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Optimizing a class of linear multi-step methods for the approximate solution of the radial Schrödinger equation and related problems with respect to phase-lag

Research Article

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Abstract: In this paper we consider a methodology of optimization of the efficiency of a numerical method for the approximate solution of the radial Schrödinger equation and related problems. More specifically, we show how the methodology of vanishing of the phase-lag and its derivatives optimizes the behaviour of a numerical method.

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1. Introduction

The radial Schrödinger equation is used as the basis of the mathematical model of many problems in quantum mechanics, theoretical physics and chemistry, electronics and elsewhere in sciences and engineering. This equation can be written as:

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

The above equation expresses the model for a particle in a central potential field where r is the radial variable [see 1, 2].

In (1) we have the following terms:

- The function $T(r) = \frac{l(l+1)}{r^2} + V(r)$ is called the effective potential. This satisfies $T(r) \to 0$ as $r \to \infty$;

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- 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.

It is mentioned here that the models which are given via the radial Schrödinger equation are boundary-value problems. In these cases the boundary conditions are:

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

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

There has been an extended investigation on the development of numerical methods for the solution of the Schrödinger equation through the last few decades. The aim of this research is the obtain fast and reliable algorithms for the numerical solution of the Schrödinger equation and related problems (see for example [3–32]. More specifically:

- In [1, 3, 19] the authors present detailed reviews of the current research on the subject of this paper.
- In [16] the authors present a new methodology for the development of numerical methods for problems related to the form (1). This methodology produces generators of numerical methods. The generation of these methods is, generally, based on a property called "phase-lag" which is explained in detail in this paper.
- In [4–7, 17, 18, 25, 32] the well-known exponential- and trigonometrical-fitting methods are presented. Single-step and multistep methods of several orders are developed.
- In the book [10] a general description of the methodology of exponential fitting is presented.
- In [8, 15, 21] numerical methods are developed. The construction of these methods is based on a combination of the property of exponential or trigonometric fitting and P-stability.
- In [14] the stabilization of exponentially and trigonometrically-fitted four-step methods is studied.
- The following papers have studied the property of the derivatives of the phase-lag: [29, 30].
- In [12, 27, 31] some modified Runge-Kutta or Runge-Kutta-Nyström methods are constructed. The modification is based on exponential and trigonometric fitting or phase-fitting property.
- In [13, 26, 28] some modified symplectic methods are developed. These methods are for long-time integration.

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

- Methods with constant coefficients;
- Methods with coefficients depending on the frequency of the problem [1];

The purpose of this paper is to show how one can optimize the efficiency of a numerical method for the approximate solution of the radial Schrödinger equation and related problems. More specifically, we will show how the methodology of vanishing of the phase-lag and its derivatives optimize the behaviour of a numerical method. The results of this methodology are methods that are very efficient on any problem with oscillating solutions or problems with solutions containing the functions cos and sin or any combination of them. In detail, the aim of this paper is the determination of the coefficients of a numerical method in order:

1. to have the optimum algebraic order,
2. to have the phase-lag vanish,
3. and finally, to have the phase-lag's lower derivatives vanish as well,

The methodology of vanishing of the phase lag and its derivatives is based on the direct formula for the computation of the phase-lag for the $2k$-method obtained in [3].

In order to show the efficiency of the new methodology, we will study the error analysis and we will apply the investigated methods to the numerical solution of the radial Schrödinger equation.

We will consider a four-step method of sixth algebraic order developed by Wang [15]. Based on this method we will develop two optimized methods. The first one will have phase-lag and its first and second derivatives equal to zero. The second one will have phase-lag and its first, second and third derivatives equal to zero. We will investigate the stability and the error of the obtained methods.

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

Finally, we will apply both of the methods to the resonance problem of the radial Schrödinger equation. This is one of the most difficult problems arising from the one-dimensional Schrödinger equation. The paper is organized as follows:

- The Phase-Lag analysis of Symmetric Multistep Methods is presented in section 2.
- The construction of the new proposed methods is presented in section 3.
- In section 4 we present the error analysis.
- The stability analysis of the new obtained methods is presented in section 5.
- The numerical results are presented in section 6. textbf
- Finally, in section 7 we present some remarks and conclusions.

2. Phase-lag analysis of symmetric multistep methods

For the approximate solution of the initial value problem

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

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 $h = |x_{i+1} - x_i|$, $i = 01m - 1$.
If the method is symmetric, then $a_i = a_{m-i}$ and $b_i = b_{m-i}$, $i = 01\frac{m}{2}$.
When a symmetric $2k$-step method, that is for $i = -k1k$, is applied to the scalar test equation

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

a difference equation of the form

$$A_k(H)\, w_{n+k} + \ldots + A_1(H) w_{n+1} + A_0(H)\, w_n + \\ + A_1(H)\, w_{n-1} + \ldots + A_k(H)\, w_{n-k} = 0, \tag{5}$$

is obtained, where $H = \omega h$, h is the step length, and $A_0(H)$, $A_1(H)$, ..., $A_k(H)$ are polynomials of $H = \omega h$.
The characteristic equation associated with (5) is given by:

$$A_k(H)\lambda^k + \ldots + A_1(H)\lambda + A_0(H) + \\ + A_1(H)\lambda^{-1} + \ldots + A_k(H)\lambda^{-k} = 0. \tag{6}$$

Theorem 2.1.
[3] The symmetric $2k$-step method with characteristic equation given by (6) has phase-lag order q and phase-lag constant c given by:

$$-c\, H^{q+2} + O\left(H^{q+4}\right) = \\ \frac{2A_k\,(H)\,\cos\,(k\,H) + \ldots + 2A_j\,(H)\,\cos\,(j\,H) + \ldots + A_0\,(H)}{2k^2 A_k\,(H) + \ldots + 2j^2 A_j\,(H) + \ldots + 2A_1\,(H)}. \tag{7}$$

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 family of four-step methods

We consider the following family of four-step methods to integrate $w'' = f(x, w)$ first introduced by Wang [15]:

$$w_{n+2} - c_1\left(w_{n+1} + w_{n-1}\right) - 2\,a\,w_n + w_{n-2} = \\ h^2\left[b_2\left(w''_{n+2} + w''_{n-2}\right) + b_1\left(w''_{n+1} + w''_{n-1}\right) + 2b_0 w''_n\right]. \tag{8}$$

The above method is one of the families of symmetric four-step methods for the numerical solution of problems of the form $w'' = f(x, w)$. In the above general form the coefficients c_1, a and b_j, $j = 0, 1, 2$ are free parameters. In the same formula, h is the step size of the integration and n is the number of steps; i.e. w_n is the approximation of the solution in the point x_n, where $x_n = x_0 + n\,h$ and x_0 is the initial value point.

3.1. The first optimized four-step method of the family with vanished phase-lag and its first and second derivatives

Consider the method (8)
Application of the method (8) to the scalar test equation leads to the difference equation (5) with $k = 2$ and A_j, $j = 0\,(1)\,2$ given by:

$$A_0 = -2a + 2H^2 b_0, \quad A_1 = H^2 b_1 - c_1, \quad A_2 = H^2 b_2 + 1. \tag{9}$$

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

$$\lambda^2 - c_1\left(\lambda + \lambda^{-1}\right) - 2a + \lambda^{-2} + H^2\left(b_2\left(\lambda^2 + \lambda^{-2}\right)\right.$$

$$+b_1\left(\lambda+\lambda^{-1}\right)+2b_0\right). \quad (10)$$

We require equation (10) to vanish for λ_i, $i=1\,(1)\,4$ given by

$$\lambda_{1,2}=e^{\pm iH},\quad \lambda_{3,4}=-e^{\pm iH}. \quad (11)$$

The requirement leads to the system of equations:

$$\begin{aligned}
&4H^2\,b_2\,(\cos(H))^2-2H^2\,b_2+4\,(\cos(H))^2\\
&-2+2\cos(H)\;H^2\,b_1-2\cos(H)\;c_1\;-2a+2H^2\,b_0=0\\
&4H^2\,b_2\,(\cos(H))^2-2H^2\,b_2+4\,(\cos(H))^2\\
&-2+2\cos(H)\;H^2\,b_1-2\cos(H)\;c_1\;-2a+2H^2\,b_0=0\\
&4H^2\,b_2\,(\cos(H))^2-2H^2\,b_2+4\,(\cos(H))^2\\
&-2-2\cos(H)\;H^2\,b_1+2\cos(H)\;c_1\;-2a+2H^2\,b_0=0\\
&4H^2\,b_2\,(\cos(H))^2-2H^2\,b_2+4\,(\cos(H))^2\\
&-2-2\cos(H)\;H^2\,b_1+2\cos(H)\;c_1\;-2a+2H^2\,b_0=0.
\end{aligned} \quad (12)$$

Requiring the above method to have its phase-lag vanish and by using the formula (7) (for $k=2$) and (9), we have the following equation:

$$PL=\left(2\left(H^2b_2+1\right)\right)$$

$$\times\frac{\cos(2H)+2\left(H^2b_1-c_1\right)\cos(H)-2a+2H^2b_0}{8H^2b_2+8+2H^2b_1-2c_1}=0. \quad (13)$$

