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ORIGINAL PAPER

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

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Abstract In this paper we introduce a new explicit hybrid Numerov-type method. This method is of fourth algebraic order and has phase-lag and its first two derivatives equal to zero. We present a stability analysis and an error analysis based on the radial Schrödinger equation. Finally we apply the new proposed method to the resonance problem of the radial Schrödinger equation and we present the final conclusion based on the theoretical analysis and numerical results.

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

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1 Introduction

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

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

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

For the above equation (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.

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.[1]

In this paper we will use a recent methodology for the development of numerical methods for the approximate solution periodic initial-value problems. The new methodology is based on the requirement of vanishing the phase-lag and its derivatives. Based on this new methodology we will develop a two-step method which will have vanishing phase-lag and its first and second derivatives.

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

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

More specifically, we will develop a hybrid Numerov-type method with algebraic order six. The development of the new family of methods is based on the requirement of vanishing the phase-lag and its first and second derivatives.

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

We will give a comparative error analysis and a comparative stability analysis in order to study the efficiency of the new proposed method. Finally, we will apply the new method 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:

– A brief bibliography on the subject is presented in Sect. 2.
– In Sect. 3 we present the theory of the new methodology.
– In Sect. 4 we present the development of the new family of methods.
– A comparative error analysis is presented in Sect. 5.
– In Sect. 6 we will present a comparative stability analysis.
– The numerical results are presented in Sect. 7.
– Finally, in Sect. 8 remarks and conclusions are discussed.

2 Brief presentation of the literature on the subject

Large research on the algorithmic development of numerical methods for the solution of the Schrödinger equation has been done 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 [5–39]).

More specifically the last years:

– Phase-fitted methods and numerical methods with minimal phase-lag of Runge-Kutta and Runge-Kutta Nyström type have been developed in [10–26]. The research on this subject has as a scope the production of numerical methods of Runge-Kutta and Runge-Kutta Nyström type which have vanished the phase-lag and/or the amplification factor. More recently this research has also as a subject the vanishing of the derivatives of the phase-lag and/or the amplification factor of the above mentioned methods.
– In [27–35] exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are obtained. The main scope of this research subject is the development of numerical methods of Runge-Kutta and Runge-Kutta Nyström type which integrate exactly any linear combination of the functions:

$$\left\{1,\ x,\ x^2,\ x^3,\ x^m,\ \ldots,\ \exp(\pm w\,x),\ x\ \exp(\pm w\,x),\right.$$
$$\left.x^2\ \exp(\pm w\,x),\ \ldots,\ x^p\ \exp(\pm w\,x)\right\} \tag{3}$$

or the functions:

$$\left\{1,\ x,\ x^2,\ x^3,\ x^m,\ \ldots,\ \cos(w\,x),\ \sin(w\,x),\ x\ \cos(w\,x),\right.$$
$$\left.x\ \sin(w\,x),\ x^2\ \cos(w\,x),\ x^2\ \sin(w\,x),\ldots,\ x^p\ \cos(w\,x),\ x^p\ \sin(w\,x),\right\} \tag{4}$$

- Multistep phase-fitted methods and multistep methods with minimal phase-lag are developed in [40–68]. The research on this subject has as a scope the production of numerical nultistep methods of several type (linear, predictor-corrector, hybrid etc.) which have vanished the phase-lag. More recently this research has also as a subject the vanishing of the derivatives of the phase-lag of the above mentioned methods. Recently also some techniques which can optimize these methods are also obtained.
- Symplectic integrators are studied in [69–95]. The research on this subject has as a scope the production of numerical methods (Runge-Kutta and Runge-Kutta Nyström, Partitioned Runge-Kutta, differential schemes based on well known integration formulae etc.) which satisfy the symplectic properties.
- Exponentially and trigonometrically multistep methods have been developed in [96–121]. The main scope of this research subject is the development of numerical multistep methods of several type (linear, predictor-corrector, hybrid etc.) which integrate exactly any linear combination of the functions (3) or (4). We note here that recently [122] an exponentially-fitted method for the time dependent Schrödinger equation was obtained.
- Several pseudospectral methods have been studied and developed [123]
- New function fitting methods [124]
- Review papers have been written in [127–129]

We note that other special new methods have also been obtained most recently (see [125] and [126]) which will be applied in the future on the numerical solution of the Schrödinger equation and related problems.

3 Phase-lag analysis of symmetric multistep methods

In this section we present the phase-lag analysis of symmetric multistep methods. The phase-lag analysis is based on the the following steps:

- We consider a 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:

$$\phi'' = f(r, \phi) \tag{5}$$

- Since the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}, \;\; i = 0(1)\lfloor \frac{m}{2} \rfloor$.
- We apply the symmetric $2k$-step method, that is for $i = -k(1)k$, to the scalar test equation

$$\phi'' = -\omega^2 \phi \tag{6}$$

- The result of the above application is a difference equation of the form

$$\begin{aligned} &A_k(\mathrm{v})\,\phi_{n+k} + \cdots + A_1(\mathrm{v})\,\phi_{n+1} + A_0(\mathrm{v})\,\phi_n \\ &+A_1(\mathrm{v})\,\phi_{n-1} + \cdots + A_k(\mathrm{v})\,\phi_{n-k} = 0 \end{aligned} \tag{7}$$

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 (7) is given by:

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

– Therefore, we have the following theorem

Theorem 1 [41] *The symmetric $2k$-step method with characteristic equation given by (8) has phase-lag order r and phase-lag constant c given by*

$$-c\,\mathrm{v}^{r+2} + O(\mathrm{v}^{r+4}) = \frac{2\,A_k(\mathrm{v})\,\cos(k\,\mathrm{v}) + \cdots + 2\,A_j(\mathrm{v})\,\cos(j\,\mathrm{v}) + \cdots + A_0(\mathrm{v})}{2\,k^2\,A_k(\mathrm{v}) + \cdots + 2\,j^2\,A_j(\mathrm{v}) + \cdots + 2\,A_1(\mathrm{v})} \tag{9}$$

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

Remark 1 The Derivatives of the phase-lag for the multistep methods are computed based on the above direct formula (9).

4 The new family of hybrid Numerov-type low algebraic order methods

4.1 Development of the new method

In order to obtain the new method 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
   – three free parameters,
2. Computation of the Difference Equation and the Associated Characteristic Equation
3. Computation of the corresponding polynomials $A_i(\mathrm{v})$, $i = 0, 1$
4. Computation of the Corresponding Phase-lag
5. Computation of the Corresponding Derivatives of the Phase-lag (First Derivative in this case)
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 $\phi'' = f(x, \phi)$:

$$\begin{aligned}
\overline{\phi}_{n+1} &= -a_0\,\phi_n - \phi_{n-1} + a_1\,h^2\,\phi''_n \\
\widetilde{\phi}_{n+1} &= -b_0\,\phi_n - \phi_{n-1} + h^2\left[b_1\left(\overline{\phi}''_{n+1} + \phi''_{n-1}\right) + b_2\,\phi''_n\right] \\
\widehat{\phi}_n &= \phi_n - d_0\,h^2\,\left(\widetilde{\phi}''_{n+1} - 2\,\phi''_n + \phi''_{n-1}\right) \\
\phi_{n+1} + c_0\,\phi_n + \phi_{n-1} &= h^2\left[c_1\left(\widetilde{\phi}''_{n+1} + \phi''_{n-1}\right) + c_2\,\widehat{\phi}''_n\right]
\end{aligned} \tag{10}$$

