
– In Sect. 6, the stability properties of the new produced method are investigated.
– In Sect. 7, the numerical results are presented.
– Finally, in Sect. 8, remarks and conclusions are mentioned.

2 Bibliography relevant on the subject of the paper

The last decades much research has been done on the development of computationally efficient and reliable algorithms for the numerical solution of the one-dimensional Schrödinger equation and related problems (see for example [5–93]). 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 [5–9].
– In [10–15] 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 [20–41].
– Symplectic integrators are investigated in [42–67].
– Exponentially and trigonometrically multistep methods have been produced in [68–87].
– Nonlinear methods have been studied in [34] and [88]
– Review papers have been presented in [89–93]
– Special issues and Symposia in International Conferences have been developed on this subject (see [94–98])

3 Theory on the analysis of phase-lag of symmetric multistep methods

Let us consider the approximate solution of the initial value problem

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

For the above solution let us also 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 $h = |x_{i+1} - x_i|$, $i = 0(1)m - 1$.

We consider also the case in which the method is symmetric, i.e. the case:

$$a_i = a_{m-i}\,,\; b_i = b_{m-i}\,,\; i = 0(1)\frac{m}{2}. \tag{4}$$

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

$$p'' = -w^2\, p \tag{5}$$

a difference equation of the form

$$A_m(v)\, q_{n+m} + \cdots + A_1(v)\, q_{n+1} + A_0(v)\, q_n + A_1(v)\, q_{n-1} + \cdots + A_m(v)\, q_{n-m} = 0 \tag{6}$$

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

We call characteristic equation (which is associated with (6)) the equation given by:

$$A_m(v)\, \lambda^m + \cdots + A_1(v)\, \lambda + A_0(v) + A_1(v)\, \lambda^{-1} + \cdots + A_m(v)\, \lambda^{-m} = 0 \tag{7}$$

Theorem 1 [23] *and* [26] *The symmetric* $2m$*-step method with characteristic equation given by (7) has phase-lag order* q *and phase-lag constant* c *given by:*

$$-c\, v^{q+2} + O\left(v^{q+4}\right) = \frac{2\, A_m\,(v)\, \cos\,(m\, v) + \cdots + 2\, A_j\,(v)\, \cos\,(j\, v) + \cdots + A_0\,(v)}{2\, m^2\, A_m\,(v) + \cdots + 2\, j^2\, A_j\,(v) + \cdots + 2\, A_1\,(v)} \tag{8}$$

Remark 1 The formula (8) is a direct method for the calculation of the phase-lag of any symmetric $2m$-step method.

4 Development of the new method

We consider the family of Runge–Kutta type symmetric four-step methods for the approximate solution of problems of the form $p'' = f\,(x, p)$:

$$\hat{p}_{n+2} \;=\; 2\, p_{n+1} - 2\, p_n + 2\, p_{n-1} - p_{n-2} + \frac{h^2}{6}\Big(7\, f_{n+1} - 2\, f_n + 7\, y_{n-1}\Big)$$

$$
\begin{aligned}
& p_{n+2} - 2\, p_{n+1} + a_2\, p_n - 2\, p_{n-1} + p_{n-2} \\
& \quad = h^2 \left[b_0 \left(\hat{f}_{n+2} + f_{n-2} \right) + b_1 \, (f_{n+1} + f_{n-1}) + b_2\, f_n \right]
\end{aligned} \tag{9}
$$

Notations for the above mentioned general family of methods :

- the coefficient a_2, b_0, b_1, b_2 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
- $f_n = f\,(x_n, q_n)$
- $x_n = x_0 + n\,h$ and
- x_0 is the initial value point.

If we apply the above mentioned family of methods (9) to the scalar test Eq. (5) will lead to the difference Eq. (6) with $m = 2$ and $A_j\,(v)\,,\ \ j = 0,\ 1,\ 2$ given by:

$$
\begin{aligned}
& A_2\,(v) \;=\; 1,\; A_1\,(v) \;=\; -2 + v^2 \left(b_0 \left(2 - \frac{7}{6}\,v^2 \right) + b_1 \right) \\
& A_0\,(v) = a_2 - 2\, b_0 v^2 + \frac{1}{3}\, v^4 b_0 + v^2 b_2
\end{aligned} \tag{10}
$$

Requiring the above method to have the phase-lag and its first, second and third derivatives vanished the following system of equations is obtained (using the formulae (8) (for $m = 2$) and (10)):

$$
\text{Phase-Lag} \;=\; -\frac{T_0}{-12 - 12\, b_0 v^2 + 7\, v^4 b_0 - 6\, v^2 b_1} = 0 \tag{11}
$$

where

$$
\begin{aligned}
T_0 \;=\; & 12\; (\cos(v))^2 - 6 - 12\; \cos(v) + 12\; \cos(v)\; b_0 v^2 \\
& -7\; \cos(v)\, v^4\, b_0 + 6\; \cos(v)\, v^2\, b_1 + 3\, a_2 - 6\, b_0 v^2 + v^4\, b_0 + 3\, v^2\, b_2
\end{aligned}
$$

$$
\text{First Derivative of the Phase-Lag} \;=\; \frac{T_1}{\left(-12 - 12\, b_0 v^2 + 7\, v^4 b_0 - 6\, v^2 b_1\right)^2} = 0 \tag{12}
$$

where

$$
\begin{aligned}
T_1 = & -144\; \sin(v)\; b_0 v^4\, b_1 + 84\; \sin(v)\, v^6\, b_0\, b_1 \\
& -288\; \cos(v) \sin(v)\; b_0 v^2 + 168\; \cos(v) \sin(v)\, v^4\, b_0 \\
& -144\; \cos(v) \sin(v)\, v^2\, b_1 + 144\; \sin(v) - 288\; \cos(v) \sin(v) \\
& +288\; \cos(v)\, v\, b_1 - 672\; \cos(v)\, v^3\, b_0 + 576\; \cos(v)\; b_0\, v \\
& +168\; \sin(v)\; {b_0}^2 v^6 - 49\; \sin(v)\; v^8\, {b_0}^2 - 144\; \sin(v)\; {b_0}^2\, v^4
\end{aligned}
$$

$$+336\,(\cos(v))^2\,b_0 v^3 - 288\,v\,(\cos(v))^2\,b_0$$
$$+84\,a_2\,b_0\,v^3 - 144\,v\,(\cos(v))^2\,b_1 - 36\,v\,a_2\,b_1 - 72\,v\,a_2\,b_0$$
$$+42\,v^5\,b_2\,b_0 + 12\,v^5\,b_0\,b_1 - 36\,\sin(v)\,v^4\,{b_1}^2 - 120\,v^3\,b_0 + 72\,v\,b_2$$
$$+72\,v\,b_1 - 60\,{b_0}^2\,v^5$$

$$\text{Second Derivative of the Phase-Lag} = \frac{T_2}{\left(-12-12\,b_0 v^2+7\,v^4\,b_0-6\,v^2\,b_1\right)^3} = 0 \tag{13}$$

