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A family of high-order multistep methods with vanished phase-lag and its derivatives for the numerical solution of the Schrödinger equation

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ABSTRACT

Many simulation algorithms (chemical reaction systems, differential systems arising from the modelling of transient behaviour in the process industries etc.) contain the numerical solution of systems of differential equations. For the efficient solution of the above mentioned problems, linear multistep methods or Runge–Kutta single-step methods are used. For the simulation of chemical procedures the radial Schrödinger equation is used frequently. In the present paper we will study a class of linear multistep methods. More specifically, the purpose of this paper is to develop an efficient algorithm for the approximate solution of the radial Schrödinger equation and related problems. This algorithm belongs in the category of the multistep methods. In order to produce an efficient multistep method the phase-lag property and its derivatives are used. Hence the main result of this paper is the development of an efficient multistep method for the numerical solution of systems of ordinary differential equations with oscillating or periodical solutions. The reason of their efficiency, as the analysis proved, is that the phase-lag and its derivatives are eliminated. Another reason of the efficiency of the new obtained methods is that they have high algebraic order

1. Introduction

Many simulation algorithms (chemical reaction systems, differential systems arising from the modelling of transient behaviour in process industries, etc.) contain the numerical solution of systems of differential equations. For the efficient solution of the above mentioned problems, linear multistep methods or Runge–Kutta single-step methods are used.

One of the models used frequently for the simulation of chemical procedures is the radial Schrödinger equation.

The formula of the radial Schrödinger equation can be presented as:

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

It is known that Mathematical Models in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics, etc., can be expressed via the above boundary value problem (see for example [1–4]).

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For the above Eq. (1) we have the following definitions:

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

The boundary conditions are:

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

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

Large research on the algorithmic development of numerical methods for the solution of the Schrödinger equation has been done in the last decades. The aim and scope of this research is the construction of fast and reliable algorithms for the solution of the Schrödinger equation and related problems (see for example [5–24]).

The numerical methods for the approximate solution of the Schrödinger equation and related problems can be divided into two main categories:

1. Methods with constant coefficients.
2. Methods with coefficients depending on the frequency of the problem.[2]

The main result of this paper is the development of an efficient multistep method for the numerical solution of systems of ordinary differential equations with oscillating or periodical solutions. The reason of their efficiency, as the analysis proved, is that the phase-lag and its derivatives are eliminated. Another reason of the efficiency of the new obtained methods is that they have high algebraic order.

The purpose of this paper is to extend the methodology for the development of numerical methods for the approximate solution periodic initial-value problems. The new methodology is based on the requirement of the phase-lag and its derivatives vanishing. Based on this new methodology we will develop two methods:

- The first one will have phase-lag and its first and second derivatives vanishing.
- The second one will have phase-lag and its first, second and third derivatives vanishing.

We will apply the new developed methods on the numerical solution of the radial Schrödinger equation. We will study the efficiency of the new obtained methods via:

- a comparative error analysis
- a comparative stability analysis and finally
- the numerical results produced from the numerical solution of the radial Schrödinger with application to the specific potential.

More specifically, we will develop a family of implicit symmetric ten-step methods of twelfth algebraic order. The development of the new family of methods is based on the requirement of the phase-lag and its first, second and third derivative vanishing (see above).

We will give a comparative error analysis and a comparative stability analysis in order to study the efficiency of the two new proposed methods of the family. Finally, we will apply both methods to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation.

We have organized the paper as follows:

- In Section 2 we present the theory of the new methodology.
- In Section 3 we present the development of the new family of methods.
- A comparative error analysis is presented in Section 4.
- In Section 5 we will present a comparative stability analysis.
- The numerical results are presented in Section 6.
- Finally, in Section 7 remarks and conclusions are discussed.

2. Basic theory

2.1. Definitions

We consider the numerical solution of the initial value problem over the equally spaced intervals $\{r_i\}_{i=0}^{m} \in [a, b]$ and $h = |r_{i+1} - r_i|,\ i = 0(1)m-1$:

$$\phi'' = -\omega^2 \phi. \tag{3}$$

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

The theoretical solution of Eq. (4) in an integration interval $[r_i, r_{i+1}]$, is equal to

$$\phi(\mathrm{v})_{th} = e^{\pm i\mathrm{v}} \tag{4}$$

where $\mathrm{v} = \omega h$, h is the step length.

Applying a numerical method for the approximate solution of (3), one can find the following numerical solution:

$$\phi(\mathrm{v})_{appr} = \alpha(\mathrm{v})\, e^{\pm i\theta(\mathrm{v})}. \tag{5}$$

Definition 1 ([25]). The quantity:

$$\zeta(\mathrm{v}) = 1 - \alpha(\mathrm{v}) \tag{6}$$

is called dissipation error or amplification factor.

Definition 2 ([25]). The quantity:

$$\varphi(\mathrm{v}) = \frac{\theta(\mathrm{v}) - \mathrm{v}}{\mathrm{v}} \tag{7}$$

is called dispersion or phase error or phase lag.

Remark 1. For the symmetric multistep methods it has been proved that the dissipation error is equal to zero.

2.2. Phase-lag analysis of symmetric multistep methods

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

$$\phi'' = f(r, \phi). \tag{8}$$

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

When a symmetric $2k$-step method, that is for $i = -k(1)k$, is applied to the scalar test equation (3) a difference equation of the form

$$A_k(\mathrm{v})\phi_{n+k} + \cdots + A_1(\mathrm{v})\phi_{n+1} + A_0(\mathrm{v})\phi_n + A_1(\mathrm{v})\phi_{n-1} + \cdots + A_k(\mathrm{v})\phi_{n-k} = 0 \tag{9}$$

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

The characteristic equation associated with (9) is given by:

$$A_k(\mathrm{v})\lambda^k + \cdots + A_1(\mathrm{v})\lambda + A_0(\mathrm{v}) + A_1(\mathrm{v})\lambda^{-1} + \cdots + A_k(\mathrm{v})\lambda^{-k} = 0. \tag{10}$$

Theorem 1 ([22]). *The symmetric $2k$-step method with characteristic equation given by (10) has phase-lag order r and phase-lag constant c given by*

$$-c\mathrm{v}^{r+2} + O(\mathrm{v}^{r+4}) = \frac{2A_k(\mathrm{v})\cos(k\mathrm{v}) + \cdots + 2A_j(\mathrm{v})\cos(j\mathrm{v}) + \cdots + A_0(\mathrm{v})}{2k^2A_k(\mathrm{v}) + \cdots + 2j^2A_j(\mathrm{v}) + \cdots + 2A_1(\mathrm{v})}. \tag{11}$$

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

3. The new family of ten-step methods

3.1. Development of the new methods

In order to obtain the new methods the following algorithm is applied:

1. General Requirements for the New Proposed Method.
   We require the new proposed methods to have:
   - the maximum algebraic order and
   - a number of free parameters (for the first method of the family we require three free parameters while for the second method of the family we require four free parameters).
2. Computation of the Difference Equation and the Associated Characteristic Equation.
3. Computation of the corresponding polynomials $A_i(\mathrm{v})$, $i = 0(1)5$.

4. Computation of the Corresponding Phase-lag.
5. Computation of the Corresponding Derivatives of the Phase-lag (First, Second, etc. Derivatives).
6. Demand for the satisfaction of the appropriate relations—Determination of the coefficients of the new proposed methods.
7. Taylor series expansions of the obtained coefficients.
8. Computation of the Local Truncation Error.

We introduce the following family of methods to integrate $p'' = f(x, p)$:

$$\sum_{i=1}^{5} a_i\left(\phi_{n+i} + \phi_{n-i}\right) + a_0\phi_n = h^2\left[\sum_{i=1}^{5} b_i\left(\phi''_{n+i} + \phi''_{n-i}\right) + b_0\phi''_n\right] \tag{12}$$

where $a_5 = 1$.

3.2. First method of the family—a method with phase-lag and its first two derivatives vanishing

Requiring the above method (12) to have the maximum algebraic order with three free parameter, the following relations are obtained:

$$\begin{aligned}
&a_0 = 0, \quad a_1 = 0, \quad a_2 = -1, \quad a_3 = 2, \quad a_4 = -2,\\
&b_3 = \frac{6937}{960} - \frac{9}{4}b_2 - \frac{45}{14}b_1 - \frac{25}{14}b_0,\\
&b_4 = -\frac{497}{90} + \frac{64}{21}b_1 + \frac{5}{3}b_2 + \frac{25}{14}b_0,\\
&b_5 = \frac{5173}{2880} - \frac{5}{12}b_2 - \frac{5}{6}b_1 - \frac{1}{2}b_0.
\end{aligned} \tag{13}$$

The application of the above method to the scalar test equation (3) gives the following difference equation:

$$\sum_{i=1}^{5} A_i(\mathrm{v})\left(\phi_{n+i} + \phi_{n-i}\right) + A_0(\mathrm{v})\phi_n = 0 \tag{14}$$

where $\mathrm{v} = \omega h$, h is the step length and $A_i(\mathrm{v}),\ i = 0(1)5$ are polynomials of v.