4.2 The new method with vanished phase-lag and its first two derivatives

Requiring the above method (10) to have the maximum algebraic order with two free parameter, the following relations are obtained:

$$a_0 = -2,\ a_1 = 1,\ b_0 = -2,\ b_1 = \frac{1}{12},\ b_2 = \frac{5}{6},\ c_0 = -2 \tag{11}$$

The application of the above method to the scalar test equation (6) gives the following difference equation:

$$A_1(\mathrm{v})\left(\phi_{n+1} + \phi_{n-1}\right) + A_0(\mathrm{v})\,\phi_n = 0 \tag{12}$$

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

The characteristic equation associated with (12) is given by:

$$A_1(\mathrm{v})\left(\lambda + \lambda^{-1}\right) + A_0(\mathrm{v}) = 0 \tag{13}$$

where

$$\begin{aligned}
A_0(\mathrm{v}) &= -2 + \mathrm{v}^2\left[c_1\left(2 - \mathrm{v}^2\left(1 - \frac{1}{12}\,\mathrm{v}^2\right)\right)\right. \\
&\quad \left. + c_2\left(1 - d_0\mathrm{v}^4\left(1 - \frac{1}{12}\,\mathrm{v}^2\right)\right)\right] \\
A_1(\mathrm{v}) &= 1
\end{aligned} \tag{14}$$

By applying $k = 1$ in the formula (9), we have that the phase-lag is equal to:

$$\begin{aligned}
phl = \cos(\mathrm{v}) - 1 + \frac{1}{2}\,\mathrm{v}^2\left[c_1\left(2 - \mathrm{v}^2\left(1 - \frac{1}{12}\,\mathrm{v}^2\right)\right)\right. \\
\left. + c_2\left(1 - d_0\mathrm{v}^4\left(1 - \frac{1}{12}\,\mathrm{v}^2\right)\right)\right]
\end{aligned} \tag{15}$$

The phase-lag's first derivative is given by:

$$\begin{aligned} \dot{phl} = & -\sin(\mathrm{v}) + \mathrm{v}\left[c_1\left(2 - \mathrm{v}^2\left(1 - \frac{1}{12}\mathrm{v}^2\right)\right)\right. \\ & \left. + c_2\left(1 - d_0\mathrm{v}^4\left(1 - \frac{1}{12}\mathrm{v}^2\right)\right)\right] + \frac{1}{2}\mathrm{v}^2\left[c_1\left(-2\,\mathrm{v}\left(1 - \frac{1}{12}\mathrm{v}^2\right) + \frac{1}{6}\mathrm{v}^3\right)\right. \\ & \left. + c_2\left(-4\,d_0\mathrm{v}^3\left(1 - \frac{1}{12}\mathrm{v}^2\right) + \frac{1}{6}\,d_0\mathrm{v}^5\right)\right] \end{aligned} \tag{16}$$

The phase-lag's second derivative is given by:

$$\begin{aligned} \ddot{phl} = & -\cos(\mathrm{v}) + c_1\left[2 - \mathrm{v}^2\left(1 - \frac{1}{12}\mathrm{v}^2\right)\right] + c_2\left[1 - d_0\mathrm{v}^4\left(1 - \frac{1}{12}\mathrm{v}^2\right)\right] \\ & + 2\,\mathrm{v}\left[c_1\left[-2\,\mathrm{v}\left(1 - \frac{1}{12}\mathrm{v}^2\right) + \frac{1}{6}\mathrm{v}^3\right] + c_2\left[-4\,d_0\mathrm{v}^3\left(1 - \frac{1}{12}\mathrm{v}^2\right)\right.\right. \\ & \left.\left. + \frac{1}{6}\,d_0\mathrm{v}^5\right]\right] + \frac{1}{2}\mathrm{v}^2\left[c_1\left(-2 + \mathrm{v}^2\right) + c_2\left[-12\,d_0\mathrm{v}^2\left(1 - \frac{1}{12}\mathrm{v}^2\right) + \frac{3}{2}\,d_0\mathrm{v}^4\right]\right] \end{aligned} \tag{17}$$

Demanding the phase-lag and the first and second derivatives of the phase-lag to be vanished we find out that:

$$\begin{aligned} c_1 &= \frac{T_0}{\mathrm{v}^8 - 12\,\mathrm{v}^6 + 48\,\mathrm{v}^4} \\ c_2 &= \frac{T_1}{12\,\mathrm{v}^8 - 144\,\mathrm{v}^6 + 576\,\mathrm{v}^4} \\ d_0 &= \frac{T_2}{T_3} \\ T_0 &= -3\cos(\mathrm{v})\,\mathrm{v}^4 + 27\,\mathrm{v}^3\sin(\mathrm{v}) - 48\,\mathrm{v}^2 + 72\cos(\mathrm{v})\,\mathrm{v}^2 \\ &\quad - 168\,\mathrm{v}\sin(\mathrm{v}) + 288 - 288\cos(\mathrm{v}) \\ T_1 &= \mathrm{v}^8\cos(\mathrm{v}) - 13\,\mathrm{v}^7\sin(\mathrm{v}) + 48\,\mathrm{v}^6 - 72\cos(\mathrm{v})\,\mathrm{v}^6 \\ &\quad + 264\,\mathrm{v}^5\sin(\mathrm{v}) + 984\cos(\mathrm{v})\,\mathrm{v}^4 - 768\,\mathrm{v}^4 - 1944\,\mathrm{v}^3\sin(\mathrm{v}) \\ &\quad + 4608\,\mathrm{v}^2 - 5184\cos(\mathrm{v})\,\mathrm{v}^2 + 4032\,\mathrm{v}\sin(\mathrm{v}) - 6912 + 6912\cos(\mathrm{v}) \\ T_2 &= 24\cos(\mathrm{v})\,\mathrm{v}^4 - 168\,\mathrm{v}^3\sin(\mathrm{v}) + 288\,\mathrm{v}^2 \\ &\quad - 432\cos(\mathrm{v})\,\mathrm{v}^2 + 720\,\mathrm{v}\sin(\mathrm{v}) + 1152\cos(\mathrm{v}) - 1152 \\ T_3 &= \mathrm{v}^{10}\cos(\mathrm{v}) - 13\,\mathrm{v}^9\sin(\mathrm{v}) + 48\,\mathrm{v}^8 - 72\,\mathrm{v}^8\cos(\mathrm{v}) \\ &\quad + 264\,\mathrm{v}^7\sin(\mathrm{v}) + 984\cos(\mathrm{v})\,\mathrm{v}^6 - 768\,\mathrm{v}^6 - 1944\,\mathrm{v}^5\sin(\mathrm{v}) \\ &\quad + 4608\,\mathrm{v}^4 - 5184\cos(\mathrm{v})\,\mathrm{v}^4 + 4032\,\mathrm{v}^3\sin(\mathrm{v}) - 6912\,\mathrm{v}^2 + 6912\cos(\mathrm{v})\,\mathrm{v}^2 \end{aligned} \tag{18}$$

