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ORIGINAL PAPER

A new methodology for the development of numerical methods for the numerical solution of the Schrödinger equation

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Abstract In the present paper we introduce a new methodology for the construction of numerical methods for the approximate solution of the one-dimensional Schrödinger equation. The new methodology is based on the requirement of vanishing the phase-lag and its derivatives. The efficiency of the new methodology is proved via error analysis and numerical applications.

Keywords Numerical solution · Schrödinger equation · Multistep methods · Hybrid methods · P-stability · Phase-lag · Phase-fitted

1 Introduction

The radial Schrödinger equation can be written as:

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

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Many problems 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]).

We give the definitions of some terms of (1):

- 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 last years an extended study on the development of numerical methods for the solution of the Schrödinger equation has been done. The aim of this research is the development of fast and reliable methods for the solution of the Schrödinger equation and related problems (see for example [5–18], [19–124]).

We can divide the numerical methods for the approximate solution of the Schrödinger equation and related problems into two main categories:

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

The purpose of this paper is to introduce a new methodology for the construction of numerical methods for the approximate solution of the one-dimensional Schrödinger equation and related problems. The new methodology is based on the requirement of vanishing the phase-lag and its derivatives. The efficiency of the new methodology will be studied via the error analysis and the application of the investigated methods to the numerical solution of the radial Schrödinger equation.

More specifically, we will develop a family of hybrid Numerov-type methods of sixth algebraic order. The development of the new family is based on the requirement of vanishing the phase-lag and its derivatives. We will investigate the stability and the error of the methods of the new family. Finally, we will apply both categories of methods the new obtained method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. The paper is organized as follows. In Sect. 2 we present the theory of the new methodology. In Sect. 3 we present the development of the new family of methods. The error analysis is presented in Sect. 4. In Sect. 5 we will investigate the stability properties of the new developed methods. In Sect. 6 the numerical results are presented. Finally, in Sect. 7 remarks and conclusions are discussed.

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

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

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

consider a multistep method with m steps which can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h = |x_{i+1} - x_i|,\ \ i = 0(1)m - 1$.

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

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

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

a difference equation of the form

$$\begin{aligned} A_k(H)\, y_{n+k} + \cdots + A_1(H)\, y_{n+1} + A_0(H)\, y_n \\ + A_1(H)\, y_{n-1} + \cdots + A_k(H)\, y_{n-k} = 0 \end{aligned} \tag{5}$$

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

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

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

$$+A_k(H)\, \lambda^{-k} = 0 \tag{7}$$

Theorem 1 [97] *The symmetric $2k$-step method with characteristic equation given by (6) has phase-lag order q and phase-lag constant c given by*

$$-cH^{q+2}+O(H^{q+4})=\frac{2A_k(H)\cos(k\,H)+\cdots+2A_j(H)\cos(j\,H)+\cdots+A_0(H)}{2k^2 A_k(H)+\cdots+2j^2 A_j(H)+\cdots+2A_1(H)} \tag{8}$$

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 numerov-type hybrid methods—construction of the new methods

3.1 First method of the family

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

$$\begin{aligned} \overline{y}_n &= y_n - a_0\, h^2\, \left(y''_{n+1} - 2\, y''_n + y''_{n-1}\right) \\ y_{n+1} + c_1\, y_n + y_{n-1} &= h^2 \left[b_0\, \left(y''_{n+1} + y''_{n-1}\right) + b_1 \overline{y}''_n\right] \end{aligned} \tag{9}$$

The application of the above method to the scalar test Eq. 4 gives the following difference equation:

$$A_1(H)\, y_{n+1} + A_0(H)\, y_n + A_1(H)\, y_{n-1} = 0$$

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

The characteristic equation associated with (10) is given by:

$$A_1(H)\, \lambda + A_0(H) + A_1(H)\, \lambda^{-1} = 0 \tag{10}$$

where

$$\begin{aligned} A_1(H) &= 1 + H^2\, b_0 + H^4\, b_1\, a_0 \\ A_0(H) &= c_1 + H^2\, b_1 - 2\, H^4\, b_1\, a_0 \end{aligned}$$

By applying $k = 1$ in the formula (8), we have that the phase-lag is equal to:

$$\begin{aligned} phl &= \frac{2\, A_1(H)\, \cos(H) + A_0(H)}{2\, A_1(H)} \\ &= \frac{1}{2}\, \frac{2\, (1 + H^2\, b_0 + H^4\, b_1\, a_0)\cos(H) + c_1 + H^2\, b_1 - 2\, H^4\, b_1\, a_0}{1 + H^2\, b_0 + H^4\, b_1\, a_0} \end{aligned} \tag{11}$$

We demand that the phase-lag is equal to zero and we consider that:

$$b_0 = \frac{1}{12}, \quad b_1 = \frac{5}{6}, \quad c_1 = -2 \tag{12}$$

Then we find out that:

$$a_0 = \frac{-12\cos(H) - \cos(H)\, H^2 + 12 - 5\, H^2}{10\cos(H)\, H^4 - 10\, H^4} \tag{13}$$

For small values of $|H|$ the formulae given by (13) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} a_0 &= \frac{1}{200} + \frac{1}{5040}\, H^2 + \frac{1}{144000}\, H^4 + \frac{1}{4435200}\, H^6 \\ &\quad + \frac{691}{99066240000}\, H^8 + \frac{1}{4790016000}\, H^{10} \\ &\quad + \frac{3617}{592812380160000}\, H^{12} + \frac{43867}{250445794959360000}\, H^{14} \\ &\quad + \frac{174611}{35213055381504000000}\, H^{16} + \cdots \end{aligned} \tag{14}$$

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

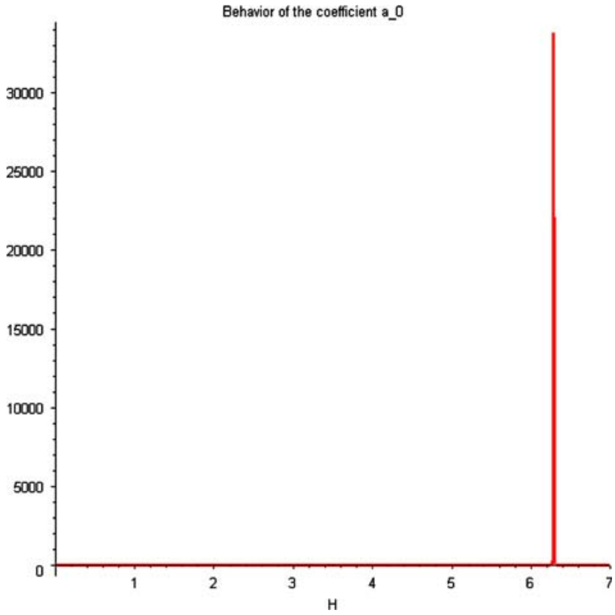

Fig. 1 Behavior of the coefficient a_0 of the new method given by (13) for several values of H

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

$$\mathrm{LTE} = \frac{h^8}{6048}\left(y_n^{(8)} + \omega^2\ y_n^{(6)}\right) \tag{15}$$

Remark 1 The method developed in this section is the same with the obtained by Simos in [111].

3.2 Second method of the family

Consider the family of methods presented in (9).

The application of the above method to the scalar test Eq. 4 gives the difference Eq. 10 and the characteristic Eq. 10.

By applying $k = 1$ in the formula (8), we have that the phase-lag is given by (11). The first derivative of the phase-lag is given by:

$$\begin{aligned}
\dot{phl} &= \frac{1}{2}\,\frac{T_4 - 2\,\mathrm{T}_0\sin(H) + 2\,H b_1 - 8\,H^3\,b_1\,a_0}{\mathrm{T}_0} \\
&\quad -\frac{1}{2}\,\frac{(2\,\mathrm{T}_0\cos(H) + c_1 + H^2\,b_1 - 2\,H^4\,b_1\,a_0)\,(2\,H\,b_0 + 4\,H^3\,b_1\,a_0)}{\mathrm{T}_0{}^2} \\
\mathrm{T}_0 &= 1 + H^2\,b_0 + H^4\,b_1\,a_0 \\
\mathrm{T}_4 &= 2\,(2\,H\,b_0 + 4\,H^3\,b_1\,a_0)\cos(H)
\end{aligned} \tag{16}$$

We demand that the phase-lag and its derivative are equal to zero and we consider that:

$$b_0 = \frac{1}{12}, \quad b_1 = \frac{5}{6} \tag{17}$$

Then we find out that:

$$\begin{aligned} a_0 &= \frac{-\sin(H)\,H^2 + 10\,H + 2\cos(H)\,H - 12\sin(H)}{10\sin(H)\,H^4 - 40\cos(H)\,H^3 + 40\,H^3} \\ c_1 &= (24\cos(2\,H) + 24 - 48\cos(H) + H^2\cos(2\,H) \\ &\quad - 9\,H^2 + 8\cos(H)\,H^2 - 6\,H^3\sin(H) \\ &\quad - 12\sin(H)\,H)/(6\sin(H)\,H - 24\cos(H) + 24) \end{aligned} \tag{18}$$

For small values of $|H|$ the formulae given by (19) are subject to heavy cancelations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} a_0 &= \frac{1}{200} + \frac{1}{3780}\,H^2 + \frac{73}{5443200}\,H^4 + \frac{509}{769824000}\,H^6 \\ &\quad + \frac{2833543}{88268019840000}\,H^8 + \frac{4912333}{3177648714240000}\,H^{10} \\ &\quad + \frac{288303913}{3889442026229760000}\,H^{12} + \frac{165095552521}{4655662105397022720000}\,H^{14} \\ &\quad + \frac{15619496804053}{9218210968686104985600000}\,H^{16} + \cdots \end{aligned} \tag{19}$$

$$\begin{aligned} c_1 - 2 &+ \frac{1}{18144}\,H^8 + \frac{13}{16329600}\,H^{10} + \frac{31}{461894400}\,H^{12} \\ &+ \frac{308851}{105921623808000}\,H^{14} + \frac{537907}{3813178457088000}\,H^{16} + \cdots \end{aligned} \tag{20}$$

The behavior of the coefficients is given in the following Fig. 2.