Demanding that the method have the first derivative of the phase-lag vanish as well, we have the equation

$$DPL=-\frac{T_0}{\left(4H^2b_2+4+H^2b_1-c_1\right)^2}=0, \quad (14)$$

where T_0 is given in Appendix A and DPL is the first derivative of the phase-lag.
We now require the method to have the second derivative of the phase-lag vanish. So, the following equation must hold:

$$DDPL=-\frac{T_1}{\left(4H^2b_2+4+H^2b_1-c_1\right)^3}=0, \quad (15)$$

where T_1 is given in Appendix A and $DDPL$ is the second derivative of the phase-lag.
Finally, we require that the following equation for the algebraic order of the method be satisfied:

$$-c_1-480\,b_2-30\,b_1+64=0. \quad (16)$$

Requiring now that the coefficients of the new proposed method satisfy equations (12-16), we obtain the following coefficients of the new developed method:

$$a=\frac{T_2}{T_3},\; b_0=\frac{T_4}{H^2T_3},\; b_1=\frac{T_5}{H^2\,T_7}$$
$$b_2=\frac{T_6}{H^2\,T_7},\; c_1=\frac{T_8}{T_7}, \quad (17)$$

where T_i, $i=2(1)8$ are given in Appendix A.
For some values of $|\omega|$ the formulae given by (17) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned}
a=\;&1-\frac{16}{15}H^2+\frac{8}{75}H^4+\frac{148}{23625}H^6-\frac{4141}{1063125}H^8\\
&+\frac{955687}{1403325000}H^{10}-\frac{297490217}{1277025750000}H^{12}\\
&+\frac{18086804381}{229864635000000}H^{14}-\frac{9919447519843}{351692891550000000}H^{16}\\
&+\frac{111882884929434331}{11226037098276000000000}H^{18}-\cdots
\end{aligned}$$

$$\begin{aligned}
b_0=\;&\frac{13}{15}-\frac{97}{225}H^2+\frac{929}{15750}H^4-\frac{2134}{354375}H^6\\
&+\frac{2426981}{5613300000}H^8-\frac{823920869}{7662154500000}H^{10}\\
&+\frac{10072052201}{306486180000000}H^{12}-\frac{77815891499}{6512831325000000}H^{14}\\
&+\frac{188490352877235953}{44904148393104000000000}H^{16}\\
&-\frac{110629794429351244 87}{7409184484862160000000000}H^{18}+\cdots
\end{aligned}$$

$$\begin{aligned}
b_1=\;&\frac{16}{15}-\frac{8}{75}H^2-\frac{148}{23625}H^4+\frac{766}{1063125}H^6-\frac{173953}{350831250}H^8\\
&+\frac{48838523}{319256437500}H^{10}-\frac{3271214939}{57466158750000}H^{12}\\
&+\frac{1748709749617}{87923222887500000}H^{14}-\frac{19892214158592739}{2806509274569000000000}H^{16}\\
&+\frac{40780273165103291}{1624821158961000000000}H^{18}-\cdots
\end{aligned}$$

$$\begin{aligned}
b_2=\;&\frac{1}{15}+\frac{1}{225}H^2+\frac{29}{47250}H^4-\frac{34}{1063125}H^6+\frac{165527}{5613300000}H^8\\
&-\frac{65342923}{7662154500000}H^{10}+\frac{2978183801}{919458540000000}H^{12}\\
&-\frac{14123908819}{12560460412500000}H^{14}+\frac{1387045152692327}{3454165261008000000000}H^{16}
\end{aligned}$$

$$\frac{1052830607333183729}{7409184484862160000000000}\,H^{18}+\cdots$$

$$c_1=\frac{16}{15}H^2-\frac{8}{75}H^4-\frac{148}{23625}H^6+\frac{766}{1063125}H^8$$
$$-\frac{173953}{350831250}H^{10}+\frac{48838523}{319256437500}H^{12}$$
$$-\frac{3271214939}{57466158750000}H^{14}+\frac{1748709749617}{87923222887500000}H^{16}$$
$$-\frac{19892214158592739}{2806509274569000000000}H^{18}+\cdots. \quad (18)$$

The behavior of the coefficients is shown in Figure 1.
In this figure, the logarithm of the coefficients is computed. From these figures, it is clear that, for some values of H, the denominator of the coefficients becomes extremely small.
The local truncation error of the new proposed method is given by:

$$LTE=-\frac{2h^8}{945}$$
$$\times\left(w_n^{(8)}-6\omega^4 w_n^{(4)}-8\omega^6 w_n^{(2)}-3\omega^8 w_n\right)+O\left(h^{10}\right). \quad (19)$$

3.2. The second optimized four-step method of the family with vanished phase-lag and its first, second and third derivatives

Consider the method (8).
Application of the method (8) to the scalar test equation leads to the difference equation (5) with $k=2$ and $A_j,\ \ j=0\,(1)\,2$ given by (9).
The characteristic equation associated with the difference equation is given by (10).
We require equation (10) to vanish for $\lambda_i,\ \ i=1\,(1)\,4$ given by (11). This requirement leads to the system of equations (12).
Requiring the above method to have a vanishing phase-lag and by using the formula (7) (for $k=2$) and (9) we have the equation (13). Demanding the method to have the first derivative of the phase-lag vanish as well, we have the equation (14). We require the method to have the second derivative of the phase-lag vanish as well. So, the equation (15) must hold.
Finally, we require the method to have the third derivative of the phase-lag vanish as well. This leads to the following equation:

$$DDDPL=\frac{T_9}{\left(4H^2b_2+4+H^2b_1-c_1\right)^4}, \quad (20)$$

where T_9 is given in Appendix B and $DDDPL$ is the third derivative of the phase-lag.
Requiring now that the coefficients of the new proposed method satisfy equations (12), (13), (14), (15) and (20),

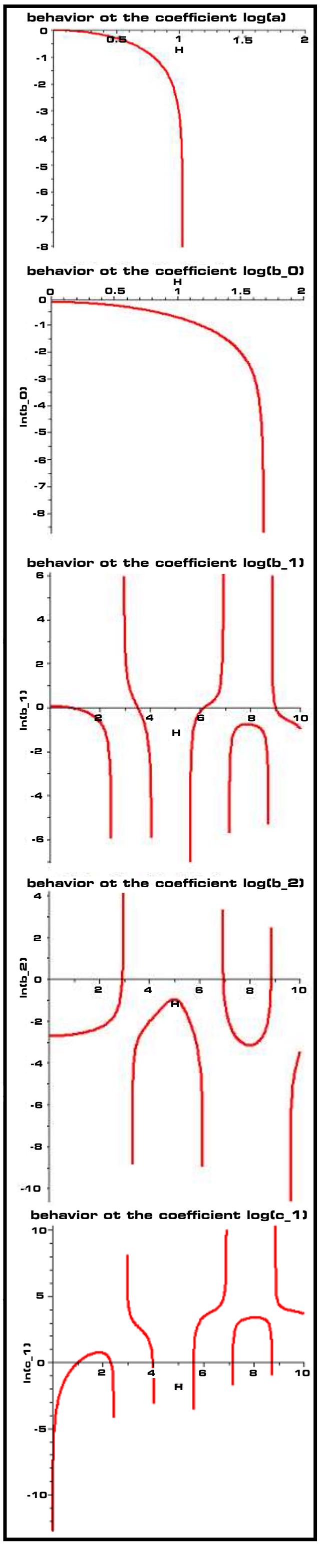

Figure 1. Behavior of the coefficients of the new proposed method given by (17) for several values of $H=\omega h$.

we obtain the following coefficients of the new developed method:

$$a = \frac{T_{10}}{2\,T_{11}},\; b_0 = \frac{T_{12}}{2\,H^2\,T_{11}},\; b_1 = \frac{T_{13}}{H^2\,T_{11}} \quad b_2 = \frac{T_{14}}{H^2\,T_{11}},\; c_1 = \frac{T_{13}}{T_{11}}, \tag{21}$$

where T_j, $j = 10(1)14$ are given in Appendix B.
For some values of $|\omega|$, the formulae given by (21) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned}
a &= 1 - \frac{16}{15}H^2 + \frac{664}{4725}H^4 - \frac{926}{70875}H^6 - \frac{107596}{245581875}H^8 \\
&- \frac{230302}{5320940625}H^{10} - \frac{243473998}{15084866671875}H^{12} \\
&- \frac{1060706246}{349694636484375}H^{14} - \frac{165481909105144}{25324361032243710937 5}H^{16} \\
&- \frac{522728140703554}{3798654154836556640625}H^{18} + \dots \\
b_0 &= \frac{13}{15} - \frac{71}{175}H^2 + \frac{3853}{70875}H^4 - \frac{361079}{81860625}H^6 \\
&+ \frac{8199329}{47888465625}H^8 - \frac{57996277}{5028288890625}H^{10} \\
&- \frac{549582701}{549520143046875}H^{12} - \frac{6954522582727}{2813817892471523437 5}H^{14} \\
&- \frac{197158329783313}{3798654154836556640625}H^{16} \\
&- \frac{1304859934871828869}{1192587471910936957324218 75}H^{18} + \dots \\
b_1 &= \frac{16}{15} - \frac{664}{4725}H^2 + \frac{926}{70875}H^4 + \frac{367471}{245581875}H^6 \\
&+ \frac{14980541}{42567525000}H^8 + \frac{17699317093}{241357866750000}H^{10} \\
&+ \frac{3764629780309}{246185024085000000}H^{12} \\
&+ \frac{103545916633420307}{32415182121271950000000}H^{14} \\
&+ \frac{520148933496074671 7}{777964370910526800000000 0}H^{16} \\
&+ \frac{186636827158360547918 41}{1332228623167417575600000000 00}H^{18} + \dots \\
b_2 &= 1/15 + \frac{61}{4725}H^2 + \frac{67}{23625}H^4 + \frac{150971}{245581875}H^6 \\
&+ \frac{6264343}{47888465625}H^8 + \frac{415793123}{15084866671875}H^{10} \\
&+ \frac{22255266331}{3846641001328125}H^{12} + \frac{307189404737519}{25324361032243710937 5}H^{14} \\
&+ \frac{45995031648199}{180888293087455078125}H^{16} \\
&+ \frac{19070620752836776681}{357776241573281087197265625}H^{18} + \dots \\
c_1 &= \frac{16}{15}H^2 - \frac{664}{4725}H^4 + \frac{926}{70875}H^6 + \frac{367471}{245581875}H^8 \\
&+ \frac{14980541}{42567525000}H^{10} + \frac{17699317093}{241357866750000}H^{12} \\
&+ \frac{3764629780309}{246185024085000000}H^{14} \\
&+ \frac{103545916633420307}{32415182121271950000000}H^{16} \\
&+ \frac{5201489334960746717}{7779643709105268000000000}H^{18} + \dots \;.
\end{aligned} \tag{22}$$

The behavior of the coefficients is shown in Figure 2.
In this figure, the logarithm of the coefficients is computed. From these figures, it is clear that for some values of H the denominator of the coefficients becomes extremely small.
The local truncation error of the new proposed method is given by:

$$LTE = -\frac{2h^8}{945} \times \left(w_n^{(8)} + 4\omega^2 w_n^{(2)} + 6\omega^4 w_n^{(4)} + 4\omega^6 w_n^{(2)} + \omega^8 w_n\right) + O\left(h^{10}\right). \tag{23}$$

4. Error Analysis

We will study the following methods:

4.1. Classical method (i.e. the method (8) with constant coefficients)

$$LTE_{CL} = -\frac{2h^8}{945} w_n^{(8)} + O\left(h^{10}\right). \tag{24}$$

4.2. Method developed by Wang [see 15]

$$LTE_{Wang[15]} = \frac{2h^8}{945}\left(\omega^8 w_n - w_n^{(8)}\right) + O\left(h^{10}\right). \tag{25}$$