The characteristic equation associated with (14) is given by:

$$\sum_{i=1}^{5} A_i(\mathrm{v})\left(\lambda^i + \lambda^{-i}\right) + A_0(\mathrm{v}) = 0 \tag{15}$$

where

$$\begin{aligned}
&A_0(\mathrm{v}) = \mathrm{v}^2 b_0, \qquad A_1(\mathrm{v}) = \mathrm{v}^2 b_1\\
&A_2(\mathrm{v}) = -1 + \mathrm{v}^2 b_2, \qquad A_3(\mathrm{v}) = 2 + \mathrm{v}^2\left(\frac{6937}{960} - \frac{9}{4}b_2 - \frac{45}{14}b_1 - \frac{25}{14}b_0\right)\\
&A_4(\mathrm{v}) = -2 + \mathrm{v}^2\left(-\frac{497}{90} + \frac{64}{21}b_1 + \frac{5}{3}b_2 + \frac{25}{14}b_0\right)\\
&A_5(\mathrm{v}) = 1 + \mathrm{v}^2\left(\frac{5173}{2880} - \frac{5}{12}b_2 - \frac{5}{6}b_1 - \frac{1}{2}b_0\right).
\end{aligned} \tag{16}$$

By applying $k = 5$ in the formula (11), we have that the phase-lag is equal to:

$$\mathrm{phl} = \frac{T_0}{T_1} \tag{17}$$

$$\begin{aligned}
T_0 \;=\; & 2\left[1 + \mathrm{v}^2\left(\frac{5173}{2880} - \frac{5}{12}b_2 - \frac{5}{6}b_1 - \frac{1}{2}b_0\right)\right]\cos(5\mathrm{v})\\
&+ 2\left[-2 + \mathrm{v}^2\left(-\frac{497}{90} + \frac{64}{21}b_1 + \frac{5}{3}b_2 + \frac{25}{14}b_0\right)\right]\cos(4\mathrm{v})\\
&+ 2\left[2 + \mathrm{v}^2\left(\frac{6937}{960} - \frac{9}{4}b_2 - \frac{45}{14}b_1 - \frac{25}{14}b_0\right)\right]\cos(3\mathrm{v}) + 2\left(-1 + \mathrm{v}^2 b_2\right)\cos(2\mathrm{v}) + 2\mathrm{v}^2 b_1\cos(\mathrm{v}) + \mathrm{v}^2 b_0
\end{aligned}$$

$$T_1 = 14 + 50v^2\left(\frac{5173}{2880} - \frac{5}{12}b_2 - \frac{5}{6}b_1 - \frac{1}{2}b_0\right) + 32v^2\left(-\frac{497}{90} + \frac{64}{21}b_1 + \frac{5}{3}b_2 + \frac{25}{14}b_0\right) + 18v^2\left(\frac{6937}{960} - \frac{9}{4}b_2 - \frac{45}{14}b_1 - \frac{25}{14}b_0\right) + 8v^2b_2 + 2v^2b_1.$$

The phase-lag's first and second derivatives can be produced from the above relation.
Demanding the phase-lag and the first and second derivatives of the phase to vanish we find out that:

$$b_0 = \frac{1}{480}\frac{T_8}{v^4T_9} \tag{18}$$

$$\begin{aligned}T_8 = {} & -4680 - 150480\sin(v)\cos(v)^3 v + 46680\sin(v) v\cos(v) + 76800\sin(v)\cos(v)^7 v \\ & + 261120\sin(v)\cos(v)^6 v + 25920\sin(v)\cos(v)^5 v - 38400\sin(v)\cos(v)^8 v \\ & - 310080\sin(v)\cos(v)^4 v + 97320\sin(v) v\cos(v)^2 - 8880\sin(v) v + 27720\cos(v) v^2 \\ & - 19257v^4\cos(v) - 42840\cos(v)^2 v^2 + 53760\cos(v)^7 v^2 + 48076\cos(v)^7 v^4 \\ & + 182952\cos(v)^6 v^4 + 141120\cos(v)^6 v^2 + 277081\cos(v)^5 v^4 \\ & + 78960\cos(v)^5 v^2 - 110880\cos(v)^4 v^2 + 182574\cos(v)^4 v^4 \\ & - 160440\cos(v)^3 v^2 + 11620\cos(v)^3 v^4 - 45234\cos(v)^2 v^4 \\ & - 57600\cos(v)^8 - 15480\cos(v) - 151200\cos(v)^4 - 272160\cos(v)^5 \\ & + 161280\cos(v)^6 + 12600v^2 - 2772v^4 + 52200\cos(v)^2 \\ & - 115200\cos(v)^9 + 299520\cos(v)^7 + 103320\cos(v)^3\end{aligned}$$

$$T_9 = \cos(v)^7 - 3\cos(v)^6 + \cos(v)^5 + 5\cos(v)^4 - 5\cos(v)^3 - \cos(v)^2 + 3\cos(v) - 1$$

$$b_1 = -\frac{1}{960}\frac{T_{10}}{v^4T_9} \tag{19}$$

$$\begin{aligned}T_{10} = {} & -8280 - 276960\sin(v)\cos(v)^3 v + 82200\sin(v) v\cos(v) + 88320\sin(v)\cos(v)^7 v \\ & + 452160\sin(v)\cos(v)^6 v + 106080\sin(v)\cos(v)^5 v \\ & - 57600\sin(v)\cos(v)^8 v - 550800\sin(v)\cos(v)^4 v + 172440\sin(v) v\cos(v)^2 \\ & - 15840\sin(v) v + 47880\cos(v) v^2 - 39102v^4\cos(v) - 78120\cos(v)^2 v^2 + 73920\cos(v)^7 v^2 \\ & + 66528\cos(v)^7 v^4 + 291186\cos(v)^6 v^4 + 231840\cos(v)^6 v^2 + 467292\cos(v)^5 v^4 \\ & + 164640\cos(v)^5 v^2 - 176400\cos(v)^4 v^2 + 318451\cos(v)^4 v^4 \\ & - 286440\cos(v)^3 v^2 + 34482\cos(v)^3 v^4 - 77210\cos(v)^2 v^4 \\ & - 126720\cos(v)^8 - 27000\cos(v) - 292320\cos(v)^4 - 448560\cos(v)^5 \\ & + 332640\cos(v)^6 + 22680v^2 - 3227v^4 + 94680\cos(v)^2 \\ & - 172800\cos(v)^9 + 469440\cos(v)^7 + 178920\cos(v)^3\end{aligned}$$

$$b_2 = \frac{1}{240}\frac{T_{11}}{v^4T_9} \tag{20}$$

$$\begin{aligned}T_{11} = {} & -1440 - 2880\sin(v) v + 8280\cos(v) v^2 - 5712v^4\cos(v) - 16200\cos(v)^2 v^2 + 5280\cos(v)^7 v^2 \\ & + 5453\cos(v)^7 v^4 + 32718\cos(v)^6 v^4 + 29520\cos(v)^6 v^2 + 68432\cos(v)^5 v^4 \\ & + 35520\cos(v)^5 v^2 - 17280\cos(v)^4 v^2 + 56490\cos(v)^4 v^4 - 49080\cos(v)^3 v^2 \\ & + 7427\cos(v)^3 v^4 - 12684\cos(v)^2 v^4 + 28080\sin(v) v\cos(v)^2 + 67680\sin(v)\cos(v)^6 v \\ & + 14640\sin(v) v\cos(v) + 41520\sin(v)\cos(v)^5 v - 53880\sin(v)\cos(v)^3 v \\ & - 87480\sin(v)\cos(v)^4 v - 5760\sin(v)\cos(v)^8 v - 1920\sin(v)\cos(v)^7 v \\ & - 4320\cos(v) - 58680\cos(v)^4 - 57960\cos(v)^5 + 71280\cos(v)^6 \\ & - 28800\cos(v)^8 + 3960v^2 - 924v^4 + 17640\cos(v)^2 \\ & - 17280\cos(v)^9 + 53280\cos(v)^7 + 26280\cos(v)^3 .\end{aligned}$$

