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ORIGINAL PAPER

New high order multiderivative explicit four-step methods with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation. Part I: Construction and theoretical analysis

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Abstract In this paper we develop and study new high algebraic order multiderivative explicit four-step method with phase-lag and its first, second and third derivatives equal to zero. For the produced methods we investigate their errors and stability. Based on the above mentioned analysis we will arrive to some remarks and conclusions about their the efficiency to the numerical integration of the radial Schrödinger equation.

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

Mathematics Subject Classification 65L05

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1 Introduction

In this paper we will investigate the approximate solution of the one-dimensional time independent Schrödiner equation. The radial Schrödinger equation can be written as the following boundary value problem:

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

Astronomy, astrophysics, quantum mechanics, quantum chemistry, celestial mechanics, electronics physical chemistry and chemical physics are some of the many scientific areas of applied sciences in which the mathematical models of their problems can be expressed with the above mentioned boundary value problem (see for example [1–4])

For the above boundary value problem (1) there are the following notations:

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

The boundary conditions are:

$$p(0) = 0, \tag{2}$$

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

In this paper we will study a family of multiderivative high algebraic order explicit methods. The idea is a procedure in order to maximize the efficiency of a numerical scheme for the approximate solution of the Schrödinger equation and related problems with periodic or oscillating solutions. More specifically we will develop three methods of this family. In the first the phase-lag and its first derivative are vanished. In the second the phase-lag and its first and second derivatives are vanished and finally in the third scheme the phase-lag and its first, second and third derivatives are vanished.

We note here that any problem with periodic or oscillating solutions or any problem with solution which contains the functions cos and sin or any problem with solution that is a combination of them can be solved effectively using numerical methods which have been produced the methodology mentioned above.

Therefore, the aim of this paper is the calculation of the coefficients of the new obtained family of multiderivative high algebraic order explicit methods in order:

- to have the highest possible algebraic order
- to have the phase-lag vanished
- to have the derivative of the phase-lag (first, first and second or first, second and third respectively) vanished as well

The methodology for the development of the new proposed methods is based on the calculation of the phase-lag and its derivatives. For this purpose we use the direct formula for the determination of the phase-lag for $2m$-method (see [26] and [29]). Therefore, the procedure of vanishing of the phase lag and its first, second and third derivatives is based on the previously mentioned direct formula.

In the present paper (Part I) the new family of multiderivative high algebraic order explicit methods are developed and studied theoretically. More specifically, the investigation of the effectiveness of the new proposed schemes will be based on the investigation of the local truncation error and of the stability analysis of the new proposed methods.

In a future paper (Part II) we will present the implementation of the new obtained formulae (using several new schemes for the computation of the first derivative) and we will also apply the obtained methods to the resonance problem of the radial time independent Schrödinger equation.

The format of the paper is given below:

- In Sect. 2 a bibliography relevant on the subject of the paper is presented
- The phase-lag analysis of symmetric $2k$-methods is described in Sect. 3.
- The new family of multiderivative high algebraic order explicit four-step methods is constructed in Sect. 4.
- A comparative error analysis is studied in Sect. 5.
- The stability properties of the new developed methods are presented in Sect. 6.
- Finally, in Sect. 7 we present remarks and conclusions.

2 Bibliography relevant on the subject of the paper

In order to obtain efficient, fast and reliable algorithms for the approximate solution of the radial Schrödinger equation and related problems, much research has been done the last decades (see for example [5–101]). In the following, we mention some bibliography:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge-Kutta and Runge-Kutta Nyström type have been obtained in [5–11].
- In [12–17] exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are constructed.
- Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [23–47].
- Symplectic integrators are investigated in [48–72].
- Exponentially and trigonometrically multistep methods have been produced in [73–92].
- Nonlinear methods have been studied in [93] and [94]
- Review papers have been presented in [95–99]
- Special issues and Symposia in International Conferences have been developed on this subject (see [102–108])

Recently several multiderivative methods has been constructed (see [109–118]). The most of them are implicit and P-stable. However, we know that P-stability is a very useful property for stiff oscillatory problems and no for problems of the form of the radial Schrödinger equation and related problems.

3 Basic theory on the phase-lag analysis of symmetric multistep methods

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

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

In the case of symmetric multistep methods, the following relations are hold:

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

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

$$q'' = -\omega^2 q \tag{5}$$

a difference equation of the form

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

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

The characteristic equation associated with (6) is given by:

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

Theorem 1 [26] *and* [29] *The symmetric $2m$-step method with characteristic equation given by (7) has phase-lag order p and phase-lag constant c given by:*

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

The formula mentioned in the above theorem is a direct method for the computation of the phase-lag of any symmetric $2m$- step method.

4 Development of the new family of multiderivative methods

Consider the following family of multiderivative eighth algebraic order explicit four-step methods for the numerical solution of problems of the form $q'' = f(x, q)$:

$$q_{n+2} + a_1 q_{n+1} + a_0 q_n + a_1 q_{n-1} + q_{n-2} = h^2 \left[b_1 (f_{n+1} + f_{n-1}) + b_0 f_n \right] + h^4 \left[c_1 (g_{n+1} + g_{n-1}) + c_0 g_n \right] \quad (9)$$

In the above general form :

- the coefficient b_0, b_1, c_0, c_1, a_0 and a_1 are free parameters,
- h is the step size of the integration,
- n is the number of steps,
- $q_{n\pm i}$ is the approximation of the solution on the point $x_{n\pm i}$, $i = 0(1)2$
- $f_{n\pm i} = q''(x_{n\pm i})$, $i = 0(1)2$
- $g_{n\pm i} = q^{(4)}(x_{n\pm i})$, $i = 0(1)2$
- $x_i = x_0 + i\, h$ and
- x_0 is the initial value point.

4.1 First method of the family

Considering that:

$$\begin{aligned} a_1 &= -2\, a_0 = 2 \\ b_1 &= 1 - \frac{1}{2} b_0 \\ c_1 &= \frac{1}{12} - \frac{1}{2} c_0 + \frac{1}{4} b_0 \end{aligned} \quad (10)$$

and applying the method (9) to the scalar test equation (5) we have the difference equation (6) with $m = 2$ and $A_j(v)$, $j = 0(1)2$ given by:

$$\begin{aligned} A_2(\mathrm{v}) &= 1 \\ A_1(\mathrm{v}) &= -2 + \mathrm{v}^2 \left(1 - \frac{1}{2} b_0\right) - \mathrm{v}^4 \left(\frac{1}{12} - \frac{1}{2} c_0 + \frac{1}{4} b_0\right) \\ A_0(\mathrm{v}) &= 2 + \mathrm{v}^2 b_0 - \mathrm{v}^4 c_0 \end{aligned} \quad (11)$$

where $\mathrm{v} = \omega\, h$

Demanding now the above mentioned method with the coefficients (10) to have its phase-lag vanished and using the formulae (8) (for $m = 2$) and (11), the following equation is obtained:

$$\text{Phase} - \text{Lag} = -\frac{\mathrm{T}_0}{-24 - 12\,\mathrm{v}^2 + 6\,\mathrm{v}^2 \mathrm{b}_0 + \mathrm{v}^4 - 6\,\mathrm{v}^4 \mathrm{c}_0 + 3\,\mathrm{v}^4 \mathrm{b}_0} = 0 \quad (12)$$

where

$$
\begin{aligned}
T_0 = {} & 24\ (\cos(\mathrm{v}))^2 - 24\ \cos(\mathrm{v}) + 12\ \cos(\mathrm{v})\,\mathrm{v}^2 \\
& - 6\ \cos(\mathrm{v})\,\mathrm{v}^2 b_0 - \cos(\mathrm{v})\,\mathrm{v}^4 + 6\ \cos(\mathrm{v})\,\mathrm{v}^4 c_0 \\
& - 3\ \cos(\mathrm{v})\,\mathrm{v}^4 b_0 + 6\,\mathrm{v}^2 b_0 - 6\,\mathrm{v}^4 c_0
\end{aligned}
$$

Requiring now the method to have the first derivative of the phase-lag vanished as well, the following equation is obtained:

$$
\begin{aligned}
& \text{First Derivative of the Phase} - \text{Lag} \\
& = \frac{T_1}{\left(-24 - 12\,\mathrm{v}^2 + 6\,\mathrm{v}^2 b_0 + \mathrm{v}^4 - 6\,\mathrm{v}^4 c_0 + 3\,\mathrm{v}^4 b_0\right)^2} = 0
\end{aligned} \tag{13}
$$

where

$$
\begin{aligned}
T_1 = {} & 96\ (\cos(\mathrm{v}))^2\,\mathrm{v}^3 - 576\,\mathrm{v}\,(\cos(\mathrm{v}))^2 \\
& + 12\,\mathrm{v}^5 b_0 + 36\,\mathrm{v}^5 {b_0}^2 - 144\,\mathrm{v}^5 c_0 + 288\,\mathrm{v} b_0 - 576\,\mathrm{v}^3 c_0 + 12\ \sin(\mathrm{v})\,\mathrm{v}^8 c_0 \\
& - 144\ \sin(\mathrm{v})\,\mathrm{v}^6 c_0 - 36\ \sin(\mathrm{v})\,\mathrm{v}^4 {b_0}^2 - 36\ \sin(\mathrm{v})\,\mathrm{v}^6 {b_0}^2 \\
& - 6\ \sin(\mathrm{v})\,\mathrm{v}^8 b_0 - 36\ \sin(\mathrm{v})\,\mathrm{v}^8 {c_0}^2 - 9\ \sin(\mathrm{v})\,\mathrm{v}^8 {b_0}^2 \\
& - 576\ (\cos(\mathrm{v}))^2\,\mathrm{v}^3 c_0 + 288\ (\cos(\mathrm{v}))^2\,\mathrm{v}^3 b_0 \\
& + 288\,\mathrm{v}\,(\cos(\mathrm{v}))^2\, b_0 + 48\ \cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^4 \\
& - 576\ \cos(\mathrm{v})\,\mathrm{v} b_0 + 1152\ \cos(\mathrm{v})\,\mathrm{v}^3 c_0 - 576\ \cos(\mathrm{v})\,\mathrm{v}^3 b_0 \\
& - 576\ \cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^2 + 60\ \sin(\mathrm{v})\,\mathrm{v}^6 b_0 \\
& + 144\ \sin(\mathrm{v})\,\mathrm{v}^4 b_0 + 576\ \sin(\mathrm{v}) + 1152\ \cos(\mathrm{v})\,\mathrm{v} \\
& - 192\ \cos(\mathrm{v})\,\mathrm{v}^3 - 1152\ \cos(\mathrm{v})\sin(\mathrm{v}) + 24\ \sin(\mathrm{v})\,\mathrm{v}^6 \\
& - \sin(\mathrm{v})\,\mathrm{v}^8 - 144\ \sin(\mathrm{v})\,\mathrm{v}^4 + 72\ \sin(\mathrm{v})\,\mathrm{v}^6 b_0 c_0 \\
& + 36\ \sin(\mathrm{v})\,\mathrm{v}^8 c_0 b_0 + 288\ \cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^2 b_0 \\
& - 288\ \cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^4 c_0 + 144\ \cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^4 b_0
\end{aligned}
$$