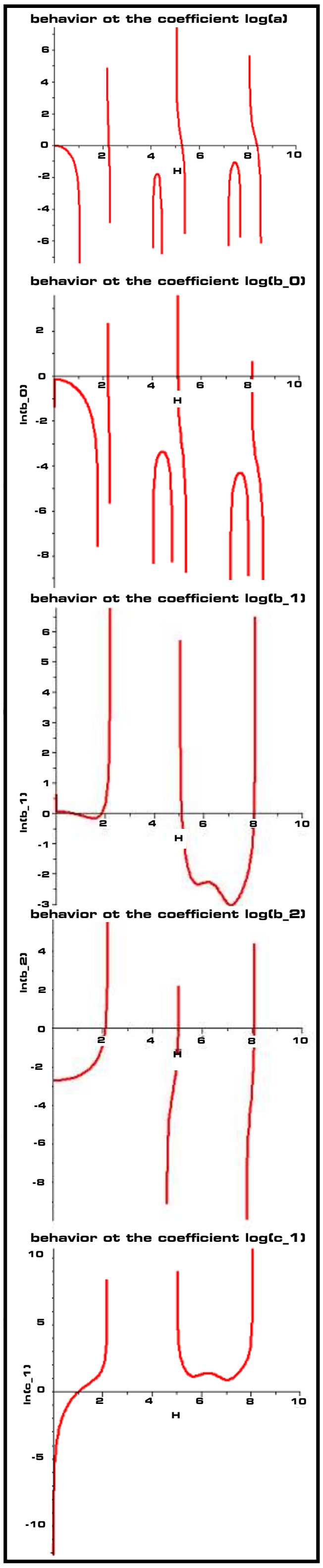

Figure 2. Behavior of the coefficients of the new proposed method given by (21) for several values of $H = \omega\, h$.

4.3. New method with vanished phase-lag and its first and second derivatives (developed in section 3.1)

$$LTE_{NMI} = -\frac{2h^8}{945}$$

$$\times\ \left(w_n^{(8)} - 6\omega^4 w_n^{(4)} - 8\omega^6 w_n^{(2)} - 3\omega^8 w_n\right) + O\left(h^{10}\right). \quad (26)$$

4.4. New method with vanished phase-lag and its first, second and third derivatives (developed in section 3.2)

$$LTE_{NMII} = -\frac{2h^8}{945}$$

$$\times\ \left(w_n^{(8)} + 4\omega^2 w_n^{(2)} + 6\omega^4 w_n^{(4)} + 4\omega^6 w_n^{(2)} + \omega^8 w_n\right) + O\left(h^{10}\right). \quad (27)$$

The error analysis is based on the following steps:

- The radial time independent Schrödinger equation is of the form

$$w''(x) = f(x)\ w(x). \quad (28)$$

- Based on the paper of Ixaru and Rizea [6], the function f(x) can be written in the form:

$$f(x) = g(x) + G, \quad (29)$$

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

- We express the derivatives $w_n^{(i)}$, $i = 2, 3, 4, \ldots,$ which are terms of the local truncation error formulae, in terms of equation (29). 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.

We use the procedure mentioned above and the formulae:

$$w_n^{(2)} = (V(x) - V_c + G)\ w(x)$$

$$w_n^{(4)} = \left(\frac{d^2}{dx^2}\, V(x)\right)\ w(x) + 2\left(\frac{d}{dx}\, V(x)\right)\left(\frac{d}{dx}\, w(x)\right)$$

$$+ (V(x) - V_c + G)\left(\frac{d^2}{dx^2}\, w(x)\right)$$

$$w_n^{(6)} = \left(\frac{d^4}{dx^4}\,V(x)\right)\,w(x) + 4\,\left(\frac{d^3}{dx^3}\,V(x)\right)\,\left(\frac{d}{dx}\,w(x)\right)$$
$$+3\,\left(\frac{d^2}{dx^2}\,V(x)\right)\,\left(\frac{d^2}{dx^2}\,w(x)\right) + 4\,\left(\frac{d}{dx}\,V(x)\right)^2\,w(x)$$
$$+6\,(V(x) - V_c + G)\,\left(\frac{d}{dx}\,V(x)\right)\,\left(\frac{d}{dx}\,w(x)\right)$$
$$+4\,(V(x) - V_c + G)\,w(x)\,\left(\frac{d^2}{dx^2}\,V(x)\right)$$
$$+\,(V(x) - V_c + G)^2\,\left(\frac{d^2}{dx^2}\,w(x)\right)\,\ldots\,. \qquad (30)$$

So, from the above expressions we have the formulae of Local Truncation Error presented in the Appendix C.
We consider two cases in terms of the value of E:

1. 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 trigonometrically-fitted methods.
2. $G >> 0$ or $G << 0$. Then $|G|$ is a large number.

Hence, we have the following asymptotic expansions of the local truncation errors:

4.5. Classical method

$$LTE_{CL} = h^8\,\left(-\frac{2}{945}\,w\,(x)\;G^4 + \ldots\right) + O\left(h^{10}\right). \qquad (31)$$

4.6. Method developed by Wang [see 15]

$$LTE_{Wang[15]} = h^8\left[-\frac{8}{945}\,g\,(x)\,w\,(x)\;G^3 + \ldots\right] + O\left(h^{10}\right). \qquad (32)$$

4.7. New method with vanished phase-lag and its first and second derivatives (developed in section 3.1)

$$LTE_{NMI} = h^8\left[-\frac{32}{945}\,\left(\frac{d^2}{dx^2}g\,(x)\right)\,w\,(x)\;G^2 + \cdots\right] + O\left(h^{10}\right). \qquad (33)$$

4.8. New method with vanished phase-lag and its first, second and third derivatives (developed in section 3.2)

$$LTE_{NMII} = h^8\Bigg[\left(-\frac{8}{315}\,\left(\frac{d^4}{dx^4}g\,(x)\right)\,w\,(x)\right.$$
$$-\frac{16}{945}\,\left(\frac{d^3}{dx^3}g\,(x)\right)\,\frac{d}{dx}w\,(x)$$
$$-\frac{32}{945}\,g\,(x)\,w\,(x)\,\frac{d^2}{dx^2}g\,(x)$$
$$\left.-\frac{8}{315}\,\left(\frac{d}{dx}g\,(x)\right)^2\,w\,(x)\right)\,G\Bigg] + O\left(h^{10}\right). \qquad (34)$$

From the above equations we have the following theorem:

Theorem 4.1.
For the Classical Four-Step Method the error increases as the fourth power of G. For the Method developed by Wang [15], the error increases as the third power of G. For the New Method with Vanished Phase-Lag and its First and Second Derivatives (developed in section 3.1, the error increases as the second power of G. Finally, for the New Method with Vanished Phase-Lag and its First, Second and Thirds Derivatives (developed in section 3.2), the error increases as the first power of G. So, for the numerical solution of the time independent radial Schrödinger equation the New Method with Vanished Phase-Lag and its First, Second and Thirds Derivatives is the most accurate one, especially for large values of $|G| = |V_c - E|$.

5. Stability analysis

Applying the new method to the scalar test equation:

$$w'' = -q^2 w, \qquad (35)$$

we obtain the following difference equation:

$$A_2\,(z,H)\,\left(w_{n+2} + w_{n-2}\right)$$
$$+\,A_1\,(z,H)\,\left(w_{n+1} + w_{n-1}\right) + A_0\,(z,H)\;w_n = 0, \qquad (36)$$

where

$$A_0\,(z,H) \;=\; -2\,a + 2z^2 b_0,$$
$$A_1\,(z,H) \;=\; z^2 b_1 - c_1,\;\; A_2\,(z,H) = z^2 b_2 + 1, \qquad (37)$$

where $H = \omega h$, $z = q\,h$.
The corresponding characteristic equation is given by:

$$A_2\,(z,H)\,\left(\lambda^4 + 1\right) + A_1\,(z,H)\,\left(\lambda^3 + \lambda\right) + A_0\,(z,H)\;\lambda^2 = 0. \qquad (38)$$

Theorem 5.1.
(see [9]) A symmetric four-step method with the characteristic equation given by (38) is said to have a nonzero interval of periodicity $\left(0, z_0^2\right)$ if, for all $z \in \left(0, z_0^2\right)$ the following relations hold:

$$P_1\left(z, H\right) \geq 0,\ P_2\left(z, H\right) \geq 0,\ P_3\left(z, H\right) \geq 0,$$
$$P_2\left(z, H\right)^2 - 4\,P_1\left(z, H\right)\,P_3\left(z, H\right) \geq 0, \qquad (39)$$

where:

$$\begin{aligned} P_1\left(z, H\right) &= 2\,A_2\left(z, H\right) - 2\,A_1\left(z, H\right) + A_0\left(z, H\right) \geq 0, \\ P_2\left(z, H\right) &= 12\,A_2\left(z, H\right) - 2\,A_0\left(z, H\right) \geq 0, \\ P_3\left(z, H\right) &= 2\,A_2\left(z, H\right) + 2\,A_1\left(z, H\right) + A_0\left(z, H\right) \geq 0, \quad (40) \\ N\left(z, H\right) &= P_2\left(z, H\right)^2 - 4\,P_1\left(z, H\right)\,P_3\left(z, H\right) \geq 0. \end{aligned}$$

Definition 1.
A method is called singularly almost P-stable if and only if its interval of periodicity is equal to $(0, \infty) - S$ [2] when the frequency of the exponential fit or phase fit is the same as the frequency of the scalar test equation, i.e. $H = z$.