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

$$\mathrm{LTE} = \frac{h^8}{18144}\left(3\;y_n^{(8)} + 4\,\omega^2\;y_n^{(6)} + \omega^8\;y_n\right) \tag{21}$$

3.3 Third method of the family

Consider the family of methods presented in (9).

The application of the above method to the scalar test Eq. 4 gives the difference Eq. 10 and the characteristic Eq. 10.

By applying $k = 1$ in the formula (8), we have that the phase-lag is given by (11). The first derivative of the phase-lag is given by (16). The second derivative of the phase-lag can be written as:

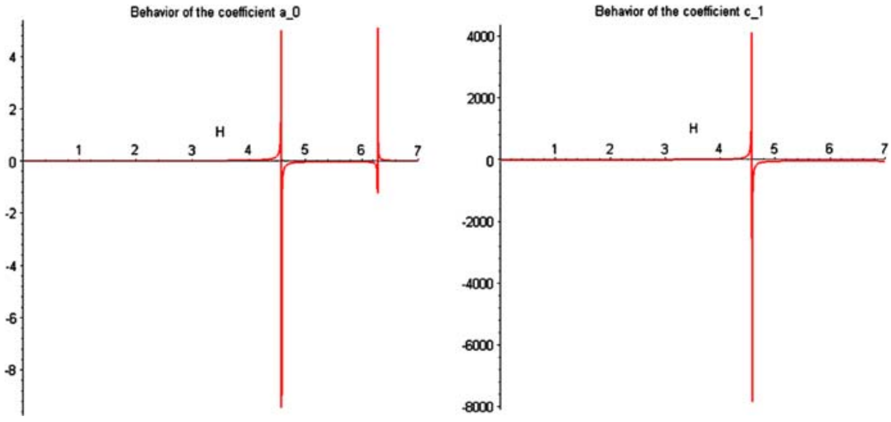

Fig. 2 Behavior of the coefficients of the new method given by (19) for several values of H

$$
\ddot{phl} = \frac{1}{2}\,\frac{T_3 - 4\,\mathrm{T}_2\sin(H) - 2\,\mathrm{T}_1\cos(H) + 2\,b_1 - 24\,b_1\,a_0\,H^2}{\mathrm{T}_1} - \frac{(2\,\mathrm{T}_2\cos(H) - 2\,\mathrm{T}_1\sin(H) + 2\,H\,b_1 - 8\,H^3\,b_1\,a_0)\,\mathrm{T}_2}{\mathrm{T}_1{}^2} + \frac{(2\,\mathrm{T}_1\cos(H) + c_1 + H^2\,b_1 - 2\,H^4\,b_1\,a_0)\,\mathrm{T}_2{}^2}{\mathrm{T}_1{}^3} - \frac{1}{2}\,\frac{(2\,\mathrm{T}_1\cos(H) + c_1 + H^2\,b_1 - 2\,H^4\,b_1\,a_0)\,(2\,b_0 + 12\,b_1\,a_0\,H^2)}{\mathrm{T}_1{}^2}
$$

$$
\begin{aligned}
\mathrm{T}_1 &= 1 + H^2\,b_0 + H^4\,b_1\,a_0\\
\mathrm{T}_2 &= 2\,H\,b_0 + 4\,H^3\,b_1\,a_0\\
\mathrm{T}_3 &= 2\,(2\,b_0 + 12\,b_1\,a_0\,H^2)\cos(H)
\end{aligned}
\tag{22}
$$

We demand that the phase-lag and its first and second derivative are equal to zero and we consider that:

$$
b_0 = \frac{1}{12} \tag{23}
$$

Then we find out that:

$$
\begin{aligned}
a_0 = \frac{1}{2}&\Big(\cos(H)\,H^3 + 12\cos(H)\,H - 12\sin(H) + 3\sin(H)\,H^2\Big)\\
&/\Big(\Big(\cos(H)^2\,H^3 + 16\cos(H)^2\,H + 5\cos(H)\,H^2\sin(H)\\
&+72\cos(H)\sin(H) + 2\cos(H)\,H^3 + 32\cos(H)\,H\\
&+\ 2\sin(H)\,H^2 - 48\,H - 2\,H^3 - 72\sin(H)\Big)\,H^2\Big)
\end{aligned}
$$

$$
\begin{aligned}
c_1 &= \frac{1}{6}\Big(24\cos(H)^2\,H^2+\cos(H)^2\,H^4+96\cos(H)^2\\
&\quad +\cos(H)\sin(H)\,H^3+12\cos(H)\,H^2\\
&\quad -24\cos(H)\sin(H)\,H-96\cos(H)+\cos(H)\,H^4\\
&\quad -\sin(H)\,H^3-2\,H^4-60\sin(H)\,H-48\,H^2\Big)\,/\\
&\quad \Big(\cos(H)\,H^2+7\sin(H)\,H+8-8\cos(H)\Big)\\
b_1 &= -\frac{1}{6}\Big(\cos(H)^2\,H^3+16\cos(H)^2\,H+5\cos(H)\,H^2\sin(H)\\
&\quad +72\cos(H)\sin(H)+2\cos(H)\,H^3\\
&\quad +32\cos(H)\,H+2\sin(H)\,H^2-48\,H-2\,H^3-72\sin(H)\Big)\\
&\quad /\Big(H\Big(\cos(H)\,H^2+7\sin(H)\,H+8-8\cos(H)\Big)\Big)
\end{aligned} \tag{24}
$$

For small values of $|H|$ the formulae given by (24) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
a_0 &= \frac{1}{200}+\frac{1}{2520}\,H^2+\frac{31}{907200}\,H^4+\frac{1229}{1197504000}\,H^6\\
&\quad +\frac{18427}{980755776000}\,H^8-\frac{669341}{98075577600000}\,H^{10}\\
&\quad -\frac{13764419}{25184162304000000}\,H^{12}-\frac{281298850211}{5747730994317312000000}\,H^{14}\\
&\quad -\frac{161773544323}{1034591578977116160000000}\,H^{16}+\cdots\\
c_1 &= -2-\frac{1}{6048}\,H^8-\frac{17}{2721600}\,H^{10}-\frac{43}{57480192}\,H^{12}\\
&\quad -\frac{1515133}{23538138624000}\,H^{14}-\frac{25819}{4483454976000}\,H^{16}+\cdots\\
b_1 &= \frac{5}{6}+\frac{1}{3024}\,H^6+\frac{11}{725760}\,H^8+\frac{2353}{1437004800}\,H^{10}\\
&\quad +\frac{186533}{1307674368000}\,H^{12}+\frac{112457}{8826801984000}\,H^{14}\\
&\quad +\frac{1635421}{1440534083788800}\,H^{16}+\cdots
\end{aligned} \tag{25}
$$

The behavior of the coefficients is given in the following Fig. 3.

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

$$
\mathrm{LTE} = \frac{h^8}{6048}\left(y_n^{(8)}+2\,\omega^2\;y_n^{(6)}-2\omega^6\,y_n^{(2)}-\omega^8\,y_n\right) \tag{26}
$$

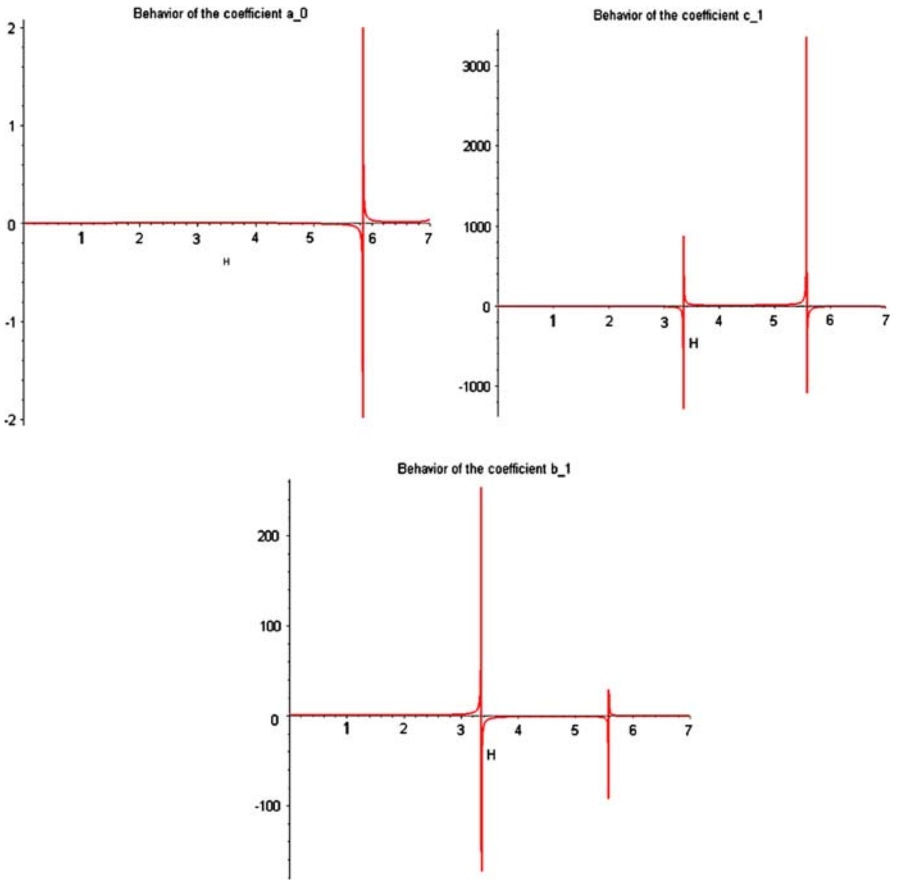

Fig. 3 Behavior of the coefficients of the new method given by (24) for several values of H

3.4 Fourth method of the family

Consider the family of methods presented in (9).

The application of the above method to the scalar test Eq. 4 gives the difference Eq. 10 and the characteristic Eq. 10.