where

$$T_2 = -3456 - 16128\,\sin(v)\,b_0 v^3 - 2592\,v^2\,(\cos(v))^2\,{b_1}^2$$
$$+3456\,(\cos(v))^2\,b_0 + 24192\,\cos(v)\sin(v)\,{b_0}^2 v^5 - 9408\,\cos(v)\sin(v)\,{b_0}^2 v^7$$
$$-10368\,(\cos(v))^2\,{b_0}^2 v^2 - 3024\,\cos(v)\,{b_0}^3 v^8 + 1728\,\cos(v)\,{b_0}^3 v^6$$
$$+432\,\cos(v)\,v^4\,{b_1}^2 + 13824\,\sin(v)\,{b_0}^2 v^3$$
$$+1764\,\cos(v)\,{b_0}^3 v^{10} - 24192\,\sin(v)\,{b_0}^2 v^5$$
$$+9408\,\sin(v)\,v^7\,{b_0}^2 - 343\,\cos(v)\,v^{12}\,{b_0}^3$$
$$+216\,\cos(v)\,v^6\,{b_1}^3 + 3456\,\sin(v)\,v^3\,{b_1}^2$$
$$+6912\,(\cos(v))^2\,v^2\,b_1 + 25056\,(\cos(v))^2\,{b_0}^2 v^4 - 19824\,(\cos(v))^2\,v^6\,{b_0}^2$$
$$+2352\,(\cos(v))^2\,v^8\,{b_0}^2 + 1728\,(\cos(v))^2\,v^4\,{b_1}^2 - 864\,b_1 + 4536\,a_2\,{b_0}^2 v^4$$
$$-2592\,a_2\,{b_0}^2 v^2 + 5184\,\cos(v)\,v^2\,{b_1}^2 + 20736\,\cos(v)\,{b_0}^2 v^2$$
$$-34560\,\cos(v)\,{b_0}^2 v^4 + 216\,v^6\,{b_0}^2\,b_1 - 252\,{b_0}^2 v^8\,b_1 - 648\,v^2 a_2\,{b_1}^2$$
$$-2940\,v^6 a_2\,{b_0}^2 - 252\,b_2 v^6\,b_0\,b_1 - 2592\,a_2\,b_0 v^2\,b_1$$
$$-882\,b_2 v^8\,{b_0}^2 - 72\,b_0 v^6\,{b_1}^2 - 504\,b_2 v^6\,{b_0}^2 - 3024\,a_2\,b_0 v^2$$
$$+6912\,\sin(v)\,v\,b_1 + 2016\,v^6\,b_0\,b_1 + 13824\,\sin(v)\,b_0 v + 1260\,v^8\,{b_0}^3$$
$$+720\,v^6\,{b_0}^3 + 1728\,(\cos(v))^2\,b_1 - 3456\,\cos(v)\,b_1$$
$$-3456\,\cos(v)\sin(v)\,{b_1}^2 v^3 - 6912\,v\cos(v)\sin(v)\,b_1$$
$$-13824\,\cos(v)\sin(v)\,{b_0}^2 v^3 + 16128\,\cos(v)\sin(v)\,b_0 v^3$$
$$-13824\,v\cos(v)\sin(v)\,b_0 + 20736\,\cos(v)\,b_0 v^2\,b_1 - 16416\,\cos(v)\,v^4\,b_0\,b_1$$
$$+1296\,\cos(v)\,b_0 v^6\,{b_1}^2 + 13824\,\sin(v)\,b_0 v^3\,b_1 + 2268\,v^4 a_2\,b_0\,b_1$$
$$-1008\,\cos(v)\,v^6\,b_0\,b_1 + 2592\,\cos(v)\,{b_0}^2 v^6\,b_1 - 3024\,\cos(v)\,{b_0}^2 v^8\,b_1$$
$$+882\,\cos(v)\,v^{10}\,{b_0}^2\,b_1 - 756\,\cos(v)\,v^8\,b_0\,{b_1}^2 - 12096\,\sin(v)\,v^5\,b_0\,b_1$$
$$+15984\,(\cos(v))^2\,v^4\,b_0\,b_1 - 4032\,(\cos(v))^2\,v^6\,b_0\,b_1$$
$$-10368\,(\cos(v))^2\,b_0 v^2\,b_1 - 6048\,v^4\,b_2\,b_0 + 2592\,v^2\,b_2\,b_0$$
$$-8424\,v^4\,b_0\,b_1 + 2592\,b_0 v^2\,b_1 + 1296\,v^2\,b_2\,b_1 + 1296\,v^2\,{b_1}^2$$
$$+864\,a_2\,b_0 + 432\,a_2\,b_1 - 1296\,{b_0}^2 v^4 + 8232\,v^6\,{b_0}^2 - 6912\,\cos(v)\,b_0$$
$$-864\,v^4\,{b_1}^2 - 1176\,v^8\,{b_0}^2 - 2592\,b_0 v^2 + 4032\,v^4\,b_0 - 3456\,v^2\,b_1$$
$$+588\,\cos(v)\,{b_0}^2 v^8 + 21504\,\cos(v)\,{b_0}^2 v^6 - 8064\,(\cos(v))^2\,v^4\,b_0$$

$$
\begin{aligned}
&+1728\ (\cos(v))^2\ b_0 v^2 + 1008\ \cos(v)\, v^4\, b_0 \\
&+22464\ \cos(v)\ b_0 v^2 - 864\ \cos(v)\, v^2\, b_1 \\
&-13824\ \cos(v)\sin(v)\ b_0 v^3\, b_1 + 12096\ \cos(v)\sin(v)\ b_0 v^5\, b_1 - 864\, b_2 \\
&-1728\ \cos(v) + 6912\ (\cos(v))^2
\end{aligned}
$$

$$
\text{Third Derivative of the Phase-Lag} = -\frac{T_3}{\left(-12 - 12\ b_0 v^2 + 7\, v^4\, b_0 - 6\, v^2\, b_1\right)^4} = 0 \tag{14}
$$

where

$$
\begin{aligned}
T_3 = {}& 919296\ \cos(v)\sin(v)\, v^6\, {b_0}^2 - 169344\ \cos(v)\sin(v)\ {b_0}^2 v^8 \\
&-787968\ \cos(v)\sin(v)\ {b_0}^2 v^4 - 1244160\ \cos(v)\ b_0 v^3\, b_1 \\
&-435456\ \cos(v)\, v^5\, b_0\, b_1 + 829440\ \cos(v)\ b_0 v - 290304\ \cos(v)\, v^3\, b_0 \\
&+124416\ \cos(v)\, v\, b_1 - 248832\ \cos(v)\sin(v)\ b_0 \\
&-24192\ \sin(v)\ b_0 v^4 - 124416\, v^3\, b_2\, {b_0}^2 + 124416\ \cos(v)\, v^3\, {b_1}^2 \\
&-2985984\ \cos(v)\ {b_0}^2 v^3 + 2515968\ \cos(v)\ {b_0}^2 v^5 + 338688\ \cos(v)\, v^7\, {b_0}^2 \\
&-124416\ {b_0}^2 v^3\, b_1 - 31104\, v^3\, b_2\, {b_1}^2 - 124416\, b_0 v^3\, {b_1}^2 \\
&+290304\, v^5\, b_2\, {b_0}^2 + 331776\, b_0 v^5\, {b_1}^2 + 663552\ {b_0}^2 v^5\, b_1 \\
&+62208\, v\, b_2\, b_1 + 124416\, v\, b_2\, b_0 - 423360\, v^7\, b_2\, {b_0}^2 + 124416\, b_0 v\, b_1 \\
&-93312\ \sin(v)\, v^4\, {b_1}^3 + 254016\, v^7 a_2\, {b_0}^3 - 123480\, v^9 a_2\, {b_0}^3 \\
&-362880\, v^3\, b_2\, b_0 - 883008\ {b_0}^2 v^7\, b_1 - 20736\ \cos(v)\sin(v)\, v^6\, {b_1}^3 \\
&-1907712\ \cos(v)\sin(v)\, v^6\, {b_0}^3 + 1899072\ \cos(v)\sin(v)\, v^8\, {b_0}^3 \\
&-663264\ \cos(v)\sin(v)\ {b_0}^3 v^{10} \\
&-21168\ \sin(v)\, v^{10}\, {b_0}^2\, b_1 + 18144\ \sin(v)\, v^8\, b_0\, {b_1}^2 + 72576\ \sin(v)\ {b_0}^3 v^{10}\, b_1 \\
&-41472\ \sin(v)\ {b_0}^3 v^8\, b_1 - 10368\ \sin(v)\ b_0 v^8\, {b_1}^3 + 36288\ \sin(v)\ {b_0}^2 v^{10}\, {b_1}^2 \\
&-42336\ \sin(v)\ {b_0}^3 v^{12}\, b_1 + 870912\ (\cos(v))^2\, v^5\, b_0\, b_1 \\
&-124416\ (\cos(v))^2\ b_0 v^3\, b_1 + 290304\ (\cos(v))^2\ {b_1}^2 v^7\, b_0 \\
&-423360\ (\cos(v))^2\ b_1 v^9\, {b_0}^2 - 663552\ (\cos(v))^2\ b_0 v^5\, {b_1}^2 \\
&+497664\ \cos(v)\sin(v)\ {b_0}^2 v^2 + 20736\ \sin(v)\, v^2\, b_1 - 338688\ \sin(v)\ {b_0}^2 v^6 \\
&+124416\ \cos(v)\sin(v)\ {b_1}^2 v^2 + 290304\ \sin(v)\ {b_0}^2 v^4 \\
&+580608\ (\cos(v))^2\ b_0 v^3 - 248832\, v\, (\cos(v))^2\ b_1 \\
&-787968\, v\, (\cos(v))^2\ b_0 - 72576\, v\, a_2\, b_0 \\
&-435456\, v^5\, b_0\, b_1 + 82944\, b_0 v^3\, b_1 - 995328\ \cos(v)\ {b_0}^3 v^3 \\
&+2571264\ \cos(v)\ {b_0}^3 v^5 + 373248\ \cos(v)\sin(v)\ b_0 v^2 \\
&+290304\ \cos(v)\sin(v)\, v^4\, b_0 \\
&-248832\ \cos(v)\sin(v)\, v^2\, b_1 + 145152\ \sin(v)\ b_0 v^4\, b_1 - 829440\ \sin(v)\ b_0 v^2
\end{aligned}
$$