Based on (37), the stability polynomials (40) for the new developed methods are given by:

$$\begin{aligned} P_1\left(z, H\right) &= 2\left(1 + c_1 - a\right) + 2z^2\left(b_2 - b_1 + b_0\right), \\ P_2\left(z, H\right) &= 4\left(3 + a\right) + 4z^2\left(3b_2 - b_0\right), \\ P_3\left(z, H\right) &= 2\left(1 - c_1 - a\right) + 2z^2\left(b_2 + b_1 + b_0\right), \qquad (41) \\ N\left(z, H\right) &= 16\left(8 + 8a + c_1^2\right) + 16z^4\left(8b_2^2 + b_1^2 - 8b_2 b_0\right) \\ &\quad + 32z^2\left(8b_2 - 4b_0 + 4b_2 a - c_1 b_1\right). \end{aligned}$$

In Figure 3 we present the $z - H$ plane for the Method of Wang [15]. In Figure 4 we present the $z - H$ plane for the New Method with Vanished Phase-Lag and its First and Second Derivatives produced in section 3.1. Finally, in the Figure 5 we present the $z - H$ plane for the New Method with Vanished Phase-Lag and its First, Second and Third Derivatives produced in section 3.2 .
A method is P-stable if the $z - H$ plane is completely shadowed. It can be seen the following:

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

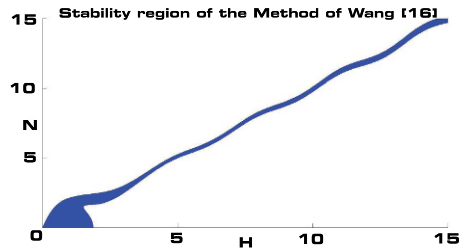

Figure 3. $z - H$ plane of the method of Wang [15].

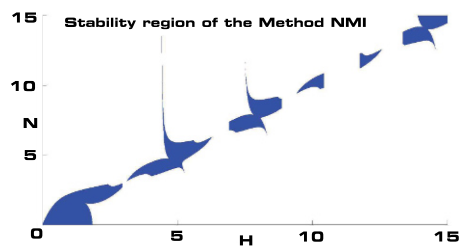

Figure 4. $z - H$ plane of the method NMI produced in section 3.1.

- Based on Figures 3, 4 and 5, we can say that the method of Wang [15], the method developed in section 3.1, and the methods developed in section 3.2 are not P-stable (i.e. there are areas in Figures 3, 4, 5 that are white and in which the conditions of P-stability are not satisfied).
- In the case where the frequency of the exponential fit is equal to the frequency of the scalar test equation, we have the following comments:

  1. For the method developed in section 3.1: The method is almost P-stable i.e. has interval of periodicity equal to $(0, +\infty) - S$, where S is

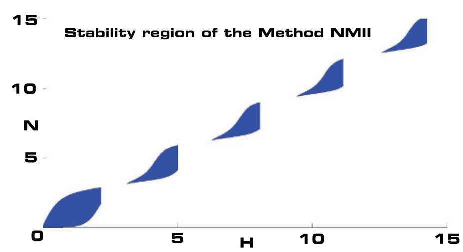

Figure 5. $z - H$ plane of the method NMII produced in section 3.2.

a set of distinct points and more specifically:

$$S = \Big\{ 0.5184149637,\ 2.741022548, 3.492878707, 6.050937628, 6.501344160, 9.313248407, 9.524522115, \ldots \Big\}. \quad (42)$$

2. For the method developed in section 3.2: The method is almost P-stable i.e. has interval of periodicity equal to $(0, +\infty) - Q$, where Q is a set of distinct points and more specifically:

$$Q = \Big\{ 0.5184149637,\ 1.518034031, 1.622122697, 3.135616028, 3.147943251,\ 3.540487604, 5.934268142, 6.273131380,\ 6.293127605, \ldots \Big\}. \quad (43)$$

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. Hence, it is necessary to observe the surroundings of the first diagonal of the $z - H$ plane.

6. Numerical results

In order to investigate the efficiency of the new developed methods, we illustrate them

- for the radial time-independent Schrödinger equation and
- for a nonlinear problem with oscillating solution.

6.1. The radial Schrödinger equation

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

$$\omega = \sqrt{|q(r)|} = \sqrt{|V(r) - E|}, \quad (44)$$

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

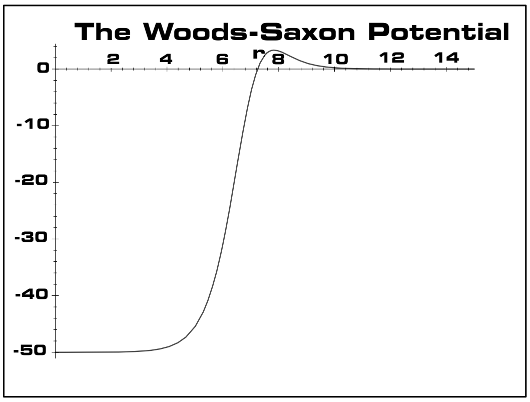

Figure 6. The Woods-Saxon potential.

6.1.1. *Woods-Saxon potential*

We use as a potential the well known Woods-Saxon form which can be written as

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2}, \quad (45)$$

with $y = \exp\left[\frac{r-R_0}{a}\right]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$. The behavior of Woods-Saxon potential is shown in Figure 6.

It is well known that for some potentials, such as the Woods-Saxon potential, the definition of the parameter ω is given not as a function of r but as based on some critical points which have been defined from the investigation of the appropriate potential (see [7] for details).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows [see for details 1, 5, 6]:

$$\omega = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h, \\ \sqrt{-25+E}, & \text{for } r = 6.5, \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h, \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15]. \end{cases} \quad (46)$$

For example, at the point of the integration region $r = 6.5$, the value of ω is equal to: $\sqrt{-25+E}$. So, $H = \omega\, h = \sqrt{-25+E}\, h$. At the point of the integration region $r = 6.5 - 3\,h$, the value of ω is equal to: $\sqrt{-50+E}$, etc.

6.1.2. *Radial Schrödinger equation – the resonance problem*

We consider the numerical solution of the radial Schrödinger equation (1) in the well-known case of the Woods-Saxon potential (45). In order to solve this problem numerically, we must 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 $r \in [0, 15]$. We consider equation (1) in a rather large domain of energies, i.e. $E \in [1, 1000]$.
In the case of positive energies, $E = k^2$, the potential decays faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation effectively reduces to

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0, \qquad (47)$$

for r greater than some value R.
The above equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus, the solution of equation (1) (when $r \to \infty$), has the asymptotic form

$$q(r) \approx Akrj_l(kr) - Bkrn_l(kr)$$

$$\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kx - \frac{l\pi}{2}\right)\right], \qquad (48)$$

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

$$\tan \delta_l = \frac{q(r_2)S(r_1) - q(r_1)S(r_2)}{q(r_1)C(r_1) - q(r_2)C(r_2)}, \qquad (49)$$

for distinct points r_1 and r_2 in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$), $S(r) = krj_l(kr)$, and $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need $q_j,\ \ j = 0(1)3$ before starting a four-step method. From the initial condition we obtain q_0. The values $q_i,\ \ i = 1(1)3$ are obtained by using high order Runge-Kutta-Nyström methods [see 22, 24]. With these starting values, we evaluate the phase shift δ_l at r_4 of the asymptotic region.
For positive energies, we have the so-called resonance problem. This 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.
The boundary conditions for this problem are:

$$q(0) = 0, \ q(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \qquad (50)$$

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

- the Classical Four-Step method of Henrici [9], which is indicated as Method MH
- the P-stable four-step method developed by Wang [15], which is indicated as Method MW
- the newly developed four-step method with vanished phase-lag and its first and second derivatives (obtained in section 3.1, which is indicated as Method NMI
- the newly developed four-step method with vanished phase-lag and its first, second and third derivatives (obtained in section 3.2, which is indicated as Method NMII.

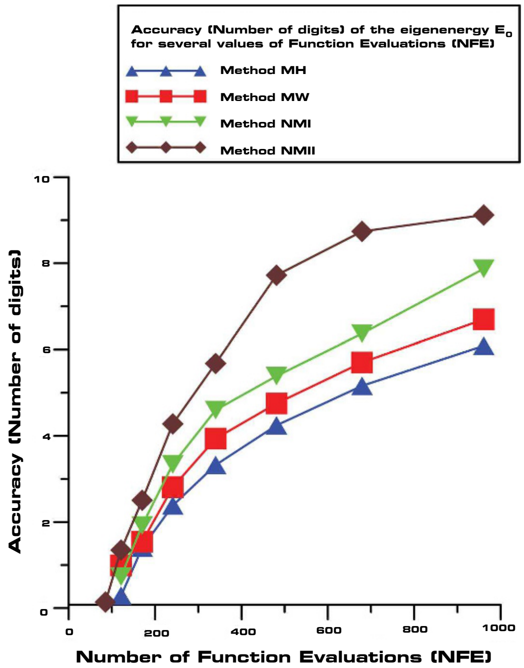

Figure 7. Accuracy (Digits) for several values of NFE for the eigenvalue $E_0 = 53.588872$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0.

The computed eigenenergies are compared with reference values[3]. In Figures 7, 8, 9 and 10, we present the maximum absolute error $log_{10}(Err)$, where

$$Err = |E_{calculated} - E_{accurate}|, \qquad (51)$$

for the eigenenergies $E_0 = 53.588872$, $E_1 = 163.215341$, $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of NFE = Number of Function Evaluations. We note that the NFE counts the computational cost for

[3] *The reference values are computed using the well known four-step method of Henrici [9] with small step size for the integration.*

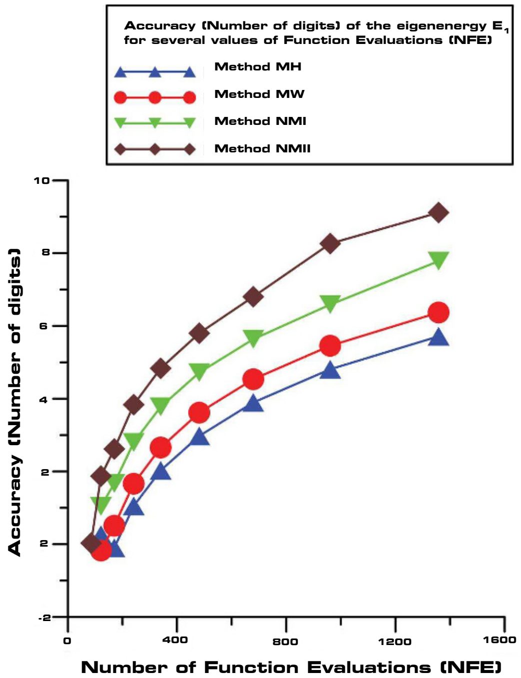

Figure 8. Accuracy (Digits) for several values of NFE for the eigenvalue $E_1 = 163.215341$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0.

