

On Eight-Step Methods with Vanished Phase-Lag and Its Derivatives for the Numerical Solution of the Schrödinger Equation

Ibraheem Alolyan^a, Theodore E. Simos^{1b}

^a*Department of Mathematics, College of Sciences,
King Saud University, P. O. Box 2455, Riyadh 11451,
Saudi Arabia*

^b*Department of Mathematics, College of Sciences,
King Saud University, P. O. Box 2455, Riyadh 11451,
Saudi Arabia and Laboratory of Computational Sciences,
Department of Computer Science and Technology,
Faculty of Sciences and Technology, University of Peloponnese,
GR-221 00 Tripolis, Greece*

E-mail addresses: `tsimos.conf@gmail.com`, `tsimos@mail.ariadne-t.gr`

(Received December 23, 2010)

Abstract

In this review paper:

- We develop new tenth algebraic order eight-step methods with vanished phase-lag and its first, second, third, fourth and fifth derivatives.
- We study all alternative methods which satisfy the above requirements.
- We compare the eight-step method with well known multistep methods in the literature.

The study of the methods is based on error analysis, stability analysis and comparison with other methods. The investigated methods are applied for the numerical integration of the radial Schrödinger equation .

¹Highly Cited Researcher, Active Member of the European Academy of Sciences and Arts
Active Member of the European Academy of Sciences Corresponding Member of European Academy of Arts, Sciences and Humanities

1. INTRODUCTION

The radial Schrödinger equation can be written as:

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

It is known from the literature that via the above boundary value problem, many mathematical models in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc. can be expressed (see for example [1] - [4]).

For the above equation (1) we have the following definitions:

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

The boundary conditions are:

$$y(0) = 0 \quad (2)$$

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

In the last decades, a large research on the development of numerical methods for the approximate solution of the Schrödinger equation has been done. The construction of fast and reliable numerical methods for the efficient solution of the Schrödinger equation and related problems is the main aim and scope of this research (see for example [5] - [85]).

More specifically the last decade:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge-Kutta and Runge-Kutta Nyström type have been developed in [10]- [27].
- In [28] - [33] exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are obtained.
- Multistep phase-fitted methods and multistep methods with minimal phase-lag are developed in [38] - [60].

- Symplectic integrators are studied in [61] - [80].
- Exponentially and trigonometrically multistep methods have been developed in [81] - [108].
- Nonlinear methods have been studied in [109] and [110]
- Review papers have been written in [111] - [115]
- Special issues and Symposia in International Conferences have been created on this subject (see [116] - [122])

The numerical methods for the approximate solution of the Schrödinger equation belong into two main categories:

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

The purpose of this paper is to produce tenth algebraic order eight-step methods with vanished phase-lag and its first, second, third, fourth and fifth derivatives, to study all the alternative methods which satisfy the above requirements and finally to compare the eight-step method with well known multistep methods in the literature. We will apply the new obtained methods together with other well known methods in the literature to the numerical solution of the resonance problem of the radial Schrödinger equation. From theoretical analysis and numerical applications, we will extract very useful conclusions.

More precisely, in this paper we will study a family of implicit symmetric eight-step methods of tenth algebraic order. The logic for the development of the new family is based on the requirement of vanishing the phase-lag and its first, second, third, fourth and fifth derivatives. Based on the above logic, three methods of the above family will be developed. The difference between these methods is the selection of free parameters of the family of methods. So, in one of the them we select as free parameters the coefficients of the right hand side of the family of methods. In the other two, we select as free parameters the coefficients of the left hand side of the family of methods. For all of these methods, we will present stability and error analysis. Finally, we will apply the new proposed

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

methods to the eigenvalue and resonance problem of the radial Schrödinger equation. We note that resonance problem is one of the most difficult problems arising from the radial Schrödinger equation.

The paper is organized as follows:

- In Section 2, we present the theory of the new methodology.
- In Section 3, we present the development of the new family of methods.
- A comparative error analysis and its conclusions are presented in Section 4.
- In Section 5, we will investigate the stability properties of the new developed methods. In the same section a comparative analysis of the main properties of some well known methods is also presented.
- In Section 6, numerical results are presented.
- Remarks and conclusions are discussed in Section 7.
- General comments are presented in Section 8.
- Finally in the Appendices we present the coefficients of all the methods obtained in this paper and also the analytic expansions for the errors for several methods.

2. PHASE-LAG ANALYSIS OF SYMMETRIC MULTISTEP METHODS

For the numerical solution of the initial value problem

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

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

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

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

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

a difference equation of the form

$$\begin{aligned} A_k(v) p_{n+k} + \dots + A_1(v) p_{n+1} + A_0(v) p_n + \\ + A_1(v) p_{n-1} + \dots + A_k(v) p_{n-k} = 0 \end{aligned} \quad (5)$$

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

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

$$A_k(v) \lambda^k + \dots + A_1(v) \lambda + A_0(v) + A_1(v) \lambda^{-1} + \dots + A_k(v) \lambda^{-k} = 0 \quad (6)$$

Theorem 1. [37] *The symmetric $2k$ -step method with characteristic equation given by (6) has phase-lag order r and phase-lag constant c given by*

$$-c v^{r+2} + O(v^{r+4}) = \frac{2 A_k(v) \cos(kv) + \dots + 2 A_j(v) \cos(jv) + \dots + A_0(v)}{2 k^2 A_k(v) + \dots + 2 j^2 A_j(v) + \dots + 2 A_1(v)} \quad (7)$$

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

Remark 1. *The First, Second, Third, Fourth and Fifth Derivatives of the phase-lag for the multistep methods are computed based on the above direct formula (7).*

3. THE NEW FAMILY OF EIGHT-STEP TENTH ALGEBRAIC ORDER METHODS

3.1 The Method of the Family with Vanished Phase-lag and its First Four Derivatives

Let us consider the following family of eight-step methods to integrate $p'' = f(x, p)$:

$$\sum_{i=1}^4 a_i (p_{n+i} + p_{n-i}) + a_0 p_n = h^2 \left[\sum_{i=1}^4 b_i (p''_{n+i} + p''_{n-i}) + b_0 p''_n \right] \quad (8)$$

Let us also consider the following conditions :

$$a_0 = 0, a_1 = -1, a_2 = 2, a_3 = -2, a_4 = 1. \quad (9)$$

For the above method to require:

- the maximum algebraic order and
- five free parameters, in order the phase-lag and its first, second, third and fourth derivatives to be vanished.

Now we apply the above method to the scalar test equation (4) and we get the following difference equation:

$$\sum_{i=1}^4 A_i(v) (p_{n+i} + p_{n-i}) + A_0 p_n = 0 \quad (10)$$

where $v = \omega h$, h is the step length and $A_i(v)$, $i = 0(1)4$ are polynomials of v .