$$
\begin{aligned}
&-31104\,\sin(v)\,{b_0}^2 v^8 {b_1}^2-124416\,\cos(v)\,v^3\,{b_1}^3+145152\,v^5\,b_2\,b_1\,b_0\\
&-124416\,v^3\,b_2\,b_0\,b_1-145152\,{b_1}^2 v^7\,b_0\\
&+211680\,b_1 v^9\,{b_0}^2-1536192\,\sin(v)\,{b_0}^3 v^8+451584\,\sin(v)\,{b_0}^3 v^{10}\\
&+8232\,\sin(v)\,{b_0}^3 v^{12}-1658880\,(\cos(v))^2\,{b_0}^3 v^5\\
&+995328\,\cos(v)\,{b_0}^2 v-497664\,\sin(v)\,{b_0}^2 v^2\\
&+1411200\,\cos(v)\,{b_0}^3 v^9+197568\,(\cos(v))^2\,{b_0}^3 v^{11}-2612736\,\cos(v)\,{b_0}^3 v^7\\
&+31104\,{b_1}^3 v^5-98784\,{b_0}^3 v^{11}+32928\,\cos(v)\sin(v)\,v^{12}\,{b_0}^3\\
&-124416\,\cos(v)\sin(v)\,v^4\,{b_1}^2+211680\,\cos(v)\,v^9\,{b_0}^2\,b_1\\
&-145152\,\cos(v)\,v^7\,b_0\,{b_1}^2+6048\,\sin(v)\,v^{10}\,b_0\,{b_1}^3\\
&-10584\,\sin(v)\,v^{12}\,{b_0}^2\,{b_1}^2+8232\,\sin(v)\,v^{14}\,{b_0}^3\,b_1\\
&+1669248\,(\cos(v))^2\,{b_0}^2 v^7\,b_1-1907712\,(\cos(v))^2\,{b_0}^2 v^5\,b_1\\
&+746496\,\cos(v)\sin(v)\,{b_0}^3 v^4+93312\,v^4\cos(v)\sin(v)\,{b_1}^3\\
&+373248\,v^3\,(\cos(v))^2\,b_0\,{b_1}^2\\
&+746496\,v^3\,(\cos(v))^2\,{b_0}^2\,b_1-497664\,v\,(\cos(v))^2\,b_0\,b_1\\
&-746496\,\cos(v)\,v^3\,{b_1}^2\,b_0-290304\,v^5 a_2\,{b_0}^3+15552\,v^3 a_2\,{b_1}^3\\
&+1700352\,\sin(v)\,{b_0}^3 v^6-746496\,\sin(v)\,{b_0}^3 v^4+248832\,\cos(v)\,v\,{b_1}^2\\
&-124416\,\sin(v)\,v^2\,{b_1}^2-1596672\,\cos(v)\,{b_0}^2 v^7\,b_1+767232\,\cos(v)\,b_0 v^5\,{b_1}^2\\
&-1119744\,\sin(v)\,{b_0}^2 v^4\,b_1-1492992\,\cos(v)\,{b_0}^2 v^3\,b_1\\
&-559872\,\sin(v)\,v^4\,{b_1}^2\,b_0-124416\,v a_2\,b_0\,b_1\\
&-21168\,b_2\,b_1 v^9\,{b_0}^2+20736\,\sin(v)\\
&+746496\,v^3\,(\cos(v))^2\,{b_0}^2+217728\,a_2\,b_0 v^3\,b_1-290304\,v^5 a_2\,{b_0}^2\,b_1\\
&+127008\,v^7 a_2\,{b_0}^2\,b_1-72576\,v^5 a_2\,b_0\,{b_1}^2+186624\,v^3 a_2\,{b_0}^2\,b_1\\
&+93312\,v^3 a_2\,b_0\,{b_1}^2-42336\,b_2\,{b_0}^3 v^9-24696\,v^{11}\,b_2\,{b_0}^3\\
&+124416\,v^3 a_2\,{b_0}^3-7056\,{b_0}^3 v^{11}\,b_1-6048\,{b_0}^2 v^9\,{b_1}^2\\
&-31104\,v a_2\,{b_1}^2-124416\,v a_2\,{b_0}^2-677376\,(\cos(v))^2\,{b_0}^2 v^7\\
&+48384\,(\cos(v))^2\,{b_0}^2 v^5+497664\,v^3\,(\cos(v))^2\,{b_0}^3-124416\,v\,(\cos(v))^2\,{b_1}^2\\
&-497664\,v\,(\cos(v))^2\,{b_0}^2-124416\,\cos(v)\sin(v)\,b_1-42336\,\sin(v)\,{b_0}^4 v^{12}\\
&-2401\,\sin(v)\,v^{16}\,{b_0}^4-98784\,\cos(v)\,v^{11}\,{b_0}^3\\
&-1296\,\sin(v)\,v^8\,{b_1}^4+31104\,\cos(v)\,v^5\,{b_1}^3\\
&-248832\,v^3\,(\cos(v))^2\,{b_1}^2+62208\,v^3\,(\cos(v))^2\,{b_1}^3-338688\,{b_0}^3 v^7\\
&+599760\,{b_0}^3 v^9+248832\,{b_0}^3 v^5+62208\,v\,{b_1}^2+124416\,v^3\,{b_1}^2\\
&+35280\,{b_0}^4 v^{11}-290304\,v^3\,b_0+124416\,v\,b_1-31104\,v^3\,{b_1}^3+60480\,{b_0}^4 v^9\\
&+124416\,\sin(v)\,b_1+393984\,{b_0}^2 v^3-266112\,{b_0}^2 v^5+338688\,v^7\,{b_0}^2\\
&+352512\,b_0 v-165888\,\cos(v)\sin(v)+248832\,\sin(v)\,b_0+18144\,{b_0}^3 v^9\,b_1\\
&+1119744\,\cos(v)\sin(v)\,{b_0}^2 v^4\,b_1+559872\,\cos(v)\sin(v)\,b_0 v^4\,{b_1}^2\\
&-559872\,\cos(v)\sin(v)\,b_0 v^6\,{b_1}^2+290304\,\cos(v)\sin(v)\,v^6\,b_0\,b_1\\
&+1094688\,\cos(v)\sin(v)\,{b_0}^2 v^8\,b_1-84672\,\cos(v)\sin(v)\,v^{10}\,{b_0}^2\,b_1
\end{aligned}
$$

$$+72576\,\cos(v)\sin(v)\,v^8\,b_0\,b_1{}^2 - 1990656\,\cos(v)\sin(v)\,v^6\,b_0{}^2\,b_1$$
$$-642816\,\cos(v)\sin(v)\,b_0 v^4\,b_1 + 497664\,\cos(v)\sin(v)\,b_0 v^2\,b_1$$
$$-497664\,\sin(v)\,b_0 v^2\,b_1 + 995328\,\cos(v)\,b_0 v\,b_1$$
$$+1679616\,\sin(v)\,b_0{}^2 v^6\,b_1 - 731808\,\sin(v)\,b_0{}^2 v^8\,b_1$$
$$+404352\,\sin(v)\,b_0 v^6\,b_1{}^2 + 2695680\,\cos(v)\,b_0{}^2 v^5\,b_1 - 423360\,v^5 a_2\,b_0{}^2$$
$$+435456\,v^3 a_2\,b_0{}^2 + 2177280\,(\cos(v))^2\,b_0{}^3 v^7 - 1340640\,(\cos(v))^2\,b_0{}^3 v^9$$
$$-62208\,(\cos(v))^2\,b_1{}^3 v^5 - 5184\,\sin(v)\,v^6\,b_1{}^3 + 16464\,\sin(v)\,b_0{}^4 v^{14}$$
$$-20736\,\sin(v)\,b_0{}^4 v^8 + 48384\,\sin(v)\,b_0{}^4 v^{10}$$

The solution of the above system of Eqs. (11)–(14) gives the following coefficients of the new obtained method:

$$a_2 = \frac{T_4}{D_0},\; b_0 = \frac{T_5}{D_1},\; b_1 = \frac{T_6}{v^3\,D_0},\; b_2 = \frac{T_7}{v^3\,D_0} \tag{15}$$

where:

$$\begin{aligned}
T_4 = {} & 432 + 3060\,\cos(v)\,v^2 - 3756\,v\sin(v) \\
& -394\,\cos(v)\,v^4 + 3788\,v^3\sin(v) - 98\,\sin(v)\,v^5 \\
& +252\,\cos(5\,v) + 144\,\cos(2\,v) - 4752\,v^2 + 3216\,v^2\cos(2\,v) \\
& -785\,v^3\sin(3\,v) - 1292\,v^3\sin(2\,v) + 24\,v^4\cos(2\,v) \\
& +2073\,v\sin(3\,v) - 172\,v^4\cos(3\,v) - 2472\,v\sin(2\,v) \\
& +16\,v^5\sin(2\,v) + 96\,v^2\cos(4\,v) + 7\,v^5\sin(5\,v) \\
& -91\,v^5\sin(3\,v) + 35\,v^3\sin(5\,v) - 147\,v\sin(5\,v) \\
& +10\,v^4\cos(4\,v) + 14\,v^4\cos(5\,v) + 189\,v^2\cos(5\,v) \\
& +516\,v\sin(4\,v) + 70\,v^3\sin(4\,v) + 4\,v^5\sin(4\,v) \\
& -2385\,v^2\cos(3\,v) - 144\,\cos(v) + 62\,v^4 - 576\,\cos(4\,v) \\
& -108\,\cos(3\,v) \\
T_5 = {} & -150\,\cos(v)\,v^2 + 6\,v^2\cos(3\,v) + 36\,\cos(v) \\
& -36\,\cos(3\,v) + 60\,v^2 - 12\,v^3\sin(3\,v) - 36\,v^3\sin(v) \\
& -36 + 36\,\cos(2\,v) - 36\,v\sin(3\,v) + 108\,v\sin(v) + 12\,v^2\cos(2\,v) \\
T_6 = {} & 1368\,v - 3636\,v^3 + 497\,v^5 - 308\,\cos(v)\,v^5 + 972\,\cos(v)\,v^3 \\
& -720\,\cos(v)\,v + 2916\,\sin(v)\,v^2 - 588\,v^3\cos(4\,v) \\
& -804\,\sin(v)\,v^4 - 648\,\sin(v) + 252\,v^5\cos(2\,v) \\
& -360\,v\cos(4\,v) - 108\,v^2\sin(3\,v) + 56\,v^6\sin(2\,v) \\
& -132\,v^4\sin(3\,v) - 77\,v^5\cos(4\,v) + 2208\,v^3\cos(2\,v) \\
& -1008\,v\cos(2\,v) - 2064\,v^2\sin(2\,v) + 432\,\sin(2\,v) \\
& -120\,v^2\sin(4\,v) + 720\,v\cos(3\,v) - 28\,v^5\cos(3\,v)
\end{aligned}$$