Demanding now the coefficients of the new proposed method to satisfy the Eqs. (12–13), the following coefficients of the new developed method are produced:

$$
\begin{aligned}
b_0 &= \frac{T_2}{D_2} \\
c_0 &= \frac{T_3}{D_3}
\end{aligned} \tag{14}
$$

where:

$$
\begin{aligned}
T_2 = {} & 12\ \sin(\mathrm{v})\,\mathrm{v}^2 + 24\,\mathrm{v}^2 \sin(2\,\mathrm{v}) - 3\,\mathrm{v}^5 \\
& - \mathrm{v}^5 \cos(2\,\mathrm{v}) + 36\,\mathrm{v}^3 - 18\,\mathrm{v} - 6\,\mathrm{v}\cos(4\,\mathrm{v})
\end{aligned}
$$

$$
\begin{aligned}
&+24\,\mathrm{v}\cos(2\,\mathrm{v})+12\,\mathrm{v}^3\cos(2\,\mathrm{v})+48\,\cos(\mathrm{v})\,\mathrm{v}^3\\
&-4\,\mathrm{v}^5\cos(\mathrm{v})+12\,\mathrm{v}^2\sin(3\,\mathrm{v})\\
&+24\,\sin(4\,\mathrm{v})-48\,\sin(2\,\mathrm{v})\\
D_2 &= 9\,\mathrm{v}^5+3\,\mathrm{v}^5\cos(2\,\mathrm{v})+12\,\mathrm{v}^5\cos(\mathrm{v})\\
&+6\,\mathrm{v}^2\sin(3\,\mathrm{v})-18\,\sin(\mathrm{v})\,\mathrm{v}^2\\
T_3 &= -12+17\,\cos(\mathrm{v})\,\mathrm{v}^4+3\,\mathrm{v}^3\sin(4\,\mathrm{v})-6\,\mathrm{v}^3\sin(2\,\mathrm{v})\\
&+\mathrm{v}^5\sin(2\,\mathrm{v})-12\,\mathrm{v}\sin(3\,\mathrm{v})+36\,\mathrm{v}\sin(\mathrm{v})\\
&+12\,\mathrm{v}^4\cos(2\,\mathrm{v})+6\,\mathrm{v}^3\sin(3\,\mathrm{v})-18\,\mathrm{v}^3\sin(\mathrm{v})\\
&+7\,\mathrm{v}^4\cos(3\,\mathrm{v})+6\,\mathrm{v}\sin(4\,\mathrm{v})-12\,\mathrm{v}\sin(2\,\mathrm{v})\\
&+12\,\mathrm{v}^2\cos(4\,\mathrm{v})-24\,\cos(3\,\mathrm{v})-12\,\mathrm{v}^2+12\,\mathrm{v}^4\\
&+24\,\cos(\mathrm{v})+2\,\sin(\mathrm{v})\,\mathrm{v}^5+12\,\cos(4\,\mathrm{v})\\
D_3 &= -3\,\mathrm{v}^7\sin(2\,\mathrm{v})-6\,\cos(\mathrm{v})\,\mathrm{v}^4+6\,\mathrm{v}^4\cos(3\,\mathrm{v})\\
&-6\,\sin(\mathrm{v})\,\mathrm{v}^7+12\,\mathrm{v}^4-12\,\mathrm{v}^4\cos(2\,\mathrm{v})
\end{aligned}
$$

For some values of $|\omega|$ the formulae given by (14) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_0 &= \frac{73}{63}-\frac{6149}{39690}\,\mathrm{v}^2+\frac{407821}{55010340}\,\mathrm{v}^4-\frac{356245907}{1802138738400}\,\mathrm{v}^6\\
&+\frac{732677171}{227069481038400}\,\mathrm{v}^8-\frac{1807959364469}{53502111122267808000}\,\mathrm{v}^{10}\\
&+\frac{29775965158673}{128084054026709132352000}\,\mathrm{v}^{12}\\
&-\frac{44482808159047}{40153431673827666754560000}\,\mathrm{v}^{14}\\
&+\frac{1170845203904512391}{267522318833740177407589509120000}\,\mathrm{v}^{16}\\
&-\frac{210549800202926021}{13483124869220504941342511259648000}\,\mathrm{v}^{18}+\cdots\\
c_0 &= \frac{1783}{3780}-\frac{6149}{95256}\,\mathrm{v}^2+\frac{45043357}{13202481600}\,\mathrm{v}^4-\frac{2041915597}{21625664860800}\,\mathrm{v}^6\\
&+\frac{42873654301}{27248337724608000}\,\mathrm{v}^8-\frac{425373820477}{25681013338688547840}\,\mathrm{v}^{10}\\
&+\frac{1429904421004901}{12296069186564076705792000}\,\mathrm{v}^{12}\\
&-\frac{51821034133265101}{100704806637959788220436480000}\,\mathrm{v}^{14}\\
&+\frac{97639044339445475527}{32102678260048821288910741094400000}\,\mathrm{v}^{16}\\
&+\frac{5767389410511169547\,9}{4044937460766151482402753377894400000}\,\mathrm{v}^{18}+\cdots
\end{aligned}
\tag{15}
$$

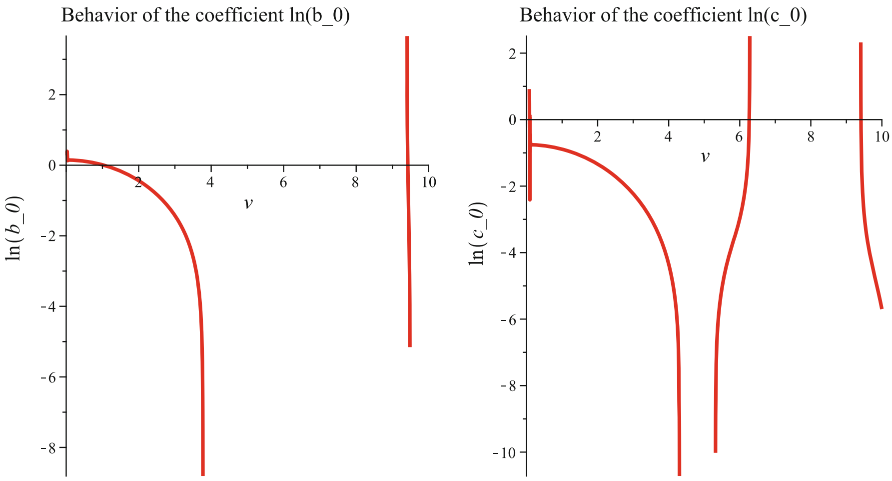


Fig. 1 Behavior of the coefficients of the new proposed method given by (14) for several values of $v = \omega h$

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

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

$$LTE_{NMI} = -\frac{614\, h^{10}}{38102400} \left(q_n^{(10)} + 2\, \omega^2 q_n^{(8)} + \omega^4 q_n^{(6)} \right) + O\left(h^{12}\right) \tag{16}$$

4.2 Second method of the family

Considering now that:

$$\begin{aligned} a_1 &= -2\; a_0 \;=\; 2 \\ b_1 &= 1 - \frac{1}{2}\, b_0 \end{aligned} \tag{17}$$

and applying the method (9) to the scalar test equation (5) we have the difference equation (6) with $m = 2$ and $A_j\,(v)\,,\, j = 0(1)2$ given by:

$$\begin{aligned} A_2\,(\mathrm{v}) &= 1 \\ A_1\,(\mathrm{v}) &= -2 + \mathrm{v}^2 \left(1 - \frac{1}{2}\, b_0\right) - \mathrm{v}^4 c_1 \\ A_0\,(\mathrm{v}) &= 2 + \mathrm{v}^2 b_0 - \mathrm{v}^4 c_0 \end{aligned} \tag{18}$$

where $\mathrm{v} = \omega\, h$

We demand now the method (9) with coefficients (17) to have its phase-lag vanished. Using the formulae (8) (for $m = 2$) and (18), the following equation is obtained:

$$\text{Phase} - \text{Lag} = -\frac{\mathrm{T}_4}{-4 - 2\,\mathrm{v}^2 + \mathrm{v}^2\mathrm{b}_0 + 2\,\mathrm{v}^4\mathrm{c}_1} = 0 \qquad (19)$$

where

$$T_4 = 4\,(\cos(\mathrm{v}))^2 - 4\,\cos(\mathrm{v}) + 2\,\mathrm{v}^2\cos(\mathrm{v}) - \cos(\mathrm{v})\,\mathrm{v}^2 b_0 - 2\,\cos(\mathrm{v})\,\mathrm{v}^4 c_1 + \mathrm{v}^2 b_0 - \mathrm{v}^4 c_0$$

We require now the method (9) with coefficients (17 to have the first derivative of the phase-lag vanished as well. The following equation is hold:

$$\text{First Derivative of the Phase} - \text{Lag} = \frac{\mathrm{T}_5}{\left(-4 - 2\,\mathrm{v}^2 + \mathrm{v}^2\mathrm{b}_0 + 2\,\mathrm{v}^4\mathrm{c}_1\right)^2} = 0 \qquad (20)$$

where

$$\begin{aligned} T_5 = {} & 8\,\cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^2 b_0 + 16\,\cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^4 c_1 \\ & -4\,\sin(\mathrm{v})\,\mathrm{v}^6 b_0 c_1 + 8\,\mathrm{v} b_0 - 16\,\mathrm{v}^3 c_0 - 32\,\cos(\mathrm{v})\sin(\mathrm{v}) \\ & +32\,\cos(\mathrm{v})\,\mathrm{v} - 16\,\mathrm{v}\,(\cos(\mathrm{v}))^2 - 4\,\mathrm{v}^5 c_0 - 4\,\sin(\mathrm{v})\,\mathrm{v}^4 \\ & +16\,\sin(\mathrm{v}) - 16\,\cos(\mathrm{v})\,\mathrm{v} b_0 - 64\,\cos(\mathrm{v})\,\mathrm{v}^3 c_1 + 8\,\mathrm{v}\,(\cos(\mathrm{v}))^2\, b_0 \\ & +32\,(\cos(\mathrm{v}))^2\,\mathrm{v}^3 c_1 + 4\,\mathrm{v}^5 b_0 c_1 + 2\,\mathrm{v}^5 c_0 b_0 \\ & -16\,\cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^2 + 4\,\sin(\mathrm{v})\,\mathrm{v}^4 b_0 + 8\,\sin(\mathrm{v})\,\mathrm{v}^6 c_1 \\ & -\sin(\mathrm{v})\,\mathrm{v}^4 {b_0}^2 - 4\,\sin(\mathrm{v})\,\mathrm{v}^8 {c_1}^2 \end{aligned}$$