The characteristic equation associated with (10) can be written as:

$$\sum_{i=1}^4 A_i(v) (\lambda^i + \lambda^{-i}) + A_0 = 0 \quad (11)$$

where

$$\begin{aligned} A_0 &= v^2 b_0 \\ A_1 &= -1 + v^2 b_1 \\ A_2 &= 2 + v^2 b_2 \\ A_3 &= -2 + v^2 b_3 \\ A_4 &= 1 + v^2 b_4 \end{aligned} \quad (12)$$

We apply now the direct formula for the computation of the phase-lag (7) for $k = 4$ and for A_j , $j = 0, 1, \dots, 4$ given by (12). This leads to the following equation:

$$\begin{aligned} phl &= \left[2(1 + v^2 b_4) \cos(4v) + 2(-2 + v^2 b_3) \cos(3v) + 2(2 + v^2 b_2) \cos(2v) \right. \\ &\quad \left. + 2(-1 + v^2 b_1) \cos(v) + v^2 b_0 \right] / \left(10 + 32v^2 b_4 + 18v^2 b_3 + 8v^2 b_2 + 2v^2 b_1 \right) \end{aligned} \quad (13)$$

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

$$\begin{aligned}
 p\ddot{h}l = & \left[4v b_4 \cos(4v) - 8(1 + v^2 b_4) \sin(4v) + 4v b_3 \cos(3v) \right. \\
 & - 6(-2 + v^2 b_3) \sin(3v) + 4v b_2 \cos(2v) - 4(2 + v^2 b_2) \sin(2v) \\
 & \left. + 4v b_1 \cos(v) - 2(-1 + v^2 b_1) \sin(v) + 2v b_0 \right] / \\
 & \left(10 + 32v^2 b_4 + 18v^2 b_3 + 8v^2 b_2 + 2v^2 b_1 \right) - \left[2(1 + v^2 b_4) \cos(4v) \right. \\
 & + 2(-2 + v^2 b_3) \cos(3v) + 2(2 + v^2 b_2) \cos(2v) + 2(-1 + v^2 b_1) \cos(v) \\
 & \left. + v^2 b_0 \right] \left(64v b_4 + 36v b_3 + 16v b_2 + 4v b_1 \right) / \quad (14)
 \end{aligned}$$

$$\left(10 + 32v^2 b_4 + 18v^2 b_3 + 8v^2 b_2 + 2v^2 b_1 \right)^2 \quad (15)$$

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

$$\begin{aligned}
 p\ddot{h}l = & \left[4b_4 \cos(4v) - 32v b_4 \sin(4v) - 32(1 + v^2 b_4) \cos(4v) + 4b_3 \cos(3v) \right. \\
 & - 24v b_3 \sin(3v) - 18(-2 + v^2 b_3) \cos(3v) + 4b_2 \cos(2v) - 16v b_2 \sin(2v) \\
 & - 8(2 + v^2 b_2) \cos(2v) + 4b_1 \cos(v) - 8v b_1 \sin(v) - 2(-1 + v^2 b_1) \cos(v) \\
 & \left. + 2b_0 \right] / S_0 - 2 \left[4v b_4 \cos(4v) - 8(1 + v^2 b_4) \sin(4v) + 4v b_3 \cos(3v) \right. \\
 & - 6(-2 + v^2 b_3) \sin(3v) + 4v b_2 \cos(2v) - 4(2 + v^2 b_2) \sin(2v) \\
 & \left. + 4v b_1 \cos(v) - 2(-1 + v^2 b_1) \sin(v) + 2v b_0 \right] \\
 & \left(64v b_4 + 36v b_3 + 16v b_2 + 4v b_1 \right) / S_0^2 + 2 \left[2(1 + v^2 b_4) \cos(4v) \right. \\
 & + 2(-2 + v^2 b_3) \cos(3v) + 2(2 + v^2 b_2) \cos(2v) + 2(-1 + v^2 b_1) \cos(v) \\
 & \left. + v^2 b_0 \right] \left(64v b_4 + 36v b_3 + 16v b_2 + 4v b_1 \right)^2 / S_0^3 - \left[2(1 + v^2 b_4) \cos(4v) \right. \\
 & + 2(-2 + v^2 b_3) \cos(3v) + 2(2 + v^2 b_2) \cos(2v) + 2(-1 + v^2 b_1) \cos(v) \\
 & \left. + v^2 b_0 \right] \left(64b_4 + 36b_3 + 16b_2 + 4b_1 \right) / S_0^2 \\
 & S_0 = 10 + 32v^2 b_4 + 18v^2 b_3 + 8v^2 b_2 + 2v^2 b_1 \quad (16)
 \end{aligned}$$

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

$$\begin{aligned}
 p\hat{h}l = & \left[-48 b_4 \sin(4v) - 192 v b_4 \cos(4v) + 128 (1 + v^2 b_4) \sin(4v) - 36 b_3 \sin(3v) \right. \\
 & - 108 v b_3 \cos(3v) + 54 \left(-2 + v^2 b_3 \right) \sin(3v) - 24 b_2 \sin(2v) \\
 & - 48 v b_2 \cos(2v) + 16 \left(2 + v^2 b_2 \right) \sin(2v) - 12 v b_1 \cos(v) - 12 v b_1 \cos(v) \\
 & \left. + 2 \left(-1 + v^2 b_1 \right) \sin(v) \right] / S_2 - 3 \left[4 b_4 \cos(4v) - 32 v b_4 \sin(4v) \right. \\
 & - 32 \left(1 + v^2 b_4 \right) \cos(4v) + 4 b_3 \cos(3v) - 24 v b_3 \sin(3v) \\
 & - 18 \left(-2 + v^2 b_3 \right) \cos(3v) + 4 b_2 \cos(2v) - 16 v b_2 \sin(2v) \\
 & - 8 \left(2 + v^2 b_2 \right) \cos(2v) + 4 b_1 \cos(v) - 8 v b_1 \sin(v) - 2 \left(-1 + v^2 b_1 \right) \cos(v) \\
 & \left. + 2 b_0 \right] S_1 / S_2^2 + 6 \left[4 v b_4 \cos(4v) - 8 \left(1 + v^2 b_4 \right) \sin(4v) + 4 v b_3 \cos(3v) \right. \\
 & - 6 \left(-2 + v^2 b_3 \right) \sin(3v) + 4 v b_2 \cos(2v) - 4 \left(2 + v^2 b_2 \right) \sin(2v) \\
 & + 4 v b_1 \cos(v) - 2 \left(-1 + v^2 b_1 \right) \sin(v) + 2 v b_0 \left] S_1^2 / S_2^3 - 3 \left[4 v b_4 \cos(4v) \right. \\
 & - 8 \left(1 + v^2 b_4 \right) \sin(4v) + 4 v b_3 \cos(3v) - 6 \left(-2 + v^2 b_3 \right) \sin(3v) \\
 & + 4 v b_2 \cos(2v) - 4 \left(2 + v^2 b_2 \right) \sin(2v) + 4 v b_1 \cos(v) \\
 & \left. - 2 \left(-1 + v^2 b_1 \right) \sin(v) + 2 v b_0 \right] \left(64 b_4 + 36 b_3 + 16 b_2 + 4 b_1 \right) / S_2^2 \\
 & - 6 \left[2 \left(1 + v^2 b_4 \right) \cos(4v) + 2 \left(-2 + v^2 b_3 \right) \cos(3v) + 2 \left(2 + v^2 b_2 \right) \cos(2v) \right. \\
 & \left. + 2 \left(-1 + v^2 b_1 \right) \cos(v) + v^2 b_0 \right] S_1^3 / S_2^4 + 6 \left[2 \left(1 + v^2 b_4 \right) \cos(4v) \right. \\
 & + 2 \left(-2 + v^2 b_3 \right) \cos(3v) + 2 \left(2 + v^2 b_2 \right) \cos(2v) + 2 \left(-1 + v^2 b_1 \right) \cos(v) \\
 & \left. + v^2 b_0 \right] S_1 \left(64 b_4 + 36 b_3 + 16 b_2 + 4 b_1 \right) / S_2^3 \\
 & S_1 = 64 v b_4 + 36 v b_3 + 16 v b_2 + 4 v b_1 \\
 & S_2 = 10 + 32 v^2 b_4 + 18 v^2 b_3 + 8 v^2 b_2 + 2 v^2 b_1 \quad (17)
 \end{aligned}$$