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

$$
\begin{aligned}
c_1 &= \frac{1}{12} - \frac{1}{840}\,\mathrm{v}^4 - \frac{19}{64800}\,\mathrm{v}^6 - \frac{557}{11404800}\,\mathrm{v}^8 \\
&\quad - \frac{8303}{1362160800}\,\mathrm{v}^{10} - \frac{1059613}{2092278988800}\,\mathrm{v}^{12} \\
&\quad + \frac{809351}{2134124568576000}\,\mathrm{v}^{14} + \frac{12949893017}{1216451004088320000}\,\mathrm{v}^{16} + \cdots \\
c_2 &= \frac{5}{6} + \frac{1}{420}\,\mathrm{v}^4 + \frac{43}{226800}\,\mathrm{v}^6 + \frac{1}{7983360}\,\mathrm{v}^8 \\
&\quad - \frac{22301}{5448643200}\,\mathrm{v}^{10} - \frac{1065907}{1046139494400}\,\mathrm{v}^{12} \\
&\quad - \frac{180943901}{1067062284288000}\,\mathrm{v}^{14} - \frac{6436501861}{304112751022080000}\,\mathrm{v}^{16} + \cdots \\
d_0 &= \frac{1}{200} + \frac{1}{700}\,\mathrm{v}^2 + \frac{277}{1260000}\,\mathrm{v}^4 + \frac{209927}{8731800000}\,\mathrm{v}^6 \\
&\quad + \frac{1117733}{756756000000}\,\mathrm{v}^8 - \frac{733705919}{7628100480000000}\,\mathrm{v}^{10} \\
&\quad - \frac{371075765461}{7780662489600000000}\,\mathrm{v}^{12} - \frac{3059031184711277}{341493276668544000000000}\,\mathrm{v}^{14} \\
&\quad - \frac{752691356321903}{650463384130560000000000}\,\mathrm{v}^{16} + \cdots
\end{aligned}
\tag{19}
$$

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

$$
\mathrm{LTE} = -\frac{h^8}{2520}\left(y_n^{(8)} + 3\omega^2\, y_n^{(6)} + 3\,\omega^4\, y_n^{(4)} + \omega^6\, y_n^{(2)}\right) \tag{20}
$$

5 Comparative error analysis

We will study the following methods:

- The Numerov's method which is indicated as *Method I*
- The method developed by Raptis and Allison [37] which is indicated as *Method II*
- The two-step P-stable method developed by Wang [142] which is indicated as *Method III*
- The method developed by Ixaru and Rizea [136] which is indicated as *Method IV*
- The method produced by Raptis [143] which is indicated as *Method V*

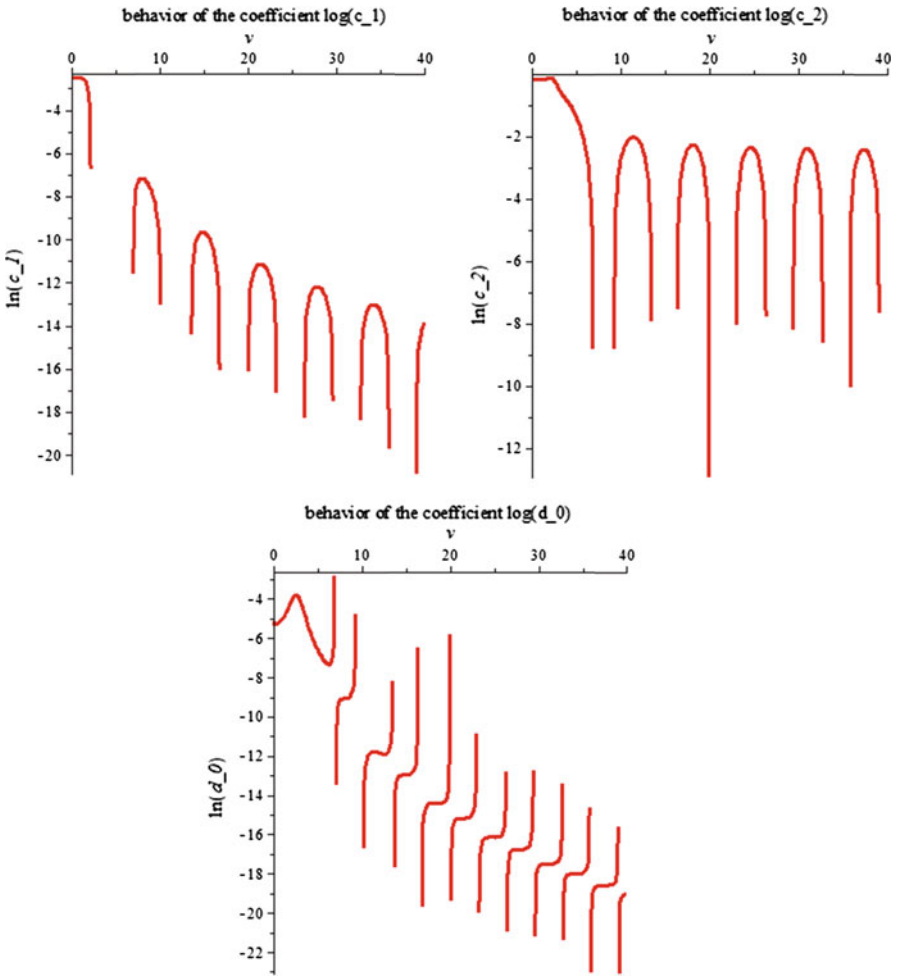

Fig. 1 Behavior of the coefficients of the new proposed method given by (18), (19) for several values of v

– The classical method of the new proposed family[2] which is indicated as *Method VI*
– The new developed two-step Numerov-type hybrid method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 4.2 which is indicated as *Method VII*

The error analysis is based on the following steps:

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

$$y''(x) = f(x)\, y(x) \tag{21}$$

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

– The function $f(x)$ is written in the form (based on the paper of Ixaru and Rizea [135]):

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

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

– Our analysis is based also 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 the equation (21). 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:

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

we obtain the expressions mentioned below (for analytic expressions of the Local Truncation Errors for the Method VI and Method VII see in Appendix A).

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 (see [139,141] and equations (47)–(48)).
THE NUMEROV'S METHOD

$$\mathrm{LTE}_{\mathrm{MethodI}} = h^6\left(-\frac{1}{240}\,y(x)\,G^3+\cdots\right) \tag{23}$$

THE METHOD OF RAPTIS AND ALLISON [37]

$$\mathrm{LTE}_{\mathrm{MethodII}} = h^6\left(-\frac{1}{240}\,g(x)\,y(x)\,G^2+\cdots\right) \tag{24}$$

THE TWO-STEP P-STABLE METHOD DEVELOPED BY WANG [142]

$$\mathrm{LTE}_{\mathrm{MethodIII}} = h^6\left(-\frac{1}{80}\,g\,(x)\,y\,(x)\;G^2+\cdots\right) \tag{25}$$

THE METHOD OF IXARU AND RIZEA [136]

$$\mathrm{LTE}_{\mathrm{MethodIV}} = h^6\left[\left(-\frac{1}{120}\left(\frac{d}{dx}g\,(x)\right)\frac{d}{dx}y\,(x) - \frac{1}{48}\left(\frac{d^2}{dx^2}g\,(x)\right)y\,(x) - \frac{1}{240}\,(g\,(x))^2\,y\,(x)\right)G+\cdots\right] \tag{26}$$

THE METHOD PRODUCED BY RAPTIS [143]

$$\mathrm{LTE}_{\mathrm{MethodV}} = h^6\left(-\frac{1}{60}\left(\frac{d^2}{dx^2}g\,(x)\right)y\,(x)\;G+\cdots\right) \tag{27}$$

THE CLASSICAL CASE OF THE FAMILY[3]

$$\mathrm{LTE}_{\mathrm{MethodVI}} = h^8\left(\frac{1}{2520}\,y\,(x)\;G^4+\cdots\right) \tag{28}$$

THE NEW DEVELOPED TWO-STEP NUMEROV-TYPE HYBRID METHOD WITH PHASE-LAG AND ITS FIRST AND SECOND DERIVATIVES EQUAL TO ZERO OBTAINED IN PARAGRAPH 4.2

$$\mathrm{LTE}_{\mathrm{MethodVII}} = h^8\left(\frac{1}{630}\left(\frac{d^2}{dx^2}g\,(x)\right)y\,(x)\;G^2+\cdots\right) \tag{29}$$