For small values of $|v|$ the formulae given by (18)–(20) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$b_0 = \frac{18117277}{5702400} - \frac{547336457}{494208000}v^2 + \frac{3988544723}{17791488000}v^4 - \frac{1060584330623}{47636709120000}v^6 + \frac{15195486142211}{14481559572480000}v^8 - \frac{591171853921499}{19115658635673600000}v^{10} + \frac{14086630076582821}{36931452484121395200000}v^{12} - \frac{17472592514198011}{42362548437668659200000}v^{14}$$

$$
\begin{aligned}
&- \frac{687773753293267}{197530511572215005184000}\mathrm{v}^{16} + \cdots \\
b_1 = &-\frac{10081177}{11404800} + \frac{547336457}{593049600}\mathrm{v}^2 - \frac{6282683567}{35582976000}\mathrm{v}^4 + \frac{883305239}{53299814400}\mathrm{v}^6 \\
&- \frac{23203291679119}{28963119144960000}\mathrm{v}^8 + \frac{166718764256269}{7646263454269440000}\mathrm{v}^{10} - \frac{33093001392989737}{73862904968242790400000}\mathrm{v}^{12} \\
&+ \frac{5766401516897381}{4801088822935781376000000}\mathrm{v}^{14} + \frac{146491245110064629}{34567839525137625907200000}\mathrm{v}^{16} + \cdots \\
b_2 = &\frac{6056249}{2851200} - \frac{547336457}{1037836800}\mathrm{v}^2 + \frac{741144379}{8895744000}\mathrm{v}^4 - \frac{61856925943}{9527341824000}\mathrm{v}^6 \\
&+ \frac{813790337461}{2413593262080000}\mathrm{v}^8 - \frac{95050599920501}{13380961044971520000}\mathrm{v}^{10} + \frac{6876481251874229}{18465726242060697600000}\mathrm{v}^{12} \\
&+ \frac{45637774138658389}{25205716320412852224000000}\mathrm{v}^{14} + \frac{1512288260037651989}{60493719168990845337600000}\mathrm{v}^{16} + \cdots .
\end{aligned} \tag{21}
$$

The behaviour of the coefficients is given in the following Fig. 1.
The local truncation error of the new proposed method is given by:

$$
\mathrm{LTE} = -\frac{547336457h^{14}}{373621248000}\left(y_n^{(14)} + 3\omega^2 y_n^{(12)} + 3\omega^4 y_n^{(10)} + \omega^6 y_n^{(8)}\right). \tag{22}
$$

3.3. Second method of the family—a method with phase-lag and its first three derivatives vanishing

Requiring the method (12) to have the maximum algebraic order with four free parameters, the following relations hold:

$$
\begin{aligned}
&a_0 = 0, \quad a_1 = 0, \quad a_2 = -1, \quad a_3 = 2, \quad a_4 = -2 \\
&b_4 = \frac{791}{108} - \frac{25}{18}b_0 - \frac{16}{9}b_3 - \frac{7}{3}b_2 - \frac{8}{3}b_1, \\
&b_5 = -\frac{413}{108} + \frac{8}{9}b_0 + \frac{7}{9}b_3 + \frac{4}{3}b_2 + \frac{5}{3}b_1.
\end{aligned} \tag{23}
$$

The application of the above method to the scalar test equation (3) gives the difference equation (14). The characteristic equation associated with (14) is given by (15) with:

$$
\begin{aligned}
&A_0(\mathrm{v}) = \mathrm{v}^2 b_0, \quad A_1(\mathrm{v}) = \mathrm{v}^2 b_1 \\
&A_2(\mathrm{v}) = -1 + \mathrm{v}^2 b_2, \quad A_3(\mathrm{v}) = 2 + \mathrm{v}^2 b_3 \\
&A_4(\mathrm{v}) = -2 + \mathrm{v}^2\left(\frac{791}{108} - \frac{25}{18}b_0 - \frac{16}{9}b_3 - \frac{7}{3}b_2 - \frac{8}{3}b_1\right) \\
&A_5(\mathrm{v}) = 1 + \mathrm{v}^2\left(-\frac{413}{108} + \frac{8}{9}b_0 + \frac{7}{9}b_3 + \frac{4}{3}b_2 + \frac{5}{3}b_1\right).
\end{aligned} \tag{24}
$$

By applying $k = 5$ in the formula (11), we have that the phase-lag is equal to:

$$
\mathrm{phl} = \frac{T_{12}}{T_{13}} \tag{25}
$$

$$
\begin{aligned}
T_{12} = &\ 2\left[1 + \mathrm{v}^2\left(-\frac{413}{108} + \frac{8}{9}b_0 + \frac{7}{9}b_3 + \frac{4}{3}b_2 + \frac{5}{3}b_1\right)\right]\cos(5\mathrm{v}) \\
&+ 2\left[-2 + \mathrm{v}^2\left(\frac{791}{108} - \frac{25}{18}b_0 - \frac{16}{9}b_3 - \frac{7}{3}b_2 - \frac{8}{3}b_1\right)\right]\cos(4\mathrm{v}) \\
&+ 2\left(2 + \mathrm{v}^2 b_3\right)\cos(3\mathrm{v}) + 2\left(-1 + \mathrm{v}^2 b_2\right)\cos(2\mathrm{v}) + 2\mathrm{v}^2 b_1 \cos(\mathrm{v}) + \mathrm{v}^2 b_0 \\
T_{13} = &\ 14 + 50\mathrm{v}^2\left(-\frac{413}{108} + \frac{8}{9}b_0 + \frac{7}{9}b_3 + \frac{4}{3}b_2 + \frac{5}{3}b_1\right) \\
&+ 32\mathrm{v}^2\left(\frac{791}{108} - \frac{25}{18}b_0 - \frac{16}{9}b_3 - \frac{7}{3}b_2 - \frac{8}{3}b_1\right) + 18\mathrm{v}^2 b_3 + 8\mathrm{v}^2 b_2 + 2\mathrm{v}^2 b_1.
\end{aligned}
$$

The phase-lag's first, second and third derivatives can be produced from the above relation.

Demanding the phase-lag and the first, second and third derivatives of the phase-lag to vanish we find out that:

$$b_0 = -\frac{1}{48}\frac{T_{21}}{v^5 T_{22}} \tag{26}$$

$$\begin{aligned}
T_{21} = {} & -396v - 288\sin(v) - 147v^5 - 252v^3 + 20216(\cos(v))^6 v^5 \\
& - 9216\sin(v)(\cos(v))^9 + 26496\sin(v)(\cos(v))^7 + 1584\sin(v)v^2 - 8064\sin(v)(\cos(v))^6 \\
& + 18432\sin(v)(\cos(v))^8 - 3024\sin(v)(\cos(v))^4 - 27648(\cos(v))^9 v \\
& + 672(\cos(v))^8 v^3 - 36288(\cos(v))^8 v + 1736(\cos(v))^8 v^5 + 2688(\cos(v))^7 v^3 \\
& + 8960(\cos(v))^7 v^5 + 27360(\cos(v))^7 v + 4704(\cos(v))^6 v^3 \\
& + 68544(\cos(v))^6 v + 3780(\cos(v))^5 v + 3696(\cos(v))^5 v^3 + 26180(\cos(v))^5 v^5 \\
& - 1092(\cos(v))^4 v^3 - 46728(\cos(v))^4 v + 20363(\cos(v))^4 v^5 \\
& + 8078(\cos(v))^3 v^5 - 4872(\cos(v))^3 v^3 - 13932(\cos(v))^3 v \\
& + 168(\cos(v))^2 v^5 - 9216\sin(v)(\cos(v))^{10} - 26208\sin(v)(\cos(v))^5 \\
& + 10224\sin(v)(\cos(v))^3 + 2160\sin(v)(\cos(v))^2 + 6912(\cos(v))^{11} v \\
& + 4608(\cos(v))^{10} v + 3528v\cos(v) + 10260v(\cos(v))^2 - 882v^5\cos(v) - 1512\cos(v)v^3 \\
& - 4032(\cos(v))^2 v^3 - 1296\cos(v)\sin(v) + 13248\sin(v)(\cos(v))^6 v^2 \\
& - 8604\sin(v)v^2(\cos(v))^2 + 1536\sin(v)(\cos(v))^{10} v^2 - 2784\sin(v)(\cos(v))^7 v^2 \\
& - 4608\sin(v)(\cos(v))^8 v^2 + 768\sin(v)(\cos(v))^9 v^2 + 2232\sin(v)v^2\cos(v) \\
& - 3048\sin(v)(\cos(v))^4 v^2 - 20796\sin(v)(\cos(v))^3 v^2 + 20472\sin(v)(\cos(v))^5 v^2
\end{aligned}$$