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

$$\begin{aligned}
 p\hat{h}l = & \left[-384 b_4 \cos(4v) + 1024 v b_4 \sin(4v) + 512 (1 + v^2 b_4) \cos(4v) \right. \\
 & -216 b_3 \cos(3v) + 432 v b_3 \sin(3v) + 162 \left(-2 + v^2 b_3 \right) \cos(3v) \\
 & -96 b_2 \cos(2v) + 128 v b_2 \sin(2v) + 32 \left(2 + v^2 b_2 \right) \cos(2v) - 24 b_1 \cos(v) \\
 & \left. + 16 v b_1 \sin(v) + 2 \left(-1 + v^2 b_1 \right) \cos(v) \right] / S_4 - 4 \left[-48 b_4 \sin(4v) \right. \\
 & -192 v b_4 \cos(4v) + 128 \left(1 + v^2 b_4 \right) \sin(4v) - 36 b_3 \sin(3v) \\
 & -108 v b_3 \cos(3v) + 54 \left(-2 + v^2 b_3 \right) \sin(3v) - 24 b_2 \sin(2v) \\
 & -48 v b_2 \cos(2v) + 16 \left(2 + v^2 b_2 \right) \sin(2v) - 12 b_1 \sin(v) - 12 v b_1 \cos(v) \\
 & \left. + 2 \left(-1 + v^2 b_1 \right) \sin(v) \right] S_6 / S_4^2 + 12 \left[4 b_4 \cos(4v) - 32 v b_4 \sin(4v) \right. \\
 & -32 \left(1 + v^2 b_4 \right) \cos(4v) + 4 b_3 \cos(3v) - 24 v b_3 \sin(3v) \\
 & -18 \left(-2 + v^2 b_3 \right) \cos(3v) + 4 b_2 \cos(2v) - 16 v b_2 \sin(2v) \\
 & -8 \left(2 + v^2 b_2 \right) \cos(2v) + 4 b_1 \cos(v) - 8 v b_1 \sin(v) - 2 \left(-1 + v^2 b_1 \right) \cos(v) \\
 & \left. + 2 b_0 \right] S_6^2 / S_4^3 - 6 \left[4 b_4 \cos(4v) - 32 v b_4 \sin(4v) - 32 \left(1 + v^2 b_4 \right) \cos(4v) \right. \\
 & + 4 b_3 \cos(3v) - 24 v b_3 \sin(3v) - 18 \left(-2 + v^2 b_3 \right) \cos(3v) + 4 b_2 \cos(2v) \\
 & -16 v b_2 \sin(2v) - 8 \left(2 + v^2 b_2 \right) \cos(2v) + 4 b_1 \cos(v) - 8 v b_1 \sin(v) \\
 & \left. - 2 \left(-1 + v^2 b_1 \right) \cos(v) + 2 b_0 \right] S_3 / S_4^2 - 24 \left[4 v b_4 \cos(4v) \right. \\
 & -8 \left(1 + v^2 b_4 \right) \sin(4v) + 4 v b_3 \cos(3v) - 6 \left(-2 + v^2 b_3 \right) \sin(3v) \\
 & + 4 v b_2 \cos(2v) - 4 \left(2 + v^2 b_2 \right) \sin(2v) + 4 v b_1 \cos(v) \\
 & -2 \left(-1 + v^2 b_1 \right) \sin(v) + 2 v b_0 \left. \right] S_6^3 / S_4^4 + 24 \left[4 v b_4 \cos(4v) \right. \\
 & -8 \left(1 + v^2 b_4 \right) \sin(4v) + 4 v b_3 \cos(3v) - 6 \left(-2 + v^2 b_3 \right) \sin(3v) \\
 & + 4 v b_2 \cos(2v) - 4 \left(2 + v^2 b_2 \right) \sin(2v) + 4 v b_1 \cos(v) \\
 & \left. - 2 \left(-1 + v^2 b_1 \right) \sin(v) + 2 v b_0 \right] S_6 S_3 / S_4^3 + \frac{24 S_5 S_6^4}{S_4^5} - \frac{36 S_5 S_6^2 S_3}{S_4^4} \\
 & \qquad \qquad \qquad + \frac{6 S_5 S_3^2}{S_4^3}
 \end{aligned} \tag{18}$$

$$\begin{aligned}
 S_3 &= 64 b_4 + 36 b_3 + 16 b_2 + 4 b_1 \\
 S_4 &= 10 + 32 v^2 b_4 + 18 v^2 b_3 + 8 v^2 b_2 + 2 v^2 b_1 \\
 S_5 &= 2 (1 + v^2 b_4) \cos(4 v) + 2 (-2 + v^2 b_3) \cos(3 v) + 2 (2 + v^2 b_2) \cos(2 v) \\
 &\quad + 2 (-1 + v^2 b_1) \cos(v) + v^2 b_0 \\
 S_6 &= 64 v b_4 + 36 v b_3 + 16 v b_2 + 4 v b_1
 \end{aligned}$$

We demand that the phase-lag and its first, second, third and fourth derivatives to be equal to zero, i.e. we demand the satisfaction of the relations (13), (15), (16), (17) and (18). Based on the above we obtain the coefficients mentioned in Appendix A.

The behavior of the coefficients is given in Figure 1.