By applying $k = 1$ in the formula (8), we have that the phase-lag is given by (11). The first derivative of the phase-lag is given by (16). The second derivative of the phase-lag is given by (23). The third derivative of the phase-lag can be written as:

$$\begin{aligned} \dddot{phl} &= \frac{1}{2}\,\frac{T_9 - 6\,\mathrm{T}_8\cos(H) + 2\,\mathrm{T}_5\sin(H) - 48\,b_1\,a_0\,H}{\mathrm{T}_5} \\ &\quad - \frac{3}{2}\,\frac{(2\,\mathrm{T}_7\cos(H) - 4\,\mathrm{T}_8\sin(H) - 2\,\mathrm{T}_5\cos(H) + 2\,b_1 - 24\,b_1\,a_0\,H^2)\,\mathrm{T}_8}{\mathrm{T}_5{}^2} \\ &\quad + \frac{3\,(2\,\mathrm{T}_8\cos(H) - 2\,\mathrm{T}_5\sin(H) + 2\,H\,b_1 - 8\,H^3\,b_1\,a_0)\,\mathrm{T}_8{}^2}{\mathrm{T}_5{}^3} \end{aligned}$$

$$
\begin{aligned}
&\quad - \frac{3}{2}\,\frac{(2\,\mathrm{T}_8\cos(H) - 2\,\mathrm{T}_5\sin(H) + 2\,H\,b_1 - 8\,H^3\,b_1\,a_0)\,\mathrm{T}_7}{{\mathrm{T}_5}^2} - \frac{3\,\mathrm{T}_6\,{\mathrm{T}_8}^3}{{\mathrm{T}_5}^4}\\
&\quad + \frac{3\,\mathrm{T}_6\,\mathrm{T}_8\,\mathrm{T}_7}{{\mathrm{T}_5}^3} - \frac{12\,\mathrm{T}_6\,b_1\,a_0\,H}{{\mathrm{T}_5}^2}\\
\mathrm{T}_5 &= 1 + H^2\,b_0 + H^4\,b_1\,a_0\\
\mathrm{T}_6 &= 2\,\mathrm{T}_5\cos(H) + c_1 + H^2\,b_1 - 2\,H^4\,b_1\,a_0\\
\mathrm{T}_7 &= 2\,b_0 + 12\,b_1\,a_0\,H^2\\
\mathrm{T}_8 &= 2\,H\,b_0 + 4\,H^3\,b_1\,a_0\\
\mathrm{T}_9 &= 48\,b_1\,a_0\,H\cos(H) - 6\,\mathrm{T}_7\sin(H)
\end{aligned}
\tag{27}
$$

We demand that the phase-lag and its first, second and third derivative are equal to zero and we find out that:

$$
\begin{aligned}
a_0 &= \frac{1}{4}\Big(3\cos(H)^2 + \cos(H)^2\,H^2 + 2\,H^2 - 3\Big)\\
&\quad \Big/ \Big(\Big(6\cos(H)^3\,H + 6\sin(H)\cos(H)^2\\
&\quad - 2\cos(H)^2\,H^2\sin(H) + \cos(H)^2\,H^3\\
&\quad + 3\cos(H)^2\,H - 6\cos(H)\sin(H)\\
&\quad - 4\cos(H)\,H^2\sin(H) - 12\cos(H)\,H + 2\,H^3\\
&\quad + 3\,H + 12\sin(H)\,H^2\Big)\,H\Big)\\
c_1 &= -2\,\Big(-12\cos(H)^3\,H + \cos(H)^2\,H^3 - 21\cos(H)^2\,H\\
&\quad - 12\sin(H)\cos(H)^2 - 4\cos(H)^2\,H^2\sin(H) + 12\cos(H)\sin(H)\\
&\quad - 8\cos(H)\,H^2\sin(H) + 24\cos(H)\,H + 2\,H^3 + 9\,H + 24\sin(H)\,H^2\Big)\\
&\quad \Big/ \Big(\cos(H)^2\,H^3 - 21\cos(H)^2\,H + 8\cos(H)\,H^2\sin(H)\\
&\quad - 12\cos(H)\,H - 12\cos(H)\sin(H) + 4\sin(H)\,H^2\\
&\quad + 33\,H + 12\sin(H) + 2\,H^3\Big)\\
b_0 &= -2\,\Big(3\cos(H)^2\,H + \cos(H)^2\,H^3 + 6\cos(H)\sin(H)\\
&\quad + 4\cos(H)\,H^2\sin(H) + 6\cos(H)\,H\\
&\quad + 2\sin(H)\,H^2 - 9\,H - 6\sin(H) + 2\,H^3\Big)\Big/\\
&\quad \Big(\Big(\cos(H)^2\,H^3 - 21\cos(H)^2\,H + 8\cos(H)\,H^2\sin(H)\\
&\quad - 12\cos(H)\,H - 12\cos(H)\sin(H)\\
&\quad + 4\sin(H)\,H^2 + 33\,H + 12\sin(H) + 2\,H^3\Big)\,H^2\Big)\\
b_1 &= 4\,\Big(6\cos(H)^3\,H + 6\sin(H)\cos(H)^2 - 2\cos(H)^2\,H^2\sin(H)\\
&\quad + \cos(H)^2\,H^3 + 3\cos(H)^2\,H - 6\cos(H)\sin(H)
\end{aligned}
$$

$$
\begin{aligned}
&- 4\cos(H)\,H^2\sin(H) - 12\cos(H)\,H + 2\,H^3 + 3\,H + 12\sin(H)\,H^2\Big) \\
&\Big/ \Big(\Big(\cos(H)^2\,H^3 - 21\cos(H)^2\,H + 8\cos(H)\,H^2\sin(H) - 12\cos(H)\,H \\
&- 12\cos(H)\sin(H) + 4\sin(H)\,H^2 + 33\,H + 12\sin(H) + 2\,H^3\Big)\,H^2\Big)
\end{aligned}
\tag{28}
$$

For small values of $|H|$ the formulae given by (28) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
a_0 &= \frac{1}{200} + \frac{1}{1260}\,H^2 + \frac{29}{504000}\,H^4 + \frac{1433}{1164240000}\,H^6 \\
&\quad - \frac{63101}{363242880000}\,H^8 - \frac{2228861}{127135008000000}\,H^{10} \\
&\quad - \frac{8804897}{77806624896000000}\,H^{12} + \frac{240953700049}{2048959660011264000000}\,H^{14} \\
&\quad + \frac{9699610781879}{8195838640045056000000000}\,H^{16} + \cdots \\
c_1 &= -2 + \frac{1}{6048}\,H^8 + \frac{1}{43200}\,H^{10} + \frac{1}{532224}\,H^{12} \\
&\quad + \frac{41}{5943974400}\,H^{14} - \frac{601}{24141680640}\,H^{16} + \cdots \\
b_0 &= \frac{1}{12} - \frac{1}{1008}\,H^4 - \frac{31}{181440}\,H^6 \\
&\quad - \frac{221}{13685760}\,H^8 - \frac{619}{1345344000}\,H^{10} \\
&\quad + \frac{25031}{174356582400}\,H^{12} + \frac{84256583}{2667655710720000}\,H^{14} \\
&\quad + \frac{1030007057}{290289444157440000}\,H^{16} + \cdots \\
b_1 &= \frac{5}{6} + \frac{1}{504}\,H^4 - \frac{29}{90720}\,H^6 \\
&\quad - \frac{3271}{47900160}\,H^8 - \frac{35293}{4540536000}\,H^{10} \\
&\quad - \frac{36019}{87178291200}\,H^{12} + \frac{47333617}{1333827855360000}\,H^{14} \\
&\quad + \frac{294008389}{24562952967168000}\,H^{16} + \cdots
\end{aligned}
\tag{29}
$$

The behavior of the coefficients is given in the following Fig. 4.

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

$$
\mathrm{LTE} = \frac{h^8}{6048}\left(y_n^{(8)} + 4\,\omega^2\ y_n^{(6)} + 6\,\omega^4\ y_n^{(4)} + 4\omega^6\,y_n^{(2)} + \omega^8\,y_n\right) \tag{30}
$$

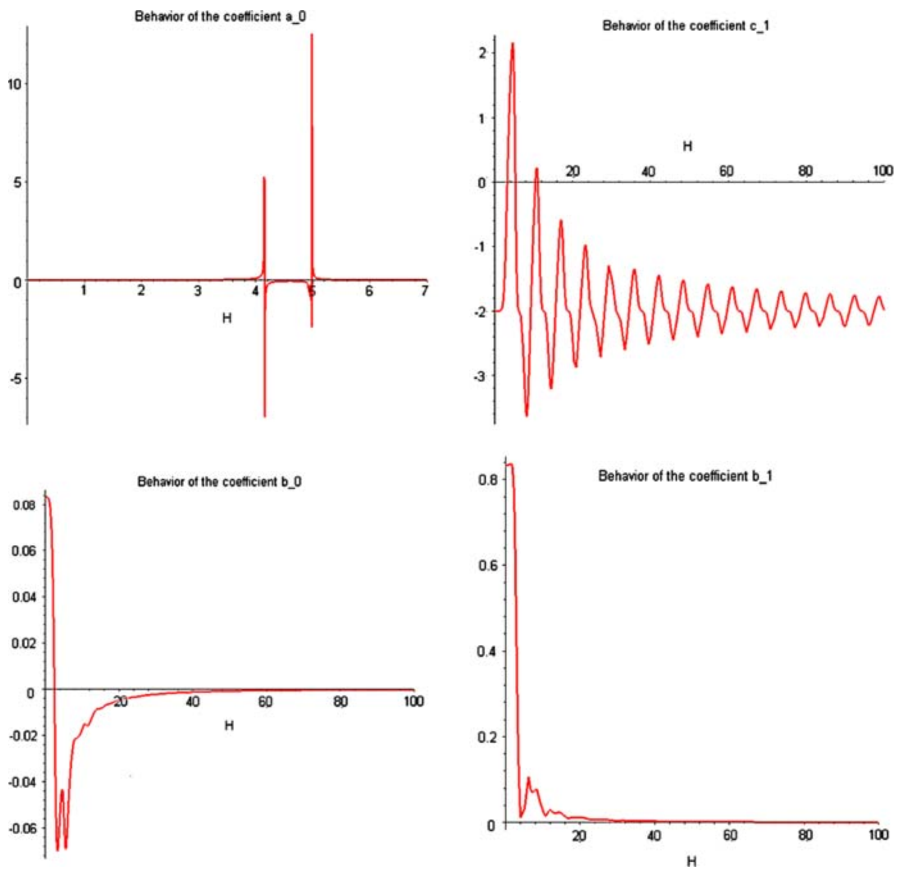

Fig. 4 Behavior of the coefficients of the new method given by (28) for several values of H