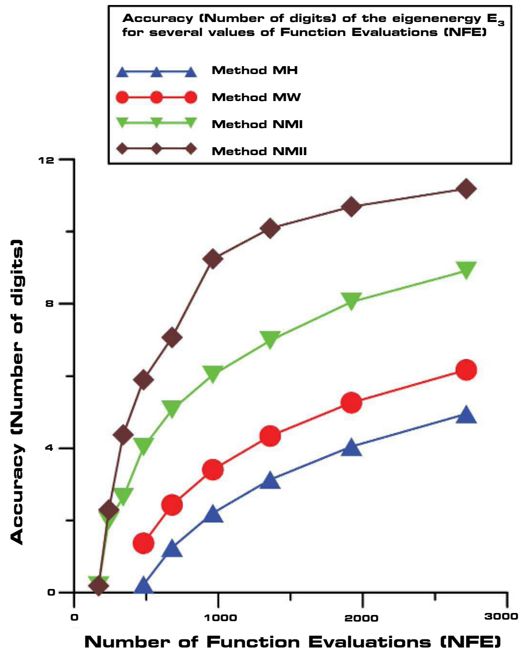

Figure 10. Accuracy (Digits) for several values of NFE for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0.

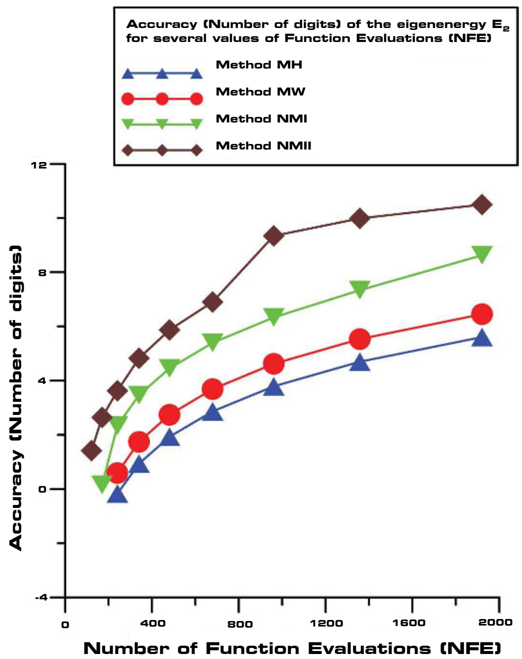

Figure 9. Accuracy (Digits) for several values of NFE for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0.

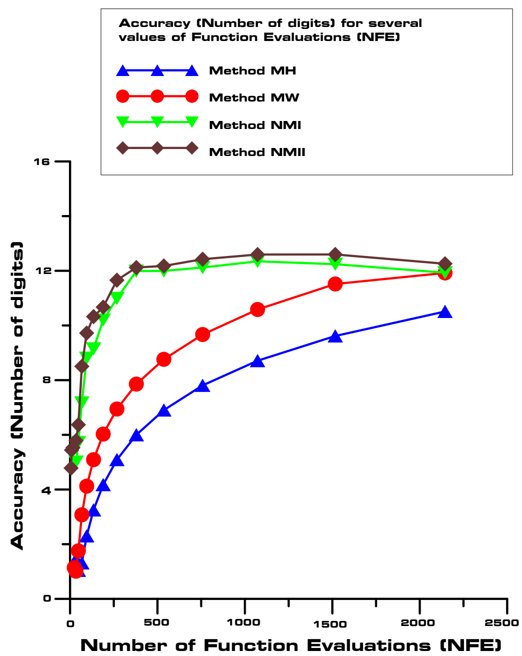

Figure 11. Accuracy (Digits) for several values of NFE for the nonlinear problem. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0.

each method. Consequently, the comparison is based on the maximum absolute error which is obtained with the specific NFE, i.e. with the specific computational cost for each method.

6.2. Nonlinear problem

Consider the second order initial-value problem

$$\psi''(t) = -100\,\psi(t) + \sin(\psi(t))\,,$$
$$\psi(0) = 0,\ \psi'(0) = 1,\ t \in [0, 20\,\pi]\,. \tag{52}$$

The theoretical solution is unknown, but we use a reference solution $\psi(20\,\pi) = 3.92823991.10^{-4}$.
For the numerical solution of the above problem, we use the methods mentioned in section 6.1.2.
The computed values $\psi(20\,\pi)$ are compared with the reference value mentioned above[4]. In Figures 11, we present the maximum absolute error $log_{10}(Err)$ where

$$Err = |\psi_{calculated} - \psi_{reference}|\,, \tag{53}$$

of the $\psi(20\,\pi)$ respectively, for several values of NFE = Number of Function Evaluations.

7. Conclusions

The purpose of this paper was the optimization of the efficiency of a numerical method for the approximate solution of the radial Schrödinger equation and related problems. We have shown how the methodology of the vanishing of the phase-lag and its derivatives optimizes the behaviour of a numerical method. The results of this methodology wer methods that are very efficient on any problem with oscillating solutions or problems with solutions containing the functions cos and sin or any combination of them.
From the results presented above, it is obvious that the theoretical results presented in the Error Analysis have been verified, i.e.

1. The P-stable four-step method developed by Wang [15] (presented in Section 3.1), which is indicated as Method MW, is much more efficient than the the Classical Four-Step method of Henrici [9], which is indicated as Method MH.

2. The newly developed four-step method with its phase-lag as well as its first and second derivatives vanished (obtained in Section 3.1 and indicated as Method NMI) is more efficient than the P-stable four-step method developed by Wang [15].

3. The most efficient method is the newly developed four-step method with its phase-lag as well as its first, second, and third derivatives vanished, (obtained in Section 3.2 and indicated as Method NMII).

[4] *The reference value was computed using the well known four-step method of Henrici [9] with small step size for the integration.*

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

References

[1] L. G. Ixaru, M. Micu, Topics in Theoretical Physics (Central Institute of Physics, Bucharest, 1978)
[2] L. D. Landau, F. M. Lifshitz, Quantum Mechanics (Pergamon, New York, 1965)
[3] T. E. Simos, P. S. Williams, On finite difference methods for the solution of the Schrödinger equation, Comput. Chem. 23, 513 (1999)
[4] A. D. Raptis, Exponential multistep methods for ordinary differential equations, Bulletin of the Greek Mathematical Society 25, 113 (1984).
[5] L .G. Ixaru, Numerical Methods for Differential Equations and Applications (Reidel, Dordrecht - Boston - Lancaster, 1984)
[6] L. G. Ixaru, M Rizea, Comput. Phys. Commun. 19, 23 (1980)
[7] T. E. Simos, P. S. Williams, MATCH Communications in Mathematical and in Computer Chemistry 45, 123 (2002).
[8] J. D. Lambert, I .A. Watson, IMA J. Appl. Math. 18, 189 (1976).
[9] P. Henrici, Discrete variable methods in ordinary differential equations (John Wiley & Sons, New York, 1962)
[10] L. G. Ixaru, G. V. Berghe, Exponential fitting (Kluwer Academic Publisher, The Netherlands, 2004)
[11] L. G. Ixaru, M. Rizea, Comput. Phys. Commun. 38, 329 (1985)

[12] A. París, L. Rández, IMA J. Appl. Math. 234, 767 (2010)
[13] M. Calvo, J. M. Franco, J. I. Montijano, L. Rández, IMA J. Appl. Math. 223, 387 (2009)
[14] T. E. Simos, Int. J. Mod. Phys. C 18, 315 (2007)
[15] Z. Wang, Comput. Phys. Commun. 171, 162 (2005)
[16] A. Konguetsof, T. E. Simos, IMA J. Appl. Math. 158, 93 (2003)
[17] R. D'Ambrosio, E. Esposito, B. Paternoster, IMA J. Appl. Math. 235, 4888 (2011)
[18] R. D'Ambrosio, M. Ferro, B. Paternoster, Math. Comput. Simulat. 81, 1068 (2011)
[19] Z. A. Anastassi, T. E. Simos, Phys. Rep. 482-483, 1 (2009)
[20] T. Lyche, Numer. Math. 19, 65 (1972)
[21] J. P. Coleman, L. G. Ixaru, IMA J. Numer. Anal. 16, 179 (1996)
[22] J. R. Dormand, P. J. Prince, Comput. Math. Appl. 14, 1007 (1988)
[23] J. R. Dormand, M. E. A. IMA J. Numer. Anal. 7, 235 (1987)
[24] J. R. Dormand, M. E. A. IMA J. Numer. Anal. 7, 423 (1987)
[25] G. A. Panopoulos, Z. A. Anastassi, T. E. Simos, J. Math. Chem. 46, 604 (2009)
[26] H. Van de Vyver, New Astronomy 10, 261 (2005)
[27] M. Calvo, J. M. Franco, J. I. Montijano, L. Rández, Comput. Phys. Commun. 181, 2044 (2010)
[28] T. E. Simos, J. Chem. Phys. 133, 104108 (2010)
[29] I. Alolyan, T. E. Simos, J. Math. Chem. 48, 925 (2010)
[30] I. Alolyan, T. Simos, J. Math. Chem. 48, 1092 (2010)
[31] R. D'Ambrosio, L. G. Ixaru, B. Paternoster, Comput. Phys. Commun. 182, 322 (2011)
[32] T. E. Simos, Acta Appl. Math. 110, 1331 (2010)