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

$$\text{LTE} = -\frac{58061 h^{12}}{31933440} \left(y_n^{(12)} + 5 \omega^2 y_n^{(10)} + 10 \omega^4 y_n^{(8)} + 10 \omega^6 y_n^{(6)} + 5 \omega^8 y_n^{(4)} + \omega^{10} y_n^{(2)} \right) \quad (19)$$

Remark 2. *The method (8) with coefficients:*

$$\begin{aligned}
 a_0 &= 0, a_1 = -1, a_2 = 2 a_3 = -2, a_4 = 1 \\
 b_0 &= \frac{17273}{72576}, b_1 = \frac{280997}{181440}, b_2 = -\frac{33961}{181440}, b_3 = \frac{173531}{181440}, b_4 = \frac{45767}{725760}
 \end{aligned} \quad (20)$$

is called **classical method** and has local truncation error which is given by:

$$\text{LTE} = -\frac{58061 h^{12}}{31933440} y_n^{(12)} \quad (21)$$

3.2 The Method of the Family with Vanished Phase-lag and its First Five Derivatives

Let us consider the following family of eight-step methods (8) to integrate $p'' = f(x, p)$.

Let us also consider the following conditions :

$$a_0 = 0, a_1 = -1, a_3 = -2, a_4 = 1. \quad (22)$$

For the above method to require:

- the maximum algebraic order and

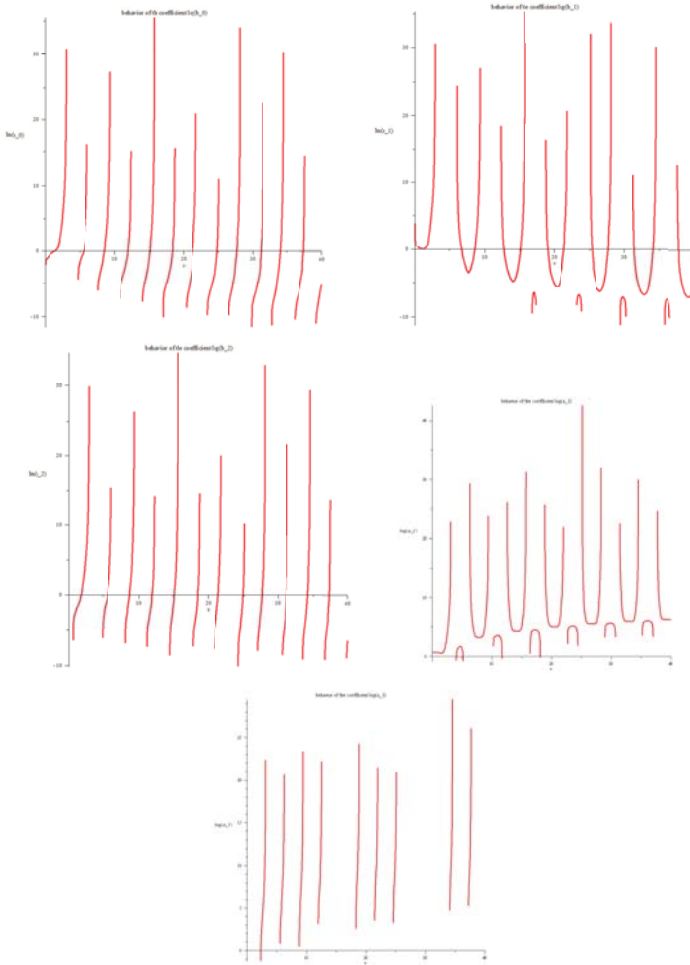


Figure 1: Behavior of the coefficients of the new proposed method given by (62)-(66) for several values of ν .

- six free parameters, in order the phase-lag and its first, second, third, fourth and fifth derivatives to be vanished.

Now we apply the above method to the scalar test equation (4) and we get the difference equation (10).

The characteristic equation associated with (10) can be written as:

$$\sum_{i=1}^4 A_i(v) \left(\lambda^i + \lambda^{-i} \right) + A_0 = 0 \quad (23)$$

where

$$\begin{aligned} A_0 &= v^2 b_0 \\ A_1 &= -1 + v^2 b_1 \\ A_2 &= a_2 + v^2 b_2 \\ A_3 &= -2 + v^2 b_3 \\ A_4 &= 1 + v^2 b_4 \end{aligned} \quad (24)$$

We apply now the direct formula for the computation of the phase-lag (7) for $k = 4$ and for A_j , $j = 0, 1, \dots, 4$ given by (24). This leads to the following equation:

$$\begin{aligned} phl &= \left[2 \left(1 + v^2 b_4 \right) \cos(4v) + 2 \left(-2 + v^2 b_3 \right) \cos(3v) \right. \\ &\quad \left. + 2 \left(a_2 + v^2 b_2 \right) \cos(2v) + 2 \left(-1 + v^2 b_1 \right) \cos(v) + v^2 b_0 \right] / \\ &\quad \left(-6 + 32 v^2 b_4 + 18 v^2 b_3 + 8 a_2 + 8 v^2 b_2 + 2 v^2 b_1 \right) \end{aligned} \quad (25)$$

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

$$\begin{aligned} p\dot{h}l &= \left[4v b_4 \cos(4v) - 8 \left(1 + v^2 b_4 \right) \sin(4v) + 4v b_3 \cos(3v) \right. \\ &\quad \left. - 6 \left(-2 + v^2 b_3 \right) \sin(3v) + 4v b_2 \cos(2v) - 4 \left(a_2 + v^2 b_2 \right) \sin(2v) \right. \\ &\quad \left. + 4v b_1 \cos(v) - 2 \left(-1 + v^2 b_1 \right) \sin(v) + 2v b_0 \right] / \\ &\quad \left(-6 + 32 v^2 b_4 + 18 v^2 b_3 + 8 a_2 + 8 v^2 b_2 + 2 v^2 b_1 \right) - \left[2 \left(1 + v^2 b_4 \right) \cos(4v) \right. \\ &\quad \left. + 2 \left(-2 + v^2 b_3 \right) \cos(3v) + 2 \left(a_2 + v^2 b_2 \right) \cos(2v) + 2 \left(-1 + v^2 b_1 \right) \cos(v) \right. \\ &\quad \left. + v^2 b_0 \right] \left(64v b_4 + 36v b_3 + 16v b_2 + 4v b_1 \right) / \\ &\quad \left(-6 + 32 v^2 b_4 + 18 v^2 b_3 + 8 a_2 + 8 v^2 b_2 + 2 v^2 b_1 \right)^2 \end{aligned} \quad (26)$$