4 Error analysis

We will study the following methods:

- The First Method of the Family (mentioned as $PL1$)
- The Second Method of the Family (mentioned as $PL2$)
- The Third Method of the Family (mentioned as $PL3$)
- The Fourth Method of the Family (mentioned as $PL4$)

The error analysis is based on the following steps:

- The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x)\, y(x) \tag{31}$$

- Based on the paper of Ixaru and Rizea [20], the function f(x) can be written in the form:

$$f(x) = g(x) + G \tag{32}$$

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

- We express the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of the Eq. 31. 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:

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

we obtain the following expressions:

The first method of the family

$$\begin{aligned}
\mathrm{LTE}_{\mathrm{PL1}} &= h^8\Bigg[-\frac{1}{6048}\,\mathrm{g}(x)\,\mathrm{y}(x)\,G^3 + \Bigg(-\frac{5}{2016}\left(\frac{d^2}{dx^2}\mathrm{g}(x)\right)\mathrm{y}(x)\\
&\quad - \frac{1}{1008}\left(\frac{d}{dx}\mathrm{g}(x)\right)\left(\frac{d}{dx}\mathrm{y}(x)\right) - \frac{1}{2016}\,\mathrm{g}(x)^2\,\mathrm{y}(x)\Bigg)G^2\\
&\quad + \Bigg(-\frac{5}{2016}\left(\frac{d^4}{dx^4}\mathrm{g}(x)\right)\mathrm{y}(x) - \frac{5}{1512}\left(\frac{d^3}{dx^3}\mathrm{g}(x)\right)\left(\frac{d}{dx}\mathrm{y}(x)\right)\\
&\quad - \frac{1}{336}\,\mathrm{g}(x)\left(\frac{d}{dx}\mathrm{y}(x)\right)\left(\frac{d}{dx}\mathrm{g}(x)\right) - \frac{37}{6048}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d^2}{dx^2}\mathrm{g}(x)\right)
\end{aligned}$$

$$
\begin{aligned}
&-\frac{1}{252}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)^2 \mathrm{y}(x)-\frac{1}{2016}\,\mathrm{g}(x)^3\,\mathrm{y}(x)\Bigg)\,G\\
&-\frac{1}{6048}\left(\frac{d^6}{dx^6}\,\mathrm{g}(x)\right)\mathrm{y}(x)-\frac{1}{1008}\left(\frac{d^5}{dx^5}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\\
&-\frac{1}{378}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d^4}{dx^4}\,\mathrm{g}(x)\right)-\frac{5}{2016}\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right)^2\mathrm{y}(x)\\
&-\frac{13}{3024}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\mathrm{y}(x)\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right)\\
&-\frac{1}{252}\,\mathrm{g}(x)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right)\\
&-\frac{1}{504}\,\mathrm{g}(x)^2\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\\
&-\frac{1}{126}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right)\\
&-\frac{11}{3024}\,\mathrm{g}(x)^2\,\mathrm{y}(x)\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right)-\frac{1}{216}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d}{dx}\,\mathrm{g}(x)\right)^2\\
&-\frac{1}{6048}\,\mathrm{g}(x)^4\,\mathrm{y}(x)\Bigg]
\end{aligned}
\tag{33}
$$

The second method of the family

$$
\begin{aligned}
\mathrm{LTE}_{\mathrm{PL2}} &= h^8\Bigg[\Bigg(\frac{19}{9072}\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right)\mathrm{y}(x)+\frac{1}{1512}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\\
&+\frac{1}{3024}\,\mathrm{g}(x)^2\,\mathrm{y}(x))\,G^2+\Bigg(\frac{11}{4536}\left(\frac{d^4}{dx^4}\,\mathrm{g}(x)\right)\mathrm{y}(x)\\
&+\frac{1}{324}\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)+\frac{1}{378}\,\mathrm{g}(x)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\\
&+\frac{13}{2268}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right)+\frac{17}{4536}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)^2\mathrm{y}(x)\\
&+\frac{1}{2268}\,\mathrm{g}(x)^3\,\mathrm{y}(x)\Bigg)\,G+\frac{1}{6048}\left(\frac{d^6}{dx^6}\,\mathrm{g}(x)\right)\mathrm{y}(x)\\
&+\frac{1}{1008}\left(\frac{d^5}{dx^5}\,\mathrm{g}(x)\right)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)+\frac{1}{378}\,\mathrm{g}(x)\,\mathrm{y}(x)\left(\frac{d^4}{dx^4}\,\mathrm{g}(x)\right)\\
&+\frac{5}{2016}\left(\frac{d^2}{dx^2}\,\mathrm{g}(x)\right)^2\mathrm{y}(x)+\frac{13}{3024}\left(\frac{d}{dx}\,\mathrm{g}(x)\right)\mathrm{y}(x)\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right)\\
&+\frac{1}{252}\,\mathrm{g}(x)\left(\frac{d}{dx}\,\mathrm{y}(x)\right)\left(\frac{d^3}{dx^3}\,\mathrm{g}(x)\right)
\end{aligned}
$$

$$+\frac{1}{504}\,g(x)^2\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d}{dx}\,g(x)\right)$$
$$+\frac{1}{126}\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right)$$
$$+\frac{11}{3024}\,g(x)^2\,y(x)\left(\frac{d^2}{dx^2}\,g(x)\right)$$
$$\left.+\frac{1}{216}\,g(x)\,y(x)\left(\frac{d}{dx}\,g(x)\right)^2+\frac{1}{6048}\,g(x)^4\,y(x)\right] \tag{34}$$

The third method of the family

$$\begin{aligned}
\mathrm{LTE}_{PL3} = h^8 \Bigg[& \frac{1}{756}\left(\frac{d^2}{dx^2}\,g(x)\right)y(x)\,G^2 \\
& +\left(\frac{1}{432}\left(\frac{d^4}{dx^4}\,g(x)\right)y(x)+\frac{1}{378}\left(\frac{d^3}{dx^3}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\right. \\
& +\frac{1}{504}\,g(x)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d}{dx}\,g(x)\right) \\
& +\frac{5}{1008}\,g(x)\,y(x)\left(\frac{d^2}{dx^2}\,g(x)\right)+\frac{5}{1512}\left(\frac{d}{dx}\,g(x)\right)^2 y(x) \\
& \left.+\frac{1}{3024}\,g(x)^3\,y(x)\right)G+\frac{1}{6048}\left(\frac{d^6}{dx^6}\,g(x)\right)y(x) \\
& +\frac{1}{1008}\left(\frac{d^5}{dx^5}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right) \\
& +\frac{1}{378}\,g(x)\,y(x)\left(\frac{d^4}{dx^4}\,g(x)\right) \\
& +\frac{5}{2016}\left(\frac{d^2}{dx^2}\,g(x)\right)^2 y(x)+\frac{13}{3024}\left(\frac{d}{dx}\,g(x)\right)y(x)\left(\frac{d^3}{dx^3}\,g(x)\right) \\
& +\frac{1}{252}\,g(x)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^3}{dx^3}\,g(x)\right) \\
& +\frac{1}{504}\,g(x)^2\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d}{dx}\,g(x)\right) \\
& +\frac{1}{126}\left(\frac{d}{dx}\,g(x)\right)\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d^2}{dx^2}\,g(x)\right) \\
& +\frac{11}{3024}\,g(x)^2\,y(x)\left(\frac{d^2}{dx^2}\,g(x)\right) \\
& \left.+\frac{1}{216}\,g(x)\,y(x)\left(\frac{d}{dx}\,g(x)\right)^2+\frac{1}{6048}\,g(x)^4\,y(x)\right]
\end{aligned} \tag{35}$$

The fourth method of the family

$$\begin{aligned}
\mathrm{LTE}_{\mathrm{PL4}} &= h^8 \Bigg[\left(\frac{1}{504} \left(\frac{d^4}{dx^4}\, g(x) \right) y(x) + \frac{1}{756} \left(\frac{d^3}{dx^3}\, g(x) \right) \left(\frac{d}{dx}\, y(x) \right) \right. \\
&\quad \left. + \frac{1}{378}\, g(x)\, y(x) \left(\frac{d^2}{dx^2}\, g(x) \right) + \frac{1}{504} \left(\frac{d}{dx}\, g(x) \right)^2 y(x) \right) G \\
&\quad + \frac{1}{6048} \left(\frac{d^6}{dx^6}\, g(x) \right) y(x) + \frac{1}{1008} \left(\frac{d^5}{dx^5}\, g(x) \right) \left(\frac{d}{dx}\, y(x) \right) \\
&\quad + \frac{1}{378}\, g(x)\, y(x) \left(\frac{d^4}{dx^4}\, g(x) \right) + \frac{5}{2016} \left(\frac{d^2}{dx^2}\, g(x) \right)^2 y(x) \\
&\quad + \frac{13}{3024} \left(\frac{d}{dx}\, g(x) \right) y(x) \left(\frac{d^3}{dx^3}\, g(x) \right) \\
&\quad + \frac{1}{252}\, g(x) \left(\frac{d}{dx}\, y(x) \right) \left(\frac{d^3}{dx^3}\, g(x) \right) \\
&\quad + \frac{1}{504}\, g(x)^2 \left(\frac{d}{dx}\, y(x) \right) \left(\frac{d}{dx}\, g(x) \right) \\
&\quad + \frac{1}{126} \left(\frac{d}{dx}\, g(x) \right) \left(\frac{d}{dx}\, y(x) \right) \left(\frac{d^2}{dx^2}\, g(x) \right) \\
&\quad + \frac{11}{3024}\, g(x)^2\, y(x) \left(\frac{d^2}{dx^2}\, g(x) \right) \\
&\quad + \frac{1}{216}\, g(x)\, y(x) \left(\frac{d}{dx}\, g(x) \right)^2 + \frac{1}{6048}\, g(x)^4\, y(x) \Bigg]
\end{aligned} \tag{36}$$