$$T_{22} = (\cos(v))^8 - 2(\cos(v))^7 - 2(\cos(v))^6 + 6(\cos(v))^5 - 6(\cos(v))^3 + 2(\cos(v))^2 + 2\cos(v) - 1$$

$$b_1 = \frac{1}{96}\frac{T_{23}}{v^5 T_{22}} \tag{27}$$

$$\begin{aligned}
T_{23} = {} & -756v - 528\sin(v) - 420v^3 - 19968\sin(v)(\cos(v))^9 + 52608\sin(v)(\cos(v))^7 \\
& + 2860\sin(v)v^2 - 12096\sin(v)(\cos(v))^6 + 26112\sin(v)(\cos(v))^8 - 5376\sin(v)(\cos(v))^4 \\
& - 42624(\cos(v))^9 v + 672(\cos(v))^8 v^3 - 75456(\cos(v))^8 v + 2072(\cos(v))^8 v^5 \\
& + 4032(\cos(v))^7 v^3 + 12432(\cos(v))^7 v^5 + 45360(\cos(v))^7 v + 8400(\cos(v))^6 v^3 \\
& + 124992(\cos(v))^6 v + 32620(\cos(v))^6 v^5 + 7056(\cos(v))^5 v + 6720(\cos(v))^5 v^3 \\
& + 45920(\cos(v))^5 v^5 - 1596(\cos(v))^4 v^3 - 79776(\cos(v))^4 v \\
& + 35399(\cos(v))^4 v^5 + 13454(\cos(v))^3 v^5 - 7896(\cos(v))^3 v^3 - 25668(\cos(v))^3 v \\
& + 924(\cos(v))^2 v^5 - 12288\sin(v)(\cos(v))^{10} - 47712\sin(v)(\cos(v))^5 + 17328\sin(v)(\cos(v))^3 \\
& + 4176\sin(v)(\cos(v))^2 + 9216(\cos(v))^{11} v + 13824(\cos(v))^{10} v + 6660v\cos(v) + 17172v(\cos(v))^2 \\
& - 1246v^5\cos(v) - 2856\cos(v)v^3 - 7056(\cos(v))^2 v^3 - 2256\cos(v)\sin(v) + 37400\sin(v)(\cos(v))^5 v^2 \\
& + 23904\sin(v)(\cos(v))^6 v^2 + 2048\sin(v)(\cos(v))^{10} v^2 - 8192\sin(v)(\cos(v))^8 v^2 \\
& - 16560\sin(v)v^2(\cos(v))^2 - 9056\sin(v)(\cos(v))^7 v^2 + 2944\sin(v)(\cos(v))^9 v^2 \\
& - 35348\sin(v)(\cos(v))^3 v^2 + 4096\sin(v)v^2\cos(v) - 4096\sin(v)(\cos(v))^4 v^2 - 455v^5
\end{aligned}$$

$$b_2 = -\frac{1}{24}\frac{T_{24}}{v^5 T_{22}} \tag{28}$$

$$\begin{aligned}
T_{24} = {} & -144v - 800\sin(v)(\cos(v))^8 v^2 + 4140(\cos(v))^5 v - 60v^3 - 49v^5 + 2712\sin(v)(\cos(v))^6 v^2 \\
& - 3032\sin(v)(\cos(v))^7 v^2 + 7604\sin(v)(\cos(v))^5 v^2 + 128\sin(v)(\cos(v))^{10} v^2 \\
& - 6080\sin(v)(\cos(v))^3 v^2 + 832\sin(v)(\cos(v))^9 v^2 + 712\sin(v)v^2\cos(v) \\
& - 3168\sin(v)v^2(\cos(v))^2 + 572\sin(v)(\cos(v))^4 v^2 - 96\sin(v) - 3840\sin(v)(\cos(v))^9 \\
& + 9696\sin(v)(\cos(v))^7 + 520\sin(v)v^2 + 432\sin(v)(\cos(v))^6 + 1344\sin(v)(\cos(v))^8 \\
& - 1776\sin(v)(\cos(v))^4 - 3600(\cos(v))^9 v - 24(\cos(v))^8 v^3 - 15120(\cos(v))^8 v \\
& + 384(\cos(v))^7 v^3 + 1036(\cos(v))^7 v^5 + 2844(\cos(v))^7 v + 1224(\cos(v))^6 v^3 + 22320(\cos(v))^6 v \\
& + 4046(\cos(v))^6 v^5 + 1200(\cos(v))^5 v^3 + 6664(\cos(v))^5 v^5 + 84(\cos(v))^4 v^3 \\
& - 13356(\cos(v))^4 v + 5929(\cos(v))^4 v^5 + 2674(\cos(v))^3 v^5 - 1032(\cos(v))^3 v^3 \\
& - 5184(\cos(v))^3 v + 154(\cos(v))^2 v^5 - 768\sin(v)(\cos(v))^{10} - 8400\sin(v)(\cos(v))^5 \\
& + 2928\sin(v)(\cos(v))^3 + 864\sin(v)(\cos(v))^2 + 576(\cos(v))^{11} v + 3456(\cos(v))^{10} v + 1224v\cos(v) \\
& + 2844v(\cos(v))^2 - 294v^5\cos(v) - 552\cos(v)v^3 - 1224(\cos(v))^2 v^3 - 384\cos(v)\sin(v)
\end{aligned}$$

$$b_3 = \frac{1}{192}\frac{T_{25}}{v^5 T_{22}} \tag{29}$$

$$\begin{aligned}
T_{25} = {} & -684v + 3072\sin(v)(\cos(v))^8 v^2 + 2304\sin(v)(\cos(v))^9 v^2 - 14616\sin(v)v^2(\cos(v))^2 \\
& - 6336\sin(v)(\cos(v))^6 v^2 - 26460\sin(v)(\cos(v))^3 v^2 + 2640\sin(v)v^2\cos(v) \\
& - 14592\sin(v)(\cos(v))^7 v^2 + 15600\sin(v)(\cos(v))^4 v^2 + 36000\sin(v)(\cos(v))^5 v^2 \\
& - 9216\sin(v)(\cos(v))^9 + 27648\sin(v)(\cos(v))^7 + 2388\sin(v)v^2 \\
& + 21888\sin(v)(\cos(v))^6 - 9216\sin(v)(\cos(v))^8 - 16992\sin(v)(\cos(v))^4 + 6912(\cos(v))^9 v \\
& - 384(\cos(v))^8 v^3 - 48384(\cos(v))^8 v + 768(\cos(v))^7 v^3 - 32544(\cos(v))^7 v \\
& + 2784(\cos(v))^6 v^3 + 80064(\cos(v))^6 v + 6216(\cos(v))^6 v^5 + 49464(\cos(v))^5 v \\
& + 19936(\cos(v))^5 v^5 + 3108(\cos(v))^4 v^3 - 52200(\cos(v))^4 v \\
& + 23023(\cos(v))^4 v^5 + 11158(\cos(v))^3 v^5 - 888(\cos(v))^3 v^3 - 29268(\cos(v))^3 v \\
& + 1456(\cos(v))^2 v^5 - 28800\sin(v)(\cos(v))^5 + 11952\sin(v)(\cos(v))^3 \\
& + 4752\sin(v)(\cos(v))^2 + 9216(\cos(v))^{10} v + 5436v\cos(v) \\
& + 11988v(\cos(v))^2 - 854v^5\cos(v) - 2952\cos(v)v^3 - 5472(\cos(v))^2 v^3 \\
& - 1584\cos(v)\sin(v) - 455v^5 - 36v^3 + 3072(\cos(v))^5 v^3 - 432\sin(v) \quad .
\end{aligned}$$