Demanding now for the method (9) with coefficients (17) the second derivative of the phase-lag to be vanished as well, the following equation is obtained:

$$\text{Second Derivative of the Phase} - \text{Lag} = \frac{\mathrm{T}_6}{\left(-4 - 2\,\mathrm{v}^2 + \mathrm{v}^2\mathrm{b}_0 + 2\,\mathrm{v}^4\mathrm{c}_1\right)^3} = 0 \qquad (21)$$

where

$$\begin{aligned} T_6 = {} & -128 + 512\,\cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^3 c_1 - 32\,\cos(\mathrm{v})\sin(\mathrm{v})\,{b_0}^2\mathrm{v}^3 \\ & -12\,\cos(\mathrm{v})\,\mathrm{v}^{10} b_0 {c_1}^2 - 6\,\cos(\mathrm{v})\,\mathrm{v}^8 {b_0}^2 c_1 - 192\,\cos(\mathrm{v})\sin(\mathrm{v})\,b_0\mathrm{v}^5 c_1 \\ & +128\,\sin(\mathrm{v})\,\mathrm{v}^3 + 16\,\cos(\mathrm{v})\,\mathrm{v}^4 + 160\,\cos(\mathrm{v})\,\mathrm{v}^2 + 288\,\cos(\mathrm{v})\,\mathrm{v}^4 b_0 c_1 \\ & +16\,\mathrm{v}^6\cos(\mathrm{v})\,b_0 c_1 - 144\,\mathrm{v}^4\,(\cos(\mathrm{v}))^2\, b_0 c_1 - 192\,\cos(\mathrm{v}) \\ & +160\,\mathrm{v}^6 c_0 c_1 + 192\,\mathrm{v}^2 c_0 + 320\,(\cos(\mathrm{v}))^2 - 32\,b_0 - 12\,\cos(\mathrm{v})\,\mathrm{v}^6 b_0 \\ & +64\,(\cos(\mathrm{v}))^2\,\mathrm{v}^8 {c_1}^2 - 128\cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^3 \\ & -64\,(\cos(\mathrm{v}))^2\,\mathrm{v}^4 b_0 + 4\mathrm{v}^4\cos(\mathrm{v})\,{b_0}^2 + 2\mathrm{v}^6 c_0 {b_0}^2 + 32\mathrm{v}^4 b_0 + 64\mathrm{v}^6 c_1 - 8\mathrm{v}^4 {b_0}^2 \end{aligned}$$

$$
\begin{aligned}
&-32\,v^8 c_1{}^2 - 32\,v^4 + 6\,\cos(v)\,v^6 b_0{}^2 - 24\,\cos(v)\,v^8 c_1 \\
&+128\,\cos(v)\sin(v)\,v^3 b_0 + 384\,\cos(v)\sin(v)\,v^5 c_1 \\
&+128\,v\cos(v)\sin(v)\,b_0 + 8\,v^6 c_0 + 192\,\sin(v)\,v^5 b_0 c_1 \\
&-40\,v^6 b_0 c_1 - 128\,v^2 + 24\,\cos(v)\,v^{10} c_1{}^2 - 128\,\sin(v)\,v^3 b_0 \\
&-384\,\sin(v)\,v^5 c_1 - 192\,v^4 b_0 c_1 - 128\,\sin(v)\,v b_0 \\
&-512\,\sin(v)\,v^3 c_1 + 768\,\cos(v)\,v^2 c_1 + 4\,v^6 b_0{}^2 c_1 - 24\,v^8 b_0 c_1{}^2 \\
&-8\,v^6 c_0 b_0 - 12\,v^8 c_0 b_0 c_1 - \cos(v)\,v^6 b_0{}^3 + 32\,\sin(v)\,v^3 b_0{}^2 \\
&-8\,\cos(v)\,v^{12} c_1{}^3 + 256\,\sin(v)\,v^7 c_1{}^2 - 384\,(\cos(v))^2\,v^2 c_1 \\
&-256\,\cos(v)\sin(v)\,v^7 c_1{}^2 + 64\,(\cos(v))^2\,v^6 b_0 c_1 \\
&+24\,\cos(v)\,v^8 b_0 c_1 + 48\,\cos(v)\,v^2 b_0{}^2 + 640\,\cos(v)\,v^6 c_1{}^2 \\
&+24\,v^8 c_0 c_1 - 32\,v^6\cos(v)\,c_1 - 32\,v^2\,(\cos(v))^2\,b_0 \\
&-16\,v^4\cos(v)\,b_0 + 16\,(\cos(v))^2\,v^4 b_0{}^2 \\
&-128\,(\cos(v))^2\,v^6 c_1 + 32\,v^4\,(\cos(v))^2\,c_1 \\
&-320\,v^6\,(\cos(v))^2\,c_1{}^2 - 24\,v^2\,(\cos(v))^2\,b_0{}^2 \\
&+160\,(\cos(v))^2\,v^2 + 112\,v^2 b_0 + 128\,v^4 c_1 + 48\,v^4 c_0 - 24\,v^2 b_0{}^2 \\
&+16\,v^8\cos(v)\,c_1{}^2 - 256\,v\cos(v)\sin(v) - 544\,\cos(v)\,v^4 c_1 \\
&-176\,\cos(v)\,v^2 b_0 + 64\,(\cos(v))^2\,v^4 + 8\,\cos(v)\,v^6 \\
&+256\,\sin(v)\,v + 64\,\cos(v)\,b_0 - 32\,(\cos(v))^2\,b_0 - 24\,v^4 c_0 b_0
\end{aligned}
$$

Demanding now the coefficients of the new proposed method to satisfy the Eqs. (19–21), the following coefficients of the new developed method are produced:

$$
\begin{aligned}
b_0 &= \frac{T_7}{D_7} \\
c_0 &= \frac{T_8}{D_8} \\
c_1 &= \frac{T_9}{D_8}
\end{aligned}
\tag{22}
$$

where:

$$
\begin{aligned}
T_7 = &-6\,v^3 + 2\,v^3\cos(2\,v) - 6\,v^2\sin(2\,v) + 2\,v^2\sin(3\,v) \\
&-6\,\sin(v)\,v^2 + 24\,v - 28\,v\cos(v) + 12\,v\cos(3\,v) \\
&-8\,v\cos(2\,v) + 40\,\sin(2\,v) - 20\,\sin(v) - 20\,\sin(3\,v) \\
D_7 = &-3\,v^3 + v^3\cos(2\,v) + 2\,v^3\cos(v) - 3\,v^2\sin(2\,v) + 6\,\sin(v)\,v^2 \\
T_8 = &-56 - 30\,\cos(v)\,v^2 + 32\,\cos(3\,v) + 6\,v^2\cos(3\,v) + v^2\cos(4\,v) \\
&-4\,v^2\cos(2\,v) - 2\,v\sin(2\,v) + 2\,v^3\sin(2\,v) + 6\,v\sin(3\,v) \\
&-5\,v\sin(4\,v) - 8\,\cos(4\,v) + 2\,v^3\sin(3\,v) + 2\,v^4\cos(2\,v) \\
&+27\,v^2 - 6\,v^4 + 6\,\sin(v)\,v - 6\,\sin(v)\,v^3 - 64\,\cos(2\,v) + 96\,\cos(v)
\end{aligned}
$$

$$D_8 = -3\,v^6 + v^6 \cos(2\,v) + 2\,\cos(v)\,v^6 - 3\,v^5 \sin(2\,v) + 6\,\sin(v)\,v^5$$

$$\begin{aligned} T_9 = {} & 2\,\cos(v)\,v^2 - 32 + 56\,\cos(v) + 2\,v^4 \cos(v) \\ & -34\,v \sin(2\,v) - 6\,v^2 + 10\,v^2 \cos(2\,v) - 32\,\cos(2\,v) \\ & + \sin(v)\,v^3 - v^3 \sin(3\,v) + 12\,v \sin(3\,v) \\ & +32\,\sin(v)\,v + 8\,\cos(3\,v) - 6\,v^2 \cos(3\,v) \end{aligned}$$

For some values of $|\omega|$ the formulae given by (14) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} b_0 = {} & \frac{73}{63} - \frac{6149}{26460}\,v^2 + \frac{218831}{12224520}\,v^4 - \frac{22640473}{44497252800}\,v^6 \\ & + \frac{8949037}{1121330770560}\,v^8 - \frac{31318112381}{440346593598912000}\,v^{10} \\ & + \frac{15652468501}{2342643877946211840 0}\,v^{12} \\ & + \frac{6303015333211}{2558167114717263329280000}\,v^{14} \\ & + \frac{39685750300249}{25092077317832898587934720 0}\,v^{16} \\ & + \frac{9867027018400309}{2283379035922793771502059520000}\,v^{18} + \cdots \\ c_0 = {} & \frac{1783}{3780} - \frac{6149}{63504}\,v^2 + \frac{12361969}{1466942400}\,v^4 - \frac{163198697}{400475275200}\,v^6 \\ & + \frac{4360326853}{336399231168000}\,v^8 - \frac{1034989297373}{352277274879129600 0}\,v^{10} \\ & + \frac{1663920138763}{330726194533582848000}\,v^{12} \\ & - \frac{1399007428451}{2093045821132306360320 0}\,v^{14} \\ & + \frac{131090624936954117}{1812205584065709342461952 00000}\,v^{16} \\ & - \frac{168587575500807313}{2740054843107352525802471424 0000}\,v^{18} + \cdots \\ c_1 = {} & \frac{1037}{7560} - \frac{6149}{635040}\,v^2 + \frac{767891}{2933884800}\,v^4 - \frac{18821}{4550855400}\,v^6 \\ & + \frac{23366087}{672798462336000}\,v^8 - \frac{525200129}{1409109099516518400}\,v^{10} \\ & - \frac{4784004499}{2248938122828363366400}\,v^{12} \\ & - \frac{939656429263}{9209401612982147985408000}\,v^{14} \end{aligned}$$