$$
\begin{aligned}
&+180\, v^3 \cos(3\,v) + 67\, v^4 \sin(4\,v) + 490\, v^4 \sin(2\,v)\\
&+14\, v^6 \sin(4\,v) - 216\, \sin(4\,v) + 216\, \sin(3\,v)\\
T_7 = &-72\, v + 3372\, v^3 - 148\, v^5 - 168\, v^2 \sin(5\,v) - 28\, v^4 \sin(5\,v)\\
&-7\, v^6 \sin(5\,v) + 504\, v \cos(5\,v) + 84\, v^3 \cos(5\,v)\\
&-38\, \cos(v)\, v^5 + 648\, \cos(v)\, v^3 - 1080\, \cos(v)\, v\\
&+21\, v^5 \cos(5\,v) + 1344\, \sin(v)\, v^2 + 98\, v^6 \sin(v)\\
&+228\, v^3 \cos(4\,v) - 3988\, \sin(v)\, v^4 + 648\, \sin(v)\\
&-48\, v^5 \cos(2\,v) - 792\, v \cos(4\,v) + 1464\, v^2 \sin(3\,v)\\
&-32\, v^6 \sin(2\,v) + 832\, v^4 \sin(3\,v) + 4\, v^5 \cos(4\,v)\\
&-4752\, v^3 \cos(2\,v) + 864\, v \cos(2\,v) - 1944\, v^2 \sin(2\,v)\\
&+91\, v^6 \sin(3\,v) - 432\, \sin(2\,v) + 540\, v^2 \sin(4\,v)\\
&+576\, v \cos(3\,v) + 113\, v^5 \cos(3\,v) + 1860\, v^3 \cos(3\,v)\\
&-108\, v^4 \sin(4\,v) + 1128\, v^4 \sin(2\,v) - 8\, v^6 \sin(4\,v)\\
&+216\, \sin(4\,v) - 216\, \sin(3\,v)
\end{aligned}
$$

$$
\begin{aligned}
D_0 = &-72 - 7\, v^4 \cos(3\,v) - 77\, \cos(v)\, v^4 - 77\, v^3 \sin(3\,v)\\
&+315\, v^2 \cos(3\,v) - 252\, \cos(3\,v) + 48\, v \sin(2\,v)\\
&-8\, v^3 \sin(2\,v) + 525\, v \sin(3\,v) + 48\, v^2 \cos(2\,v)\\
&+72\, \cos(2\,v) - 245\, v^3 \sin(v) - 651\, \cos(v)\, v^2\\
&-2247\, v \sin(v) + 252\, \cos(v)\\
D_1 = &\;56\, v^5 \sin(2\,v) - 84\, v^3 \sin(2\,v) - 24\, \cos(v)\, v^4\\
&+35\, v^6 + 7\, v^6 \cos(2\,v) + 8\, \sin(v)\, v^5 + 315\, v^4\\
&-147\, v^4 \cos(2\,v) + 24\, v^3 \sin(v)
\end{aligned}
$$

For some values of $|w|$ the formulae given by (15) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
a_2 = &\;2 + \frac{751}{302400}\, v^8 - \frac{1529}{9072000}\, v^{10}\\
&+ \frac{1414837}{125737920000}\, v^{12} - \frac{70831729}{49037788800000}\, v^{14}\\
&- \frac{91935504629}{494300911104000000}\, v^{16} - \frac{1035153325523}{420155774438400000000}\, v^{18} + \cdots\\
b_0 = &\;\frac{3}{40} - \frac{751}{75600}\, v^2 + \frac{337}{1134000}\, v^4\\
&+ \frac{271429}{15717240000}\, v^6 + \frac{874647199}{196151155200000}\, v^8\\
&+ \frac{8713539283}{15446903472000000}\, v^{10} + \frac{1889753409197}{420155774438400000}\, v^{12}
\end{aligned}
$$

$$
-\frac{151273220882233}{829828662304561920000000} v^{14} - \frac{4683107434641043 67}{612796550624907264000000000} v^{16}
$$

$$
-\frac{2423453940641512667722 69}{15006223211357791571558400000000000} v^{18} + \cdots
$$

$$
b_1 = \frac{13}{15} + \frac{751}{18900} v^2 - \frac{5213}{324000} v^4
- \frac{269117}{1964655000} v^6 - \frac{30404441}{1114495200000} v^8
+ \frac{11251277021}{2808527904000000} v^{10} + \frac{25084215673501}{21007788721920000000} v^{12}
+ \frac{1545501689550498247}{829828662304561920000000} v^{14} + \frac{598699993342795769}{311185748364210720000000000} v^{16}
+ \frac{3469065660246423295009 99}{37515558028394478928896000000000000} v^{18} + \cdots
$$

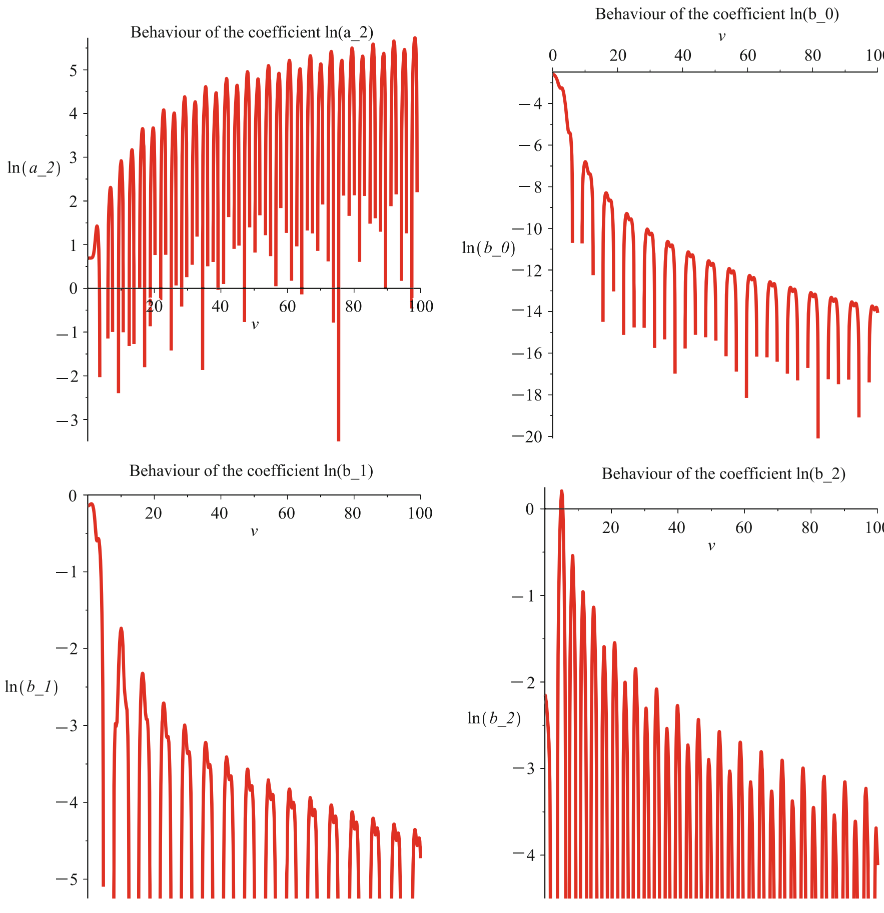

Fig. 1 Behavior of the coefficients of the new proposed method given by (15) for several values of $v = wh$

$$
\begin{aligned}
b_2 = {} & \frac{7}{60} - \frac{751}{12600}\, v^2 + \frac{11939}{378000}\, v^4 \\
& - \frac{25394981}{2619540000}\, v^6 + \frac{1634664971}{3632428800000}\, v^8 \\
& - \frac{188369586949}{5148967824000000}\, v^{10} + \frac{52861588469201}{2100778872192000000}\, v^{12} \\
& + \frac{152908220668984553}{345761942626900800000000}\, v^{14} + \frac{134285140595563303 67}{1896751228124712960000000 00}\, v^{16} \\
& + \frac{17782272829435032786724 91}{2501037201892965261926400000000 00}\, v^{18} + \cdots
\end{aligned} \tag{16}
$$

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

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

$$
LTE_{OptMeth} = \frac{751\, h^8}{302400} \left(p_n^{(8)} + 4\, w^2\, p_n^{(6)} + 6\, w^4\, p_n^{(4)} + 4\, w^6\, p_n^{(2)} + w^8\, p_n + \right) + O\left(h^{10}\right) \tag{17}
$$

5 Comparative error analysis

We will investigate the following methods:

5.1 Classical method (i.e. the method (9) with constant coefficients)

$$
LTE_{CL} = -\frac{751\, h^8}{302400}\, p_n^{(8)} + O\left(h^{10}\right) \tag{18}
$$