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

Table 1 Comparative error analysis for the methods mentioned in Sect. 4

Method	Algebraic order	Order of G	CFAE
Method I	4	3	$-\frac{1}{240}$
Method II	4	2	$-\frac{1}{240}$
Method III	4	2	$-\frac{1}{80}$
Method IV	4	1	$-\frac{1}{120}$
Method V	4	1	$-\frac{1}{60}$
Method VI	6	4	$\frac{1}{2520}$
Method VII	6	2	$\frac{1}{630}$

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

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

Theorem 2

- *For the two-step Numerov's fourth algebraic order method the error increases as the third power of G*
- *For the two-step exponentially-fitted fourth algebraic order method developed by Raptis and Allison* [37] *the error increases as the second power of G*
- *For the two-step P-stable fourth algebraic order method developed by Wang* [142] *the error increases as the second power of G*
- *For the two-step exponentially-fitted fourth algebraic order method developed by Ixaru and Rizea* [136] *the error increases as the first power of G*
- *For the two-step exponentially-fitted fourth algebraic order method developed by Raptis* [143] *the error increases as the first power of G*
- *For the classical sixth algebraic order method of the new proposed family*[4] *the error increases as the fourth power of G*
- *Finally, for the new developed two-step Numerov-type sixth algebraic order hybrid method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 4.2 the error increases as the second power of G*

So, for the numerical solution of the time independent radial Schrödinger equation the new proposed method produced in this paper (*Sect.* 4.2) *is the most accurate Method , especially for large values of* $|\ G\ | = |\ V_c - E\ |$, *since it is of a sixth algebraic order method for which the error increases as the second power of G.*

6 Stability analysis

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

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

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 (10), with the coefficients (18) is applied to the scalar test equation:

$$\psi'' = -t^2\psi, \tag{30}$$

where $t \neq \omega$.

We obtain the following difference equation:

$$\begin{aligned} A_k(s,\mathrm{v})\,\psi_{n+k} + \cdots + A_1(s,\mathrm{v})\,\psi_{n+1} + A_0(s,\mathrm{v})\,\psi_n \\ + A_1(s,\mathrm{v})\,\psi_{n-1} + \cdots + A_k(s,\mathrm{v})\,\psi_{n-k} = 0 \end{aligned} \tag{31}$$

where $s = t\,h$, 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 polynomials $A_i(s,\mathrm{v})$, $i = 0(1)5$ for the two methods of the family are presented in Appendix C.

The characteristic equation associated with (31) is given by:

$$A_k(s,\mathrm{v})\,\vartheta^k + \cdots + A_1(s,\mathrm{v})\,\vartheta + A_0(s,\mathrm{v}) + A_1(s,\mathrm{v})\,\vartheta^{-1} + \cdots + A_k(s,\mathrm{v})\,\vartheta^{-k} = 0 \tag{32}$$

Definition 1 (*see* [36]) A symmetric $2k$-step method with the characteristic equation given by (32) 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

$$z_{1,2} = e^{\pm i\,\zeta(t\,h)},\ |z_i| \leq 1, \quad i = 3, 4 \tag{33}$$

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

Definition 2 (*see* [36]) 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 $(0, \infty) - S$[5] 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 Fig. 2 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.

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

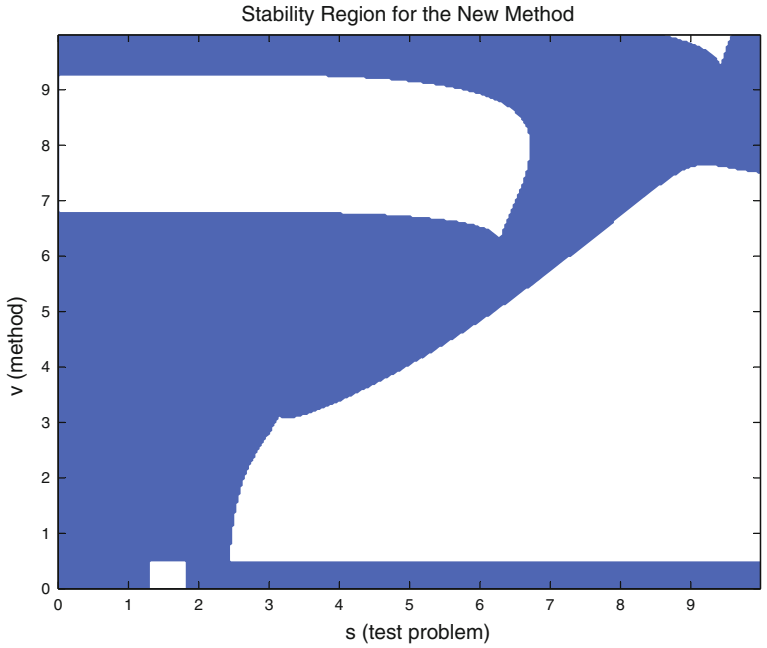

Fig. 2 $s-$ v plane of the New Method produced in Sect. 4.2

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 $s-v$ 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 $s-v$ plane), it is easy to see that the interval of periodicity of the new obtained method is equal to: $(0,\infty)-Q$ (where where $Q=k\,\Pi,\ k=0,1,2,\ldots$) i.e the new proposed method is singularly almost P-stable.

From the above analysis we have the following theorem:

Theorem 3 *The method* (10) *with the coefficients given by* (18) *and* (19) *is of sixth algebraic order, has the phase-lag and its first and second derivatives equal to zero and has an interval of periodicity equals to:* $(0,\infty)-Q$ (*where* $Q=k\,\Pi,\ k=0,1,2,\ldots$).

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

7 Numerical results: conclusion

We apply the new proposed method to the radial time independent Schrödinger equation. This application is used in order to illustrate the efficiency of the new proposed method.

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

Method	Interval of periodicity
Method I	$(0, 6)$
Method II	$(0, \infty) - S_1$
Method III	$(0, \infty) - S_2$
Method IV	$(0, \infty) - S_3$
Method V	$(0, \infty) - S_4$
Method VI	$(0, 5.92)$
Method VII	$(0, \infty) - Q$

The sets S_i, $i = 1(1)4$ and Q are sets of of distinct points

The application of the new obtained method to the to the radial Schrödinger equation requires the value of parameter v. For any mathematical model which can be expressed problem with equations of the form of the radial Schrödinger equation given by (1) the parameter v is given by

$$\mathrm{v} = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{34}$$

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

7.1 Woods-Saxon potential

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

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\left(1+z\right)^2} \tag{35}$$

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

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

It is well known, from the literature, 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 [136]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [136]):

$$\mathrm{v} = \begin{cases} \sqrt{-50+E}, & \text{for } x \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } x = 6.5-h \\ \sqrt{-25+E}, & \text{for } x = 6.5 \\ \sqrt{-12.5+E}, & \text{for } x = 6.5+h \\ \sqrt{E}, & \text{for } x \in [6.5+2h, 15] \end{cases} \tag{36}$$