Appendix A

$$T_0 = 4\sin(H)H^2 b_1 + 4\sin(H)\cos(H)H^4 b_2 b_1$$
$$+32\sin(H)\cos(H)H^2 b_2 + 16\sin(H)\cos(H)$$
$$-4\sin(H)\, c_1 - 4\sin(H)\cos(H)c_1 + \sin(H)\, c_1^2$$
$$+16\sin(H)\cos(H)H^4 b_2^2 + 4\sin(H)\cos(H)\, H^2 b_1$$
$$+\sin(H)\, H^4 b_1^2 - 4\sin(H)\cos(H)H^2 b_2 c_1$$
$$+4\sin(H)\, H^4 b_1 b_2 - 2\sin(H)\, H^2 b_1 c_1$$
$$-4\sin(H)\, c_1 H^2 b_2 - 8H b_1\cos(H)$$
$$+4(\cos(H))^2\, H b_1 + 4(\cos(H))^2\, H b_2 c_1$$
$$-8H\cos(H)\, c_1 b_2 - 8H a b_2$$
$$-2H b_2 c_1 + 2H b_0 c_1 - 2H b_1 - 8H b_0 - 2H a b_1 \quad (54)$$

$$T_1 = -64 + 8\cos(H)\, c_1^2 + 96H^2 b_0 b_2 + 96H^2 a b_2^2$$
$$+6H^2 a b_1^2 + 8a b_2 c_1 + 8H^4 b_1 b_2 c_1$$
$$-32\cos(H)\, H^2 b_2 c_1 + 32\cos(H)\, H^4 b_2 b_1$$
$$-128(\cos(H))^2\, c_1 H^2 b_2 + 8(\cos(H))^2\, H^6 b_2 b_1^2$$
$$+8(\cos(H))^2\, H^2 b_2 c_1^2 - 16(\cos(H))^2\, H^2 b_1 c_1$$
$$-192H^2 b_2 - 16\cos(H)\, c_1 - 32H^2 b_1 - 16H b_1\sin(H)\, c_1$$
$$+64H^3 b_1\sin(H)\, b_2 + 48H^2 a b_1 b_2 - 16H\sin(H)\, c_1^2 b_2$$
$$+96H^2\cos(H)\, c_1 b_2^2 + 32c_1 - 8b_1 + 128(\cos(H))^2$$
$$+2b_1 c_1 - 32b_1\cos(H) + 16b_0 c_1 + \cos(H)\, H^6 b_1^3$$
$$+8\cos(H)\, c_1^2 b_2 + 24\cos(H)\, H^2 b_1^2 - 32\cos(H)\, c_1 b_2$$
$$+8\cos(H)\, H^4 b_1^2 + 24b_0 H^2 b_1 + 8\cos(H)\, b_1 c_1$$
$$-2b_0 c_1^2 - \cos(H)\, c_1^3 + 2b_2 c_1^2 - 16\sin(H)\cos(H)\, b_1^2 H^3$$
$$-16(\cos(H))^2\, H^4 b_1 b_2 c_1 + 6H^2 b_2 b_1 c_1$$
$$-64H^3 b_2\sin(H)\cos(H)\, b_1 + 16H\sin(H)\cos(H)\, b_1 c_1$$
$$-64H^3 b_2^2\sin(H)\cos(H)\, c_1 - 64H\sin(H)\cos(H)\, b_1$$
$$+24H^2 b_2 b_1 + 24b_2^2 c_1 H^2 - 4H^6 b_2 b_1^2 - 32H^6 b_2^2 b_1$$
$$+16\cos(H)\, H^2 b_1 + 384H^2 b_2(\cos(H))^2$$
$$+64(\cos(H))^2\, H^2 b_1 - 12(\cos(H))^2\, H^2 b_1^2$$
$$+384(\cos(H))^2\, H^4 b_2^2 + 8(\cos(H))^2\, H^4 b_1^2$$
$$-4(\cos(H))^2\, b_1 c_1 + 16(\cos(H))^2\, b_2 c_1$$
$$-4(\cos(H))^2\, b_2 c_1^2 + 128(\cos(H))^2\, H^6 b_2^3$$
$$+64c_1 H^2 b_2 + 64H b_1\sin(H) - 16\cos(H)\, b_1 c_1 H^2$$
$$+24\cos(H)\, b_1 c_1 H^2 b_2 + 16H^3 b_1\sin(H)\, c_1 b_2$$
$$-16\cos(H)\, H^4 b_1 c_1 b_2 + 96\cos(H)\, H^2 b_1 b_2$$
$$-24b_0 c_1 H^2 b_2 - 6b_0 H^2 b_1 c_1 - 16H^3 b_2\sin(H)\cos(H)\, b_1 c_1$$
$$+8H^2 b_1 c_1 - 64H^4 b_1 b_2 - 8b_2 c_1 - 4H^4 b_1^2 - 192H^4 b_2^2$$
$$+2a b_1 c_1 + 16H^3 b_1^2\sin(H) - 3\cos(H)\, H^4 b_1^2 c_1$$
$$+3\cos(H)\, H^2 b_1 c_1^2 - 16\cos(H)\, c_1 H^4 b_2^2 + 8\cos(H)\, c_1^2 H^2 b_2$$
$$+64H\sin(H)\, c_1 b_2 + 64\sin(H)\, c_1 b_2^2 H^3 - 48(\cos(H))^2\, b_2^2 c_1 H^2$$

$$+64\,(\cos(H))^2\, H^6\, b_2^2\, b_1 - 48\,(\cos(H))^2\, H^2\, b_2\, b_1$$
$$-64\,(\cos(H))^2\, H^4\, b_2^2\, c_1 + 128\,(\cos(H))^2\, H^4\, b_1\, b_2$$
$$-64\,H^6\, b_2^3 + 6\,H^2\, b_1^2 - 32\,b_0 - 32\,a\, b_2 - 8\,a\, b_1 - 4\,c_1^2$$
$$+16\,(\cos(H))^2\, b_1 - 64\,(\cos(H))^2\, c_1 + 8\,(\cos(H))^2\, c_1^2$$
$$-64\,H\, b_2 \sin(H) \cos(H)\, c_1 + 16\,H\, b_2 \sin(H)\, \cos(H)\, c_1^2$$
$$-12\,(\cos(H))^2\, H^2\, b_2\, b_1\, c_1 + 32\,H^4\, b_2^2\, c_1 - 4\,H^2\, b_2\, c_1^2$$
$$+\,16\,\cos(H)\, H^6\, b_1\, b_2^2 + 8\,\cos(H)\, H^6\, b_1^2\, b_2 \qquad (55)$$

$$T_2 = 180\,H + 1440\,\sin(H) + 6\,H^3 - 192\,\sin(H)\, H^2$$
$$-1920\,H\cos(H) - 256\,\cos(H)\, H^3 + 3\,H^2 \sin(4\,H)$$
$$-2\,H^3\,\cos(4\,H) - 60\,H\cos(4\,H)$$
$$-\,192\,H^2 \sin(3\,H) - 480\,\sin(3\,H) + 90\,\sin(4\,H) \qquad (56)$$

$$T_3 = 4\,H^3 \cos(2\,H) + 6\,H^2 \sin(2\,H) + 120\,H\cos(2\,H)$$
$$+\,180\,\sin(2\,H) - 1920\,\sin(H) \qquad (57)$$

$$T_4 = 180\,H + 480\,\sin(H) + 6\,H^3 - 320\,\sin(H)\, H^2$$
$$-1920\,H\cos(H) - 256\,\cos(H)\, H^3 - H^2 \sin(4\,H)$$
$$-2\,H^3 \cos(4\,H) - 60\,H\cos(4\,H)$$
$$-\,64\,H^2 \sin(3\,H) + 480\,\sin(3\,H) - 30\,\sin(4\,H) \qquad (58)$$

$$T_5 = 128\,H^3 \cos(2\,H) + 192\,H^2 \sin(2\,H)$$
$$+\,960\,H\cos(2\,H) - 480\,\sin(2\,H) \qquad (59)$$

$$T_6 = -2\,H^3 \cos(2\,H) + H^2 \sin(2\,H) - 128\,\sin(H)\, H^2$$
$$-\,60\,H\cos(2\,H) + 30\,\sin(2\,H) \qquad (60)$$

$$T_7 = 2\,H^3 \cos(2\,H) + 3\,H^2 \sin(2\,H)\;\; + 60\,H\cos(2\,H)$$
$$+\,90\,\sin(2\,H) - 960\,\sin(H) \qquad (61)$$

$$T_8 = 128\,H^3 \cos(2\,H) + 192\,H^2 \sin(2\,H)$$
$$+\,960\,H\,\cos(2\,H) - 480\,\sin(2\,H) \qquad (62)$$

Appendix B

$$T_9 = 64\,\sin(H)\, H^2\, b_1 + 192\,H^3\, b_2\, b_1^2 + 384\,H^3\, b_2^2\, b_1$$
$$-384\,b_1\,\sin(H) - 384\,b_0\, b_2^2\, c_1\, H^3 - 24\,b_0\, b_1^2\, H^3\, c_1$$
$$-96\,H\, b_0\, b_2\, c_1^2 - 24\,H\, b_0\, b_1\, c_1^2 + 1536\,H^3\, a\, b_2^3$$
$$+24\,H^3\, a\, b_1^3 - 1536\,H\, a\, b_2^2 - 96\,H\, a\, b_1^2 - 24\,H^5$$
$$b_1^3\,\cos(H) + 12\,\sin(H)\, H^6\, b_1^3 + \sin(H)\, H^8\, b_1^4 - 24\,\sin(H)\, c_1^3$$
$$b_2 + 192\,\sin(H)\, b_1\, c_1 - 384\,\sin(H)\, c_1\, b_2 - 384\,H\, b_1^2\,\cos(H)$$
$$+192\,\sin(H)\, H^2\, b_1^2 + 96\,H^3\, b_1^3\,\cos(H) + 72\,\sin(H)\, H^4\, b_1^3$$
$$+192\,\sin(H)\, c_1^2\, b_2 - 24\,\sin(H)\, b_1\, c_1^2 - 192\,b_0\, b_2\, H^3\, b_1\, c_1$$
$$+192\,H\, a\, b_1\, b_2\, c_1 + 576\,\sin(H)\, b_1 H^4\, b_2^2\, c_1$$
$$-48\,\sin(H)\, b_1\, H^2 b_2\, c_1^2 + 72\,\sin(H)\, b_1^2\, H^4\, b_2\, c_1 - 192\,H^5\, b_1$$
$$\cos(H)\, b_2^2\, c_1 + 48\,H^3\, b_1\,\cos(H)\, b_2\, c_1^2 - 24\,H^5\, b_1^2\,\cos(H)\, b_2\, c_1$$
$$-192\,\sin(H)\, H^4\, b_1\, c_1\, b_2 - 96\,\sin(H)\, H^6\, b_1\, b_2^2\, c_1$$
$$+36\,\sin(H)\, H^4\, b_1\, b_2\, c_1^2 - 36\,\sin(H)\, H^6\, b_1^2\, b_2\, c_1$$
$$+96\,H\,\cos(H)\, b_1\, b_2\, c_1^2 + 768\,\cos(H)\, b_1\, b_2^2\, c_1\, H^3$$
$$+96\,\cos(H)\, b_1^2\, b_2\, H^3\, c_1 - 12\,\sin(H)\, c_1^3 + \sin(H)$$
$$c_1^4 + 1152\,H^3\, a\, b_2^2\, b_1 + 288\,H^3\, a\, b_2\, b_1^2 + 384\,H\, a\, b_2^2\, c_1$$
$$+24\,H\, a\, b_1^2 c_1 - 768\,H\, a\, b_1\, b_2 - 384\,\cos(H)\, c_1\, b_2^3\, H^5$$
$$+192\,\cos(H)\, c_1^2\, b_2^2\, H^3 - 24\,H\,\cos(H)\, c_1^3\, b_2 - 24\,H\, b_1$$
$$\cos(H)\, c_1^2 - 192\,H^5\, b_1^2\,\cos(H)\, b_2 + 48\,H^3\, b_1^2\,\cos(H)\, c_1$$
$$-384\,H^5\, b_1\,\cos(H)\, b_2^2 + 36\,\sin(H)\, H^2\, b_1\, c_1^2$$
$$+96\,\sin(H)\, H^6\, b_1^2\, b_2 - 36\,\sin(H)\, H^4\, b_1^2\, c_1$$
$$+192\,\sin(H)\, H^6\, b_1\, b_2^2 + 64\,\sin(H)\, H^8\, b_1\, b_2^3$$
$$-4\,\sin(H)\, H^2\, b_1\, c_1^3 - 4\,\sin(H)\, H^6\, b_1^3\, c_1$$
$$+6\,\sin(H)\, H^4\, b_1^2\, c_1^2 + 48\,\sin(H)\, H^8\, b_1^2\, b_2^2$$
$$+12\,\sin(H)\, H^8\, b_1^3\, b_2 + 96\,\sin(H)\, c_1^2\, H^2\, b_2$$
$$-192\,\sin(H)\, c_1\, H^4\, b_2^2 - 64\,\sin(H)\, c_1\, H^6\, b_2^3$$
$$+48\,\sin(H)\, c_1^2\, H^4\, b_2^2 - 12\,\sin(H)\, c_1^3\, H^2\, b_2$$
$$-192\,H^2 \sin(H)\, c_1^2\, b_2^2 + 1152\,H^4 \sin(H)\, c_1\, b_2^3$$
$$+1536\,H^3 \cos(H)\, c_1\, b_2^3 + 384\,H\cos(H)\, c_1^2\, b_2^2$$