For small values of $|v|$ the formulae given by (26)–(29) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned}
b_0 = {} & \frac{18117277}{5702400} - \frac{547336457}{370656000}v^2 + \frac{3962346469}{8895744000}v^4 - \frac{116550460207}{1488647160000}v^6 \\
& + \frac{83803131439129}{9654373048320000}v^8 - \frac{420395172804467}{682702094131200000}v^{10} + \frac{607852721579988701}{18465726242060697600000}v^{12} \\
& - \frac{361940606600619341}{3600816617201836032000000}v^{14} + \frac{27619257622207333}{4489329808459431936000000}v^{16} + \cdots \\
b_1 = {} & -\frac{10081177}{11404800} + \frac{547336457}{444787200}v^2 - \frac{18717059431}{53374464000}v^4 + \frac{27383413801}{476367091200}v^6 \\
& - \frac{1035327626828773}{173778714869760000}v^8 + \frac{4645144731473}{10923233506099200}v^{10} - \frac{770986892016568637}{36931452484121395200000}v^{12} \\
& + \frac{261424539473820839}{3086414243315859456000000}v^{14} - \frac{5710129260292811569}{34567839525137625907200000}v^{16} + \cdots \\
b_2 = {} & \frac{6056249}{2851200} - \frac{547336457}{778377600}v^2 + \frac{1403003699}{8491392000}v^4 - \frac{2021599429}{95273418240}v^6 + \frac{536896133041987}{304112751022080000}v^8 \\
& - \frac{26719018155653}{223016017416192000}v^{10} + \frac{3323984311926673}{710222040079257600000}v^{12} - \frac{76743438942516257}{236303590503870489600000}v^{14} \\
& - \frac{7108094900546776489}{604937191689908453376000000}v^{16} + \cdots \\
b_3 = {} & -\frac{8790917}{22809600} + \frac{547336457}{2075673600}v^2 - \frac{9959676119}{249080832000}v^4 + \frac{757223293}{272209766400}v^6 - \frac{44881181749919}{270322445352960000}v^8 \\
& - \frac{1147417492703}{5352384417988608000}v^{10} - \frac{6888378190068871}{10551843566891827200000}v^{12} - \frac{33024377725008451}{43836028383326699520000}v^{14} \\
& - \frac{7084715188436265629}{691356790502752518144000000}v^{16} + \cdots .
\end{aligned} \tag{30}$$

The behaviour of the coefficients is given in the following Fig. 2.
The local truncation error of the new proposed method is given by:

$$\mathrm{LTE} = -\frac{547336457h^{14}}{373621248000}\left(y_n^{(14)} + 4\omega^2 y_n^{(12)} + 6\omega^4 y_n^{(10)} + 4\omega^6 y_n^{(8)} + \omega^8 y_n^{(6)}\right). \tag{31}$$

4. Comparative error analysis

We will study the following methods:

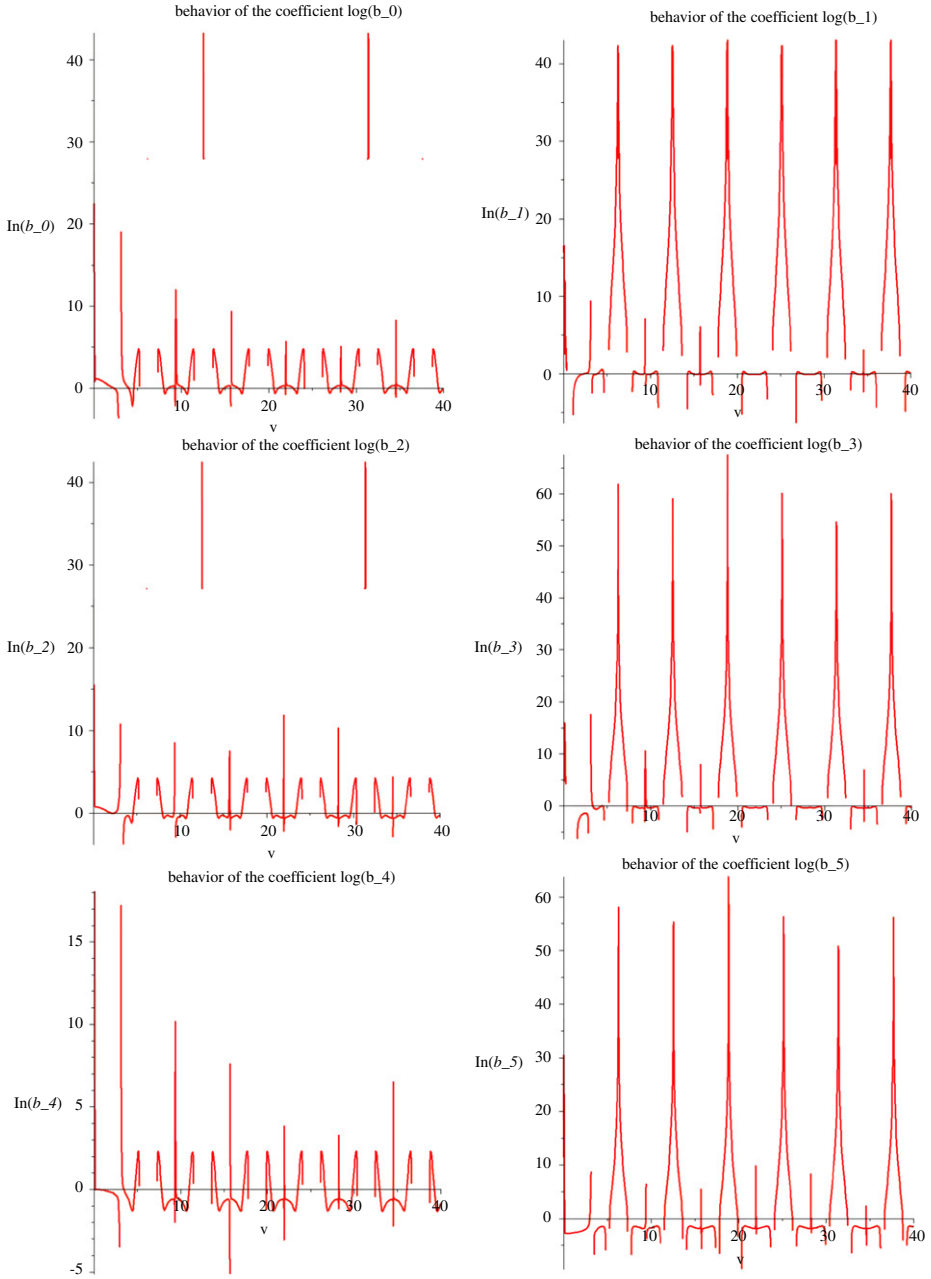

Fig. 1. Behaviour of the coefficients of the new proposed method developed in Section 3.2 for several values of v.

- The eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] which is indicated as QT10.
- The ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] which is indicated as QT12.
- The twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21] which is indicated as QT14.
- The classical ten-step method of the family of methods mentioned in paragraph 3 which is indicated as CL.
- The method with vanished phase-lag produced by Alolyan and Simos [23] which is indicated as PF.
- The method with vanished phase-lag and its first derivative produced by Alolyan and Simos [23] which is indicated as PFDF.
- The new developed ten-step method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 3.2 which is indicated as PFDF12.
- The new developed ten-step method with phase-lag and its first, second and third derivatives equal to zero obtained in paragraph 3.3 which is indicated as PFDF123.