5.2 The method with vanished phase-lag and its first and second derivatives developed in [39]

$$
LTE_{MethI} = -\frac{751\, h^8}{302400} \left(p_n^{(8)} + 3\, w^2\, p_n^{(6)} + 3\, w^4\, p_n^{(4)} + w^6\, p_n^{(2)} \right) + O\left(h^{10}\right) \tag{19}
$$

5.3 The new proposed method with vanished phase-lag and its first, second and third derivatives developed in Section 4

$$
LTE_{MethII} = \frac{751\, h^8}{302400} \left(p_n^{(8)} + 4\, w^2\, p_n^{(6)} + 6\, w^4\, p_n^{(4)} + 4\, w^6\, p_n^{(2)} + w^8\, p_n + \right) + O\left(h^{10}\right) \tag{20}
$$

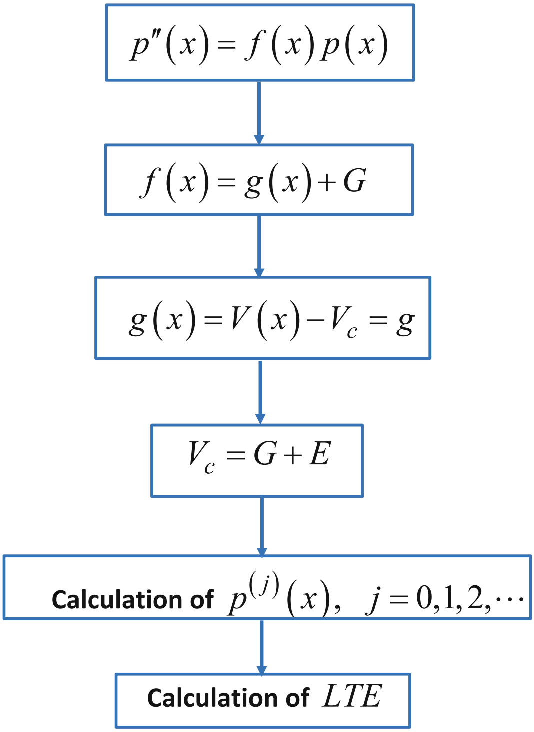

Fig. 2 Flowchart for the error analysis

The error analysis is based on Flowchart mentioned in the Fig. 2.
Using the procedure mentioned above and the formulae:

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

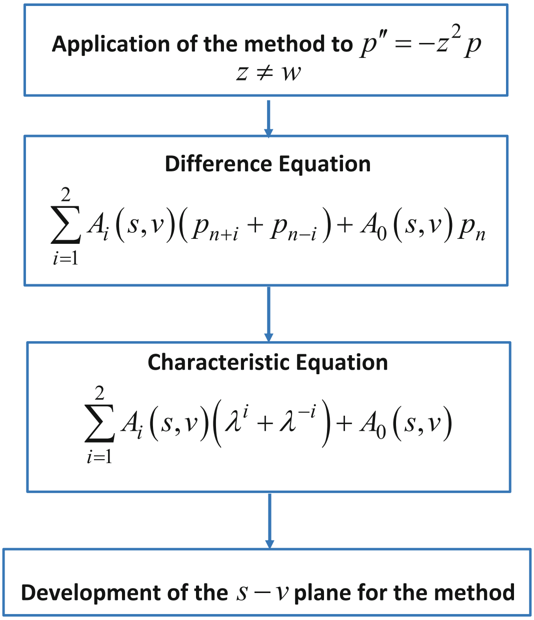

Fig. 3 Flowchart for the stability analysis

$$
\begin{aligned}
&+ (V(x) - V_c + G)^2 \left(\frac{d^2}{dx^2} p(x)\right) \\
&\cdots \\
p_n^{(8)} = &\left(\frac{d^6}{dx^6} g(x)\right) p(x) + 6 \left(\frac{d^5}{dx^5} g(x)\right) \frac{d}{dx} p(x) \\
&+16\ (g(x) + G)\, p(x) \frac{d^4}{dx^4} g(x) + 26 \left(\frac{d}{dx} g(x)\right) p(x) \\
&\frac{d^3}{dx^3} g(x) + 24\ (g(x) + G) \left(\frac{d}{dx} p(x)\right) \frac{d^3}{dx^3} g(x) \\
&+15 \left(\frac{d^2}{dx^2} g(x)\right)^2 p(x) + 48 \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} p(x)\right) \\
&\frac{d^2}{dx^2} g(x) + 22\ (g(x) + G)^2\, p(x) \frac{d^2}{dx^2} g(x) \\
&+28\ (g(x) + G)\, p(x) \left(\frac{d}{dx} g(x)\right)^2 + 12\ (g(x) + G)^2 \\
&\left(\frac{d}{dx} p(x)\right) \frac{d}{dx} g(x) + (g(x) + G)^4\, p(x)
\end{aligned}
\tag{21}
$$

we obtain the expressions of the Local Truncation Errors. For the methods mentioned above the expression can be found in the "Appendix".

In order to study the Local Truncation Errors we examine 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.
- $G \gg 0$ 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

$$LTE_{CL} = h^8 \left(\frac{751}{302400}\, p\,(x)\;G^4 + \cdots \right) + O\left(h^{10}\right) \tag{22}$$

5.5 The method with vanished phase-lag and its first and second derivatives developed in [39]

$$LTE_{MethI} = h^8 \left[\left(\frac{751}{75600} \left(\frac{d^2}{dx^2} g\,(x) \right) p\,(x) \right) G^2 + \cdots \right] + O\left(h^{10}\right) \tag{23}$$

5.6 The new proposed method with vanished phase-lag and its first, second and third derivatives developed in Section 4

$$\begin{aligned} LTE_{MethII} = h^8 \Bigg[\Bigg(& \frac{751}{25200} \left(\frac{d^4}{dx^4} g\,(x) \right) p\,(x) + \frac{751}{37800} \left(\frac{d^3}{dx^3} g\,(x) \right) \frac{d}{dx} p\,(x) \\ & + \frac{751}{18900}\, g\,(x)\, p\,(x)\, \frac{d^2}{dx^2} g\,(x) + \frac{751}{25200} \left(\frac{d}{dx} g\,(x) \right)^2 p\,(x) \Bigg) G + \cdots \Bigg] + O\left(h^{10}\right) \end{aligned} \tag{24}$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Hybrid Four-Step Method the error increases as the fourth power of G. For the the method with vanished phase-lag and its first and second derivatives developed in* [39]*, the error increases as the second power of G. For the new obtained method with vanished phase-lag and its first, second and third derivatives developed in this paper, the error increases as the first power of G.*

So, for the numerical solution of the time independent radial Schrödinger equation the New Proposed 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

Applying the new obtained method to the scalar test equation:

$$p'' = -z^2\, p. \tag{25}$$

we obtain the following difference equation:

$$A_2\,(s,v)\;(p_{n+2}+p_{n-2}) + A_1\,(s,v)\;(p_{n+1}+p_{n-1}) + A_0\,(s,v)\;p_n = 0 \tag{26}$$

where

$$A_2\,(s,v) \;=\; 1,\;\; A_1 \;=\; -2\,\frac{T_8}{D_2\,v^3},\;\; A_0 \;=\; -2\,\frac{T_9}{D_2\,v^3} \tag{27}$$

where

$$\begin{aligned}
T_8 = {} & 14\,v^6 + 12\,v^3\sin(v) + 4\,\sin(v)\,v^5 - 12\,\cos(v)\,v^4 + 231\,v^4 - 147\,(\cos(v))^2\,v^4 \\
& -28\,v^4s^2 + 42\,s^4\cos(v) + 21\,s^4\,(\cos(v))^2 + 102\,v^2s^2 + 14\,s^4v^2 + 7\,(\cos(v))^2\,v^6 \\
& -42\,(\cos(v))^3\,s^4 - 84\,(\cos(v))^3\,v^2s^2 - 84\,\cos(v)\,v^3\sin(v) + 119\,v^4s^2\cos(v) \\
& -256\,v^3\sin(v)\,s^2 + 7\,s^4\,(\cos(v))^2\,v^2 - 96\,\cos(v)\,v^2s^2 - 35\,(\cos(v))^3\,s^2v^4 \\
& -42\,s^4\,(\cos(v))^2\,v\sin(v) + 168\,(\cos(v))^2\,s^2v\sin(v) - 14\,s^4\,(\cos(v))^2\,v^3\sin(v) \\
& +196\,(\cos(v))^2\,v^3s^2\sin(v) + 14\,(\cos(v))^2\,v^5s^2\sin(v) - 24\,\cos(v)\,v^3s^2\sin(v) \\
& -108\,\cos(v)\,s^2v\sin(v) - 21\,s^4 + 42\,s^4v\sin(v) - 14\,(\cos(v))^2\,v^4s^2 \\
& +56\,\cos(v)\,v^5\sin(v) \\
& +7\,(\cos(v))^3\,s^4v^2 - 49\,s^4\cos(v)\,v^2 + 12\,v\sin(v)\,s^2 \\
& -7\,s^4v^3\sin(v) + 6\,(\cos(v))^2\,v^2s^2 + 7\,v^5s^2\sin(v) \\
T_9 = {} & 548\,\cos(v)\,v^5\sin(v) + 348\,(\cos(v))^2\,v^2s^2 + 96\,(\cos(v))^3\,v^2s^2 \\
& +14\,\sin(v)\,(\cos(v))^3\,v^7 - 12\,s^4v\sin(v) - 2\,s^4\,(\cos(v))^2\,v^2 \\
& +2\,s^4v^3\sin(v) + 60\,\cos(v)\,v^3\sin(v) \\
& -20\,(\cos(v))^3\,s^2v^4 - 4\,v^5s^2\sin(v) + 336\,v^3\sin(v)\,s^2 - 168\,\sin(v)\,(\cos(v))^3\,v^3 \\
& +4\,(\cos(v))^2\,v^7\sin(v) + 192\,(\cos(v))^2\,v^3\sin(v) + 4\,(\cos(v))^2\,v^5\sin(v) \\
& +6\,s^4 - 249\,v^4 - 6\,s^4\,(\cos(v))^2 + 12\,v^2s^2 - 4\,s^4v^2 - 331\,(\cos(v))^2\,v^6 - 10\,v^6\cos(v) \\
& +12\,(\cos(v))^3\,s^4 + 108\,(\cos(v))^3\,v^4 + 22\,(\cos(v))^3\,v^6 - 42\,(\cos(v))^4\,v^4 \\
& +70\,(\cos(v))^4\,v^6 - 12\,v^3\sin(v) - 328\,\sin(v)\,v^5 - 288\,\cos(v)\,v^4 + 399\,(\cos(v))^2\,v^4 \\
& -202\,v^4s^2 + 2\,v^7\sin(v) - 12\,s^4\cos(v) + 56\,\cos(v)\,v^5s^2\sin(v) \\
& -184\,\cos(v)\,v^3s^2\sin(v) - 24\,\cos(v)\,s^2v\sin(v) \\
& -14\,\sin(v)\,(\cos(v))^3\,s^2v^5 - 56\,\sin(v)\,(\cos(v))^3\,s^2v^3 \\
& -336\,\sin(v)\,(\cos(v))^3\,s^2v
\end{aligned}$$