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

$$\begin{aligned}
 p\ddot{h}l = & \left[4b_4 \cos(4v) - 32v b_4 \sin(4v) - 32(1 + v^2 b_4) \cos(4v) + 4b_3 \cos(3v) \right. \\
 & - 24v b_3 \sin(3v) - 18(-2 + v^2 b_3) \cos(3v) + 4b_2 \cos(2v) - 16v b_2 \sin(2v) \\
 & \left. - 8T_1 \cos(2v) + 4b_1 \cos(v) - 8v b_1 \sin(v) - 2(-1 + v^2 b_1) \cos(v) + 2b_0 \right] / \\
 & T_0 - 2 \left[4v b_4 \cos(4v) - 8(1 + v^2 b_4) \sin(4v) + 4v b_3 \cos(3v) \right. \\
 & - 6(-2 + v^2 b_3) \sin(3v) + 4v b_2 \cos(2v) - 4T_1 \sin(2v) + 4v b_1 \cos(v) \\
 & \left. - 2(-1 + v^2 b_1) \sin(v) + 2v b_0 \right] \left(64v b_4 + 36v b_3 + 16v b_2 + 4v b_1 \right) / T_0^2 \\
 & + 2 \left[2(1 + v^2 b_4) \cos(4v) + 2(-2 + v^2 b_3) \cos(3v) + 2T_1 \cos(2v) \right. \\
 & \left. + 2(-1 + v^2 b_1) \cos(v) + v^2 b_0 \right] \left(64v b_4 + 36v b_3 + 16v b_2 + 4v b_1 \right)^2 / T_0^3 \\
 & - \left[2(1 + v^2 b_4) \cos(4v) + 2(-2 + v^2 b_3) \cos(3v) + 2T_1 \cos(2v) \right. \\
 & \left. + 2(-1 + v^2 b_1) \cos(v) + v^2 b_0 \right] \left(64b_4 + 36b_3 + 16b_2 + 4b_1 \right) / T_0^2 \\
 & T_0 = -6 + 32v^2 b_4 + 18v^2 b_3 + 8a_2 + 8v^2 b_2 + 2v^2 b_1 \\
 & T_1 = a_2 + v^2 b_2 \quad (27)
 \end{aligned}$$

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

$$\begin{aligned}
 p\hat{h}l = & \left[-48b_4 \sin(4v) - 192v b_4 \cos(4v) + 128(1 + v^2 b_4) \sin(4v) - 36b_3 \sin(3v) \right. \\
 & - 108v b_3 \cos(3v) + 54(-2 + v^2 b_3) \sin(3v) - 24b_2 \sin(2v) \\
 & - 48v b_2 \cos(2v) + 16T_4 \sin(2v) - 12b_1 \sin(v) - 12v b_1 \cos(v) \\
 & \left. + 2(-1 + v^2 b_1) \sin(v) \right] / T_3 - 3 \left[4b_4 \cos(4v) - 32v b_4 \sin(4v) \right. \\
 & \left. - 32(1 + v^2 b_4) \cos(4v) + 4b_3 \cos(3v) - 24v b_3 \sin(3v) \right]
 \end{aligned}$$

$$\begin{aligned}
& -18 \left(-2 + v^2 b_3 \right) \cos(3v) + 4 b_2 \cos(2v) - 16 v b_2 \sin(2v) - 8 T_4 \cos(2v) \\
& \quad + 4 b_1 \cos(v) - 8 v b_1 \sin(v) - 2 \left(-1 + v^2 b_1 \right) \cos(v) + 2 b_0 \left[T_2/T_3^2 \right. \\
& \quad \quad \left. + 6 \left[4 v b_4 \cos(4v) - 8 \left(1 + v^2 b_4 \right) \sin(4v) + 4 v b_3 \cos(3v) \right. \right. \\
& \quad \quad \left. - 6 \left(-2 + v^2 b_3 \right) \sin(3v) + 4 v b_2 \cos(2v) - 4 T_4 \sin(2v) + 4 v b_1 \cos(v) \right. \\
& \quad \quad \left. \left. - 2 \left(-1 + v^2 b_1 \right) \sin(v) + 2 v b_0 \right] T_2^2/T_3^3 - 3 \left[4 v b_4 \cos(4v) \right. \right. \\
& \quad \quad \left. - 8 \left(1 + v^2 b_4 \right) \sin(4v) + 4 v b_3 \cos(3v) - 6 \left(-2 + v^2 b_3 \right) \sin(3v) \right. \\
& \quad \quad \left. + 4 v b_2 \cos(2v) - 4 T_4 \sin(2v) + 4 v b_1 \cos(v) - 2 \left(-1 + v^2 b_1 \right) \sin(v) \right. \\
& \quad \quad \left. \left. + 2 v b_0 \right] \left(64 b_4 + 36 b_3 + 16 b_2 + 4 b_1 \right) / T_3^2 - 6 \left[2 \left(1 + v^2 b_4 \right) \cos(4v) \right. \right. \\
& \quad \quad \left. + 2 \left(-2 + v^2 b_3 \right) \cos(3v) + 2 T_4 \cos(2v) + 2 \left(-1 + v^2 b_1 \right) \cos(v) + v^2 b_0 \right] T_2^3 / \\
& \quad \quad T_3^4 + 6 \left[2 \left(1 + v^2 b_4 \right) \cos(4v) + 2 \left(-2 + v^2 b_3 \right) \cos(3v) + 2 T_4 \cos(2v) \right. \\
& \quad \quad \left. \left. + 2 \left(-1 + v^2 b_1 \right) \cos(v) + v^2 b_0 \right] T_2 \left(64 b_4 + 36 b_3 + 16 b_2 + 4 b_1 \right) / T_3^3 \right. \\
& \quad \quad \quad \left. T_2 = 64 v b_4 + 36 v b_3 + 16 v b_2 + 4 v b_1 \right. \\
& \quad \quad \quad T_3 = -6 + 32 v^2 b_4 + 18 v^2 b_3 + 8 a_2 + 8 v^2 b_2 + 2 v^2 b_1 \\
& \quad \quad \quad \left. T_4 = a_2 + v^2 b_2 \right] \quad (28)
\end{aligned}$$

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

$$\begin{aligned}
\hat{p} \hat{h} l = & \left[-384 b_4 \cos(4v) + 1024 v b_4 \sin(4v) + 512 \left(1 + v^2 b_4 \right) \cos(4v) \right. \\
& - 216 b_3 \cos(3v) + 432 v b_3 \sin(3v) + 162 \left(-2 + v^2 b_3 \right) \cos(3v) \\
& - 96 b_2 \cos(2v) + 128 v b_2 \sin(2v) + 32 T_7 \cos(2v) - 24 b_1 \cos(v) \\
& \left. + 16 v b_1 \sin(v) + 2 \left(-1 + v^2 b_1 \right) \cos(v) \right] / T_6 - 4 \left[-48 b_4 \sin(4v) \right. \\
& - 192 v b_4 \cos(4v) + 128 \left(1 + v^2 b_4 \right) \sin(4v) - 36 b_3 \sin(3v) \\
& \left. - 108 v b_3 \cos(3v) + 54 \left(-2 + v^2 b_3 \right) \sin(3v) - 24 b_2 \sin(2v) \right.
\end{aligned}$$