$$-1536\,H\cos(H)\;c_1\,b_2^2 - 1536\,H\,b_1\cos(H)\;b_2$$
$$+768\sin(H)\;H^2\,b_1\,b_2 + 1536\,H^3\,b_1\cos(H)\;b_2^2$$
$$+768\,H^3\,b_1^2\cos(H)\;b_2 + 96\,H\,b_1^2\cos(H)\;c_1$$
$$+1152\sin(H)\;H^4\,b_1\,b_2^2 + 576\sin(H)\;H^4\,b_1^2\,b_2$$
$$-48\sin(H)\;H^2\,b_1^2\,c_1 + 768\sin(H)\;c_1\,b_2^2\,H^2$$
$$-72\sin(H)\cos(H)\;b_2\,H^4\,b_1^2\,c_1$$
$$+48\sin(H)\cos(H)\;b_2\,H^2\,b_1\,c_1^2$$
$$-576\sin(H)\cos(H)\;b_2^2\,H^4\,b_1\,c_1$$
$$-768\sin(H)\cos(H)\;H^4\,b_2\,b_1\,c_1$$
$$-48\sin(H)\cos(H)\,H^6\,b_2\,b_1^2\,c_1$$
$$+48\sin(H)\cos(H)\;H^4\,b_2\,b_1\,c_1^2$$
$$-384\sin(H)\cos(H)\,H^6\,b_2^2\,b_1\,c_1$$
$$-384\,H^5\,b_2^3\,c_1 + 192\sin(H)\cos(H)\;c_1^2 - 16\sin(H)\cos(H)\;c_1^3$$
$$+384\sin(H)\cos(H)\;b_1 + 48\,H^3\,b_1^2\,c_1 + 384\,b_2^3\,c_1\,H^3$$
$$+96\,H\,b_2^2\,c_1^2 - 24\,H\,b_1\,c_1^2 - 384\,H^5\,b_2^2\,b_1 - 192\,H^5\,b_2\,b_1^2$$
$$-24\,H\,b_2\,c_1^3 - 1152\sin(H)\cos(H)\;b_2^3\,H^4\,c_1$$
$$+192\sin(H)\cos(H)\;b_2^2\,H^2\,c_1^2 + 384\sin(H)\cos(H)\;H^2\,b_2\,c_1^2$$
$$+2304\sin(H)\cos(H)\;H^6\,b_2^2\,b_1 - 2304\sin(H)\cos(H)\;H^4\,b_2^2\,c_1$$
$$+384\sin(H)\cos(H)\;H^6\,b_2\,b_1^2 + 16\sin(H)\cos(H)\;H^8\,b_2\,b_1^3$$
$$-16\sin(H)\cos(H)\;H^2\,b_2\,c_1^3 + 768\sin(H)\cos(H)\;H^8\,b_2^3\,b_1$$
$$-768\sin(H)\cos(H)\;H^6\,b_2^3\,c_1 + 192\sin(H)\cos(H)\;H^8\,b_2^2\,b_1^2$$
$$+192\sin(H)\cos(H)\;H^4\,b_2^2\,c_1^2 - 384\sin(H)\cos(H)\;H^2\,b_1\,c_1$$
$$-48\sin(H)\cos(H)\;H^4\,b_1^2\,c_1 + 48\sin(H)\cos(H)\;H^2\,b_1\,c_1^2$$
$$+48\,H^2\sin(H)\cos(H)\;b_1^2\,c_1 - 768\sin(H)\cos(H)\;H^2\,b_2\,b_1$$
$$-1152\sin(H)\cos(H)\;H^4\,b_2^2\,b_1 - 768\sin(H)\cos(H)\;H^2\,b_2^2\,c_1$$
$$-576\sin(H)\cos(H)\;H^4\,b_2\,b_1^2 - 192\sin(H)\cos(H)\;b_2\,c_1^2$$
$$+24\sin(H)\cos(H)\;b_2\,c_1^3 + 4096\sin(H)\cos(H)\;H^6\,b_2^3$$
$$+1024\sin(H)\cos(H)\;H^8\,b_2^4 + 192\sin(H)\cos(H)\;H^4\,b_1^2$$
$$+16\sin(H)\cos(H)\;H^6\,b_1^3 - 72\,H^4\sin(H)\cos(H)\;b_1^3$$
$$+24\sin(H)\cos(H)\;b_1\,c_1^2 + 384\sin(H)\cos(H)\;b_2\,c_1$$
$$-192\sin(H)\cos(H)\;b_1^2\,H^2 - 192\sin(H)\cos(H)\;b_1\,c_1$$

$$-24\,b_1^3\,H^5 + 24\,H^3\,b_1^3 - 24\,H^5\,b_2\,b_1^2\,c_1 + 48\,H^3\,b_1\,b_2\,c_1^2$$
$$-192\,H^5\,b_2^2\,b_1\,c_1 + 24\,H\,b_2\,b_1\,c_1^2 + 192\,H^3\,b_2^2\,b_1\,c_1$$
$$+24\,H^3\,b_2\,b_1^2\,c_1 + 192\,H^3\,b_2^2\,c_1^2 + 24\,H\,b_1^2\,c_1 + 48\,(\cos(H))^2$$
$$H^5\,b_2\,b_1^2\,c_1 - 96\,(\cos(H))^2\;H^3\,b_1\,b_2\,c_1^2 + 384\,(\cos(H))^2\;H^5$$
$$b_2^2\,b_1\,c_1 - 48\,(\cos(H))^2\;H\,b_2\,b_1\,c_1^2 - 384\,(\cos(H))^2\;H^3\,b_2^2$$
$$b_1\,c_1 - 48\,(\cos(H))^2\;H^3\,b_2\,b_1^2\,c_1 - 48\,(\cos(H))^2\;H^3\,b_1^3$$
$$+384\,(\cos(H))^2\;H^3\,b_1^2 + 192\,(\cos(H))^2\;H\,b_1^2 + 48\,(\cos(H))^2$$
$$b_1^3\,H^5 - 384\,(\cos(H))^2\;H^3\,b_2\,b_1^2 - 768\,(\cos(H))^2\;H^3\,b_2^2\,b_1$$
$$+768\,(\cos(H))^2\;H^5\,b_2^3\,c_1 - 96\,(\cos(H))^2\;H^3\,b_1^2\,c_1$$
$$-768\,(\cos(H))^2\;b_2^3\,c_1\,H^3 - 192\,(\cos(H))^2\;H\,b_2^2\,c_1^2$$
$$+48\,(\cos(H))^2\;H\,b_1\,c_1^2 + 768\,(\cos(H))^2\;H^5\,b_2^2\,b_1$$
$$+384\,(\cos(H))^2\;H^5\,b_2\,b_1^2 + 48\,(\cos(H))^2\;H\,b_2\,c_1^3$$
$$-384\,(\cos(H))^2\;H^3\,b_2^2\,c_1^2 - 48\,(\cos(H))^2\;H\,b_1^2\,c_1$$
$$+1536\,(\cos(H))^2\;H^3\,b_1\,b_2 - 384\,(\cos(H))^2\;H\,b_1\,c_1$$
$$-384\,(\cos(H))^2\;H\,c_1^2\,b_2 + 1536\,(\cos(H))^2\;c_1\,b_2^2\,H^3$$
$$+768\,(\cos(H))^2\;H\,b_2\,b_1 + 768\,(\cos(H))^2\;b_2^2\,c_1\,H$$
$$-64\sin(H)\;c_1 + 48\sin(H)\;c_1^2 - 768\sin(H)\cos(H)\;c_1$$
$$-384\,H\,b_2\,c_1 + 768\,(\cos(H))^2\;H\,b_1$$
$$+768\,(\cos(H))^2\;H\,b_2\,c_1$$
$$+192\sin(H)\,H^4\,b_1\,b_2 - 96\sin(H)\;H^2\,b_1\,c_1$$
$$-192\sin(H)\;c_1\,H^2\,b_2 - 384\,H\cos(H)\;c_1\,b_2$$
$$-384\,H\,b_1\cos(H) + 48\sin(H)\;H^4\,b_1^2 - 384\,H\,b_1$$
$$+2304\sin(H)\cos(H)\;H^4\,b_2\,b_1$$
$$-2304\sin(H)\cos(H)\;H^2\,b_2\,c_1$$
$$+1024\sin(H)\cos(H) + 4096\sin(H)\cos(H)\;H^2\,b_2$$
$$+6144\sin(H)\cos(H)\;H^4\,b_2^2 + 768\sin(H)\cos(H)\;H^2\,b_1$$
$$-1536\,H\,b_0\,b_2 - 384\,H\,b_0\,b_1 + 1536\,H^3\,b_0\,b_2^2$$
$$+96\,H^3\,b_0\,b_1^2 + 768\,H^3\,b_0\,b_2\,b_1 + 768\,H\,b_0\,b_2\,c_1$$
$$+192\,H\,b_0\,b_1\,c_1 - 192\,H^3\,b_1^2 - 768\,H^3\,b_1\,b_2$$
$$+192\,H\,b_1\,c_1 + 192\,H\,c_1^2\,b_2 - 768\,c_1\,b_2^2\,H^3$$
$$-768\,H^3\,b_1\cos(H)\;b_2 + 192\,H\,b_2\cos(H)\;c_1^2$$