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 $\mid G \mid$ is a large number. So, we have the following asymptotic expansions of the Eqs. 33, 34, 35 and 36.
  The first method of the family

$$\mathrm{LTE}_{\mathrm{PL1}} = h^8 \left(-\frac{1}{6048}\, g(x)\, y(x)\, G^3 + \cdots \right) \tag{37}$$

The second method of the family

$$\begin{aligned}
\mathrm{LTE}_{\mathrm{PL2}} = h^8 & \left(\frac{19}{9072} \left(\frac{d^2}{dx^2}\, g(x) \right) y(x) + \frac{1}{1512} \left(\frac{d}{dx}\, g(x) \right) \left(\frac{d}{dx}\, y(x) \right) \right. \\
& \left. + \frac{1}{3024}\, g(x)^2\, y(x) \right) G^2 + \cdots \Bigg)
\end{aligned} \tag{38}$$

The third method of the family

$$\mathrm{LTE_{PL3}} = h^8 \left(\frac{1}{756} \left(\frac{d^2}{dx^2}\, \mathrm{g}(x) \right) \mathrm{y}(x)\, G^2 + \cdots \right) \tag{39}$$

The fourth method of the family

$$\begin{aligned}\mathrm{LTE_{PL4}} &= h^8 \left(\left(\frac{1}{504} \left(\frac{d^4}{dx^4}\, \mathrm{g}(x) \right) \mathrm{y}(x) + \frac{1}{756} \left(\frac{d^3}{dx^3}\, \mathrm{g}(x) \right) \left(\frac{d}{dx}\, \mathrm{y}(x) \right) \right.\right. \\ &\quad \left.\left. + \frac{1}{378}\, \mathrm{g}(x)\, \mathrm{y}(x) \left(\frac{d^2}{dx^2}\, \mathrm{g}(x) \right) + \frac{1}{504} \left(\frac{d}{dx}\, \mathrm{g}(x) \right)^2 \mathrm{y}(x) \right) G + \cdots \right)\end{aligned} \tag{40}$$

From the above equations we have the following theorem:

Theorem 2 *For the First Method of the New Family of Methods the error increases as the third power of G. For the Second and Third Methods of the New Family of Methods the error increases as the second power of G. For the Fourth Method of the New Family of Methods the error increases as the first power of G. It is easy one to see that the coefficient of the second power of G in the case of the second method of the New Family of Methods is* 1.583333333 *times larger than the coefficient of the second power of G in the case of the third method of the New Family of Methods. So, for the numerical solution of the time independent radial Schrödinger equation the new obtained Fourth Method of the New Family of Methods is the most accurate one, especially for large values of $\mid G \mid = \mid V_c - E \mid$.*

5 Stability analysis

We apply the new family of methods to the scalar test equation:

$$y'' = -t^2 y, \tag{41}$$

where $t \neq \omega$. We obtain the following difference equation:

$$A_1(H, s)\, y_{n+1} + A_0(H, s)\, y_n + A_1(H, s)\, y_{n-1} = 0$$

where $s = t\,h$, h is the step length and $A_0(H, s)$ and $A_1(H, s)$ are polynomials of s.

The characteristic equation associated with (42) is given by:

$$A_1(H, s)\, s + A_0(H, s) + A_1(H, s)\, s^{-1} = 0 \tag{42}$$

where

$$\begin{aligned} A_1(H, s) &= 1 + s^2\, b_0 + s^4\, b_1\, a_0 \\ A_0(H, s) &= c_1 + s^2\, b_1 - 2\, s^4\, b_1\, a_0 \end{aligned} \tag{43}$$

Definition 1 (*see [125]*) A symmetric four-step method with the characteristic equation given by (42) is said to have an *interval of periodicity* $\left(0, w_0^2\right)$ if, for all $w \in \left(0, w_0^2\right)$, the roots $z_i,\ i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i\,\theta(t\,h)}, \quad |z_i| \leq 1, \quad i = 3, 4 \tag{44}$$

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

Definition 2 (*see [125]*) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Theorem 3 (see [126]) *A symmetric two-step method with the characteristic equation given by (42) is said to have a nonzero interval of periodicity* $\left(0, s_0^2\right)$ *if, for all* $s \in \left(0, s_0^2\right)$ *the following relations are hold*

$$P_1(H, s) > 0,\ P_2(H, s) > 0, \tag{45}$$

where $H = \omega\,h$, $s = t\,h$ *and:*

$$\begin{aligned} P_1(H, s) &= A_0(H, s) + 2\,A_1(H, s) > 0, \\ P_2(H, s) &= A_0(H, s) - 2\,A_1(H, s) > 0, \end{aligned} \tag{46}$$

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S^2$ only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $H = s$.

Based on (43) the stability polynomials (46) for the new developed methods take the form:

$$\begin{aligned} P_1(H, s) &= c_1 + v^2\,b_1 + 2 + 2\,v^2\,b_0, \\ P_2(H, s) &= c_1 + v^2\,b_1 - 4\,v^4\,b_1\,a_0 - 2 - 2\,v^2\,b_0 \end{aligned} \tag{47}$$

In Figs. 5, 6, 7 and 8 we present the s–H planes for the methods developed in this paper. A shadowed area denotes the s–H region where the method is unstable, while a white area denotes the region where the method is stable. In Fig. 5 we present the s–H plane for the first method of the new family of method developed in this paper (Sect. 3.1). In Fig. 6 we present the s–H plane for the second method of the new family of method developed in this paper (Sect. 3.2). In Fig. 7 we present the s–H plane for the third method of the new family of method developed in this paper (Sect. 3.3). Finally, in Fig. 8 we present the s–H plane for the fourth method of the new family of method developed in this paper (Sect. 3.4).

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 $H = s$, we have the following figure for the stability polynomials of the new developed methods. A method is P-stable if the s–H plane

[2] where S is a set of distinct points.

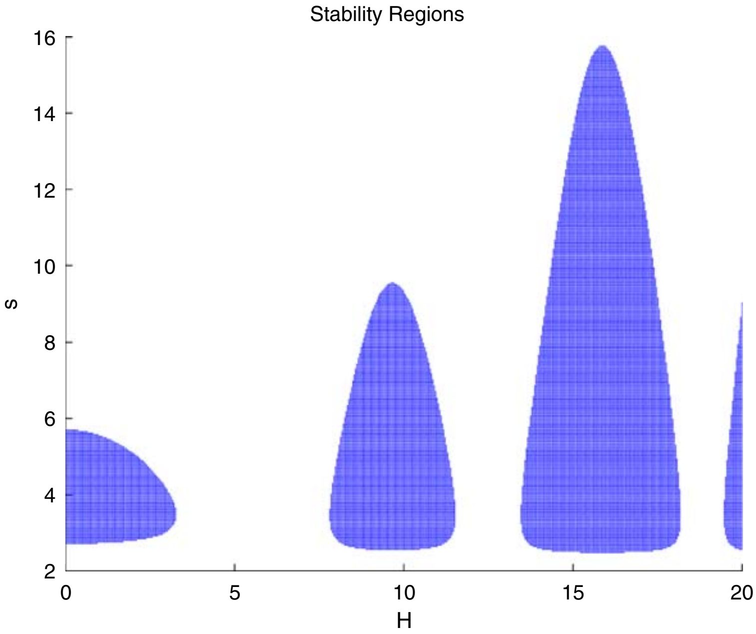

Fig. 5 s–H plane of the first method of the new family of method developed in this paper (Sect. 3.1)

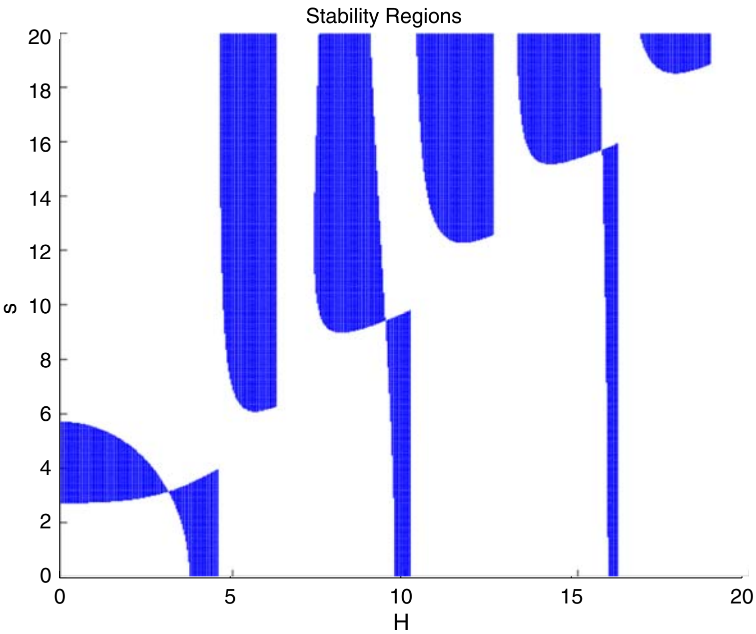

Fig. 6 s–H plane of the second method of the new family of method developed in this paper (Sect. 3.2)

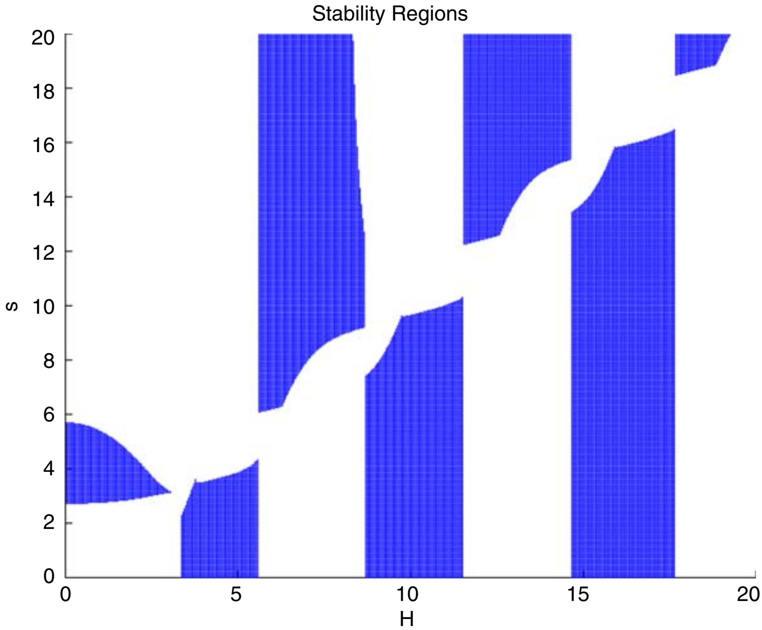

Fig. 7 s–H plane of the third method of the new family of method developed in this paper (Sect. 3.3)