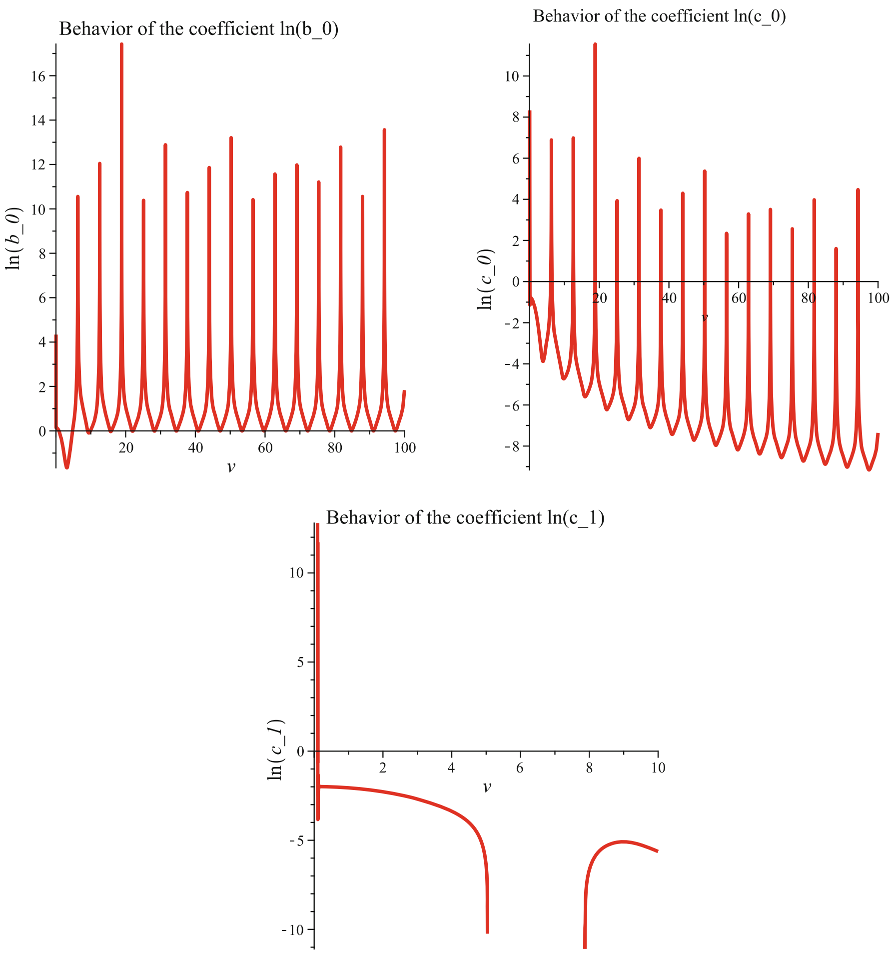


Fig. 2 Behavior of the coefficients of the new proposed method given by (22) for several values of $v = \omega h$

$$
-\frac{993383534961577}{362441116813141868492390400000}\,\mathrm{v}^{16}
-\frac{4228645637016869}{548010968621470505160494284800000}\,\mathrm{v}^{18}+\cdots \tag{23}
$$

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

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

$$
LTE_{NMII} = -\frac{614\,h^{10}}{38102400}\left(q_n^{(10)} + 3\,\omega^2 q_n^{(8)} + 3\,\omega^4 q_n^{(6)} + \omega^6 q_n^{(4)}\right) + O\left(h^{12}\right) \tag{24}
$$

4.3 Third method of the family

Considering now that:

$$a_1 = -2 \; a_0 = 2 \tag{25}$$

and applying the method (9) to the scalar test equation (5) we have the difference equation (6) with $m = 2$ and $A_j(v)$, $j = 0(1)2$ given by:

$$\begin{aligned} A_2(\mathrm{v}) &= 1 \\ A_1(\mathrm{v}) &= -2 + \mathrm{v}^2 b_1 - \mathrm{v}^4 c_1 \\ A_0(\mathrm{v}) &= 2 + \mathrm{v}^2 b_0 - \mathrm{v}^4 c_0 \end{aligned} \tag{26}$$

where $\mathrm{v} = \omega\, h$

We demand now the method (9) with coefficients (25) to have its phase-lag vanished. Using the formulae (8) (for $m = 2$) and (18), the following equation is hold:

$$\mathrm{Phase-Lag} = -\frac{1}{2}\,\frac{\mathrm{T}_{10}}{-2 - \mathrm{v}^2\mathrm{b}_1 + \mathrm{v}^4\mathrm{c}_1} = 0 \tag{27}$$

where

$$T_{10} = 4\,(\cos(v))^2 - 4\cos(v) + 2\cos(v)\,v^2 b_1 - 2\cos(v)\,v^4 c_1 + v^2 b_0 - v^4 c_0$$

We require now the method (9) with coefficients (25 to have the first derivative of the phase-lag vanished as well. The following equation is obtained:

$$\mathrm{First\ Derivative\ of\ the\ Phase-Lag} = \frac{\mathrm{T}_{11}}{\left(-2 - \mathrm{v}^2\mathrm{b}_1 + \mathrm{v}^4\mathrm{c}_1\right)^2} = 0 \tag{28}$$

where

$$\begin{aligned} T_{11} = &-4\cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^2 b_1 + 4\cos(\mathrm{v})\sin(\mathrm{v})\,\mathrm{v}^4 c_1 + 2\sin(\mathrm{v})\,\mathrm{v}^6 b_1 c_1 \\ &+2\,\mathrm{v}\, b_0 - 4\,\mathrm{v}^3 c_0 - 8\cos(\mathrm{v})\sin(\mathrm{v}) + 8\cos(\mathrm{v})\,\mathrm{v}\, b_1 - 16\cos(\mathrm{v})\,\mathrm{v}^3 c_1 \\ &-\sin(\mathrm{v})\,\mathrm{v}^4 {b_1}^2 - \sin(\mathrm{v})\,\mathrm{v}^8 {c_1}^2 + \mathrm{v}^5 b_0 c_1 - \mathrm{v}^5 c_0 b_1 \\ &-4\,\mathrm{v}\,(\cos(\mathrm{v}))^2\, b_1 + 8\,(\cos(\mathrm{v}))^2\,\mathrm{v}^3 c_1 + 4\sin(\mathrm{v}) \end{aligned}$$

Demanding now for the method (9) with coefficients (17 the second derivative of the phase-lag to be vanished as well, the following equation is obtained:

$$\mathrm{Second\ Derivative\ of\ the\ Phase-Lag} = \frac{\mathrm{T}_{12}}{\left(-2 - \mathrm{v}^2\mathrm{b}_1 + \mathrm{v}^4\mathrm{c}_1\right)^3} = 0 \tag{29}$$

where

$$
\begin{aligned}
T_{12} = & -16 + 4\,\cos(\mathrm{v})\,\mathrm{v}^4 c_1 - 16\,\cos(\mathrm{v})\,b_1 - 12\,\mathrm{v}^2\,(\cos(\mathrm{v}))^2\,{b_1}^2 \\
& -40\,\mathrm{v}^6\,(\cos(\mathrm{v}))^2\,{c_1}^2 + 32\,(\cos(\mathrm{v}))^2\,\mathrm{v}^2 b_1 - 32\,(\cos(\mathrm{v}))^2\,\mathrm{v}^4 c_1 \\
& + 8\,(\cos(\mathrm{v}))^2\,\mathrm{v}^4 {b_1}^2 + 2\,\cos(\mathrm{v})\,\mathrm{v}^4 {b_1}^2 + 8\,(\cos(\mathrm{v}))^2\,\mathrm{v}^8 {c_1}^2 \\
& +2\,\cos(\mathrm{v})\,\mathrm{v}^8 {c_1}^2 + 16\,\sin(\mathrm{v})\,\mathrm{v}^3 {b_1}^2 + \cos(\mathrm{v})\,\mathrm{v}^6 {b_1}^3 - \cos(\mathrm{v})\,\mathrm{v}^{12} {c_1}^3 \\
& +32\,\sin(\mathrm{v})\,\mathrm{v}^7 {c_1}^2 + 24\,\cos(\mathrm{v})\,\mathrm{v}^2 {b_1}^2 - 48\,(\cos(\mathrm{v}))^2\,\mathrm{v}^2 c_1 + 80\,\cos(\mathrm{v})\,\mathrm{v}^6 {c_1}^2 \\
& -3\,b_0 \mathrm{v}^8 {c_1}^2 + \mathrm{v}^6 c_0 {b_1}^2 + 48\cos(\mathrm{v})\,\sin(\mathrm{v})\,b_1 \mathrm{v}^5 c_1 + 20\,\mathrm{v}^6 c_0 c_1 + 32\sin(\mathrm{v})\,\mathrm{v} b_1 \\
& + 8\mathrm{v}^6 b_1 c_1 - 64\sin(\mathrm{v})\,\mathrm{v}^3 c_1 + 96\,\cos(\mathrm{v})\,\mathrm{v}^2 c_1 + 24\,\mathrm{v}^2 c_0 - 4\,\cos(\mathrm{v})\,\mathrm{v}^2 b_1 \\
& -72\,\cos(\mathrm{v})\,\mathrm{v}^4 b_1 c_1 + 36\,\mathrm{v}^4\,(\cos(\mathrm{v}))^2\,b_1 c_1 - 16\,(\cos(\mathrm{v}))^2\,\mathrm{v}^6 b_1 c_1 \\
& -4\,\cos(\mathrm{v})\,\mathrm{v}^6 b_1 c_1 - 3\,\cos(\mathrm{v})\,\mathrm{v}^8 {b_1}^2 c_1 + 3\,\cos(\mathrm{v})\,\mathrm{v}^{10} b_1 {c_1}^2 \\
& -48\,\sin(\mathrm{v})\,\mathrm{v}^5 b_1 c_1 + 64\,\cos(\mathrm{v})\,\sin(\mathrm{v})\,\mathrm{v}^3 c_1 - 16\,\cos(\mathrm{v})\,\sin(\mathrm{v})\,{b_1}^2 \mathrm{v}^3 \\
& -32\cos(\mathrm{v})\,\sin(\mathrm{v})\,\mathrm{v}^7 {c_1}^2 - 32\mathrm{v}\cos(\mathrm{v})\,\sin(\mathrm{v})\,b_1 + 8\,(\cos(\mathrm{v}))^2\,b_1 - 8\cos(\mathrm{v}) \\
& +32\,(\cos(\mathrm{v}))^2 - 16\,\mathrm{v}^2 b_1 + 16\,\mathrm{v}^4 c_1 - 4\,b_0 + 6\,\mathrm{v}^2 b_0 b_1 + 6\,\mathrm{v}^4 c_0 b_1 \\
& -24\,\mathrm{v}^4 b_0 c_1 - 4\,\mathrm{v}^4 {b_1}^2 - 4\,\mathrm{v}^8 {c_1}^2 - b_0 \mathrm{v}^6 b_1 c_1 + 3\,\mathrm{v}^8 c_0 b_1 c_1
\end{aligned}
$$