$$
\begin{aligned}
&+12\,s^4\,(\cos(v))^2\,v\sin(v)+216\,(\cos(v))^2\,s^2 v\sin(v)+4\,s^4\,(\cos(v))^2\,v^3\sin(v)\\
&-72\,(\cos(v))^2\,v^3 s^2\sin(v)-8\,(\cos(v))^2\,v^5 s^2\sin(v)\\
&-4\,v^4 s^2\cos(v)-312\,\cos(v)\,v^2 s^2\\
&-56\,v^7\sin(v)\cos(v)+14\,s^4\cos(v)\,v^2-2\,(\cos(v))^3\,s^4 v^2\\
&-140\,\sin(v)\,(\cos(v))^3\,v^5+214\,(\cos(v))^2\,v^4 s^2+192\,v^6\\
D_2 =\ &7\,(\cos(v))^2\,v^3-147\,(\cos(v))^2\,v+56\,\cos(v)\,v^2\sin(v)\\
&-84\,\sin(v)\cos(v)-12\,\cos(v)\,v+12\,\sin(v)+4\,\sin(v)\,v^2+231\,v+14\,v^3
\end{aligned}
$$

and $s = z\,h$.

Remark 2 The frequency of the scalar test Eq. (25), z, is not equal with the frequency of the scalar test Eq. (5), w, i.e. $z \neq w$.

The corresponding characteristic equation is given by:

$$A_2(s,v)\left(\lambda^4+1\right)+A_1(s,v)\left(\lambda^3+\lambda\right)+A_0(s,v)\,\lambda^2 = 0 \tag{28}$$

Definition 1 (see [16]) A symmetric $2k$-step method with the characteristic equation given by (7) 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

$$\lambda_{1,2} = e^{\pm i\,\zeta(s)},\ |\lambda_i| \leq 1,\ i = 3, 4, \ldots \tag{29}$$

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

The stability analysis is shown on Flowchart mentioned in the Fig. 3.

Definition 2 (see [16]) 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. 4 we present the s–v plane for the 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**.

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 $s = v$ (i.e. see the surroundings of the first diagonal of the s–v plane), it is easy to see that the interval of periodicity of the new method developed in Sect. 4 is equal to: $(0, 36.83054610)$.

From the above analysis we have the following theorem:

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

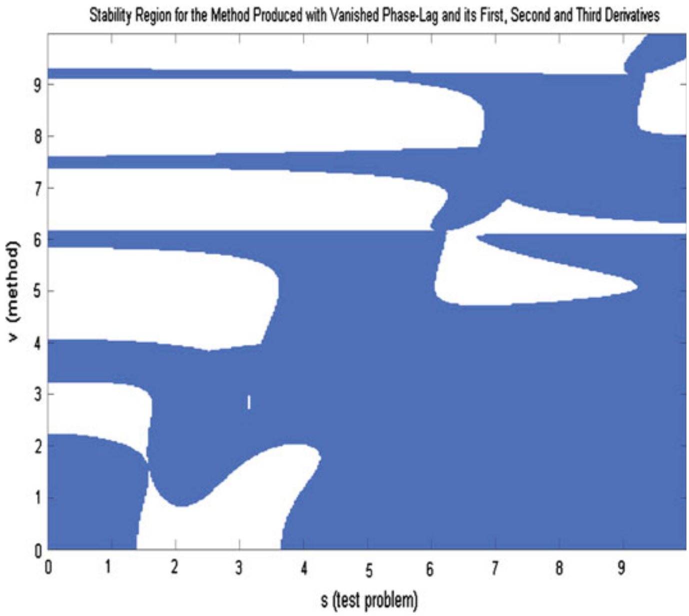

Fig. 4 s–v plane of the the new developed method

Theorem 3 *The method developed in* Sect. 4 *is of sixth 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, 36.83054610).

7 Numerical results

We test the efficiency of the new proposed method using the numerical solution of the the radial time-independent Schrödinger Eq. (1).

Since the new obtained method belongs to the category of the frequency dependent methods, we must define the value of parameter w. This in order to be possible the application of the new method to the one-dimensional Schrödinger equation. Based on (1), the parameter w is given by (for the case $l = 0$):

$$w = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{30}$$

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

7.1 Woods-Saxon potential

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

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{31}$$

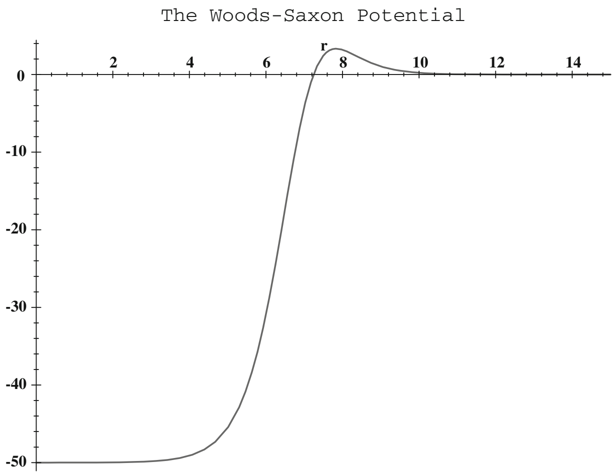

Fig. 5 The Woods-Saxon potential

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. 5.

It is known that for some potentials, such as the Woods-Saxon potential, the definition of parameter w can be given also based on some critical points which have been determined from the study of the appropriate potential (see for details [92]).

For the purpose of obtaining our numerical results, it is appropriate to choose v as follows (see for details [1] and [68]):

$$w = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{32}$$

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, we consider the numerical solution of the radial time independent Schrödinger Eq. (1) in the known case of the Woods-Saxon potential (31). The numerical solution of this problem requires the approximation of the true (infinite) interval of integration by a finite interval. For our numerical purposes, 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

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{33}$$

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.

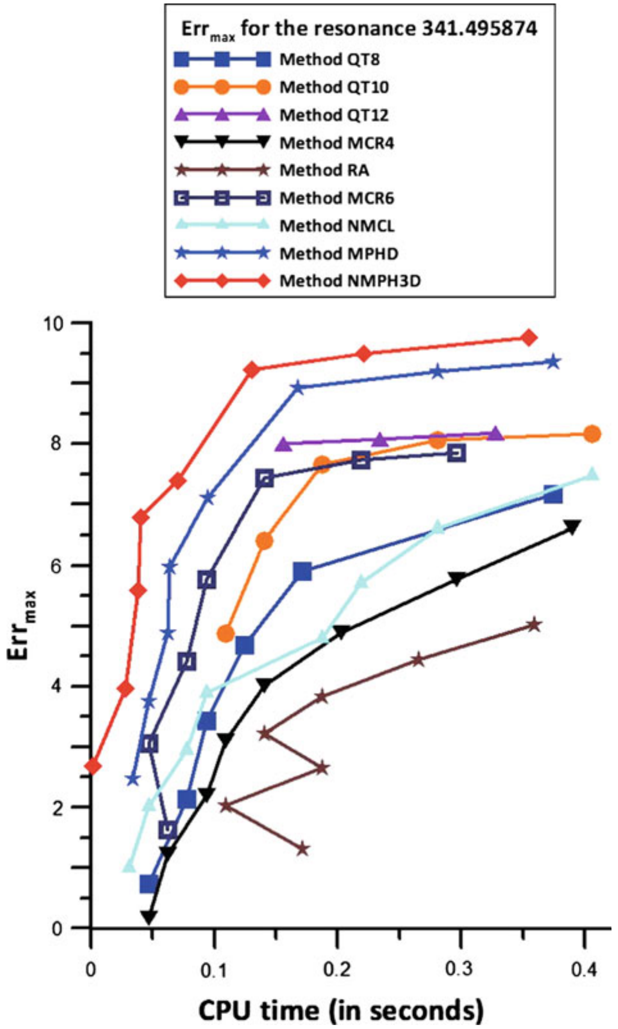

Fig. 6 Accuracy (Digits) for several values of *CPU* Time (in seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