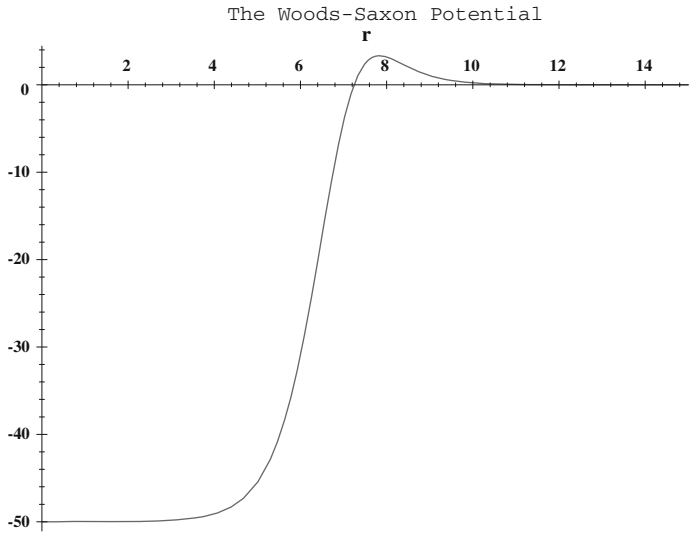

Fig. 3 The Woods-Saxon potential

7.2 Radial Schrödinger equation: the resonance problem

We consider the numerical solution of the radial time independent Schrödinger equation (1) in the well-known case of the Woods-Saxon potential (35). It is known that the interval of integration for these kind of problems is equal to $[0, \infty]$. For the numerical solution of the above problem we need to approximate this 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

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{37}$$

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

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{38}$$

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

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{39}$$

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 we consider the present problem as an initial-value problem, we need y_0, y_1 before starting a two-step method. From the initial condition we obtain y_0. The other value can be obtained using the Runge-Kutta-Nyström methods of Dormand et al. (see [8]). 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:

$$y(0) = 0,\ y(x) = \cos\left(\sqrt{E}\times\right) \text{ for large } x. \tag{40}$$

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

- The Numerov's method which is indicated as *Method I*
- The Exponentially-fitted two-step method developed by Raptis and Allison [37] which is indicated as *Method II*
- The two-step P-stable fourth algebraic order method developed by Wang [142] which is indicated as *Method III*
- The two-step exponentially-fitted fourth algebraic order method developed by Ixaru and Rizea [136] which is indicated as *Method IV*
- The two-step exponentially-fitted fourth algebraic order method developed by Raptis [143] which is indicated as *Method V*
- The classical sixth algebraic order method of the new proposed family which is indicated as *Method VI*
- The new developed two-step Numerov-type sixth algebraic order hybrid method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 4.2 which is indicated as *Method VII*

The computed eigenenergies are compared with exact ones. In Fig. 4 we present the maximum absolute error $log_{10}\left(Err\right)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{41}$$

of the eigenenergy $E_2 = 341.495874$, for several values of CPU time (in seconds). In Fig. 5 we present the maximum absolute error $log_{10}\left(Err\right)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{42}$$

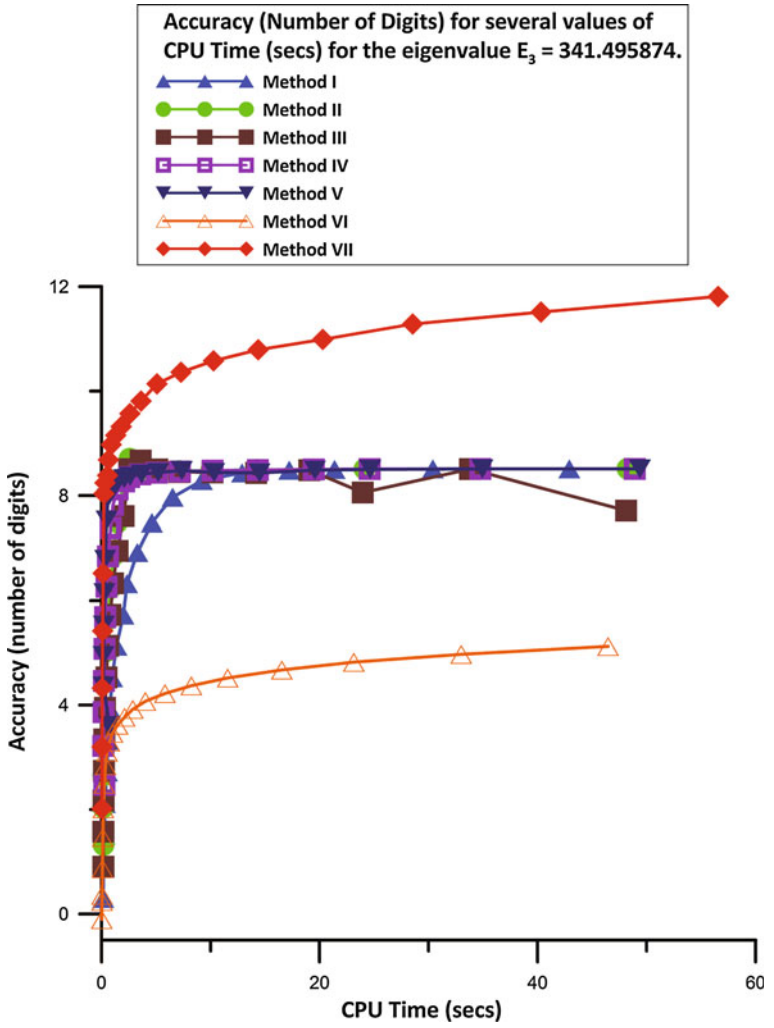

Fig. 4 Accuracy (Digits) for several values of CPU time in seconds for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this CPU time, the Accuracy (Digits) is less than 0

of the eigenenergy $E_3 = 989.701916$, for several values of CPU time (in seconds).

8 Remarks: conclusions—summaries

8.1 Remarks and conclusions

The purpose of this paper was the development of a new explicit hybrid Numerov-type method of fourth algebraic order with phase-lag and its first two derivatives equal to zero.

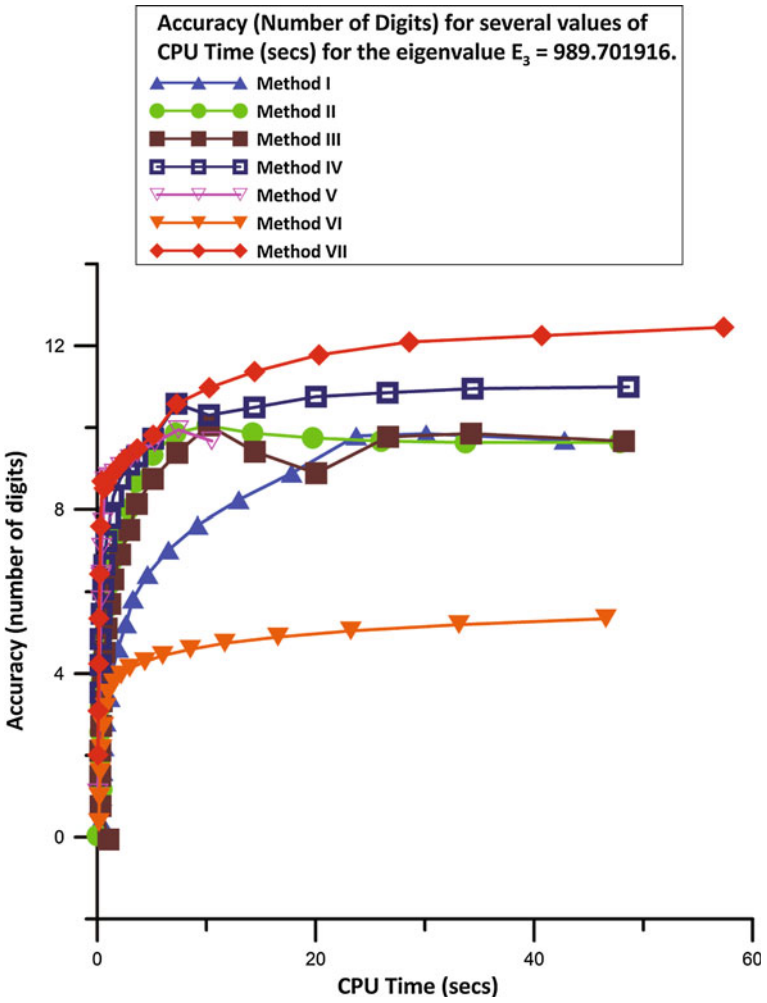

Fig. 5 Accuracy (Digits) for several values of CPU time in seconds for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this CPU time, the Accuracy (Digits) is less than 0

We have applied the new method to the resonance problem of the one-dimensional Schrödinger equation.