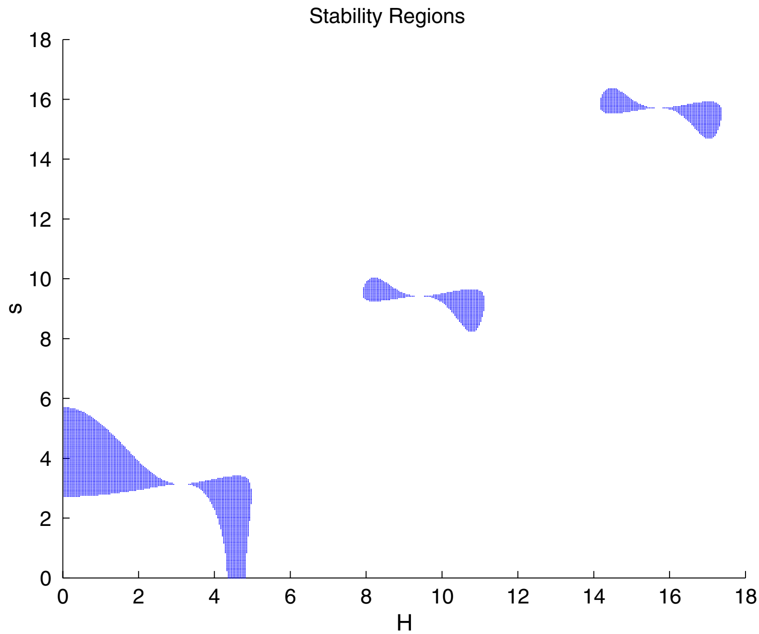

Fig. 8 s–H plane of the fourth method of the new family of method developed in this paper (Sect. 3.4)

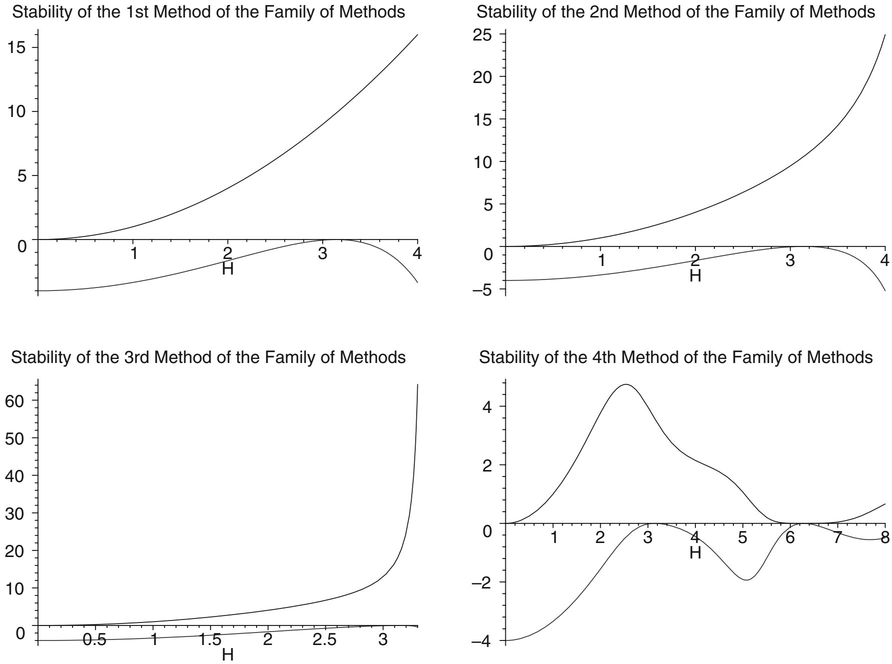

Fig. 9 Stability polynomials of the new developed methods in the case that $H = s$

is not shadowed. From the above diagrams it is easy for one to see that the interval of periodicity of all the new methods is equal to: $\left(0, \pi^2\right)$ (Fig. 9).

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 w–H plane.

6 Numerical results—conclusion

In order to illustrate the efficiency of the new methods obtained in Sects. 3.1–3.4, we apply them to the radial 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 one-dimensional Schrödinger equation given by (1) the parameter v is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{48}$$

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

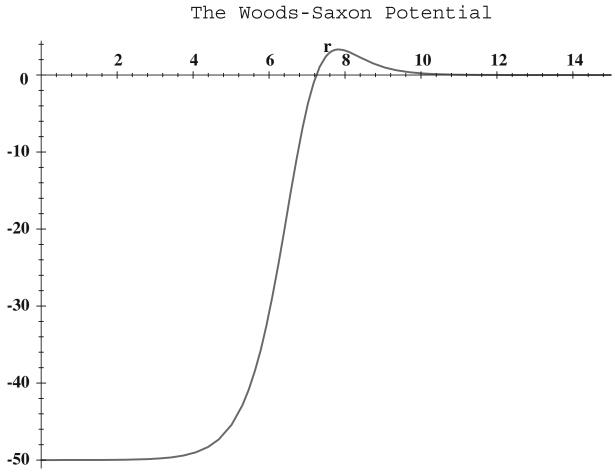

Fig. 10 The Woods-Saxon potential

6.1 Woods-Saxon potential

We use the well known Woods-Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\,(1+z)^2} \tag{49}$$

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

The behavior of Woods-Saxon potential is shown in the Fig. 10.

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 [13]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [13]):

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

6.2 Radial Schrödinger equation—the resonance problem

Consider the numerical solution of the radial time independent Schrödinger equation (1) in the well-known case of the Woods-Saxon potential (49). In order to solve this problem numerically we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration 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

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{51}$$

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

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC\left[sin\left(kx - \frac{l\pi}{2}\right) + tan\delta_l cos\left(kx - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{52}$$

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

$$tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{53}$$

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 before starting a one-step method. From the initial condition we obtain y_0. 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:

$$y(0) = 0, \;\; y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{54}$$

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 four-step method developed by Raptis [16] which is indicated as *Method II*.
- The Two-Step Numerov-type Method with minimum phase-lag produced by Chawla and Rao [127] which is indicated as *Method III*.
- The new Two-Step Numerov-Type Method with phase-lag equal to zero obtained in Sect. 3.1 which is indicated as *Method IV*.

- The new Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero obtained in Sect. 3.2 which is indicated as *Method V*.
- The new Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero obtained in Sect. 3.3 which is indicated as *Method VI*.
- The new Two-Step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero obtained in Sect. 3.4 which is indicated as *Method VII*.

The computed eigenenergies are compared with exact ones. In Fig. 11 we present the maximum absolute error $log_{10}\,(Err)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{55}$$

of the eigenenergy E_1, for several values of NFE = Number of Function Evaluations. In Fig. 12 we present the maximum absolute error $log_{10}\,(Err)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{56}$$

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

7 Conclusions

In the present paper we have developed a family of methods of sixth algebraic order for the numerical solution of the radial Schrödinger equation.

More specifically we have developed:

1. A Two-Step Numerov-Type Method with phase-lag equal to zero.
2. A Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero.
3. A Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero.
4. A Two-Step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero.

We have applied the new method to the resonance problem of the radial Schrödinger equation.

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

- The Exponentially-fitted four-step method developed by Raptis [16] (denoted as Method II) is more efficient than the Numerov's Method (denoted Method I).
- The Two-Step Numerov-type Method with minimum phase-lag produced by Chawla and Rao [127] (Method III) is more efficient than the Exponentially-fitted four-step method developed by Raptis [16] (Method II) for the energy 163.215341 and less efficient for the energy 989.701916.
- The new developed methods are much more efficient than the older ones.
- The Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero (Method V) is more efficient than the New Two-Step Numerov-Type Method with phase-lag equal to zero (Method IV).

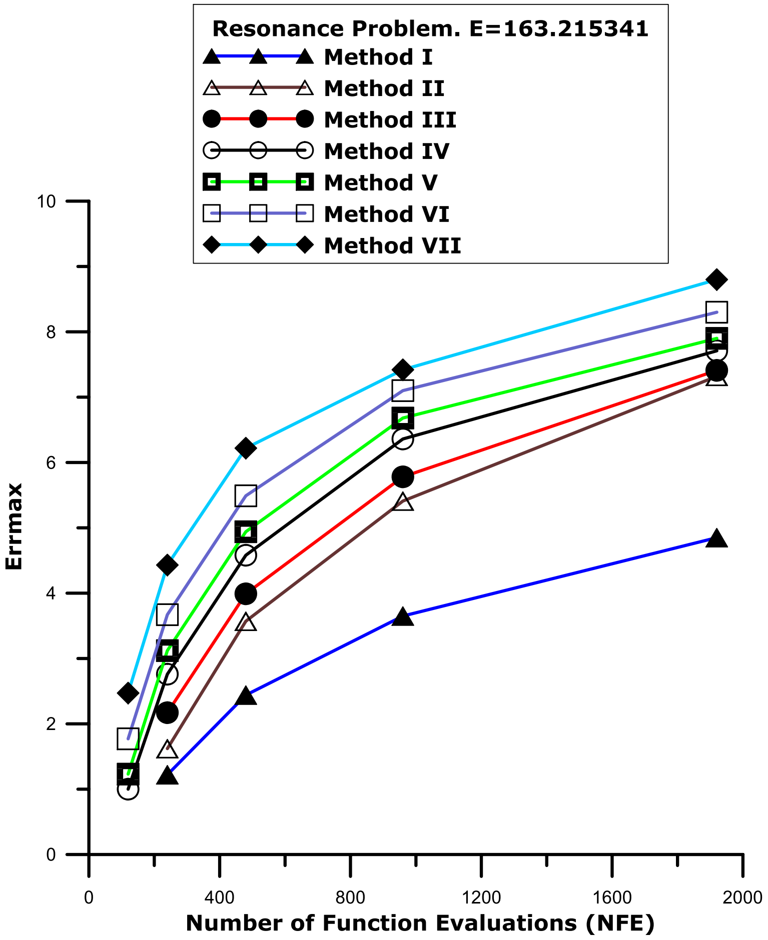

Fig. 11 Error Errmax for several values of n for the eigenvalue $E_1 = 163.215341$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

– The Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero (Method VI) is more efficient than the Two-Step Numerov-Type Method with phase-lag and its first derivative equal to zero (Method V).
– The Two-Step Numerov-Type Method with phase-lag and its first, second and third derivatives equal to zero (Method VII) is more efficient than the Two-Step Numerov-Type Method with phase-lag and its first and second derivatives equal to zero (Method VI).