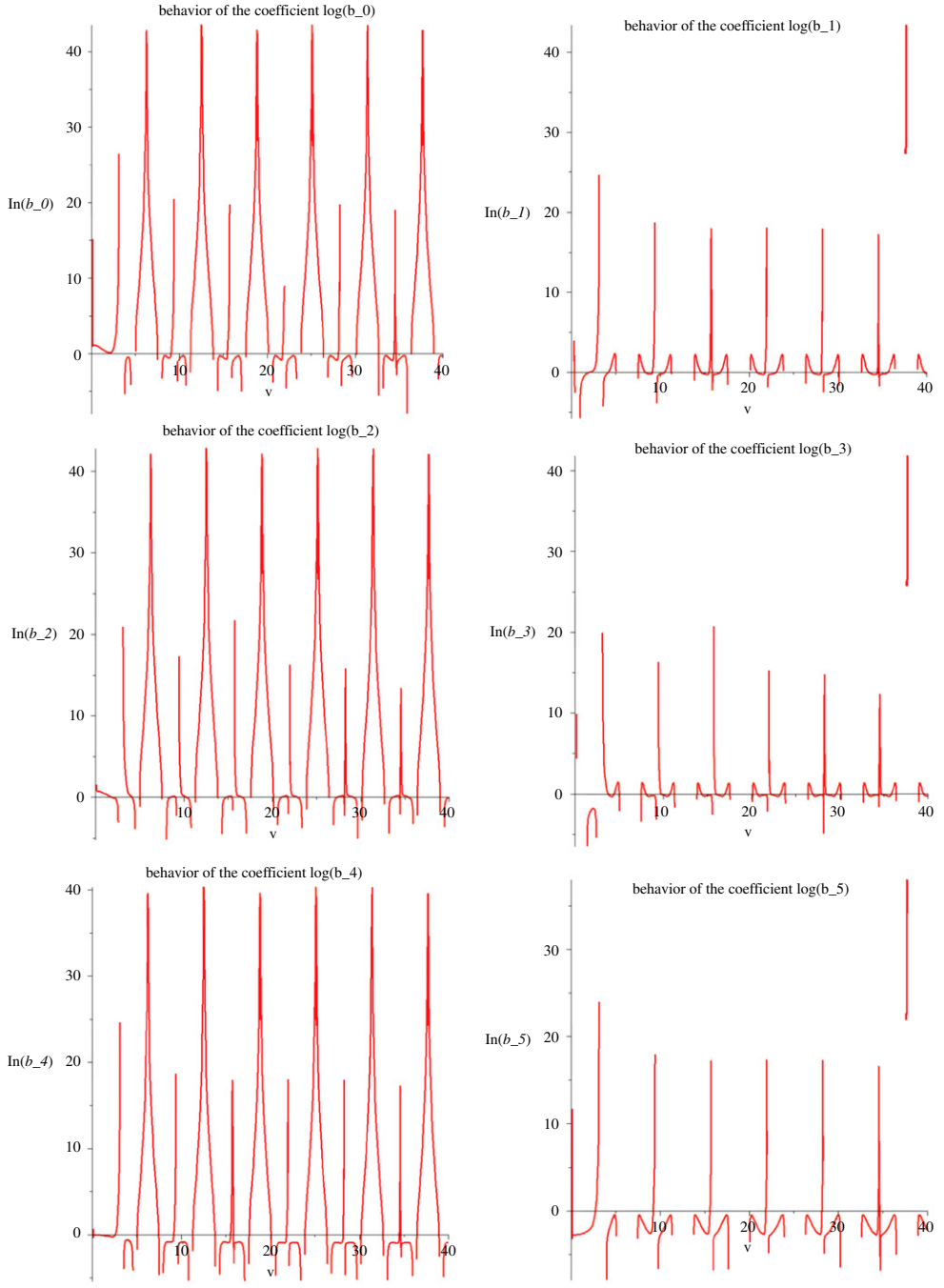

Fig. 2. Behaviour of the coefficients of the new proposed method developed in Section 3.3 for several values of v.

The error analysis is based on the following steps:

- The one-dimensional time independent Schrödinger equation is of the form

$$y''(x) = f(x)y(x). \tag{32}$$

- The function $f(x)$ is written in the form (based on the paper of Ixaru and Rizea [26]):

$$f(x) = g(x) + G \tag{33}$$

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

- Our analysis is also based on the expression of the derivatives $y_n^{(i)},\ i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of Eq. (32). The expressions are presented as polynomials of G.
- Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae.

Based on the procedure mentioned above and on the formulae:

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

we obtain the expressions mentioned below.

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

- The Energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in G are considered. Thus for these values of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G, are the same for the cases of the classical method and of the new developed methods.
- $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number.

So, we have the following asymptotic expansions of the equations produced from the Local Truncation errors and based on the above procedure.

The eight-step tenth algebraic order method developed by Quinlan and Tremaine [21]*—for the analysis of the Local Truncation Error see* [24]

$$\mathrm{LTE}_{\mathrm{QT10}} = h^{10}\left(-\frac{45767}{725760}\mathrm{y}(x)G^5 + \cdots\right). \tag{34}$$

The ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21]*—for the analysis of the Local Truncation Error see* [24]

$$\mathrm{LTE}_{\mathrm{QT12}} = h^{12}\left(-\frac{52559}{912384}\mathrm{y}(x)G^6 + \cdots\right). \tag{35}$$

The twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21]*—for the analysis of the Local Truncation Error see* [24]

$$\mathrm{LTE}_{\mathrm{QT14}} = h^{14}\left(-\frac{16301796103}{290594304000}\mathrm{y}(x)G^7 + \cdots\right). \tag{36}$$

The Classical Case of the Family[3] [23] *which is indicated as* CL

$$\mathrm{LTE}_{\mathrm{CL}} = h^{14}\left(-\frac{547336457}{373621248000}y(x)G^7 + \cdots\right). \tag{37}$$

The method with vanished phase-lag produced by Alolyan and Simos [23] *which is indicated as* PF

$$\mathrm{LTE}_{\mathrm{PF}} = h^{14}\left(-\frac{547336457}{373621248000}g(x)y(x)G^6 + \cdots\right). \tag{38}$$

[3] *Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.*

The method with vanished phase-lag and its first derivative produced by Alolyan and Simos [23] *which is indicated as* PFDF

$$\mathrm{LTE}_{\mathrm{PFDF}} = h^{14}\left[\left(-\frac{547336457}{17791488000}\left(\frac{d^2}{dx^2}g(x)\right)y(x) - \frac{547336457}{373621248000}\left(g(x)\right)^2 y(x) - \frac{547336457}{186810624000}\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}y(x)\right)G^5 + \cdots\right]. \tag{39}$$

The method with vanished phase-lag and its first and second derivatives developed in Section 3.2

$$\mathrm{LTE}_{\mathrm{PFDF12}} = h^{14}\left[\left(-\frac{547336457}{93405312000}\left(\frac{d^2}{dx^2}g(x)\right)y(x)\right)G^5 + \cdots\right]. \tag{40}$$

The method with vanished phase-lag and its first, second and third derivatives developed in Section 3.3

$$\mathrm{LTE}_{\mathrm{PFDF123}} = h^{14}\left[\left(-\frac{547336457}{6227020800}\left(\frac{d^4}{dx^4}g(x)\right)y(x) - \frac{547336457}{46702656000} \times \left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}y(x) - \frac{547336457}{31135104000}\left(\frac{d}{dx}g(x)\right)^2 y(x) - \frac{547336457}{23351328000}g(x)y(x)\frac{d^2}{dx^2}g(x)\right)G^4 + \cdots\right]. \tag{41}$$

From the above equations and Table 1 we have the following theorem:

Theorem 2.
- *For the eight-step tenth algebraic order method developed by Quinlan and Tremaine* [21] *the error increases as the fifth power of G.*
- *For the ten-step twelfth algebraic order method developed by Quinlan and Tremaine* [21] *the error increases as the sixth power of G.*
- *For the twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine* [21] *the error increases as the seventh power of G.*
- *For the twelfth algebraic order Classical Method of the Family (see* [23] *for more details) the error increases as the seventh power of G.*
- *For the twelfth algebraic order ten-step method* PF *produced by Alolyan and Simos* [23] *the error increases as the sixth power of G.*
- *For the twelfth algebraic order ten-step method* PFDF *produced by Alolyan and Simos* [23] *the error increases as the fifth power of G.*
- *For the twelfth algebraic order ten-step method* PFDF12 *produced in this paper (Section* 3.2*) the error increases as the fifth power of G.*
- *For the twelfth algebraic order ten-step method* PFDF123 *produced in this paper (Section* 3.3*) the error increases as the fourth power of G.*

So, for the numerical solution of the time independent radial Schrödinger equation the new proposed method produced in this paper (Section 3.3*) is the most accurate Method, especially for large values of* $|G| = |V_c - E|$*, since it is of a twelfth algebraic order method for which the error increases as the fourth power of G.*

5. Stability analysis

In this section we will present the stability analysis for the new method which is based on the following algorithm:

1. Application of the Proposed Method to the Scalar Test Equation.
2. Definition of the Difference Equation and the Corresponding Characteristic Equation.
3. Development of the $s - \mathrm{v}$ Plane and production of the appropriate diagrams.
4. Remarks and Conclusions.

Based on the above algorithm we have the following analysis:
The method developed in Section 3.2 or the method obtained in Section 3.3, is applied to the scalar test equation:

$$\psi'' = -t^2\psi, \tag{42}$$

where $t \neq \omega$.

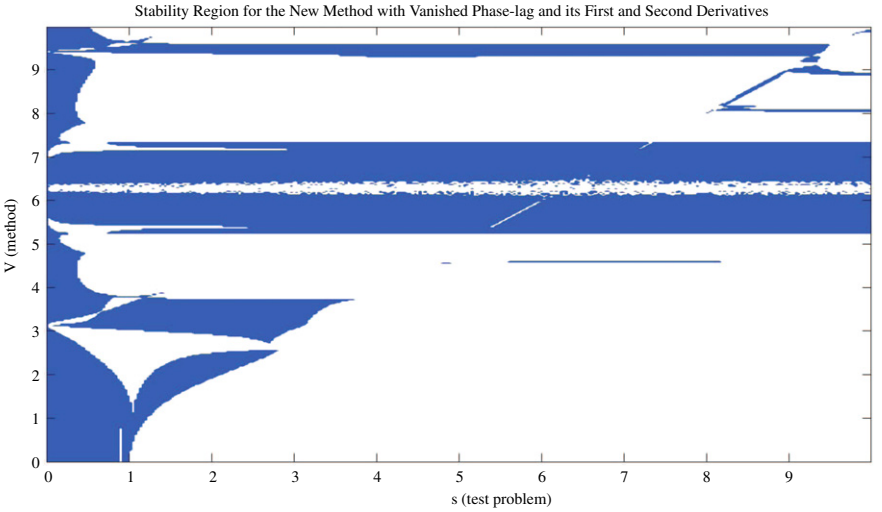

Fig. 3. $s-\mathrm{v}$ plane of the new proposed method of the family developed in Section 3.1 (mentioned as PFDF12).