$$\begin{aligned}
 & -48 \, v \, b_2 \cos(2 \, v) + 16 \, T_7 \sin(2 \, v) - 12 \, b_1 \sin(v) - 12 \, v \, b_1 \cos(v) \\
 & + 2 \left(-1 + v^2 \, b_1 \right) \sin(v) \Big] T_9/T_6^2 + 12 \left[4 \, b_4 \cos(4 \, v) - 32 \, v \, b_4 \sin(4 \, v) \right. \\
 & \quad \left. - 32 \left(1 + v^2 \, b_4 \right) \cos(4 \, v) + 4 \, b_3 \cos(3 \, v) - 24 \, v \, b_3 \sin(3 \, v) \right. \\
 & \quad \left. - 18 \left(-2 + v^2 \, b_3 \right) \cos(3 \, v) + 4 \, b_2 \cos(2 \, v) - 16 \, v \, b_2 \sin(2 \, v) - 8 \, T_7 \cos(2 \, v) \right. \\
 & \quad \left. + 4 \, b_1 \cos(v) - 8 \, v \, b_1 \sin(v) - 2 \left(-1 + v^2 \, b_1 \right) \cos(v) + 2 \, b_0 \right] T_9^2/T_6^3 \\
 & - 6 \left[4 \, b_4 \cos(4 \, v) - 32 \, v \, b_4 \sin(4 \, v) - 32 \left(1 + v^2 \, b_4 \right) \cos(4 \, v) + 4 \, b_3 \cos(3 \, v) \right. \\
 & \quad \left. - 24 \, v \, b_3 \sin(3 \, v) - 18 \left(-2 + v^2 \, b_3 \right) \cos(3 \, v) + 4 \, b_2 \cos(2 \, v) - 16 \, v \, b_2 \sin(2 \, v) \right. \\
 & \quad \left. - 8 \, T_7 \cos(2 \, v) + 4 \, b_1 \cos(v) - 8 \, v \, b_1 \sin(v) - 2 \left(-1 + v^2 \, b_1 \right) \cos(v) + 2 \, b_0 \right] T_5/T_6^2 \\
 & - 24 \left[4 \, v \, b_4 \cos(4 \, v) - 8 \left(1 + v^2 \, b_4 \right) \sin(4 \, v) + 4 \, v \, b_3 \cos(3 \, v) \right. \\
 & \quad \left. - 6 \left(-2 + v^2 \, b_3 \right) \sin(3 \, v) + 4 \, v \, b_2 \cos(2 \, v) - 4 \, T_7 \sin(2 \, v) + 4 \, v \, b_1 \cos(v) \right. \\
 & \quad \left. - 2 \left(-1 + v^2 \, b_1 \right) \sin(v) + 2 \, v \, b_0 \right] T_9^3/T_6^4 + 24 \left[4 \, v \, b_4 \cos(4 \, v) \right. \\
 & \quad \left. - 8 \left(1 + v^2 \, b_4 \right) \sin(4 \, v) + 4 \, v \, b_3 \cos(3 \, v) - 6 \left(-2 + v^2 \, b_3 \right) \sin(3 \, v) \right. \\
 & \quad \left. + 4 \, v \, b_2 \cos(2 \, v) - 4 \, T_7 \sin(2 \, v) + 4 \, v \, b_1 \cos(v) - 2 \left(-1 + v^2 \, b_1 \right) \sin(v) \right. \\
 & \quad \left. + 2 \, v \, b_0 \right] T_9 \, T_5/T_6^3 + \frac{24 \, T_8 \, T_9^4}{T_6^5} - \frac{36 \, T_8 \, T_9^2 \, T_5}{T_6^4} + \frac{6 \, T_8 \, T_5^2}{T_6^3} \quad (29)
 \end{aligned}$$

$$T_5 = 64 \, b_4 + 36 \, b_3 + 16 \, b_2 + 4 \, b_1$$

$$T_6 = -6 + 32 \, v^2 \, b_4 + 18 \, v^2 \, b_3 + 8 \, a_2 + 8 \, v^2 \, b_2 + 2 \, v^2 \, b_1$$

$$T_7 = a_2 + v^2 \, b_2$$

$$T_8 = 2 \left(1 + v^2 \, b_4 \right) \cos(4 \, v) + 2 \left(-2 + v^2 \, b_3 \right) \cos(3 \, v) + 2 \, T_7 \cos(2 \, v)$$

$$+ 2 \left(-1 + v^2 \, b_1 \right) \cos(v) + v^2 \, b_0$$

$$T_9 = 64 \, v \, b_4 + 36 \, v \, b_3 + 16 \, v \, b_2 + 4 \, v \, b_1$$

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

$$\begin{aligned}
p\check{h}l = & \left[2560\,b_4\sin(4\,v) + 5120\,v\,b_4\cos(4\,v) - 2048\left(1+v^2\,b_4\right)\sin(4\,v) \right. \\
& + 1080\,b_3\sin(3\,v) + 1620\,v\,b_3\cos(3\,v) - 486\left(-2+v^2\,b_3\right)\sin(3\,v) \\
& + 320\,b_2\sin(2\,v) + 320\,v\,b_2\cos(2\,v) - 64\,T_{13}\sin(2\,v) + 40\,b_1\sin(v) \\
& \left. + 20\,v\,b_1\cos(v) - 2\left(-1+v^2\,b_1\right)\sin(v) \right] / (T_{12}) - 5 \left[-384\,b_4\cos(4\,v) \right. \\
& + 1024\,v\,b_4\sin(4\,v) + 512\left(1+v^2\,b_4\right)\cos(4\,v) - 216\,b_3\cos(3\,v) \\
& + 432\,v\,b_3\sin(3\,v) + 162\left(-2+v^2\,b_3\right)\cos(3\,v) - 96\,b_2\cos(2\,v) \\
& + 128\,v\,b_2\sin(2\,v) + 32\,T_{13}\cos(2\,v) - 24\,b_1\cos(v) + 16\,v\,b_1\sin(v) \\
& \left. + 2\left(-1+v^2\,b_1\right)\cos(v) \right] T_{11}/T_{12}^2 + 20 \left[-48\,b_4\sin(4\,v) - 192\,v\,b_4\cos(4\,v) \right. \\
& + 128\left(1+v^2\,b_4\right)\sin(4\,v) - 36\,b_3\sin(3\,v) - 108\,v\,b_3\cos(3\,v) \\
& + 54\left(-2+v^2\,b_3\right)\sin(3\,v) - 24\,b_2\sin(2\,v) - 48\,v\,b_2\cos(2\,v) + 16\,T_{13}\sin(2\,v) \\
& \left. - 12\,b_1\sin(v) - 12\,v\,b_1\cos(v) + 2\left(-1+v^2\,b_1\right)\sin(v) \right] T_{11}^2/T_{12}^3 \\
-10 \left[& -48\,b_4\sin(4\,v) - 192\,v\,b_4\cos(4\,v) + 128\left(1+v^2\,b_4\right)\sin(4\,v) - 36\,b_3\sin(3\,v) \right. \\
& - 108\,v\,b_3\cos(3\,v) + 54\left(-2+v^2\,b_3\right)\sin(3\,v) - 24\,b_2\sin(2\,v) \\
& - 48\,v\,b_2\cos(2\,v) + 16\,T_{13}\sin(2\,v) - 12\,b_1\sin(v) - 12\,v\,b_1\cos(v) \\
& \left. + 2\left(-1+v^2\,b_1\right)\sin(v) \right] T_{10}/T_{12}^2 - 60 \left[4\,b_4\cos(4\,v) - 32\,v\,b_4\sin(4\,v) \right. \\
& - 32\left(1+v^2\,b_4\right)\cos(4\,v) + 4\,b_3\cos(3\,v) - 24\,v\,b_3\sin(3\,v) \\
& - 18\left(-2+v^2\,b_3\right)\cos(3\,v) + 4\,b_2\cos(2\,v) - 16\,v\,b_2\sin(2\,v) - 8\,T_{13}\cos(2\,v) \\
& \left. + 4\,b_1\cos(v) - 8\,v\,b_1\sin(v) - 2\left(-1+v^2\,b_1\right)\cos(v) + 2\,b_0 \right] T_{11}^3/T_{12}^4 \\
+60 \left[& 4\,b_4\cos(4\,v) - 32\,v\,b_4\sin(4\,v) - 32\left(1+v^2\,b_4\right)\cos(4\,v) + 4\,b_3\cos(3\,v) \right. \\
& - 24\,v\,b_3\sin(3\,v) - 18\left(-2+v^2\,b_3\right)\cos(3\,v) + 4\,b_2\cos(2\,v) - 16\,v\,b_2\sin(2\,v) \\
& \left. - 8\,T_{13}\cos(2\,v) + 4\,b_1\cos(v) - 8\,v\,b_1\sin(v) - 2\left(-1+v^2\,b_1\right)\cos(v) + 2\,b_0 \right] \\
& T_{11}\,T_{10}/T_{12}^3
\end{aligned}$$