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

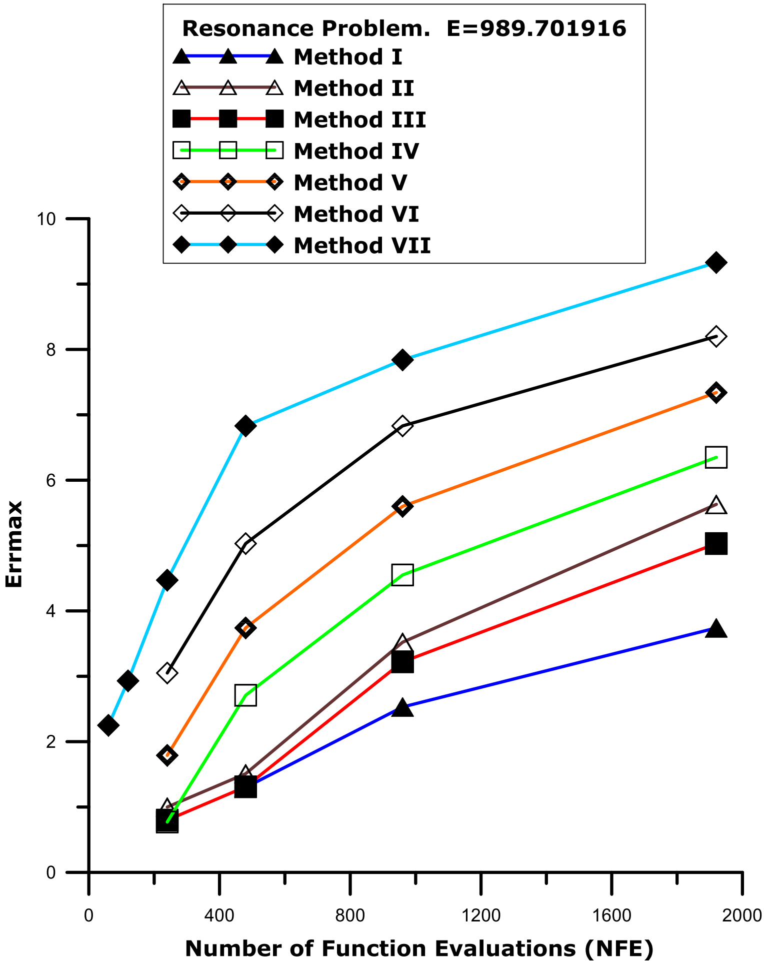

Fig. 12 Error Errmax for several values of n for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Errmax indicates that for this value of n, Errmax is positive

References

1. L.Gr. Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
2. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)
3. I. Prigogine, S. Rice (eds.), *Advances in Chemical Physics, vol. 93: New Methods in Computational Quantum Mechanics* (Wiley, 1997)
4. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
5. T.E. Simos, in Atomic Structure Computations in Chemical Modelling: Applications and Theory, ed by A. Hinchliffe, UMIST), (The Royal Society of Chemistry 2000), pp. 38–142
6. T.E. Simos, Numerical methods for 1D, 2D and 3D differential equations arising in chemical problems. Chem. Model.: Appl. Theory, Roy. Soc. Chem. **2**, 170–270 (2002)
7. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. Comput. Chem. **23**, 513–554 (1999)

8. T.E. Simos, *Numerical Solution of Ordinary Differential Equations with Periodical Solution*. Doctoral Dissertation, National Technical University of Athens, Greece, 1990 (in Greek).
9. A. Konguetsof, T.E. Simos, On the Construction of exponentially-fitted methods for the numerical solution of the Schrödinger Equation. J. Comput. Methods Sci. Eng. **1**, 143–165 (2001)
10. A.D. Raptis, A.C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **14**, 1–5 (1978)
11. A.D. Raptis, Exponential multistep methods for ordinary differential equations. Bull. Greek Math. Soc. **25**, 113–126 (1984)
12. L.Gr. Ixaru, *Numerical Methods for Differential Equations and Applications* (Reidel, Dordrecht, Boston, Lancaster 1984)
13. L.Gr. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. Comput. Phys. Commun. **19**, 23–27 (1980)
14. T.E. Simos, P.S. Williams, A New Runge-Kutta-Nystrom method with phase-lag of order infinity for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 123–137 (2002)
15. T.E. Simos, Multiderivative methods for the numerical solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **45**, 7–26 (2004)
16. A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Shrödinger equation with automatic error control. Comput. Phys. Commun. **28**, 427–431 (1983)
17. A.D. Raptis, On the numerical solution of the Schrodinger equation. Comput. Phys. Commun. **24**, 1–4 (1981)
18. Z. Kalogiratou, T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation. Appl. Math. Comput. **112**, 99–112 (2000)
19. L.Gr. Ixaru, G.V. Berghe, *Exponential Fitting, Series on Mathematics and its Applications*, vol 568 (Kluwer Academic Publisher, The Netherlands, 2004)
20. L.Gr. Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. Comput. Phys. Commun. **38**(3), 329–337 (1985)
21. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge-Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. J. Math. Chem. **41**(1), 79–100 (2007)
22. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **40** (3), 257–267 (2006)
23. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order Predictor-Corrector methods. J. Math. Chem. **40**(3), 269–293 (2006)
24. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. J. Math. Chem. **40**(3), 305–318 (2006)
25. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **37**(3), 263–270 (2005)
26. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Numerical solution of the two-dimensional time independent Schrödinger equation with Numerov-type methods. J. Math. Chem. **37**(3), 271–279 (2005)
27. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 281–293 (2005)
28. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation. J. Math. Chem. **37**(3), 295–316 (2005)
29. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **37**(3), 317–331 (2005)
30. T.E. Simos, Exponentially-fitted multiderivative methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **36**(1), 13–27 (2004)
31. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation. J. Math. Chem. **35**(1), 55–63 (2004)
32. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. J. Math. Chem. **34**(1–2), 39–58 (JUL 2003)
33. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Shrödinger equation. J. Math. Chem. **34** (1–2), 83–94 (2003)

34. J. Vigo-Aguiar J, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **32**(3), 257–270 (2002)
35. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. J. Math. Chem. **31**(4), 371–404 (2002)
36. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. J. Math. Chem. **31**(2), 135–144 (2002)
37. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nystrom methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. J. Math. Chem. **31**(2), 211–232
38. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation. J. Math. Chem. **30**(1), 121–131 (2001)
39. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. J. Math. Chem. **29**(4), 281–291 (2001)
40. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. J. Math. Chem. **29**(4), 293–305 (2001)
41. J. Vigo-Aguiar, T.E. Simos, A family of P-stable eighth algebraic order methods with exponential fitting facilities. J. Math. Chem. **29**(3), 177–189 (2001)
42. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. J. Math. Chem. **27**(4), 343–356 (2000)
43. G. Avdelas, T.E. Simos, Embedded eighth order methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **26**(4), 327–341 (1999)
44. T.E. Simos, A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation. J. Math. Chem. **25**(1), 65–84 (1999)
45. T.E. Simos, Some embedded modified Runge-Kutta methods for the numerical solution of some specific Schrödinger equations. J. Math. Chem. **24**(1–3), 23–37 (1998)
46. T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. J. Math. Chem. **21**(4), 359–372 (1997)
47. P. Amodio, I. Gladwell, G. Romanazzi, Numerical Solution of General Bordered ABD Linear Systems by Cyclic Reduction. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 5–12 (2006)
48. S.D. Capper, J.R. Cash, D.R. Moore, Lobatto-Obrechkoff Formulae for 2nd order two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 13–25 (2006)
49. S.D. Capper, D.R. Moore, On high order MIRK schemes and Hermite-Birkhoff interpolants. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 27–47 (2006)
50. J.R. Cash, N. Sumarti, T.J. Abdulla, I. Vieira, The derivation of interpolants for nonlinear two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 49–58 (2006)
51. J.R. Cash, S. Girdlestone, Variable step Runge-Kutta-Nystrf́7m methods for the numerical solution of reversible systems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 59–80 (2006)
52. J.R. Cash, F. Mazzia, Hybrid mesh selection algorithms based on conditioning for two-point boundary value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 81–90 (2006)
53. F. Iavernaro, F. Mazzia, D. Trigiante, Stability and conditioning in numerical analysis. JNAIAM J. Numer. Anal. Indust. Appl. Math **1**(1), 91–112 (2006)
54. F. Iavernaro, D. Trigiante, Discrete conservative vector fields induced by the trapezoidal method. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 113–130 (2006)
55. F. Mazzia, A. Sestini, D. Trigiante, BS linear multistep methods on non-uniform meshes. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(1), 131–144 (2006)
56. L.F. Shampine, P.H. Muir, H. Xu, A user-friendly fortran BVP solver. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(2), 201–217 (2006)
57. G. Vanden Berghe, M. Van Daele, Exponentially-fitted Störmer/Verlet methods. JNAIAM J. Numer. Anal. Indust. Appl. Math. **1**(3), 241–255 (2006)
58. L. Aceto, R. Pandolfi, D. Trigiante, Stability analysis of linear multistep methods via polynomial type variation. JNAIAM J. Numer. Anal. Indust. Appl. Math. **2**(1–2), 1–9 (2007)
59. G. Psihoyios, A block implicit advanced step-point (BIAS) algorithm for stiff differential systems. Comput. Lett. **2**(1–2), 51–58 (2006)
60. W.H. Enright, On the use of ’arc length’ and ’defect’ for mesh selection for differential equations. Comput. Lett. **1**(2), 47–52 (2005)