Based on the results presented above we have the following conclusions:

– The Numerov's Method (Method I) is much more efficient than the classical sixth algebraic order method of the new proposed family (Method VI). The reason is that for the Numerov's method (Method I) the error increases as the third power of G while for the classical sixth algebraic order method of the new proposed family (Method VI) the error increases as the fourth power of G (see Sect. 4 for more details).

- The Exponentially-fitted two-step method developed by Raptis and Allison [37] (Method II) is more efficient than the Numerov's Method (Method I). The reason is that for the Numerov's method (Method I) the error increases as the third power of G while for the method developed by Raptis and Allison (Method II) the error increases as the second power of G (see Sect. 4 for more details).
- The two-step P-stable fourth algebraic order method developed by Wang [142] (Method III) has the same approximately behavior with the the exponentially-fitted two-step method developed by Raptis and Allison [37] (Method II). The reason is that for the method developed by Raptis and Allison (Method II) the error increases as the second power of G i.e. has the same dependence with G like the two-step P-stable fourth algebraic order method developed by Wang [142] (Method III)(see Sect. 4 for more details).
- The two-step exponentially-fitted fourth algebraic order method developed by Ixaru and Rizea [136](Method IV) has the same approximately behavior with the the exponentially-fitted two-step method developed by Raptis and Allison [37] (Method II) and the two-step P-stable fourth algebraic order method developed by Wang [142] (Method III) for low energies and is more efficient than the Method II and Method III for high energies. The reason is that for the method developed by Ixaru and Rizea [136] (Method IV) the error increases as the first power of G while for the exponentially-fitted two-step method developed by Raptis and Allison [37] (Method II) and the the two-step P-stable fourth algebraic order method developed by Wang [142] (Method III) the error increases as the second power of G (see Sect. 4 for more details).
- The two-step exponentially-fitted fourth algebraic order method developed by Raptis [143] (Method V) has the same approximately behavior with the two-step exponentially-fitted fourth algebraic order method developed by Ixaru and Rizea [136](Method IV). The reason is that for the method developed by Ixaru and Rizea [136] (Method IV) the error increases as the first power of G i.e. has the same dependence with G like the exponentially-fitted two-step method developed by Raptis [143] (Method V)
- Finally, the new developed two-step Numerov-type sixth algebraic order hybrid method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 4.2 (Method VII) is much more efficient than all the other methods. The reason is that this is a sixth algebraic order method for which the error increases as the second power of G.

8.2 Summaries on the properties of the numerical methods

From the analysis presented above (comparative error analysis and comparative stability anslysis) 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. The important is the phase-lag and as many as possible derivatives to be vanished 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 explicit schemes (like the obtained in this paper) give much better results then the corresponding implicit for the numerical approximation of the radial Schrödinger equation.
- The Large Interval of Periodicity, as we have mentioned previously, doesn't play important role for the numerical solution of this category of problems.

During our research for this paper we have realized the following remark

Remark 3 The symmetric multistep methods which have the phase-lag and its derivatives equal to zero are exactly the same with the symmetric multistep methods of the same form which integrates any linear combination of the functions

$$\left\{1,\ x,\ x^2,\ x^3,\ x^m,\ \ldots,\ \cos(w\,x),\ \sin(w\,x),\ x\,\cos(w\,x),\ x\,\sin(w\,x),\right.$$
$$\left.x^2\,\cos(w\,x),\ x^2\,\sin(w\,x),\ldots,\ x^p\,\cos(w\,x),\ x^p\,\sin(w\,x),\right\} \tag{43}$$

with the following algorithm:

- The symmetric multistep method which has the phase-lag equal to zero (phase-fitted) is exactly the same with the symmetric multistep method of the same form which integrates any linear combination of the functions

$$\left\{1,\ x,\ x^2,\ x^3,\ x^m,\ \ldots,\ \cos(w\,x),\ \sin(w\,x)\right\} \tag{44}$$

- The symmetric multistep method which has the phase-lag and its first derivative equal to zero is exactly the same with the symmetric multistep method of the same form which integrates any linear combination of the functions

$$\left\{1,\ x,\ x^2,\ x^3,\ x^m,\ \ldots,\ \cos(w\,x),\ \sin(w\,x),\ x\,\cos(w\,x),\ x\,\sin(w\,x)\right\} \tag{45}$$

- The symmetric multistep method which has the phase-lag and its first and second derivative equal to zero is exactly the same with the symmetric multistep method

of the same form which integrates any linear combination of the functions

$$\left\{1,\ x,\ x^2,\ x^3,\ x^m,\ \ldots,\ \cos(w\,x),\ \sin(w\,x),\right.$$
$$\left.x\ \cos(w\,x),\ x\ \sin(w\,x),\ x^2\ \cos(w\,x),\ x^2\ \sin(w\,x)\right\} \tag{46}$$

The reason can be easily obtained from the definition of the phase-lag. In the Appendix B we prove that the above algorithm is applied for the case of Numerov's method.

All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

Appendix A

THE CLASSICAL METHOD OF THE NEW PROPOSED FAMILY[6] WHICH IS INDICATED AS *Method VI*

$$\begin{aligned}
\mathrm{LTE}_{\mathrm{MethodVI}} = h^8\Bigg[&\left(\frac{1}{2520}\,y\,(x)\right)G^4+\left(\frac{1}{630}\,g\,(x)\,y\,(x)\right)G^3\\
&+\left(\frac{11}{1260}\left(\frac{d^2}{dx^2}g\,(x)\right)y\,(x)+\frac{1}{210}\left(\frac{d}{dx}g\,(x)\right)\frac{d}{dx}y\,(x)\right.\\
&\left.+\frac{1}{420}\,(g\,(x))^2\,y\,(x)\right)G^2+\left(\frac{2}{315}\left(\frac{d^4}{dx^4}g\,(x)\right)y\,(x)\right.\\
&+\frac{1}{105}\left(\frac{d^3}{dx^3}g\,(x)\right)\frac{d}{dx}y\,(x)+\frac{1}{105}\,g\,(x)\left(\frac{d}{dx}y\,(x)\right)\frac{d}{dx}g\,(x)\\
&+\frac{11}{630}\,g\,(x)\,y\,(x)\,\frac{d^2}{dx^2}g\,(x)+\frac{1}{90}\left(\frac{d}{dx}g\,(x)\right)^2y\,(x)\\
&\left.+\frac{1}{630}\,(g\,(x))^3\,y\,(x)\right)G+\frac{1}{2520}\left(\frac{d^6}{dx^6}g\,(x)\right)y\,(x)\\
&+\frac{1}{420}\left(\frac{d^5}{dx^5}g\,(x)\right)\frac{d}{dx}y\,(x)+\frac{2}{315}\,g\,(x)\,y\,(x)\,\frac{d^4}{dx^4}g\,(x)\\
&+\frac{1}{168}\left(\frac{d^2}{dx^2}g\,(x)\right)^2y\,(x)+\frac{13}{1260}\left(\frac{d}{dx}g\,(x)\right)y\,(x)\,\frac{d^3}{dx^3}g\,(x)\\
&+\frac{1}{105}\,g\,(x)\left(\frac{d}{dx}y\,(x)\right)\frac{d^3}{dx^3}g\,(x)+\frac{1}{210}\,(g\,(x))^2\left(\frac{d}{dx}y\,(x)\right)\frac{d}{dx}g\,(x)
\end{aligned}$$