$$\begin{aligned}
 & + \frac{120 T_{15} T_{11}^4}{T_{12}^5} - \frac{180 T_{15} T_{11}^2 T_{10}}{T_{12}^4} + \frac{30 T_{15} T_{10}^2}{T_{12}^3} - \frac{120 T_{14} T_{11}^5}{T_{12}^6} \\
 & + \frac{240 T_{14} T_{11}^3 T_{10}}{T_{12}^5} - \frac{90 T_{14} T_{11} T_{10}^2}{T_{12}^4} \\
 & T_{10} = 64 b_4 + 36 b_3 + 16 b_2 + 4 b_1 \\
 & T_{11} = 64 v b_4 + 36 v b_3 + 16 v b_2 + 4 v b_1 \\
 & T_{12} = -6 + 32 v^2 b_4 + 18 v^2 b_3 + 8 a_2 + 8 v^2 b_2 + 2 v^2 b_1 \\
 & T_{13} = a_2 + v^2 b_2 \\
 & T_{14} = 2 (1 + v^2 b_4) \cos(4 v) + 2 (-2 + v^2 b_3) \cos(3 v) + 2 T_{13} \cos(2 v) \\
 & + 2 (-1 + v^2 b_1) \cos(v) + v^2 b_0 \\
 & T_{15} = 4 v b_4 \cos(4 v) - 8 (1 + v^2 b_4) \sin(4 v) + 4 v b_3 \cos(3 v) \\
 & - 6 (-2 + v^2 b_3) \sin(3 v) + 4 v b_2 \cos(2 v) - 4 T_{13} \sin(2 v) + 4 v b_1 \cos(v) \\
 & - 2 (-1 + v^2 b_1) \sin(v) + 2 v b_0
 \end{aligned} \tag{30}$$

We demand that the phase-lag and its first, second, third, fourth and fifth derivatives to be equal to zero, i.e. we demand the satisfaction of the relations (25), (26), (27), (28), (29) and (30). Based on the above we obtain the coefficients mentioned in Appendix B.

The behavior of the coefficients is given in Figure 2.

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

$$\text{LTE} = -\frac{58061 h^{12}}{31933440} \left(y_n^{(12)} + 6 \omega^2 y_n^{(10)} + 15 \omega^4 y_n^{(8)} + 20 \omega^6 y_n^{(6)} + 15 \omega^8 y_n^{(4)} + 6 \omega^{10} y_n^{(2)} + \omega^{12} y_n \right) \tag{31}$$

4. COMPARATIVE ERROR ANALYSIS

We will investigate the error for the following methods:

- The eight-step eighth algebraic order method developed by Quinlan and Tremaine [35] which is indicated as **QT9**
- The ten-step tenth algebraic order method developed by Quinlan and Tremaine [35] which is indicated as **QT11**

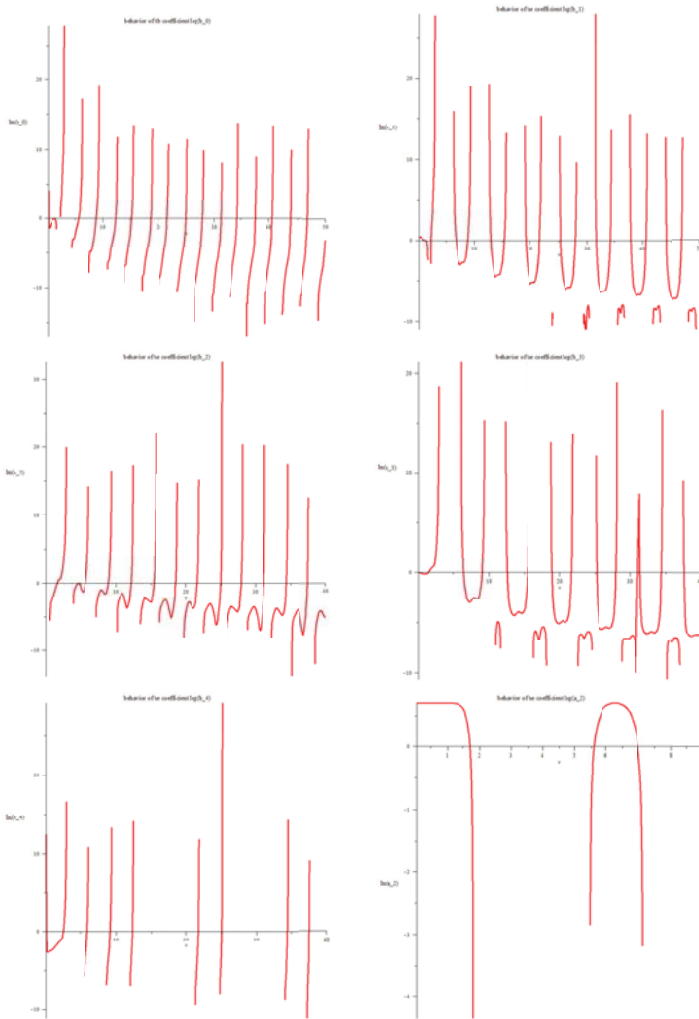


Figure 2: Behavior of the coefficients of the new proposed method given by (68)-(73) for several values of v .