Finally, we require for the new produced method the third derivative of the phase-lag to be vanished as well. Therefore, the following equation is obtained:

$$
\text{Third Derivative of the Phase} - \text{Lag} = -\frac{\mathrm{T}_{13}}{\left(-2 - \mathrm{v}^2 \mathrm{b}_1 + \mathrm{v}^4 \mathrm{c}_1\right)^4} = 0 \qquad (30)
$$

where

$$
\begin{aligned}
T_{13} = & -288\,\mathrm{v}^5 b_1 c_1 - 12\,b_0 \mathrm{v}^{11} {c_1}^3 + 96\,\cos(\mathrm{v})\,\mathrm{v} b_1 - 192\,\cos(\mathrm{v})\,\mathrm{v}^3 c_1 \\
& -96\,\cos(\mathrm{v})\,\sin(\mathrm{v})\,b_1 - 576\,\sin(\mathrm{v})\,\mathrm{v}^2 c_1 + 384\,\cos(\mathrm{v})\,\mathrm{v} c_1 \\
& +192\,\cos(\mathrm{v})\,\mathrm{v}^7 {c_1}^2 + 288\,\sin(\mathrm{v})\,\mathrm{v}^6 {b_1}^2 c_1 + 96\,\cos(\mathrm{v})\,\mathrm{v}^3 {b_1}^2 \\
& + 48\,\mathrm{v} b_0 b_1 - 240\,\mathrm{v}^3 b_0 c_1 + 480\,\mathrm{v}^5 c_0 c_1 - 48\,\mathrm{v}^3 c_0 b_1 + 12\,\mathrm{v}^9 c_0 {b_1}^2 c_1 \\
& +12\,\mathrm{v}^{11} c_0 b_1 {c_1}^2 - 288\,\cos(\mathrm{v})\,\mathrm{v}^5 b_1 c_1 - 4\,\sin(\mathrm{v})\,\mathrm{v}^6 {b_1}^3 + 4\,\sin(\mathrm{v})\,\mathrm{v}^{12} {c_1}^3 \\
& - \sin(\mathrm{v})\,\mathrm{v}^8 {b_1}^4 + 24\,\cos(\mathrm{v})\,\mathrm{v}^5 {b_1}^3 - 192\,\mathrm{v}^3\,(\cos(\mathrm{v}))^2\,{b_1}^2 \\
& +96\,(\cos(\mathrm{v}))^2\,\mathrm{v}^{11} {c_1}^3 - 384\,\mathrm{v}^7\,(\cos(\mathrm{v}))^2\,{c_1}^2 \\
& -96\,\cos(\mathrm{v})\,\mathrm{v}^7 {b_1}^2 c_1 + 120\,\cos(\mathrm{v})\,\mathrm{v}^9 b_1 {c_1}^2 \\
& +576\,\cos(\mathrm{v})\,\sin(\mathrm{v})\,\mathrm{v}^2 c_1 + 96\,\sin(\mathrm{v})\,\mathrm{v}^4 b_1 c_1 \\
& -1152\,\cos(\mathrm{v})\,\mathrm{v}^3 b_1 c_1 + 96\,\cos(\mathrm{v})\,\sin(\mathrm{v})\,{b_1}^2 \mathrm{v}^2 \\
& +192\,\cos(\mathrm{v})\,\sin(\mathrm{v})\,\mathrm{v}^6 {c_1}^2 - 96\,\sin(\mathrm{v})\,\mathrm{v}^2 {b_1}^2 \\
& -192\,\sin(\mathrm{v})\,\mathrm{v}^6 {c_1}^2 + 192\,\cos(\mathrm{v})\,\mathrm{v} {b_1}^2 + 1920\,\cos(\mathrm{v})\,\mathrm{v}^5 {c_1}^2 \\
& -72\,\sin(\mathrm{v})\,\mathrm{v}^4 {b_1}^3 - 96\,\mathrm{v}\,(\cos(\mathrm{v}))^2\,{b_1}^2 \\
& -192\,\mathrm{v} c_1\,(\cos(\mathrm{v}))^2 - 16\,\sin(\mathrm{v})\,\mathrm{v}^4 c_1 + 16\,\sin(\mathrm{v})\,\mathrm{v}^2 b_1 \\
& -192\,\mathrm{v}\,(\cos(\mathrm{v}))^2\,b_1 + 384\,(\cos(\mathrm{v}))^2\,\mathrm{v}^3 c_1
\end{aligned}
$$

$$
\begin{aligned}
&-\sin(v)\, v^{16} c_1{}^4 - 48\cos(v)\, v^{11} c_1{}^3 - 48\,(\cos(v))^2\, b_1{}^3 v^5\\
&+96\, v^5 b_0 b_1 c_1 + 96\, v^7 c_0 b_1 c_1 - 12\, b_0 b_1 v^9 c_1{}^2 + 96\, v^3 b_1{}^2 + 192\, v^7 c_1{}^2\\
&+24\, b_1{}^3 v^5 - 48\, v^{11} c_1{}^3 + 96\, v b_1 - 192\, v^3 c_1 + 16\sin(v)\\
&-96\cos(v)\sin(v)\, b_1 v^4 c_1 + 192\cos(v)\sin(v)\, v^6 b_1 c_1\\
&+48\cos(v)\sin(v)\, v^8 b_1{}^2 c_1 - 48\cos(v)\sin(v)\, v^{10} b_1 c_1{}^2\\
&-288\, v^6\cos(v)\sin(v)\, b_1{}^2 c_1 + 456\, v^8\cos(v)\sin(v)\, b_1 c_1{}^2\\
&-456\sin(v)\, v^8 b_1 c_1{}^2 + 384\cos(v)\, v^5 b_1{}^2 c_1 - 576\cos(v)\, v^7 b_1 c_1{}^2\\
&+192\,(\cos(v))^2\, b_1{}^2 v^7 c_1 - 240\,(\cos(v))^2\, b_1 v^9 c_1{}^2\\
&+240\sin(v)\, v^{10} c_1{}^3 + 480\cos(v)\, v^9 c_1{}^3 + 48\, v^3\,(\cos(v))^2\, b_1{}^3\\
&-240\, v^9\,(\cos(v))^2\, c_1{}^3 + 96\, v c_0 - 128\cos(v)\sin(v)\\
&-960\,(\cos(v))^2\, v^5 c_1{}^2 + 576\,(\cos(v))^2\, b_1 v^3 c_1\\
&+72\, v^4\cos(v)\sin(v)\, b_1{}^3 - 240\, v^{10}\cos(v)\sin(v)\, c_1{}^3\\
&-192\, v^5\,(\cos(v))^2\, b_1{}^2 c_1 + 288\, v^7\,(\cos(v))^2\, b_1 c_1{}^2\\
&+192\cos(v)\sin(v)\, v^4 c_1 - 192\cos(v)\sin(v)\, v^2 b_1\\
&-96\cos(v)\, v^3 b_1{}^3 + 96\sin(v)\, b_1 + 576\, v^5\,(\cos(v))^2\, b_1 c_1\\
&-96\cos(v)\sin(v)\, v^4 b_1{}^2 - 96\cos(v)\sin(v)\, v^8 c_1{}^2\\
&-16\cos(v)\sin(v)\, v^6 b_1{}^3 + 16\cos(v)\sin(v)\, v^{12} c_1{}^3\\
&+12\sin(v)\, v^8 b_1{}^2 c_1 - 12\sin(v)\, v^{10} b_1 c_1{}^2 + 4\sin(v)\, v^{10} b_1{}^3 c_1\\
&-6\sin(v)\, v^{12} b_1{}^2 c_1{}^2 + 4\sin(v)\, v^{14} b_1 c_1{}^3\\
&-24\, v^3 b_0 b_1{}^2 - 240\, v^7 b_0 c_1{}^2 + 120\, v^9 c_0 c_1{}^2 - 96\, b_1{}^2 v^7 c_1 + 120\, b_1 v^9 c_1{}^2
\end{aligned}
$$

Demanding now the coefficients of the new proposed method to satisfy the Eqs. (27–30), the following coefficients of the new developed method are produced:

$$
\begin{aligned}
b_0 &= \frac{T_{14}}{D_{14}}\\
b_1 &= \frac{T_{15}}{D_{14}}\\
c_0 &= \frac{T_{16}}{D_{16}}\\
c_1 &= \frac{T_{17}}{D_{17}}
\end{aligned}
\tag{31}
$$

where:

$$
\begin{aligned}
T_{14} = {} & 120 - 176\, v^2 - 120\cos(v) + 60\cos(5\,v) + 60\cos(3\,v) + 80\, v^2\cos(4\,v)\\
&-480\, v^2\cos(2\,v) + 314\, v^2\cos(3\,v) - 192\, v\sin(4\,v)\\
&-118\, v^2\cos(5\,v) + 138\, v\sin(5\,v) - 42\, v\sin(3\,v)\\
&+v^5\sin(5\,v) - 13\, v^5\sin(3\,v) + 8\, v^3\sin(4\,v)\\
&-89\, v^4\cos(3\,v) + 192\, v\sin(2\,v) - 176\, v^3\sin(2\,v) - 50\, v^3\sin(5\,v)
\end{aligned}
$$

$$+262\,v^3\sin(3\,v)+11\,v^4\cos(5\,v)-180\,\sin(v)\,v$$
$$+72\,\sin(v)\,v^3+380\,\cos(v)\,v^2-18\,\cos(v)\,v^4$$
$$-14\,\sin(v)\,v^5-120\,\cos(4\,v)$$

$$D_{14}=-11\,\cos(v)\,v^6+9\,\sin(v)\,v^5-v^6\cos(3\,v)$$
$$+v^5\sin(3\,v)+3\,\cos(v)\,v^4-9\,\sin(v)\,v^3$$
$$-3\,v^4\cos(3\,v)+3\,v^3\sin(3\,v)$$

$$T_{15}=-204\,\sin(v)\,v+52\,\sin(v)\,v^3+284\,\cos(v)\,v^2$$
$$-44\,\cos(v)\,v^4+9\,v^4\cos(4\,v)+52\,v^4\cos(2\,v)$$
$$+120\,v\sin(2\,v)-122\,v^3\sin(2\,v)+20\,v^3\sin(3\,v)$$
$$-4\,v^4\cos(3\,v)-3\,v^3\sin(4\,v)+52\,v^2\cos(4\,v)$$
$$+2\,v^5\sin(4\,v)-240\,v^2\cos(2\,v)+4\,v^2\cos(3\,v)$$
$$-108\,v\sin(4\,v)+120\,\cos(3\,v)+132\,v\sin(3\,v)-120\,\cos(v)$$
$$-100\,v^2+35\,v^4-60\,\cos(4\,v)+60+8\,v^5\sin(2\,v)$$

$$T_{16}=-24-13\,v^5\sin(3\,v)+6\,v^4\cos(5\,v)-78\,\sin(v)\,v$$
$$-10\,\sin(v)\,v^3+2\,\cos(v)\,v^2+28\,\cos(v)\,v^4$$
$$-288\,v^2\cos(2\,v)-15\,v^3\sin(5\,v)+215\,v^3\sin(3\,v)$$
$$-14\,\sin(v)\,v^5-87\,v\sin(3\,v)-13\,v^2\cos(5\,v)$$
$$-9\,v\sin(5\,v)+v^5\sin(5\,v)-12\,\cos(5\,v)+24\,\cos(v)$$
$$+32\,v^2\cos(4\,v)+192\,v\sin(2\,v)+8\,v^3\sin(4\,v)$$
$$-82\,v^4\cos(3\,v)-12\,\cos(3\,v)+64\,v^2+203\,v^2\cos(3\,v)$$
$$+24\,\cos(4\,v)-176\,v^3\sin(2\,v)$$

$$D_{16}=-11\,v^8\cos(v)+9\,v^7\sin(v)-v^8\cos(3\,v)$$
$$+v^7\sin(3\,v)+3\,\cos(v)\,v^6-9\,\sin(v)\,v^5$$
$$-3\,v^6\cos(3\,v)+3\,v^5\sin(3\,v)$$

$$T_{17}=-2\,v^4\sin(3\,v)-6\,\sin(v)\,v^4+10\,v^3+2\,v^3\cos(2\,v)$$
$$+26\,v^2\sin(3\,v)+2\,v^2\sin(v)-6\,v-42\,v\cos(2\,v)$$
$$-12\,\sin(3\,v)-12\,\sin(v)-13\,v^3\cos(v)+18\,\cos(v)\,v$$
$$-11\,v^3\cos(3\,v)+30\,v\cos(3\,v)-16\,v^2\sin(2\,v)+24\,\sin(2\,v)$$