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

$$+\frac{2}{105}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}y(x)\right)\frac{d^2}{dx^2}g(x)+\frac{11}{1260}(g(x))^2 y(x)\frac{d^2}{dx^2}g(x)$$
$$+\frac{1}{90}g(x)y(x)\left(\frac{d}{dx}g(x)\right)^2+\frac{1}{2520}(g(x))^4 y(x)\Bigg] \quad (47)$$

THE NEW DEVELOPED TWO-STEP NUMEROV-TYPE HYBRID METHOD WITH PHASE-LAG AND ITS FIRST DERIVATIVE EQUAL TO ZERO OBTAINED IN PARAGRAPH 4.2 WHICH IS INDICATED AS *Method VII*

$$\begin{aligned}\mathrm{LTE}_{\mathrm{MethodVII}} = h^8\Bigg[&\left(\frac{1}{630}\left(\frac{d^2}{dx^2}g(x)\right)y(x)\right)G^2\\
&+\left(\frac{13}{2520}\left(\frac{d^4}{dx^4}g(x)\right)y(x)+\frac{1}{210}\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}y(x)\right.\\
&+\frac{1}{420}g(x)\left(\frac{d}{dx}y(x)\right)\frac{d}{dx}g(x)+\frac{23}{2520}g(x)y(x)\frac{d^2}{dx^2}g(x)\\
&\left.+\frac{2}{315}\left(\frac{d}{dx}g(x)\right)^2 y(x)+\frac{1}{2520}(g(x))^3 y(x)\right)G\\
&+\frac{1}{2520}\left(\frac{d^6}{dx^6}g(x)\right)y(x)+\frac{1}{420}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}y(x)\\
&+\frac{2}{315}g(x)y(x)\frac{d^4}{dx^4}g(x)+\frac{1}{168}\left(\frac{d^2}{dx^2}g(x)\right)^2 y(x)\\
&+\frac{13}{1260}\left(\frac{d}{dx}g(x)\right)y(x)\frac{d^3}{dx^3}g(x)\\
&+\frac{1}{105}g(x)\left(\frac{d}{dx}y(x)\right)\frac{d^3}{dx^3}g(x)+\frac{1}{210}(g(x))^2\left(\frac{d}{dx}y(x)\right)\frac{d}{dx}g(x)\\
&+\frac{2}{105}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}y(x)\right)\frac{d^2}{dx^2}g(x)+\frac{11}{1260}(g(x))^2 y(x)\frac{d^2}{dx^2}g(x)\\
&+\frac{1}{90}g(x)y(x)\left(\frac{d}{dx}g(x)\right)^2+\frac{1}{2520}(g(x))^4 y(x)\Bigg] \quad (48)\end{aligned}$$

Appendix B: Numerov's Methods with phase-lag and its first and second derivatives equal to zero

B.1. THE PHASE-FITTED NUMEROV'S METHOD

Consider the well known Numerov's method:

$$\phi_{n+1}+c_0\phi_n+\phi_{n-1}=h^2\left[c_1\left(\phi''_{n+1}+\phi''_{n-1}\right)+c_2\phi''_n\right] \quad (49)$$

Requiring the above method (49) to have the maximum algebraic order with one free parameter, the following relations are obtained:

$$c_0 = -2, \quad c_2 := 1 - 2\,c_1 \tag{50}$$

The application of the above method to the scalar test equation (6) gives the difference equation (12) with the associated characteristic equation (13), where:

$$\begin{aligned} A_0(\mathrm{v}) &= -2 + \mathrm{v}^2\,(1 - 2\,c_1) \\ A_1(\mathrm{v}) &= 1 + \mathrm{v}^2\,c_1 \end{aligned} \tag{51}$$

By applying $k = 1$ in the formula (9), we have that the phase-lag is equal to:

$$phl = \frac{1}{2}\,\frac{2\,\left(1 + \mathrm{v}^2\,c_1\right)\cos(\mathrm{v}) - 2 + \mathrm{v}^2\,(1 - 2\,c_1)}{1 + \mathrm{v}^2\,c_1} \tag{52}$$

Demanding the phase-lag to be vanished we find out that:

$$c_1 = \frac{-2\,\cos(\mathrm{v}) + 2 - \mathrm{v}^2}{2\,\cos(\mathrm{v})\,\mathrm{v}^2 - 2\,\mathrm{v}^2} \tag{53}$$

For small values of $|\mathrm{v}|$ the formulae given by (53) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} c_1 = {} & \frac{1}{12} + \frac{1}{240}\,\mathrm{v}^2 + \frac{1}{6048}\,\mathrm{v}^4 + \frac{1}{172800}\,\mathrm{v}^6 \\ & + \frac{1}{5322240}\,\mathrm{v}^8 + \frac{691}{118879488000}\,\mathrm{v}^{10} \\ & + \frac{1}{5748019200}\,\mathrm{v}^{12} + \frac{3617}{711374856192000}\,\mathrm{v}^{14} \\ & + \frac{43867}{3005349539512320000}\,\mathrm{v}^{16} + \cdots \end{aligned} \tag{54}$$

The local truncation error of the new proposed method is given by:

$$\mathrm{LTE} = -\frac{h^6}{240}\left(y_n^{(6)} + \omega^2\,y_n^{(4)}\right) \tag{55}$$

From the above analysis it is proved the following theorem

Theorem 4 *The Numerov's method with phase-lag equal to zero is exactly the same with the method developed by Raptis and Allison [37].*

B.2. The Numerov's Method with phase- lag and its first derivative equal to zero

Consider again the well known Numerov's method (37). Requiring the method (49) to have the maximum algebraic order with two free parameter, the following relation is hold:

$$c_0 = -2 \tag{56}$$

The application of the above method to the scalar test equation (6) gives the difference equation (12) with the associated characteristic equation (13), where:

$$\begin{aligned} A_0(\mathrm{v}) &= -2 + \mathrm{v}^2 c_2 \\ A_1(\mathrm{v}) &= 1 + \mathrm{v}^2 c_1 \end{aligned} \tag{57}$$

By applying $k = 1$ in the formula (9), we have that the phase-lag is equal to:

$$phl = \frac{1}{2} \frac{2\left(1 + \mathrm{v}^2 c_1\right)\cos(\mathrm{v}) - 2 + \mathrm{v}^2 c_2}{1 + \mathrm{v}^2 c_1} \tag{58}$$

The phase-lag's first derivative is given by:

$$\dot{phl} = -\frac{\sin(\mathrm{v}) + 2\sin(\mathrm{v})\,\mathrm{v}^2 c_1 + \sin(\mathrm{v})\,\mathrm{v}^4 {c_1}^2 - \mathrm{v}\,c_2 - 2\,\mathrm{v}\,c_1}{\left(1 + \mathrm{v}^2 c_1\right)^2} \tag{59}$$