We obtain the following difference equation:

$$A_k(s,\mathrm{v})\psi_{n+k}+\cdots+A_1(s,\mathrm{v})\psi_{n+1}+A_0(s,\mathrm{v})\psi_n+A_1(s,\mathrm{v})\psi_{n-1}+\cdots+A_k(s,\mathrm{v})\psi_{n-k}=0 \tag{43}$$

where $s=th$, h is the step length and $A_0(s,\mathrm{v}), A_1(s,\mathrm{v}),\ldots,A_k(s,\mathrm{v})$ are polynomials of s and $\mathrm{v}=\omega h$ and $k=5$.

The characteristic equation associated with (43) is given by:

$$A_k(s,\mathrm{v})\vartheta^k+\cdots+A_1(s,\mathrm{v})\vartheta+A_0(s,\mathrm{v})+A_1(s,\mathrm{v})\vartheta^{-1}+\cdots+A_k(s,\mathrm{v})\vartheta^{-k}=0. \tag{44}$$

Definition 3 (*See [27]*)**.** A symmetric $2k$-step method with the characteristic equation given by (44) is said to have an *interval of periodicity* $\left(0,s_0^2\right)$ if, for all $s\in\left(0,s_0^2\right)$, the roots z_i, $i=1,2$ satisfy

$$z_{1,2}=e^{\pm i\zeta(th)},\quad |z_i|\leq 1,\ i=3,4 \tag{45}$$

where $\zeta(th)$ is a real function of th and $s=th$.

Definition 4 (*See [27]*)**.** A method is called P-stable if its interval of periodicity is equal to $(0,\infty)$.

Definition 5. A method is called singularly almost P-stable if its interval of periodicity is equal to $(0,\infty)-S$[4] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $\mathrm{v}=s$.

In Figs. 3 and 4 we present the $s-\mathrm{v}$ plane for the methods developed in this paper. A shadowed area denotes the $s-\mathrm{v}$ region where the method is stable, while a white area denotes the region where the method is unstable.

Remark 2. For the solution of the Schrödinger equation the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to observe the surroundings of the first diagonal of the $s-\mathrm{v}$ plane.

In the case that the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $\mathrm{v}=s$ (i.e. see the surroundings of the first diagonal of the $s-\mathrm{v}$ plane), it is easy to see that the interval of periodicity of the new methods is equal to: $(0,6.6)$ for the method developed in Section 3.2 and $(0,3.6)$ for the method developed in Section 3.3.

From the above analysis we have the following theorem:

Theorem 3.
- *The method developed in Section 3.2 is of twelfth algebraic order, has the phase-lag and its first and second derivatives equal to zero and has an interval of periodicity equal to:* $(0,6.6)$.
- *The method developed in Section 3.3 is of twelfth algebraic order, has the phase-lag and its first, second and third derivatives equal to zero and has an interval of periodicity equal to:* $(0,3.6)$.

Based on the analysis presented above, we studied the interval of periodicity of the eight methods mentioned in the previous paragraph. The results are presented in Table 2.

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

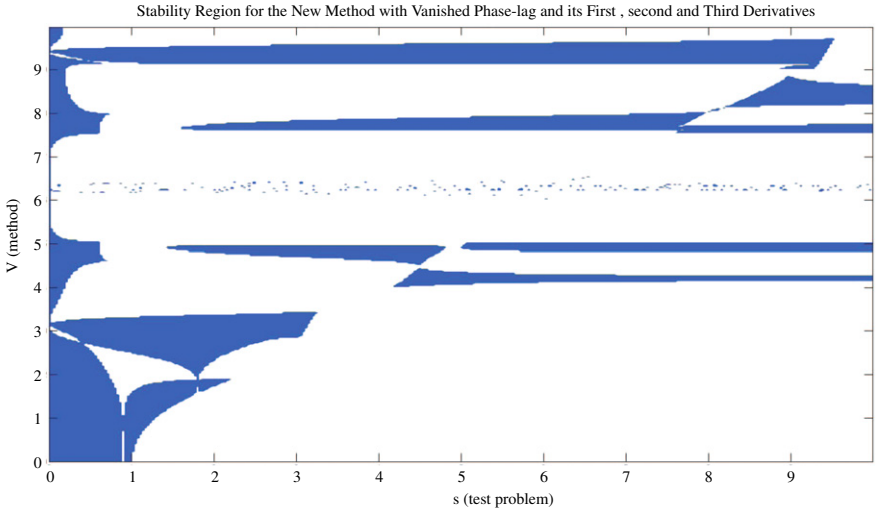

Fig. 4. $s-$ v plane of the new proposed method of the family developed in Section 3.2 (mentioned as PFDF123).

Table 1
Comparative error analysis for the methods mentioned in Section 4. We note that *CFAE* is the coefficient of the maximum power of G in the asymptotic expansion and Order of G is the order of G in the asymptotic expansion of the Local Truncation Error.

Method	Algebraic order	Order of G	CFAE
QT10	8	5	$-\frac{45767}{725760}$
QT12	10	6	$-\frac{52559}{912384}$
QT14	12	7	$-\frac{16301796103}{290594304000}$
CL	12	7	$-\frac{547336457}{373621248000}$
PF	12	6	$-\frac{547336457}{373621248000}$
PFDF	12	5	$-\frac{547336457}{17791488000}$
PFDF12	12	5	$-\frac{547336457}{93405312000}$
PFDF123	12	4	$-\frac{547336457}{6227020800}$

Table 2
Comparative stability analysis for the methods mentioned in Section 5.

Method	Interval of periodicity
QT10	(0, 0.52)
QT12	(0, 0.17)
QT14	(0, 0.046)
CL	(0, 0.8)
PF (see [23])	(0, 1.2)
PFDF (see [23])	(0, 1.5)
PFDF12 (see Section 3.2)	(0, 6.6)
PFDF123 (see Section 3.3)	(0, 3.6)

6. Numerical results—conclusion

The illustration of the efficiency of the new proposed methods obtained in Section 3 is examined by their application to the one-dimensional time independent Schrödinger equation.

In order to apply the new methods to the radial Schrödinger equation the value of parameter v is needed. For every problem of the radial Schrödinger equation given by (1) the parameter v is given by

$$\mathrm{v} = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{46}$$

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

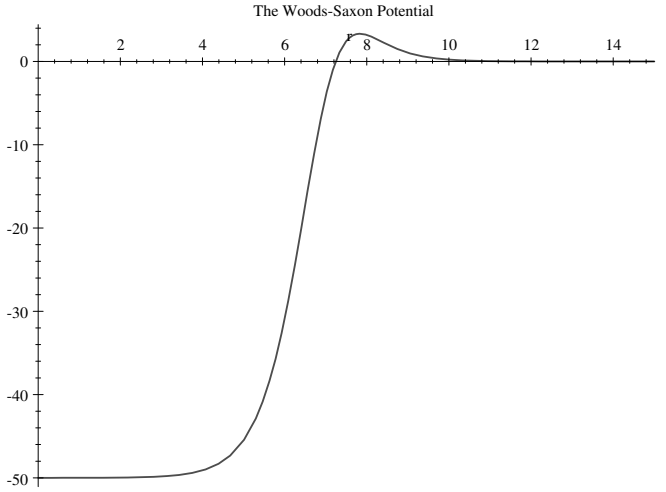

Fig. 5. The Woods–Saxon potential.

6.1. Woods–Saxon potential

In our example the well known Woods–Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a(1+z)^2} \tag{47}$$

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

The behaviour of the Woods–Saxon potential is shown in Fig. 5.

It is well known that for some potentials, such as the Woods–Saxon potential, the definition of parameter v is not given as a function of x but it is based on some critical points which have been defined from the investigation of the appropriate potential (see for details [28]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [28]):

$$\mathrm{v} = \begin{cases} \sqrt{-50+E}, & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } x = 6.5-h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5+h \\ \sqrt{E}, & \text{for } x \in [6.5+2h, 15]. \end{cases} \tag{48}$$

6.2. Radial Schrödinger equation—the resonance problem

We consider the numerical solution of the one-dimensional time independent Schrödinger equation (1) in the well-known case of the Woods–Saxon potential (47). For the numerical solution of the above problem we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical example we take the domain of integration as $x \in [0, 15]$. We consider Eq. (1) in a rather large domain of energies, i.e. $E \in [1, 1000]$.