$$D_{17}=5\,v^7+v^7\cos(2\,v)-3\,v^5+3\,v^5\cos(2\,v)$$

For some values of $|\omega|$ the formulae given by (31) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$b_0=\frac{73}{63}-\frac{6149}{19845}\,v^2+\frac{181033}{5501034}\,v^4-\frac{813877139}{901069369200}\,v^6$$
$$-\frac{26603652419}{181655584830720}\,v^8+\frac{158586653896091}{1337552778056695200 0}\,v^{10}$$
$$-\frac{119179903473797861}{2561681080534182647040 00}\,v^{12}$$

$$
\begin{aligned}
&+\frac{50497280493020337661}{4196033609914991175851520000}\,\mathrm{v}^{14}\\
&-\frac{1007769648977661056149\,01}{535044637667480354815179018240000}\,\mathrm{v}^{16}\\
&+\frac{646414400080111975225183}{168539060865256311766781390745600000}\,\mathrm{v}^{18}+\cdots\\
b_1 =\ &\frac{53}{126}+\frac{6149}{39690}\,\mathrm{v}^2-\frac{181033}{11002068}\,\mathrm{v}^4+\frac{813877139}{1802138738400}\,\mathrm{v}^6\\
&-\frac{13560456191}{1816555848307200}\,\mathrm{v}^8+\frac{165520447879}{1671940972570869000}\,\mathrm{v}^{10}\\
&+\frac{71204405959391}{39410478162064348416000}\,\mathrm{v}^{12}\\
&+\frac{1099388490275298539}{8392067219829982351703040000}\,\mathrm{v}^{14}\\
&+\frac{6110498090838379806803}{1070089275334960709630358036480000}\,\mathrm{v}^{16}\\
&+\frac{68896910412184210723097}{337078121730512623533562781491200000}\,\mathrm{v}^{18}+\cdots\\
c_0 =\ &\frac{1783}{3780}-\frac{6149}{47628}\,\mathrm{v}^2+\frac{103300271}{6601240800}\,\mathrm{v}^4-\frac{587169761}{540641621520}\,\mathrm{v}^6\\
&+\frac{2474485186517}{54496675449216000}\,\mathrm{v}^8-\frac{841049141726459}{642025333467213696000}\,\mathrm{v}^{10}\\
&+\frac{835855620562247381}{30740172966410191764480000}\,\mathrm{v}^{12}\\
&-\frac{2591855344873053593}{6294050414872486763777280000}\,\mathrm{v}^{14}\\
&+\frac{198306812857690683345253}{32102678260048821288910741094400000}\,\mathrm{v}^{16}\\
&-\frac{14683836037885912740487}{2022468730383075741201376688947200000}\,\mathrm{v}^{18}+\cdots\\
c_1 =\ &\frac{1037}{7560}-\frac{6149}{476280}\,\mathrm{v}^2+\frac{5319529}{13202481600}\,\mathrm{v}^4-\frac{5990329}{1081283243040}\,\mathrm{v}^6\\
&+\frac{11915141983}{108993350898432000}\,\mathrm{v}^8+\frac{2153559601337}{1284050666934427392000}\,\mathrm{v}^{10}\\
&+\frac{4935848837625259}{61480345932820383528960000}\,\mathrm{v}^{12}\\
&+\frac{26654638354794911}{12588100829744973527554560000}\,\mathrm{v}^{14}\\
&+\frac{1219160544823341864647}{64205356520097642577821482188800000}\,\mathrm{v}^{16}\\
&-\frac{10180749592901438674091}{4044937460766151482402753377894400000}\,\mathrm{v}^{18}+\cdots
\end{aligned}
\tag{32}
$$

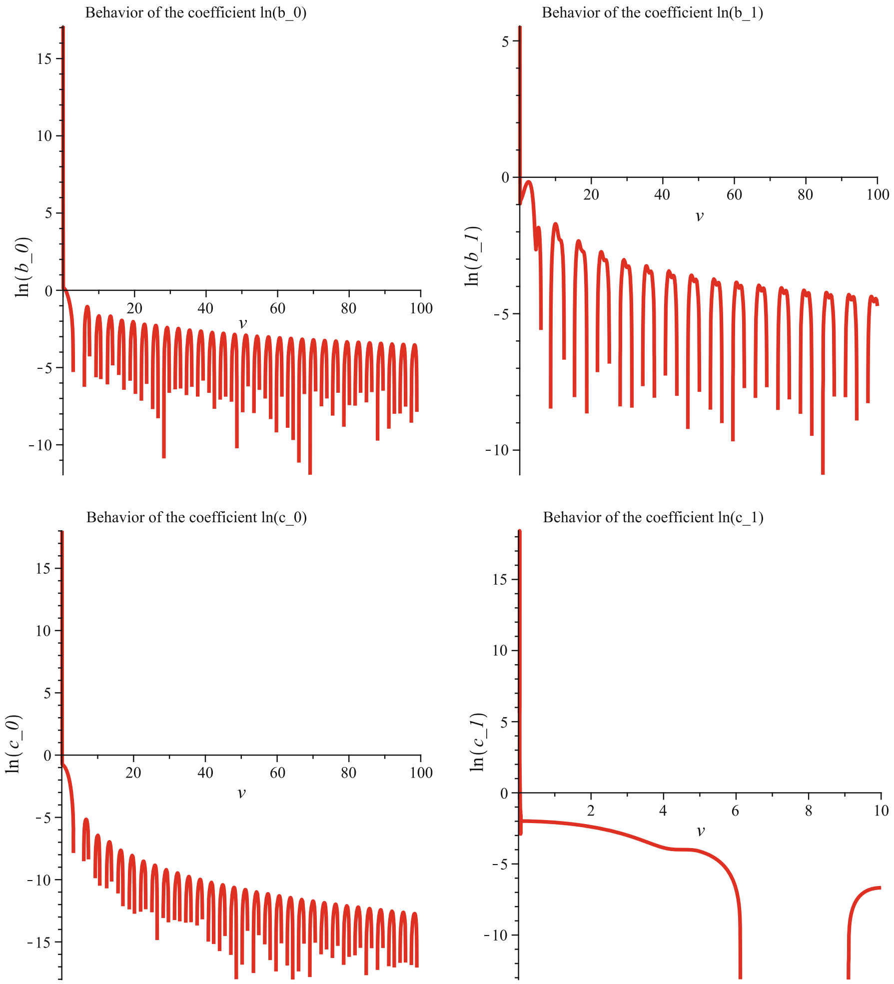


Fig. 3 Behavior of the coefficients of the new proposed method given by (31) for several values of $v = \omega h$

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

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

$$LTE_{NMIII} = -\frac{614\,h^{10}}{38102400}\left(q_n^{(10)} + 4\,\omega^2 q_n^{(8)} + 6\,\omega^4 q_n^{(6)} + 4\,\omega^6 q_n^{(4)} + \omega^8 q_n^{(2)}\right) + O\left(h^{12}\right) \tag{33}$$

5 Error analysis

In this section we will investigate the local truncation error of the following methods:

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

$$LTE_{CL} = -\frac{614\,h^{10}}{38102400}\,q_n^{(10)} + O\left(h^{12}\right) \tag{34}$$

5.2 An implicit P-stable multiderivative method (see Appendix A)

$$LTE_{W} = \frac{236\,h^{10}}{297675}\left(q_n^{(10)} + \omega^2 q_n^{(8)}\right) + O\left(h^{12}\right) \tag{35}$$

5.3 Method with vanished phase-lag and its first derivative (method (9) with coefficients given by (14))

$$LTE_{MI} = -\frac{614\,h^{10}}{38102400}\left(q_n^{(10)} + 2\,\omega^2 q_n^{(8)} + \omega^4 q_n^{(6)}\right) + O\left(h^{12}\right) \tag{36}$$

5.4 Method with vanished phase-lag and its first and second derivatives (method (9) with coefficients given by (22))

$$LTE_{NMII} = -\frac{614\,h^{10}}{38102400}\left(q_n^{(10)} + 3\,\omega^2 q_n^{(8)} + 3\,\omega^4 q_n^{(6)} + \omega^6 q_n^{(4)}\right) + O\left(h^{12}\right) \tag{37}$$

5.5 Method with vanished phase-lag and its first, second and third derivatives (method (9) with coefficients given by (31))

$$LTE_{NMIII} = -\frac{614\,h^{10}}{38102400}\left(q_n^{(10)} + 4\,\omega^2 q_n^{(8)} + 6\,\omega^4 q_n^{(6)} + 4\,\omega^6 q_n^{(4)} + \omega^8 q_n^{(2)}\right) + O\left(h^{12}\right) \tag{38}$$

The following procedure is applied :

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

$$q''(x) = f(x)\,q(x) \tag{39}$$

- Based on the paper of Ixaru and Rizea [73], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \tag{40}$$

where $g(x) = V(x) - V_c = g$, where V_c is the constant approximation of the potential and $G = \omega^2 = V_c - E$.
- We express the derivatives $q_n^{(i)}$, $i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of the Eq. (40). 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

Following the procedure mentioned above and the formulae:

$$\begin{aligned}
q_n^{(2)} &= (V(x) - V_c + G)\; q(x) \\
q_n^{(4)} &= \left(\frac{d^2}{dx^2}\, V(x)\right) q(x) + 2\left(\frac{d}{dx}\, V(x)\right)\left(\frac{d}{dx}\, q(x)\right) \\
&\quad + (V(x) - V_c + G)\left(\frac{d^2}{dx^2}\, q(x)\right) \\
q_n^{(6)} &= \left(\frac{d^4}{dx^4}\, V(x)\right) q(x) + 4\left(\frac{d^3}{dx^3}\, V(x)\right)\left(\frac{d}{dx}\, q(x)\right) \\
&\quad +3\left(\frac{d^2}{dx^2}\, V(x)\right)\left(\frac{d^2}{dx^2}\, q(x)\right) + 4\left(\frac{d}{dx}\, V(x)\right)^2 q(x) \\
&\quad +6\;(V(x) - V_c + G)\left(\frac{d}{dx}\, V(x)\right)\left(\frac{d}{dx}\, q(x)\right) \\
&\quad +4\;(V(x) - V_c + G)\; q(x)\left(\frac{d^2}{dx^2}\, V(x)\right) \\
&\quad + (V(x) - V_c + G)^2\left(\frac{d^2}{dx^2}\, q(x)\right) \ldots
\end{aligned} \tag{41}$$

we obtain the expressions of the Local Truncation Errors.