Demanding the phase-lag and its first derivative to be vanished we find out that:

$$\begin{aligned} c_1 &= \frac{-\mathrm{v}\sin(\mathrm{v}) - 2\cos(\mathrm{v}) + 2}{\sin(\mathrm{v})\,\mathrm{v}^3} \\ c_2 &= \frac{2\,\mathrm{v}\sin(\mathrm{v}) - 4\cos(\mathrm{v}) + 2\cos(2\,\mathrm{v}) + 2}{\sin(\mathrm{v})\,\mathrm{v}^3} \end{aligned} \tag{60}$$

For small values of $|\mathrm{v}|$ the formulae given by (53) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} c_1 = {} & \frac{1}{12} + \frac{1}{120}\mathrm{v}^2 + \frac{17}{20160}\mathrm{v}^4 + \frac{31}{362880}\mathrm{v}^6 \\ & + \frac{691}{79833600}\mathrm{v}^8 + \frac{5461}{6227020800}\mathrm{v}^{10} \\ & + \frac{929569}{10461394944000}\mathrm{v}^{12} + \frac{3202291}{355687428096000}\mathrm{v}^{14} \\ & + \frac{221930581}{243290200817664000}\mathrm{v}^{16} + \cdots \\ c_2 = {} & \frac{5}{6} - \frac{1}{60}\mathrm{v}^2 + \frac{5}{2016}\mathrm{v}^4 + \frac{29}{181440}\mathrm{v}^6 \end{aligned}$$

$$+\frac{139}{7983360}\,\mathrm{v}^8+\frac{5459}{3113510400}\,\mathrm{v}^{10}+\frac{185917}{1046139494400}\,\mathrm{v}^{12}+\frac{3202289}{177843714048000}\,\mathrm{v}^{14}+\frac{44386117}{24329020081766400}\,\mathrm{v}^{16}+\cdots \tag{61}$$

The local truncation error of the new proposed method is given by:

$$\mathrm{LTE}=-\frac{h^6}{240}\left(y_n^{(6)}+2\,\omega^2\,y_n^{(4)}+\omega^4\,y_n^{(2)}\right) \tag{62}$$

From the above analysis it is proved the following theorem

Theorem 5 *The Numerov's method with phase-lag and its first derivative equal to zero is exactly the same with the method developed by Ixaru and Rizea* [136].

B.3. The Numerov's Method with phase- lag and its first and second derivatives equal to zero

Consider again the well known Numerov's method (37).

The application of the above method to the scalar test equation (6) gives the difference equation (12) with the associated characteristic equation (13), where:

$$\begin{aligned} A_0(\mathrm{v}) &= c_0+\mathrm{v}^2\,c_2\\ A_1(\mathrm{v}) &= 1+\mathrm{v}^2\,c_1 \end{aligned} \tag{63}$$

By applying $k=1$ in the formula (9), we have that the phase-lag is equal to:

$$phl=\frac{1}{2}\,\frac{2\,\left(1+\mathrm{v}^2\,c_1\right)\cos\left(\mathrm{v}\right)+c_0+\mathrm{v}^2\,c_2}{1+\mathrm{v}^2\,c_1} \tag{64}$$

The phase-lag's first derivative is given by:

$$\dot{phl}=-\frac{\sin\left(\mathrm{v}\right)+2\,\sin\left(\mathrm{v}\right)\mathrm{v}^2c_1+\sin\left(\mathrm{v}\right)\mathrm{v}^4{c_1}^2-\mathrm{v}c_2+\mathrm{v}\,c_1\,c_0}{\left(1+\mathrm{v}^2c_1\right)^2} \tag{65}$$

The phase-lag's second derivative is given by:

$$\ddot{phl}=-\frac{T_4}{\left(1+\mathrm{v}^2\,c_1\right)^3} \tag{66}$$

$$\begin{aligned} T_4 &= 3\,\cos\left(\mathrm{v}\right)\mathrm{v}^2\,c_1+\cos\left(\mathrm{v}\right)+c_1\,c_0-c_2\\ &\quad+3\,\cos\left(\mathrm{v}\right)\mathrm{v}^4\,{c_1}^2+\cos\left(\mathrm{v}\right)\mathrm{v}^6\,{c_1}^3+3\,c_2\,\mathrm{v}^2\,c_1-3\,\mathrm{v}^2{c_1}^2\,c_0 \end{aligned}$$

Demanding the phase-lag and its first and second derivatives to be vanished we find out that:

$$\begin{aligned} c_0 &= \frac{-3\,\sin(2\,\mathrm{v}) - 3\,\mathrm{v} + \mathrm{v}\cos(2\,\mathrm{v})}{\mathrm{v}\cos(\mathrm{v}) + 3\,\sin(\mathrm{v})} \\ c_1 &= \frac{-\mathrm{v}\cos(\mathrm{v}) + \sin(\mathrm{v})}{\mathrm{v}^3\cos(\mathrm{v}) + 3\,\mathrm{v}^2\sin(\mathrm{v})} \\ c_2 &= \frac{3\,\mathrm{v} - \mathrm{v}\cos(2\,\mathrm{v}) - \sin(2\,\mathrm{v})}{\mathrm{v}^3\cos(\mathrm{v}) + 3\,\mathrm{v}^2\sin(\mathrm{v})} \end{aligned} \tag{67}$$

For small values of $|\mathrm{v}|$ the formulae given by (53) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} c_0 &= -2 - \frac{1}{240}\,\mathrm{v}^6 - \frac{1}{2016}\,\mathrm{v}^8 - \frac{1}{11520}\,\mathrm{v}^{10} \\ &\quad - \frac{2291}{159667200}\,\mathrm{v}^{12} - \frac{62879}{26417664000}\,\mathrm{v}^{14} \\ &\quad - \frac{2647}{6706022400}\,\mathrm{v}^{16} + \cdots \\ c_1 &= \frac{1}{12} + \frac{1}{80}\,\mathrm{v}^2 + \frac{41}{20160}\,\mathrm{v}^4 + \frac{1219}{3628800}\,\mathrm{v}^6 \\ &\quad + \frac{8887}{159667200}\,\mathrm{v}^8 + \frac{8045189}{871782912000}\,\mathrm{v}^{10} \\ &\quad + \frac{16009177}{10461394944000}\,\mathrm{v}^{12} + \frac{2707911809}{10670622842880000}\,\mathrm{v}^{14} \\ &\quad + \frac{716697321049}{17030314057236480000}\,\mathrm{v}^{16} + \cdots \\ c_2 &= \frac{5}{6} - \frac{1}{40}\,\mathrm{v}^2 + \frac{17}{2016}\,\mathrm{v}^4 + \frac{1811}{1814400}\,\mathrm{v}^6 \\ &\quad + \frac{13817}{79833600}\,\mathrm{v}^8 + \frac{12478951}{435891456000}\,\mathrm{v}^{10} \\ &\quad + \frac{24838031}{5230697472000}\,\mathrm{v}^{12} + \frac{600196633}{762187345920000}\,\mathrm{v}^{14} \\ &\quad + \frac{222395138593}{1703031405723648000}\,\mathrm{v}^{16} + \cdots \end{aligned} \tag{68}$$

The local truncation error of the new proposed method is given by:

$$\mathrm{LTE} = -\frac{h^6}{240}\left(y_n^{(6)} + 3\,\omega^2\,y_n^{(4)} + 3\,\omega^4\,y_n^{(2)} + \omega^6\,y_n\right) \tag{69}$$

From the above analysis it is proved the following theorem

Theorem 6 *The Numerov's method with phase-lag and its first and second derivatives equal to zero is exactly the same with the method developed by Raptis* [143].

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