Thus, the solution of Eq. (1) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} q(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{34}$$

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

$$\tan \delta_l = \frac{q(r_2)\, S(r_1) - q(r_1)\, S(r_2)}{q(r_1)\, C(r_1) - q(r_2)\, C(r_2)} \tag{35}$$

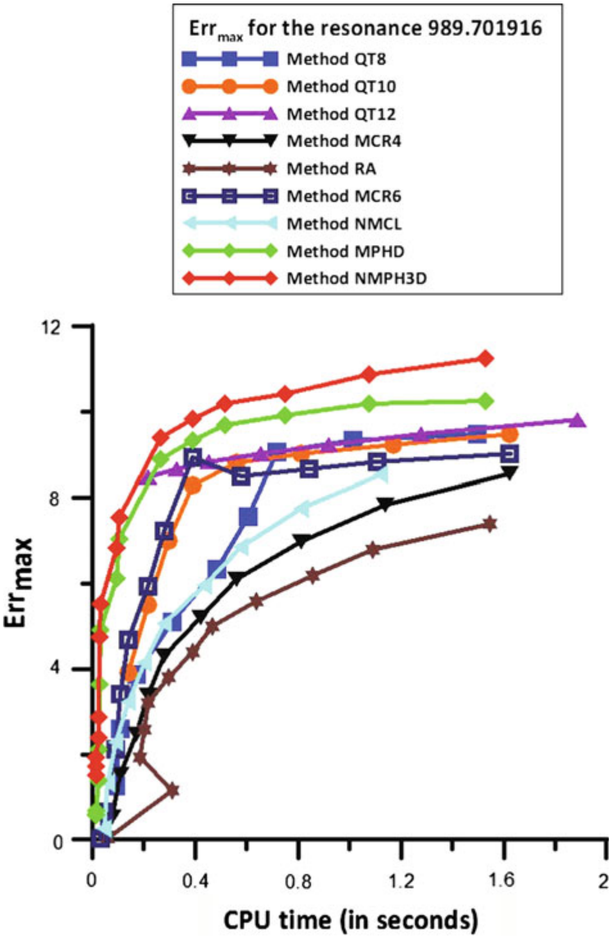

Fig. 7 Accuracy (Digits) for several values of *CPU* Time (in seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

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 [99] and [100]). 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:

$$q(0) = 0,\ q(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{36}$$

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

- The eighth order multi-step method developed by Quinlan and Tremaine [17], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [17], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [17], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [22], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [69], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [21], 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 hybrid four-step method of sixth algebraic order with vanished phase-lag and its first and second derivatives (obtained in [39]), which is indicated as **Method MPHD**
- The hybrid four-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 NMPH3D**

The computed eigenenergies are compared with reference values.[3] In Figs. 6 and 7, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

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

[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 [21] with small step size for the integration.

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 investigated a family of two-stage four-step sixth algebraic order methods and the influencing of the procedure of vanishing phase-lag and its derivatives on the efficiency of the above mentioned methods for the numerical solution of the radial Schrödinger equation and related problems. As a result of the above, a two-stage four-step sixth algebraic order methods with vanished phase-lag and its first and second derivatives was produced. 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:

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 with minimal phase-lag [22], which is indicated as **Method MCR4**. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [69], which is indicated as **Method MRA**.
2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [17], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [22], 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 [17], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [21], 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 [17], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [17], which is indicated as **Method QT10**
4. The hybrid four-step two-stage sixth algebraic order method with vanished phase-lag and its first and second derivatives (obtained in [39]), which is indicated as **Method MPHD** is more efficient than all the methods mentioned above.
5. The hybrid four-step two-stage sixth algebraic order method with vanished phase-lag and its first, second and third derivatives (obtained in Sect. 4), which is indicated as **Method NMPH3D** 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).

9 Appendix

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

$$
\begin{aligned}
\mathrm{LTE}_{\mathrm{OptMeth}} = h^8 \Bigg[& \left(\frac{751}{25200} \left(\frac{d^4}{dx^4} g(x) \right) p(x) + \frac{751}{37800} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} p(x) \right. \\
& \left. + \frac{751}{18900} g(x)\, p(x) \frac{d^2}{dx^2} g(x) + \frac{751}{25200} \left(\frac{d}{dx} g(x) \right)^2 p(x) \right) G \\
& \frac{751}{302400} \left(\frac{d^6}{dx^6} g(x) \right) p(x) + \frac{751}{50400} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} p(x) \\
& + \frac{751}{18900} g(x)\, p(x) \frac{d^4}{dx^4} g(x) + \frac{751}{20160} \left(\frac{d^2}{dx^2} g(x) \right)^2 p(x) \\
& + \frac{9763}{151200} \left(\frac{d}{dx} g(x) \right) p(x) \frac{d^3}{dx^3} g(x) + \frac{751}{12600} g(x) \left(\frac{d}{dx} p(x) \right) \frac{d^3}{dx^3} g(x) \\
& + \frac{751}{25200} (g(x))^2 \left(\frac{d}{dx} p(x) \right) \frac{d}{dx} g(x) + \frac{751}{6300} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} p(x) \right) \frac{d^2}{dx^2} g(x) \\
& + \frac{8261}{151200} (g(x))^2 p(x) \frac{d^2}{dx^2} g(x) + \frac{751}{10800} g(x)\, p(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{751}{302400} (g(x))^4 p(x) \Bigg] \qquad (38)
\end{aligned}
$$

References

1. L.G. Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
2. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)
3. I. Prigogine, S. Rice (eds.), Advances in Chemical Physics. New Methods in Computational Quantum Mechanics, 93rd edn. (Wiley, London, 1997)
4. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
5. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation. J. Math. Chem. **30**(1), 121–131 (2001)
6. K. Tselios, T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**(1), 173–181 (2005)
7. Z.A. Anastassi, T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**(1), 1–9 (2005)
8. D.F. Papadopoulos, T.E. Simos, A new methodology for the construction of optimized Runge-Kutta-Nyström methods. Int. J. Mod. Phys. C **22**(6), 623–634 (2011)
9. A.A. Kosti, Z.A. Anastassi, T.E. Simos, An optimized explicit Runge-Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems. J. Math. Chem. **47**(1), 315–330 (2010)
10. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nyström methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. J. Math. Chem. **31**(2), 211–232 (2002)
11. T.E. Simos, A fourth algebraic order exponentially-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation. IMA Journal of Numerical Analysis **21**(4), 919–931 (2001)

12. T.E. Simos, Exponentially-Fitted Runge-Kutta-Nyström Method for the Numerical Solution of Initial-Value Problems with Oscillating Solutions. Appl. Math. Lett. **15**(2), 217–225 (2002)
13. Ch. Tsitouras, T.E. Simos, Optimized Runge-Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
14. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 281–293 (2005)
15. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge-Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. J. Math. Chem. **41**(1), 79–100 (2007)
16. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
17. G.D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits. Astron. J. **100**, 1694–1700 (1990)
18. C. Tsitouras, I.T. Famelis, T.E. Simos, On modified Runge-Kutta trees and methods. Comput. Math. Appl. **62**(4), 2101–2111 (2011)
19. http://burtleburtle.net/bob/math/multistep.html
20. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. J. Math. Chem. **29**(4), 281–291 (2001)
21. M.M. Chawla, P.S. Rao, An explicit sixth–order method with phase-lag of order eight for $y'' = f(t, y)$. J. Comput. Appl. Math. **17**, 363–368 (1987)
22. M.M. Chawla, P.S. Rao, An Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems II Explicit method. J. Comput. Appl. Math. **15**, 329–337 (1986)
23. T.E. Simos, P.S. Williams, A finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**, 189–205 (1997)
24. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. J. Math. Chem. **29**(4), 293–305 (2001)
25. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. J. Math. Chem. **31**(2), 135–144 (2002)
26. A. Konguetsof, T.E. Simos, A Generator of Hybrid Symmetric Four-Step Methods for the Numerical Solution of the Schrödinger Equation. J. Comput. Appl. Math. **158**(1), 93–106 (2003)
27. T.E. Simos, I.T. Famelis, C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions. Numer. Algorithms **34**(1), 27–40 (2003)
28. D.P. Sakas, T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation. J. Comput. Appl. Math. **175**(1), 161–172 (2005)
29. T.E. Simos, Optimizing a class of linear multi-step methods for the approximate solution of the radial Schrödinger equation and related problems with respect to phase-lag. Cent. Eur. J. Phys. **9**(6), 1518–1535 (2011)
30. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 317–331 (2005)
31. H. Van de Vyver, Phase-fitted and amplification-fitted two-step hybrid methods for $y'' = f(x, y)$. J. Comput. Appl. Math. **209**(1), 33–53 (2007)
32. H. Van de Vyver, An explicit Numerov-type method for second-order differential equations with oscillating solutions. Comput. Math. Appl. **53**, 1339–1348 (2007)
33. T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation. J. Math. Chem. **46**(3), 981–1007 (2009)
34. S. Stavroyiannis, T.E. Simos, Optimization as a function of the phase-lag order of nonlinear explicit two-step P-stable method for linear periodic IVPs. Appl. Numer. Math. **59**(10), 2467–2474 (2009)
35. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A new symmetric eight-step predictor-corrector method for the numerical solution of the radial Schrödinger equation and related orbital problems. Int. J. Mod. Phys. C **22**(2), 133–153 (2011)
36. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, A symmetric eight-step predictor-corrector method for the numerical solution of the radial Schrödinger equation and related IVPs with oscillating solutions. Comput. Phys. Commun. **182**(8), 1626–1637 (2011)