Considering now two cases in terms of the value of E:

- The Energy is close to the potential, i.e., $G = V_c - E \approx 0$. Consequently, the free terms of the polynomials in G are considered only. Thus, for these values of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G are the same for the cases of the classical method and of the methods with vanished the phase-lag and its derivatives.
- $G >> 0$ or $G << 0$. Then $|G|$ is a large number.

we obtain the following asymptotic expansions of the Local Truncation Errors:

5.6 Classical eighth algebraic order multiderivative method (i.e. the method (9) with constant coefficients)

$$LTE_{CL} = -\frac{614\, h^{10}}{38102400} \left(q\,(x)\;\, G^5 + \cdots \right) + O\left(h^{12}\right) \tag{42}$$

5.7 An implicit P-stable multiderivative method (see Appendix A)

$$LTE_{W} = \frac{236\, h^{10}}{297675} \left[\left(g(x) q(x) \right) G^4 + \cdots \right] + O\left(h^{12}\right) \tag{43}$$

5.8 An eighth algebraic order multiderivative method with vanished phase-lag and its first derivative (method (9) with coefficients given by (14))

$$\begin{aligned} LTE_{MI} = -\frac{614\, h^{10}}{38102400} \Bigg[\Bigg(& 2 \left(\frac{d}{dx} g\,(x) \right) \frac{d}{dx} q\,(x) + 13 \left(\frac{d^2}{dx^2} g\,(x) \right) q\,(x) \\ & + \left(g\,(x) \right)^2 q\,(x) \Bigg) G^3 + \cdots \Bigg] + O\left(h^{12}\right) \end{aligned} \tag{44}$$

5.9 An eighth algebraic order multiderivative method with vanished phase-lag and its first and second derivatives (method (9) with coefficients given by (22))

$$LTE_{NMII} = -\frac{614\, h^{10}}{38102400} \left[\left(4 \left(\frac{d^2}{dx^2} g\,(x) \right) q\,(x) \right) G^3 + \cdots \right] + O\left(h^{12}\right) \tag{45}$$

5.10 An eighth algebraic order multiderivative method with vanished phase-lag and its first, second and third derivatives (method (9) with coefficients given by (31))

$$\begin{aligned} LTE_{NMIII} = -\frac{614\, h^{10}}{38102400} \Bigg[\Bigg(& 12 \left(\frac{d}{dx} g\,(x) \right)^2 q\,(x) + 28 \left(\frac{d^4}{dx^4} g\,(x) \right) q\,(x) \\ & + 8 \left(\frac{d^3}{dx^3} g\,(x) \right) \frac{d}{dx} q\,(x) + 16\, g\,(x)\, q\,(x) \frac{d^2}{dx^2} g\,(x) \Bigg) G^2 + \cdots \Bigg] \\ & + O\left(h^{12}\right) \end{aligned} \tag{46}$$

From the above equations, we have the following theorem:

Theorem 2 *For the classical explicit high algebraic order multiderivative four-step method the error increases as the fifth power of G. For the implicit P-stable multiderivative method (presented in the Appendix), the error increases as the fourth power of G. For the explicit high algebraic order multiderivative four-step method with vanished phase-lag and its first derivative (method (9) with coefficients given by (14)), the error increases as the third power of G. For the explicit high algebraic order multiderivative four-step method with vanished phase-lag and its first and second derivatives (method (9) with coefficients given by (22)), the error increases as the third power of G. Finally, for the explicit high algebraic order multiderivative four-step method with vanished phase-lag and its first, second and third derivatives (method (9) with coefficients given by (31)), the error increases as the second power of G. So, for the numerical solution of the time independent radial Schrödinger equation the explicit high algebraic order multiderivative four-step method with vanished phase-lag and its first, second and third derivatives (method (9) with coefficients given by (31)) is much more efficient, especially for large values of $|G| = |V_c - E|$.*

6 Stability analysis

Application of the new obtained methods to the scalar test equation:

$$q'' = -z^2\, q, \tag{47}$$

leads to the following difference equation:

$$A_2\,(\mathrm{v},\mathrm{s})\;\left(q_{n+2} + q_{n-2}\right) + A_1\,(\mathrm{v},\mathrm{s})\;\left(q_{n+1} + q_{n-1}\right) + A_0\,(\mathrm{v},\mathrm{s})\;q_n = 0 \tag{48}$$

where

$$\begin{aligned} A_2\,(\mathrm{v},\mathrm{s}) &= 1,\; A_1\,(\mathrm{v},\mathrm{s}) = a_1 + \mathrm{s}^2\, b_1 - \mathrm{s}^4\, c_1 \\ A_0\,(\mathrm{v},\mathrm{s}) &= a_0 + \mathrm{s}^2\, b_0 - \mathrm{s}^4\, c_0 \end{aligned} \tag{49}$$

where $\mathrm{s} = z\,h, z \neq \omega, T_3 = H^8 \sin(H) + 9\cos(H)\,H^7 - 33\sin(H)$ $H^6 - 48\cos(H)\,H^5 + 3\sin(H)\,H^4\mathrm{v}^4 + 15\cos(H)\,H^3\mathrm{v}^4 - 15\sin(H)\,H^2\mathrm{v}^4 -$ $\mathrm{v}^6 \sin(H)$
$H^2 - 3\,\mathrm{v}^6\cos(H)\,H + 45\sin(H)\,H^4\mathrm{v}^2 - 3\,\mathrm{v}^2\sin(H)\,H^6 - 21\,\mathrm{v}^2\cos(H)$ $H^5 + 3\,\mathrm{v}^6\sin(H)$ and $\mathrm{v} = z\,h$.

The corresponding characteristic equation is given by:

$$A_2\,(\mathrm{v},\mathrm{s})\left(\lambda^4 + 1\right) + A_1\,(\mathrm{v},\mathrm{s})\left(\lambda^3 + \lambda\right) + A_0\,(\mathrm{v},\mathrm{s})\;\lambda^2 = 0 \tag{50}$$

Definition 1 (see [18]) A symmetric $2k$-step method with the characteristic equation given by (7) is said to have an *interval of periodicity* $\left(0, \mathrm{s}_0^2\right)$ if, for all $\mathrm{s} \in \left(0, \mathrm{s}_0^2\right)$, the roots $\lambda_i,\; i = 1, 2, \ldots$ satisfy

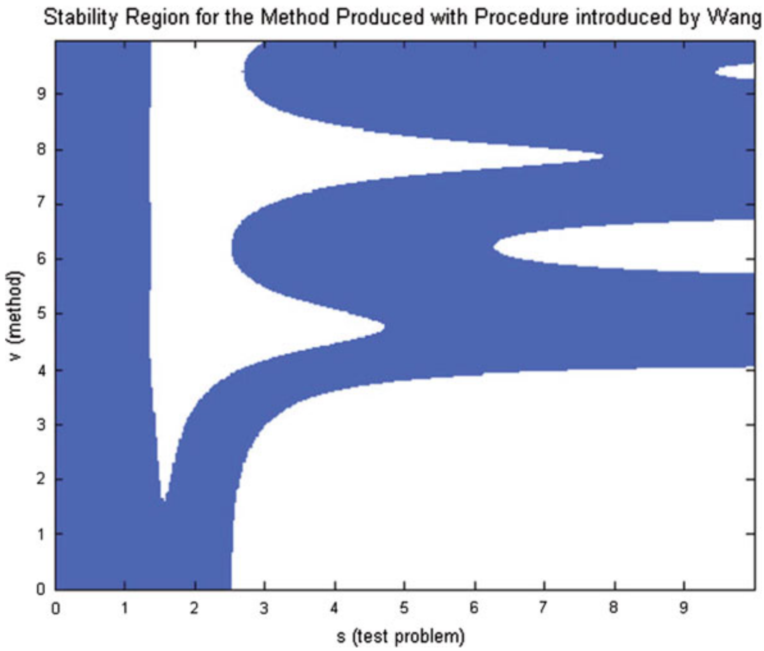


Fig. 4 s–v plane of the Implicit P-stable Multiderivative Method produced based on the procedure of Wang [88] (see Appendix A)

$$\lambda_{1,2} = e^{\pm i\,\zeta(\mathrm{v})},\ |\lambda_i| \leq 1,\ i = 3, 4, \ldots \tag{51}$$

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

Definition 2 (see [18]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S$[1] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $\mathrm{v} = \mathrm{s}$.

In Figs. 4, 5, 6 and 7 we present the s–v plane for the methods developed in this paper. A shadowed area denotes the s–v region where the methods are stable, while a white area denotes the region where the method is unstable.

Remark 1 For the solution of the Schrödinger equation the frequency of the phase 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.

Based on the analysis presented above and on the Remark 1, we studied the interval of periodicity of the following methods:

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

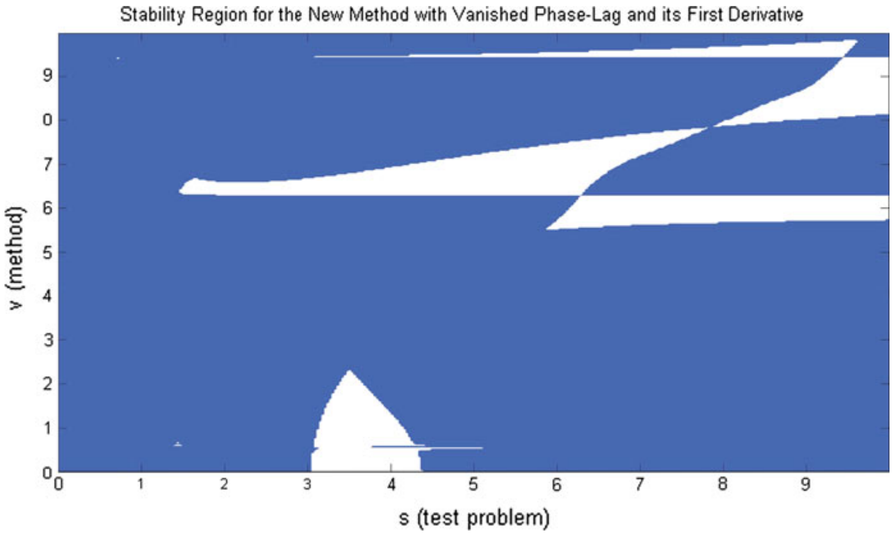


Fig. 5 s–v plane of the new developed family of methods (First Method of the Family)

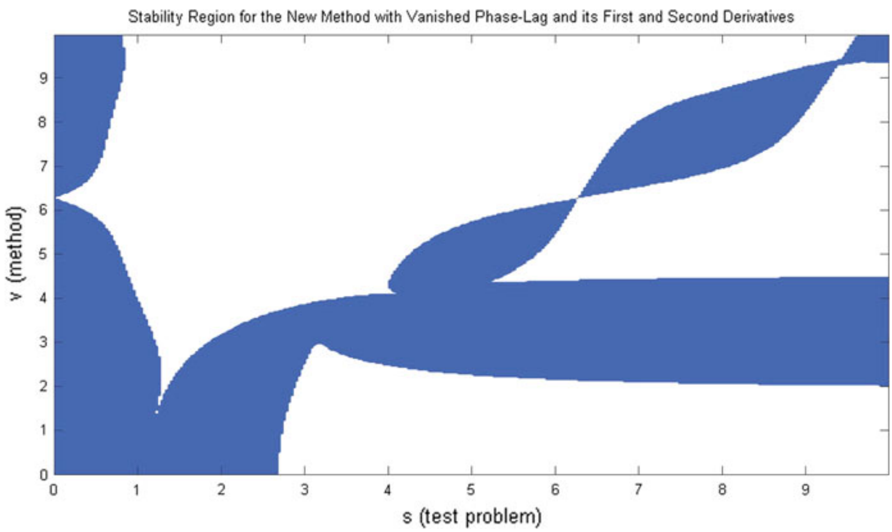


Fig. 6 s–v plane of the new developed family of methods (Second Method of the Family)