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

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{49}$$

for x greater than some value X.

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

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{50}$$

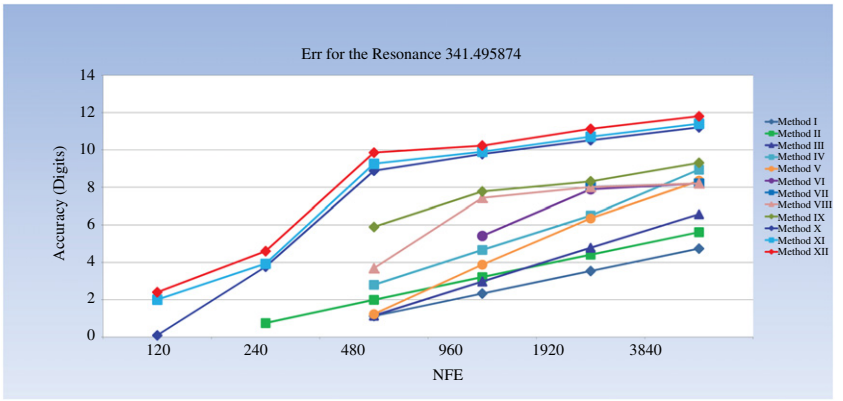

Fig. 6. Accuracy (Digits) for several values of NFE for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0.

where δ_l is the phase shift, that is calculated from the formula

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{51}$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need $y_0, y_i,\ i = 1(1)9$ before starting a ten-step method. From the initial condition we obtain y_0. The other values can be obtained using the Runge–Kutta–Nyström methods of Dormand et al. (see [29]). With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l.

For positive energies we have the so-called resonance problem. This problem consists either of finding the phase-shift δ_l or finding those E, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$. We actually solve the latter problem, known as *the resonance problem* when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

$$y(0) = 0, \qquad y(x) = \cos\left(\sqrt{E}x\right) \quad \text{for large } x. \tag{52}$$

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

- Numerov's method which is indicated as *Method* I.
- The Exponentially-fitted two-step method developed by Raptis and Allison [18] which is indicated as *Method* II.
- The Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] which is indicated as *Method* III.
- The Exponentially-fitted four-step method developed by Raptis [20] which is indicated as *Method* IV.
- The eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] which is indicated as *Method* V.
- The ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] which is indicated as *Method* VI.
- The twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21] which is indicated as *Method* VII.
- The classical ten-step method of the family of methods mentioned in paragraph 3 of [23] which is indicated as *Method* VIII.
- The ten-step method with phase-lag equal to zero (phase-fitted) obtained in [23] which is indicated as *Method* IX.
- The ten-step method with phase-lag and its first derivative equal to zero obtained in [23] which is indicated as *Method* X.
- The new developed ten-step method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 3.2 which is indicated as *Method* XI.
- The new developed ten-step method with phase-lag and its first, second and third derivatives equal to zero obtained in paragraph 3.3 which is indicated as *Method* XII.

The computed eigenenergies are compared with exact ones. In Fig. 6 we present the maximum absolute error $\log_{10}(\text{Err})$ where

$$\text{Err} = |E_{\text{calculated}} - E_{\text{accurate}}| \tag{53}$$

the eigenenergy $E_2 = 341.495874$, for several values of NFE = Number of Function Evaluations. In Fig. 7 we present the maximum absolute error $\log_{10}(\text{Err})$ where

$$\text{Err} = |E_{\text{calculated}} - E_{\text{accurate}}| \tag{54}$$

of the eigenenergy $E_3 = 989.701916$, for several values of NFE = Number of Function Evaluations.

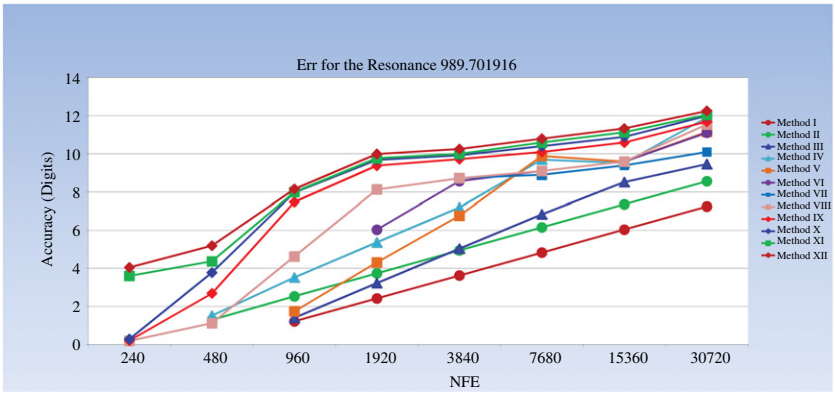

Fig. 7. Accuracy (Digits) for several values of NFE for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0.

7. Remarks – conclusions – summaries

7.1. Remarks and conclusions

The purpose of this paper was the development of two ten-step twelfth algebraic order methods with the following characteristics:

- The first method is a ten-step twelfth algebraic order method with phase-lag and its first and second derivatives equal to zero and with an interval of periodicity equal to: (0, 6.6).
- The second method is a ten-step twelfth algebraic order method with phase-lag and its first, second and third derivatives equal to zero and with an interval of periodicity equal to: (0, 3.6).

We have applied the new methods to the resonance problem of the one-dimensional Schrödinger equation.
Based on the results presented above we have the following conclusions:

- The Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) is more efficient than Numerov's Method (denoted as Method I) and for a low number of function evaluations is more efficient than the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III).
- The Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III) is more efficient than the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) for a high number of function evaluations.
- The Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III).
- The eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method V) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III) and less efficient than the Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV).
- The ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VI) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III) and the Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV) for a small number of function evaluations.
- The twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VII) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV) for a small number of function evaluations, the eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method V) for a small number of function evaluations and the ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VI) for a small number of function evaluations.

- The classical ten-step method of the family of methods mentioned in paragraph 3 (denoted as Method VIII) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III). The method is also more efficient than the Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV) for small number of function evaluations, the eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method V) for a small number of function evaluations, the ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VI) for a small number of function evaluations and the twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VII) for a small number of function evaluations.
- The ten-step phase-fitted method of the family of methods developed in [23] (denoted as Method IX) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV), the eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method V), the ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VI), the twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VII) and the classical ten-step method of the family of methods mentioned in paragraph 3 (denoted as Method VIII).
- The ten-step method of the family of methods with vanished phase-lag and its first derivative developed in [23] (denoted as Method X) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV), the eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method V), the ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VI), the twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VII) and the classical ten-step method of the family of methods mentioned in paragraph 3 (denoted as Method VIII) and the ten-step phase-fitted method of the family of methods developed in [23] (denoted as Method IX).
- The ten-step method of the family of methods with vanished phase-lag and its first and second derivatives developed in paragraph 3.2 (denoted as Method XI) is more efficient than the Numerov Method (denoted as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [18] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogiratou and Simos [19] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [20] (denoted as Method IV), the eight-step tenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method V), the ten-step twelfth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VI), the twelve-step fourteenth algebraic order method developed by Quinlan and Tremaine [21] (denoted as Method VII) and the classical ten-step method of the family of methods mentioned in paragraph 3 (denoted as Method VIII), the ten-step phase-fitted method of the family of methods developed in [23] (denoted as Method IX) and the ten-step method of the family of methods with vanished phase-lag and its first derivative developed in [23] (denoted as Method X).
- Finally, the ten-step method of the family of methods with vanished phase-lag and its first, second and third derivatives developed in paragraph 3.3 (denoted as Method XII) is much more efficient than all the other methods.

7.2. Summaries on the properties of the numerical methods

From the analysis presented above (comparative error analysis and comparative stability analysis) and from the numerical results presented above, the following summaries on the importance of the properties of the numerical methods are excluded:

- The dependence of the Algebraic Order of a Numerical Method and the parameter $G = V_c - E$ (where V_c is the constant approximation of the potential). For the same algebraic order it is important to have the minimal possible power of the parameter G. This is because in this case we have the minimal Local Truncation Error.
- The Phase-Lag and its derivatives must be equal to zero since this leads to the reduction of the power of G in the terms of the Local Truncation Error. Important is the phase-lag and as many as possible derivatives to vanish in order to have at least one order lower of the power of the parameter G than the previous known method of the same family.
- The Large Interval of Periodicity, as we have mentioned previously, does not play an important role for the numerical solution of this category of problems.

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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