61. T.E. Simos, P-stable four-step exponentially-fitted method for the numerical integration of the Schrödinger equation. Comput. Lett. **1**(1), 37–45 (2005)
62. T.E. Simos, Stabilization of a four-step exponentially-fitted method and its application to the Schrödinger equation. Int. J. Modern Phys. C **18**(3), 315–328 (2007)
63. Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems. Comput. Phys. Commun. **171**, 162–174 (2005)
64. T.E. Simos, A Runge-Kutta Fehlberg method with phase-lag of order infinity for initial value problems with oscillating solution. Comput. Math. Appl. **25**, 95–101 (1993)
65. T.E. Simos, Runge-Kutta interpolants with minimal phase-lag. Comput. Math. Appl. **26**, 43–49 (1993)
66. T.E. Simos, Runge-Kutta-Nyström interpolants for the numerical integration of special second-order periodic initial-value problems. Comput. Math. Appl. **26**, 7–15 (1993)
67. T.E. Simos, G.V. Mitsou, A family of four-step exponential fitted methods for the numerical integration of the radial Schrödinger equation. Comput. Math. Appl. **28**, 41–50 (1994)
68. T.E. Simos, G. Mousadis, A two-step method for the numerical solution of the radial Schrödinger equation. Comput. Math. Appl. **29**, 31–37 (1995)
69. G. Avdelas, T.E. Simos, Block Runge-Kutta methods for periodic initial-value problems. Comput. Math. Appl. **31**, 69–83 (1996)
70. G. Avdelas, T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **31**, 85–102 (1996)
71. G. Papakaliatakis, T.E. Simos, A new method for the numerical solution of fourth order BVPs with oscillating solutions. Comput. Math. Appl. **32**, 1–6 (1996)
72. T.E. Simos, An extended Numerov-type method for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **33**, 67–78 (1997)
73. T.E. Simos, A new hybrid imbedded variable-step procedure for the numerical integration of the Schrödinger equation. Comput. Math. Appl. **36**, 51–63 (1998)
74. T.E. Simos, Bessel and Neumann fitted methods for the numerical solution of the Schrödinger equation. Comput. Math. Appl. **42**, 833–847 (2001)
75. A. Konguetsof, T.E. Simos, An exponentially-fitted and trigonometrically-fitted method for the numerical solution of periodic initial-value problems. Comput. Math. Appl. **45**, 547–554 (2003)
76. Z.A. Anastassi, T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems. J. Comput. Appl. Math. **175**(1), 1–9 (2005)
77. G. Psihoyios, T.E. Simos, A fourth algebraic order trigonometrically fitted predictor-corrector scheme for IVPs with oscillating solutions. J. Comput. Appl. Math. **175**(1), 137–147 (2005)
78. D.P. Sakas, T.E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation. J. Comput. Appl. Math. **175**(1), 161–172 (2005)
79. K. Tselios, T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. J. Comput. Appl. Math. **175**(1), 173–181 (2005)
80. Z. Kalogiratou, T.E. Simos, Newton-Cotes formulae for long-time integration. J. Comput. Appl. Math. **158**(1), 75–82 (2003)
81. Z. Kalogiratou, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 83–92 (2003)
82. A. Konguetsof, T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **158**(1), 93–106 (2003)
83. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. J. Comput. Appl. Math. **158**(1), 135–144 (2003)
84. Ch. Tsitouras, T.E. Simos, Optimized Runge-Kutta pairs for problems with oscillating solutions. J. Comput. Appl. Math. **147**(2), 397–409 (2002)
85. T.E. Simos, An exponentially fitted eighth-order method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **108**(1–2), 177–194 (1999)
86. T.E. Simos, An accurate finite difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **91**(1), 47–61 (1998)
87. R.M. Thomas, T.E. Simos, A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **87**(2), 215–226 (1997)
88. Z.A. Anastassi, T.E. Simos, Special Optimized Runge-Kutta methods for IVPs with Oscillating Solutions. Int. J. Modern Phys. C **15**, 1–15 (2004)

89. Z.A. Anastassi, T.E. Simos, A dispersive-fitted and dissipative-fitted explicit Runge-Kutta method for the numerical solution of orbital problems. New Astronomy **10**, 31–37 (2004)
90. Z.A. Anastassi, T.E. Simos, A trigonometrically-fitted Runge-Kutta method for the numerical solution of orbital problems. New Astronomy **10**, 301–309 (2005)
91. T.V. Triantafyllidis, Z.A. Anastassi, T.E. Simos, Two optimized Runge-Kutta methods for the solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
92. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted fifth order Runge-Kutta methods for the numerical solution of the Schrödinger equation. Math. Comput. Model. **42**(7–8), 877–886 (2005)
93. Z.A. Anastassi, T.E. Simos, New trigonometrically fitted six-step symmetric methods for the efficient solution of the Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
94. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, Two new optimized eight-step symmetric methods for the efficient solution of the Schrödinger equation and related problems. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
95. Z.A. Anastassi, T.E. Simos, A six-step P-stable trigonometrically-fitted method for the numerical integration of the radial Schrödinger equation. MATCH Commun. Math. Comput. Chem. **60**, 3 (2008)
96. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. J. Math. Chem. (in Press, corrected proof)
97. T.E. Simos, P.S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **79**(2), 189–205 (1997)
98. G. Avdelas, T.E. Simos, A generator of high-order embedded P-stable methods for the numerical solution of the Schrödinger equation. J. Comput. Appl. Math. **72**(2), 345–358 (1996)
99. R.M. Thomas, T.E. Simos, G.V. Mitsou, A family of Numerov-type exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. J. Comput. Appl. Math. **67**(2), 255–270 (1996)
100. T.E. Simos, A family of 4-step exponentially fitted predictor-corrector methods for the numerical-integration of the Schrödinger-equation. J. Comput. Appl. Math. **58**(3), 337–344 (1995)
101. T.E. Simos, An explicit 4-step phase-fitted method for the numerical-integration of 2nd-order initial-value problems. J. Comput. Appl. Math. **55**(2), 125–133 (1994)
102. T.E. Simos, E. Dimas, A.B. Sideridis, A Runge-Kutta-Nyström method for the numerical-integration of special 2nd-order periodic initial-value problems. J. Comput. Appl. Math. **51**(3), 317–326 (1994)
103. A.B. Sideridis, T.E. Simos, A low-order embedded Runge-Kutta method for periodic initial-value problems. J. Comput. Appl. Math. **44**(2), 235–244 (1992)
104. T.E. Simos, A.D. Raptis, A 4th-order Bessel fitting method for the numerical-solution of the SchrÖdinger-equation. J. Comput. Appl. Math. **43**(3), 313–322 (1992)
105. T.E. Simos, Explicit 2-step methods with minimal phase-lag for the numerical-integration of special 2nd-order initial-value problems and their application to the one-dimensional Schrödinger-equation. J. Comput. Appl. Math. **39**(1), 89–94 (1992)
106. T.E. Simos, A 4-step method for the numerical-solution of the Schrödinger-equation. J. Comput. Appl. Math. **30**(3), 251–255 (1990)
107. C.D. Papageorgiou, A.D. Raptis, T.E. Simos, A method for computing phase-shifts for scattering. J. Comput. Appl. Math. **29**(1), 61–67 (1990)
108. A.D. Raptis, Two-step methods for the numerical solution of the Schrödinger equation. Computing **28**, 373–378 (1982)
109. T.E. Simos, A new Numerov-type method for computing eigenvalues and resonances of the radial Schrödinger equation. Int. J. Modern Phy. C-Phy. Comput. **7**(1), 33–41 (1996)
110. T.E. Simos, Predictor corrector phase-fitted methods for $Y'' = F(X,Y)$ and an application to the Schrödinger-equation. Int. J. Quantum Chem. **53**(5), 473–483 (1995)
111. T.E. Simos, Two-step almost P-stable complete in phase methods for the numerical integration of second order periodic initial-value problems. Int. J. Comput. Math. **46**, 77–85 (1992)
112. R.M. Corless, A. Shakoori, D.A. Aruliah, L. Gonzalez-Vega, Barycentric Hermite interpolants for event location in initial-value problems. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 1–16 (2008)
113. M. Dewar, Embedding a general-purpose numerical library in an interactive environment. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 17–26 (2008)
114. J. Kierzenka, L.F. Shampine, A BVP solver that controls residual and error. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 27–41 (2008)

115. R. Knapp, A method of lines framework in mathematica. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 43–59 (2008)
116. N.S. Nedialkov, J.D. Pryce, Solving differential algebraic equations by taylor series (III): the DAETS code. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 61–80 (2008)
117. R.L. Lipsman, J.E. Osborn, J.M. Rosenberg, The SCHOL Project at the University of Maryland: using mathematical software in the teaching of Sophomore differential equations. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 81–103 (2008)
118. M. Sofroniou, G. Spaletta, Extrapolation methods in mathematica. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 105–121 (2008)
119. R.J. Spiteri, T.-P. Ter, pythNon: a PSE for the numerical solution of nonlinear algebraic equations. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 123–137 (2008)
120. S.P. Corwin, S. Thompson, S.M. White, Solving ODEs and DDEs with impulses. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 139–149 (2008)
121. W. Weckesser, VFGEN: a code generation tool. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 151–165 (2008)
122. A. Wittkopf, Automatic code generation and optimization in maple. JNAIAM J. Numer. Anal. Indust. Appl. Math. **3**, 167–180 (2008)
123. P. Henrici, *Discrete Variable Methods in Ordinary Differential Equations*. (Wiley, 1962)
124. M.M. Chawla, Uncoditionally stable Noumerov-type methods for second order differential equations. BIT **23**, 541–542 (1983)
125. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. J. Inst. Math. Appl. **18**, 189–202 (1976)
126. A.D. Raptis, T.E. Simos, A four-step phase-fitted method for the numerical integration of second order initial-value problem. BIT **31**, 160–168 (1991)
127. M.M. Chawla, P.S. Rao, A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems. J. Comput. Appl. Math. **11(3)**, 277–281 (1984)