– The Classical Eighth Algebraic Order Multiderivative Method (i.e. the method (9) with constant coefficients) (indicated as **CL**)
– The Implicit P-stable Multiderivative Method produced based on the procedure of Wang [88] (see Appendix A) (indicated as **W**)
– The Eighth Algebraic Order Multiderivative Method with Vanished Phase-Lag and its First Derivative (method (9) with coefficients given by (14)) (indicated as **NMI**)

Table 1 Comparative stability analysis for the methods mentioned in the Sect. 5

Method	Interval of periodicity
CL	(0, 2.447172260)
W (see Appendix A)	(0, ∞)
NMI (method (9) with coefficients given by (14))	(0, 39.47841760)
NMII (method (9) with coefficients given by (14))	(0, 39.47841760)
NMIII (method (9) with coefficients given by (14))	(0, 39.47838891)

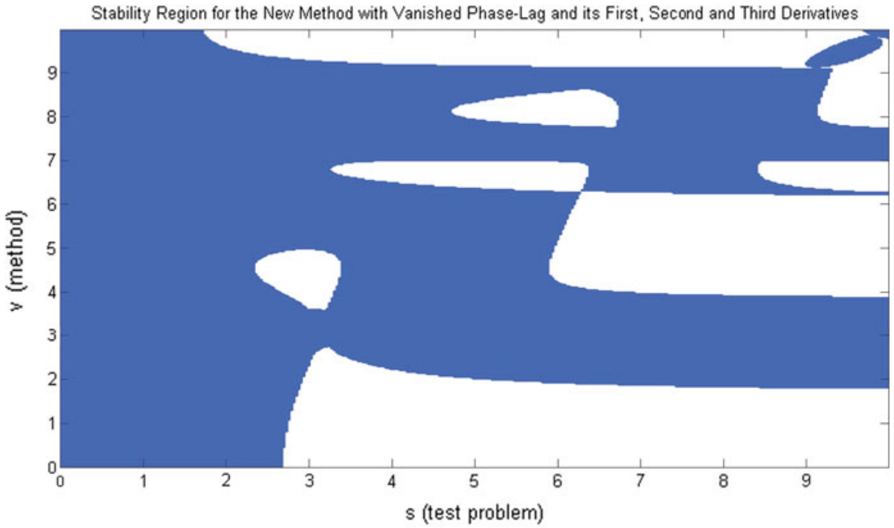


Fig. 7 s–v plane of the new developed family of methods (Third Method of the Family)

- The Eighth Algebraic Order Multiderivative Method with Vanished Phase-Lag and its First and Second Derivatives (method (9) with coefficients given by (22)) (indicated as **NMII**)
- The Eighth Algebraic Order Multiderivative Method with Vanished Phase-Lag and its First, Second and Third Derivatives (method (9) with coefficients given by (31)) (indicated as **NMIII**)

More specifically, we investigate the case that the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. the case that v = s (i.e. see the surroundings of the first diagonal of the s − v plane)

The results presented in the Table 1.

From the above analysis we have the following theorem:

Theorem 3 *For the methods developed in this paper we have the following characteristics:*

- *The Classical Eighth Algebraic Order Multiderivative Method (i.e. the method (9) with constant coefficients) (indicated as* **CL***): Algebraic Order: 8, Interval of periodicity equal to:* $(0, 2.447172260)$
- *The Implicit P-stable Multiderivative Method produced based on the procedure of Wang [88] (see Appendix A) (indicated as* **W***): Algebraic Order: 8, Interval of periodicity equal to:* $(0, \infty)$
- *The Eighth Algebraic Order Multiderivative Method with Vanished Phase-Lag and its First Derivative (method (9) with coefficients given by (14)) (indicated as* **NMI***): Algebraic Order: 8, Phase-Lag Order:* ∞*. First Derivative of Phase-Lag Order:* ∞*. Interval of periodicity equal to:* $(0, 39.47841760)$
- *The Eighth Algebraic Order Multiderivative Method with Vanished Phase-Lag and its First and Second Derivatives (method (9) with coefficients given by (22)) (indicated as* **NMII***): Algebraic Order: 8, Phase-Lag Order:* ∞*. First Derivative of Phase-Lag Order:* ∞*. Second Derivative of Phase-Lag Order:* ∞*. Interval of periodicity equal to:* $(0, 39.47841760)$
- *The Eighth Algebraic Order Multiderivative Method with Vanished Phase-Lag and its First, Second and Third Derivatives (method (9) with coefficients given by (31)) (indicated as* **NMIII***): Algebraic Order: 8, Phase-Lag Order:* ∞*. First Derivative of Phase-Lag Order:* ∞*. Second Derivative of Phase-Lag Order:* ∞*. Third Derivative of Phase-Lag Order:* ∞*. Interval of periodicity equal to:* $(0, 39.47838891)$

7 Conclusions

In this paper we developed and investigated three methods of a family of eighth algebraic order multiderivative explicit four-step methods. The constructed methods

- have the phase-lag vanished
- have the derivative of the phase-lag (first, first and second or first, second and third respectively) vanished as well

For the above mentioned methods we have presented their development and we have studied their error and stability. From the theoretical error analysis produced the result that the new obtained eighth algebraic order multiderivative explicit four-step method with phase-lag vanished and its first, second and third derivatives vanished as well, is the most accurate one for the numerical solution of the radial Schrödinger equation especially for large values of energy.

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

Appendix

An implicit P-stable multiderivative method developed using the procedure of Wang [88]

Consider the following family of multiderivative eighth algebraic order implicit four-step methods:

$$q_{n+2} + a_0\, q_n + q_{n-2} = h^2 \Big[b_2\,\left(f_{n+2} + f_{n-2}\right) + b_0\, f_n \Big] + h^4 \Big[c_2\,\left(g_{n+2} + g_{n-2}\right) + c_0\, g_n \Big] \qquad (52)$$

In the above general form :

- the coefficient b_0, b_2, c_0, c_2, a_0 and a_1 are free parameters,
- h is the step size of the integration,
- n is the number of steps,
- $q_{n\pm i}$ is the approximation of the solution on the point $x_{n\pm i}$, $i = 0(1)2$
- $f_{n\pm i} = q''\left(x_{n\pm i}\right)$, $i = 0(1)2$
- $g_{n\pm i} = q^{(4)}\left(x_{n\pm i}\right)$, $i = 0(1)2$
- $x_i = x_0 + i\,h$ and
- x_0 is the initial value point.

Considering that:

$$\begin{aligned} a_1 &= -2,\;\; b_2 = 2 - \frac{1}{2}\, b_0 \\ c_0 &= -\frac{244}{45} + \frac{5}{3}\, b_0,\;\; c_2 = -\frac{28}{45} + \frac{1}{6}\, b_0 \end{aligned} \qquad (53)$$

and applying the method (52) to the scalar test equation (5) we have the difference equation (6) and the corresponding characteristic equation (7) with $m = 2$ and $A_j\,(v)$, $j = 0(1)2$ given by:

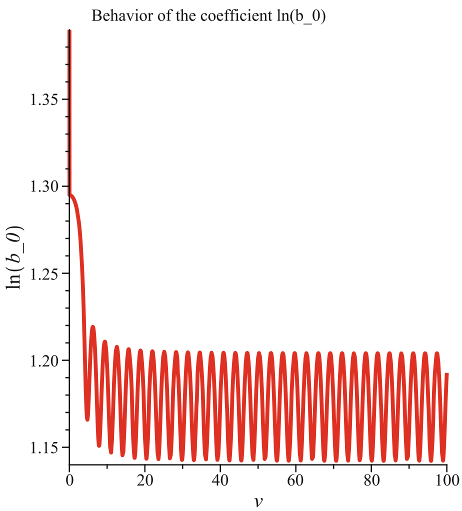
$$\begin{aligned} A_2\,(\mathrm{v}) &= 1 + \mathrm{v}^2 \left(2 - \frac{1}{2}\, b_0\right) - \mathrm{v}^4 \left(-\frac{28}{45} + \frac{1}{6}\, b_0\right) \\ A_1\,(\mathrm{v}) &= 0 \\ A_0\,(\mathrm{v}) &= -2 + \mathrm{v}^2 b_0 - \mathrm{v}^4 \left(-\frac{244}{45} + \frac{5}{3}\, b_0\right) \end{aligned} \qquad (54)$$

where $\mathrm{v} = \omega\, h$

Demanding now the roots of the corresponding characteristic equation (7) to be equal to:

$$\lambda_{1,2} = e^{\pm I\,\mathrm{v}}, \quad \lambda_{3,4} = -e^{\pm I\,\mathrm{v}} \qquad (55)$$

Fig. 8 Behavior of the coefficient of the proposed method given by (56) for several values of $\mathrm{v} = \omega\, h$



the following coefficient b_0 is obtained:

$$b_0 = \frac{2}{15}\,\frac{T_{18}}{D_{18}} \tag{56}$$

where:

$$T_{18} = 28\,\cos(2\,\mathrm{v})\,\mathrm{v}^4 + 90\,\cos(2\,\mathrm{v})\,\mathrm{v}^2 + 45\,\cos(2\,\mathrm{v}) + 122\,\mathrm{v}^4 - 45$$
$$D_{18} = \left(-3 + 3\,\cos(2\,\mathrm{v}) + 5\,\mathrm{v}^2 + \cos(2\,\mathrm{v})\,\mathrm{v}^2\right)\mathrm{v}^2$$

For some values of $|\omega|$ the formulae given by (56) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned} b_0 = {} & \frac{230}{63} - \frac{118}{19845}\,\mathrm{v}^2 - \frac{932}{2750517}\,\mathrm{v}^4 - \frac{902074}{56316835575}\,\mathrm{v}^6 \\ & - \frac{446716}{709592128245}\,\mathrm{v}^8 - \frac{4041821516}{208992621571358625}\,\mathrm{v}^{10} \\ & - \frac{1275859208}{3848679508014096525}\,\mathrm{v}^{12} \\ & + \frac{10638430144046}{1024422268045652142541875}\,\mathrm{v}^{14} \\ & + \frac{4673935681923764}{3265653306075929899994989125}\,\mathrm{v}^{16} \\ & + \frac{473590881027129748}{5143403957069589592492107871875}\,\mathrm{v}^{18} + \cdots \end{aligned} \tag{57}$$

The behavior of the above obtained coefficient is given in the Fig. 8.

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

$$LTE_W = \frac{236\,h^{10}}{297675}\left(q_n^{(10)} + \omega^2 q_n^{(8)}\right) + O\left(h^{12}\right) \tag{58}$$

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