$$+192\,H\,b_1\cos(H)\,c_1-768\,H^3\,b_2^2\cos(H)\,c_1$$

$$-384\,H\,b_2\,b_1-384\,b_2^2\,c_1\,H-96\,H\,b_1^2-192\,H^3\,b_1^2\cos(H) \quad (63)$$

$$T_{10}=9H\sin(5H)+36H\sin(H)-27H\sin(3H)$$

$$+44\cos(H)H^2+30H^2\cos(3H)-12\cos(H)$$

$$+9\cos(3H)\;-2H^2\cos(5H)+3\cos(5H) \quad (64)$$

$$T_{11}=-14\cos(H)H^2+2H^2\cos(3H)+9H\sin(3H)$$

$$-27H\sin(H)+3\cos(H)-3\cos(3H) \quad (65)$$

$$T_{12}=44\cos(H)H^2+30H^2\cos(3H)-2H^2\cos(5H)$$

$$-12\cos(H)+9\cos(3H)+3\cos(5H)+9H\sin(3H)$$

$$-12H\sin(H)-3H\sin(5H) \quad (66)$$

$$T_{13}=-40H^2-8H^2\cos(4H)+6-6\cos(4H) \quad (67)$$

$$T_{14}=14\cos(H)H^2-2H^2\cos(3H)+3H\sin(3H)$$

$$-9H\sin(H)-3\cos(H)+3\cos(3H) \quad (68)$$

Appendix C

Classical method

$$LTE_{CL}=h^8\Bigg[-\frac{2}{945}w(x)\,G^4-\frac{8}{945}g(x)\,w(x)\,G^3$$

$$+\Bigg(-\frac{44}{945}\left(\frac{d^2}{dx^2}g(x)\right)w(x)-\frac{8}{315}\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}w(x)$$

$$-\frac{4}{315}(g(x))^2\,w(x)\Bigg)G^2+\Bigg(-\frac{32}{945}\left(\frac{d^4}{dx^4}g(x)\right)w(x)$$

$$-\frac{16}{315}\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}w(x)-\frac{16}{315}g(x)\left(\frac{d}{dx}w(x)\right)$$

$$\frac{d}{dx}g(x)-\frac{88}{945}g(x)\,w(x)\,\frac{d^2}{dx^2}g(x)-\frac{8}{135}\left(\frac{d}{dx}g(x)\right)^2w(x)$$

$$-\frac{8}{945}(g(x))^3\,w(x)\Bigg)G-\frac{2}{945}\left(\frac{d^6}{dx^6}g(x)\right)w(x)$$

$$-\frac{4}{315}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}w(x)-\frac{32}{945}g(x)\,w(x)\,\frac{d^4}{dx^4}g(x)$$

$$-\frac{2}{63}\left(\frac{d^2}{dx^2}g(x)\right)^2w(x)\;-\frac{52}{945}\left(\frac{d}{dx}g(x)\right)w(x)\,\frac{d^3}{dx^3}g(x)$$

$$-\frac{16}{315}g(x)\left(\frac{d}{dx}w(x)\right)\frac{d^3}{dx^3}g(x)$$

$$-\frac{8}{315}(g(x))^2\left(\frac{d}{dx}w(x)\right)\frac{d}{dx}$$

$$g(x)-\frac{32}{315}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}w(x)\right)\frac{d^2}{dx^2}g(x)$$

$$-\frac{44}{945}(g(x))^2\,w(x)\,\frac{d^2}{dx^2}g(x)-\frac{8}{135}g(x)\,w(x)$$

$$\left(\frac{d}{dx}g(x)\right)^2\;-\frac{2}{945}(g(x))^4\,w(x)\Bigg]+O\left(h^{10}\right) \quad (69)$$

Method developed by Wang [see 15]

$$LTE_{Wang[15]}=h^8\Bigg[-\frac{8}{945}g(x)\,w(x)\,G^3$$

$$+\Bigg(-\frac{44}{945}\left(\frac{d^2}{dx^2}g(x)\right)w(x)$$

$$-\frac{8}{315}\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}w(x)\;-\frac{4}{315}(g(x))^2\,w(x)\Bigg)G^2$$

$$+\Bigg(-\frac{32}{945}\left(\frac{d^4}{dx^4}g(x)\right)w(x)-\frac{16}{315}\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}w(x)$$

$$-\frac{16}{315}g(x)\left(\frac{d}{dx}w(x)\right)\frac{d}{dx}g(x)-\frac{88}{945}g(x)\,w(x)\,\frac{d^2}{dx^2}g(x)$$

$$-\frac{8}{135}\left(\frac{d}{dx}g(x)\right)^2w(x)-\frac{8}{945}(g(x))^3\,w(x)\Bigg)G$$

$$-\frac{2}{945}\left(\frac{d^6}{dx^6}g(x)\right)w(x)-\frac{4}{315}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}w(x)$$

$$-\frac{32}{945}g(x)\,w(x)\,\frac{d^4}{dx^4}g(x)-\frac{2}{63}\left(\frac{d^2}{dx^2}g(x)\right)^2w(x)$$

$$-\frac{52}{945}\left(\frac{d}{dx}g(x)\right)w(x)\,\frac{d^3}{dx^3}g(x)-\frac{16}{315}g(x)$$

$$\times\left(\frac{d}{dx}w(x)\right)\frac{d^3}{dx^3}g(x)$$

$$-\frac{8}{315}(g(x))^2\left(\frac{d}{dx}w(x)\right)\frac{d}{dx}g(x)-\frac{32}{315}\left(\frac{d}{dx}g(x)\right)$$

$$\left(\frac{d}{dx}w(x)\right)\frac{d^2}{dx^2}g(x)\;-\frac{44}{945}(g(x))^2\,w(x)\,\frac{d^2}{dx^2}g(x)$$

$$-\frac{8}{135}g(x)\,w(x)\left(\frac{d}{dx}g(x)\right)^2-\frac{2}{945}$$

$$(g(x))^4\,w(x)\Bigg]+O\left(h^{10}\right)+O\left(h^{10}\right) \quad (70)$$

New method with vanished phase-lag and its first and second derivatives (developed in section 3.1)

$$LTE_{NMI} = h^8\Bigg[-\frac{32}{945}\left(\frac{d^2}{dx^2}g(x)\right)w(x)\,G^2$$
$$\left(-\frac{32}{945}\left(\frac{d^4}{dx^4}g(x)\right)w(x)-\frac{16}{315}\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}w(x)\right.$$
$$-\frac{16}{315}g(x)\left(\frac{d}{dx}w(x)\right)\frac{d}{dx}g(x)-\frac{88}{945}g(x)w(x)\frac{d^2}{dx^2}g(x)$$
$$\left.-\frac{8}{135}\left(\frac{d}{dx}g(x)\right)^2w(x)-\frac{8}{945}(g(x))^3w(x)\right)G$$
$$-\frac{2}{945}\left(\frac{d^6}{dx^6}g(x)\right)w(x)-\frac{4}{315}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}w(x)$$
$$-\frac{32}{945}g(x)w(x)\frac{d^4}{dx^4}g(x)-\frac{2}{63}\left(\frac{d^2}{dx^2}g(x)\right)^2w(x)$$
$$-\frac{52}{945}\left(\frac{d}{dx}g(x)\right)w(x)\frac{d^3}{dx^3}g(x)-\frac{16}{315}g(x)\left(\frac{d}{dx}w(x)\right)$$
$$\frac{d^3}{dx^3}g(x)-\frac{8}{315}(g(x))^2\left(\frac{d}{dx}w(x)\right)\frac{d}{dx}g(x)$$
$$-\frac{32}{315}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}w(x)\right)\frac{d^2}{dx^2}g(x)-\frac{44}{945}(g(x))^2$$
$$w(x)\frac{d^2}{dx^2}g(x)-\frac{8}{135}g(x)w(x)\left(\frac{d}{dx}g(x)\right)^2$$
$$-\frac{2}{945}(g(x))^4w(x)\Bigg]+O\left(h^{10}\right) \tag{71}$$

New method with vanished phase-lag and its first, second and third derivatives (developed in section 3.2)

$$LTE_{NMII} = h^8\Bigg[\Bigg(-\frac{8}{315}\left(\frac{d^4}{dx^4}g(x)\right)w(x)$$
$$-\frac{16}{945}\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}w(x)-\frac{32}{945}g(x)w(x)\frac{d^2}{dx^2}g(x)$$
$$-\frac{8}{315}\left(\frac{d}{dx}g(x)\right)^2w(x)\Bigg)G-\frac{2}{945}\left(\frac{d^6}{dx^6}g(x)\right)w(x)$$
$$-\frac{4}{315}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}w(x)-\frac{32}{945}g(x)w(x)\frac{d^4}{dx^4}g(x)$$
$$-\frac{2}{63}\left(\frac{d^2}{dx^2}g(x)\right)^2w(x)-\frac{52}{945}\left(\frac{d}{dx}g(x)\right)w(x)\frac{d^3}{dx^3}g(x)$$
$$-\frac{16}{315}g(x)\left(\frac{d}{dx}w(x)\right)\frac{d^3}{dx^3}g(x)$$
$$-\frac{8}{315}(g(x))^2\left(\frac{d}{dx}w(x)\right)\frac{d}{dx}g(x)$$
$$-\frac{32}{315}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}w(x)\right)\frac{d^2}{dx^2}g(x)$$
$$-\frac{44}{945}(g(x))^2w(x)\frac{d^2}{dx^2}g(x)$$
$$-\frac{8}{135}g(x)w(x)\left(\frac{d}{dx}g(x)\right)^2-\frac{2}{945}(g(x))^4w(x)\Bigg]+O\left(h^{10}\right) \tag{72}$$