37. T.E. Simos, Optimizing a hybrid two-step method for the numerical solution of the Schrödinger equation and related problems with respect to phase-lag. J. Appl. Math. Article ID 420387, vol. 2012 (2012).
38. T.E. Simos, A two-step method with vanished phase-lag and its first two derivatives for the numerical solution of the Schrödinger equation. J. Math. Chem. **49**(10), 2486–2518 (2011)
39. I. Alolyan, T.E. Simos, High order four-step hybrid method with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation. J. Math. Chem. (in press). doi:10.1007/s10910-012-0102-y
40. Z.A. Anastassi, T.E. Simos, A parametric symmetric linear four-step method for the efficient integration of the Schrödinger equation and related oscillatory problems. J. Comput. Appl. Math. **236**(16), 3880–3889 (2012)
41. A. Konguetsof, A new two-step hybrid method for the numerical solution of the Schrödinger equation. J. Math. Chem. **47**(2), 871–890 (2010)
42. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation. J. Math. Chem. **34**(1–2), 83–94 (2003)
43. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation. J. Math. Chem. **35**(1), 55–63 (2004)
44. T. Monovasilis, T.E. Simos, New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation. J. Math. Chem. **42**(3), 535–545 (2007)
45. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **37**(3), 263–270 (2005)
46. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **40**(3), 257–267 (2006)
47. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 83–92 (2003)
48. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high-order for long-time integration of orbital problems. Appl. Math. Lett. **22**(10), 1616–1621 (2009)
49. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
50. T.E. Simos, High order closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation. Appl. Math. Comput. **209**(1), 137–151 (2009)
51. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for the solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**(3), 787–801 (2008)
52. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation. J. Math. Chem. **44**(2), 483–499 (2008)
53. T.E. Simos, High-order closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. Comput. Phys. Commun. **178**(3), 199–207 (2008)
54. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for numerical integration of the Schrödinger equation. Computing Letters **3**(1), 45–57 (2007)
55. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. RevMexAA **42**(2), 167–177 (2006)
56. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration. Int. J. Mod. Phys C **14**(8), 1061–1074 (2003)
57. T.E. Simos, New closed Newton-Cotes type formulae as multilayer symplectic integrators. J. Chem. Phys. 133(10) Article Number: 104108(2010).
58. T.E. Simos, New stable closed Newton-Cotes trigonometrically fitted formulae for long-time integration. Abstr. Appl. Anal. Article Number: 182536, doi:10.1155/2012/182536(2012).
59. T.E. Simos, High order closed Newton-Cotes exponentially and trigonometrically fitted formulae as multilayer symplectic integrators and their application to the radial Schrödinger equation. J. Math. Chem. **50**(5), 1224–1261 (2012)
60. G. Vanden Berghe, M. Van Daele, Exponentially fitted open Newton-Cotes differential methods as multilayer symplectic integrators. J. Chem. Phys. **132**, 204107 (2010)
61. Z. Kalogiratou, T. Monovasilis, T.E. Simos, A fifth-order symplectic trigonometrically fitted partitioned Runge-Kutta method. in *International Conference on Numerical Analysis and Applied Math-*

ematics, SEP 16–20, 2007 Corfu, GREECE, Numerical Analysis and Applied Mathematics. AIP Conference Proceedings (2007) vol. 936, pp. 313–317
62. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Families of third and fourth algebraic order trigonometrically fitted symplectic methods for the numerical integration of Hamiltonian systems. Comput. Phys. Commun. **177**(10), 757–763 (2007)
63. T. Monovasilis, T.E. Simos, Symplectic methods for the numerical integration of the Schrödinger equation. Comput. Mater. Sci. **38**(3), 526–532 (2007)
64. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Computation of the eigenvalues of the Schrödinger equation by symplectic and trigonometrically fitted symplectic partitioned Runge-Kutta methods. Phys. Lett. A **372**(5), 569–573 (2008)
65. Z. Kalogiratou, T. Monovasilis, T.E. Simos, New modified Runge-Kutta-Nyström methods for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **60**(6), 1639–1647 (2010)
66. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Two new phase-fitted symplectic Partitioned Runge-Kutta Methods. Int. J. Mod. Phys. C **22**(12), 1343–1355 (2011)
67. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Symplectic partitioned Runge-Kutta methods with minimal phase-lag. Comput. Phys. Commun. **181**(7), 1251–1254 (2010)
68. L.G. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. Comput. Phys. Commun. **19**, 23–27 (1980)
69. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
70. J. Vigo-Aguiar, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **32**(3), 257–270 (2002)
71. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
72. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**(1), 137–147 (2005)
73. T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution. Appl. Math. Lett. **17**(5), 601–607 (2004)
74. T.E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation. Acta Applicandae Mathematicae **110**(3), 1331–1352 (2010)
75. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **31**(4), 371–404 (2002)
76. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. J. Math. Chem. **34**(1–2), 39–58 (2003)
77. T.E. Simos, Exponentially-fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
78. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. J. Math. Chem. **40**(3), 305–318 (2006)
79. H. Van de Vyver, A trigonometrically fitted explicit hybrid method for the numerical integration of orbital problems. Appl. Math. Comput. **189**(1), 178–185 (2007)
80. T.E. Simos, A family of four-step trigonometrically-fitted methods and its application to the Schrodinger equation. J. Math. Chem. **44**(2), 447–466 (2009)
81. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. **45**(4), 1102–1129 (2009)
82. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation. J. Math. Chem. **37**(3), 295–316 (2005)
83. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order predictor-corrector methods. J. Math. Chem. **40**(3), 269–293 (2006)
84. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**(3), 162–174 (2005)
85. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. J. Math. Chem. **27**(4), 343–356 (2000)
86. C. Tang, W. Wang, H. Yan, Z. Chen, High-order predictorcorrector of exponential fitting for the N-body problems. J. Comput. Phys. **214**(2), 505–520 (2006)

87. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions. J. Math. Chem. **46**(2), 604–620 (2009)
88. S. Stavroyiannis, T.E. Simos, A nonlinear explicit two-step fourth algebraic order method of order infinity for linear periodic initial value problems. Comput. Phys. Commun. **181**(8), 1362–1368 (2010)
89. Z.A. Anastassi, T.E. Simos, Numerical multistep methods for the efficient solution of quantum mechanics and related problems. Phys. Rep. **482**, 1–240 (2009)
90. R. Vujasin, M. Sencanski, J. Radic-Peric, M. Peric, A comparison of various variational approaches for solving the one-dimensional vibrational Schrödinger equation. MATCH Commun. Math. Comput. Chem. **63**(2), 363–378 (2010)
91. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Computers and Chemistry **23**, 513–554 (1999)
92. L. Gr Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **38**(3), 329–337 (1985)
93. J. Vigo-Aguiar, T.E. Simos, Review of multistep methods for the numerical solution of the radial Schrödinger equation. Int. J. Quantum Chem. **103**(3), 278–290 (2005)
94. T.E. Simos, G. Psihoyios, Special issue: the international conference on computational methods in sciences and engineering 2004–Preface. J. Comput. Appl. Math. **191**(2), 165–165 (2006)
95. T.E. Simos, G. Psihoyios, Special issue—selected papers of the International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003) Kastoria, Greece, 12–16 September 2003–Preface. J. Comput. Appl. Math. **175**(1), IX–IX (2005)
96. T.E. Simos, J. Vigo-Aguiar, Special issue–selected papers from the Conference on Computational and Mathematical Methods for Science and Engineering (CMMSE-2002)–Alicante University, Spain, 20–25 September 2002-Preface. J. Comput. Appl. Math. **158**(1), IX–IX (2003)
97. T.E. Simos, C. Tsitouras, Preface for the special issue numerical methods in chemistry. MATCH Commun. Math. Comput. Chem. **60**(3), 695 (2008)
98. T.E. Simos, I. Gutman, Papers presented on the International Conference on Computational Methods in Sciences and Engineering (Castoria, Greece, September 12–16, 2003). MATCH Commun. Math. Comput. Chem. **53**(2), A3–A4 (2005)
99. J.R. Dormand, M.E.A. El-Mikkawy, P.J. Prince, Families of Runge–Kutta–Nyström formulae. IMA J. Numer. Anal. **7**, 235–250 (1987)
100. J.R. Dormand, P.J. Prince, A family of embedded RungeKutta formulae. J. Comput. Appl. Math. **6**, 19–26 (1980)