- The twelve-step twelfth algebraic order method developed by Quinlan and Tremaine [35] which is indicated as **QT13**
- The eight-step eighth algebraic order method developed by Jenkins [36] which is indicated as **J9**

- The ten-step tenth algebraic order method developed by Jenkins [36] which is indicated as **J11**
- The twelve-step twelfth algebraic order method developed by Jenkins [36] which is indicated as **J13**³
- The classical eight-step method of the family of methods mentioned in paragraph 3 which is indicated as **CL**
- The method produced by Alolyan and Simos [57] which is indicated as **PLD1**
- The method produced by Alolyan and Simos [58] which is indicated as **PLD12**
- The method developed by Alolyan and Simos [59] which is indicated as **PLD123a**
- The method developed by Alolyan and Simos [59] which is indicated as **PLD123b**
- The method developed by Alolyan and Simos [59] which is indicated as **PLD123c**
- The method developed in paragraph 3.1 which is indicated as **PLD1234**
- The method developed in paragraph 3.2 which is indicated as **PLD12345**

The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x)y(x) \quad (32)$$

Based on the paper of Ixaru and Rizea [114], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \quad (33)$$

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

Now we express the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \dots$, which are terms of the local truncation error formulae, in terms of equation (32). The expressions are presented as polynomials of G .

We substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae.

³We note here that the correct coefficient is 25671199 instead of presented 25671198

Based on the procedure described above and on the formulae:

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

we obtain the expressions mentioned below for the above methods.

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

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

So, we have the following asymptotic expansions of the equations mentioned in [58] and in (75)-(77).

The eight-step eighth algebraic order method developed by Quinlan and Tremaine [35] (see for details Alolyan and Simos [58])

$$\text{LTE}_{\text{QT9}} = h^{10} \left(-\frac{45767}{725760} y(x) G^5 + \dots \right) \quad (34)$$

The ten-step tenth algebraic order method developed by Quinlan and Tremaine [35](see for details Alolyan and Simos [58])

$$\text{LTE}_{\text{QT11}} = h^{12} \left(-\frac{52559}{912384} y(x) G^6 + \dots \right) \quad (35)$$

The twelve-step twelfth algebraic order method developed by Quinlan and Tremaine [35](see for details Alolyan and Simos [58])

$$\text{LTE}_{\text{QT13}} = h^{14} \left(-\frac{16301796103}{290594304000} y(x) G^7 + \dots \right) \quad (36)$$

The eight-step eighth algebraic order method developed by Jenkins [36] (see Appendix B for details)

$$\text{LTE}_{\text{J9}} = h^{10} \left(\frac{31511}{518400} y(x) G^5 + \dots \right) \quad (37)$$

The ten-step tenth algebraic order method developed by Jenkins [36] (see Appendix B for details)

$$\text{LTE}_{\text{J11}} = h^{12} \left(\frac{3055417}{53222400} y(x) G^6 + \dots \right) \quad (38)$$

The twelve-step twelfth algebraic order method developed by Jenkins [36] (see Appendix B for details)

$$\text{LTE}_{\text{J13}} = h^{14} \left(\frac{12995034463}{237758976000} y(x) G^7 + \dots \right) \quad (39)$$

The Classical Method of the Family (see Remark 2 of paragraph 3) (see for details Alolyan and Simos [58])

$$\text{LTE}_{\text{CL}} = h^{12} \left(-\frac{58061}{31933440} y(x) G^6 + \dots \right) \quad (40)$$

The method produced by Alolyan and Simos [57] (see for details Alolyan and Simos [57])

$$\text{LTE}_{\text{PLD1}} = h^{12} \left[\left(\frac{987037}{31933440} \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \frac{58061}{15966720} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) + \frac{58061}{31933440} g(x)^2 y(x) \right) G^4 + \dots \right] \quad (41)$$

The method produced by Alolyan and Simos [58] (see for details Alolyan and Simos [58])

$$\text{LTE}_{\text{PLD12}} = h^{12} \left[\frac{58061}{7983360} G^4 \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \dots \right] \quad (42)$$

The first method developed by Alolyan and Simos in [59] (see for details Alolyan and Simos [59])

$$\begin{aligned} \text{LTE}_{\text{PLD123a}} = h^{12} & \left[G^3 \left[\frac{58061}{2661120} \left(\frac{d}{dx} g(x) \right)^2 y(x) + \frac{58061}{3991680} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) \right. \right. \\ & \left. \left. + \frac{58061}{725760} \left(\frac{d^4}{dx^4} g(x) \right) y(x) + \frac{58061}{1995840} g(x) y(x) \frac{d^2}{dx^2} g(x) \right] + \dots \right] \quad (43) \end{aligned}$$

The second and third methods developed by Alolyan and Simos in [59] (see for details Alolyan and Simos [59])

$$\begin{aligned} \text{LTE}_{\text{PLD123bc}} = h^{12} & \left[G^3 \left[\frac{58061}{177408} \left(\frac{d}{dx} g(x) \right)^2 y(x) + \frac{58061}{133056} g(x) y(x) \frac{d^2}{dx^2} g(x) \right. \right. \\ & \left. \left. + \frac{1335403}{2661120} \left(\frac{d^4}{dx^4} g(x) \right) y(x) + \frac{58061}{266112} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) \right] + \dots \right] \quad (44) \end{aligned}$$

The new proposed method developed in paragraph 3.1 (see Appendix B for details)

$$\text{LTE}_{\text{PLD1234}} = h^{12} \left[G^3 \left(-\frac{58061}{1995840} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \right) + \dots \right] \quad (45)$$

The new proposed method developed in paragraph 3.2 (see Appendix B for details)

$$\begin{aligned} \text{LTE}_{\text{PLD12345}} = h^{12} \left[G^2 \left[-\frac{58061}{133056} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \right. \right. \\ \left. -\frac{58061}{332640} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) -\frac{58061}{399168} \left(\frac{d^6}{dx^6} g(x) \right) y(x) \right. \\ \left. \left. -\frac{58061}{997920} \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} y(x) \right) -\frac{58061}{199584} \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) \right] + \dots \right] \quad (46) \end{aligned}$$

From the above equations we have the following theorem:

Theorem 2. *Based on the above error analysis and on formulae (34) - (45), we have:*

- *For the eight-step eighth algebraic order methods developed by Quinlan and Tremaine [35] and Jenkins [36], the error increases as the fifth power of G*
- *For the ten-step tenth algebraic order method developed by Quinlan and Tremaine [35] and Jenkins [36], the error increases as the sixth power of G*
- *For the twelve-step twelfth algebraic order method developed by Quinlan and Tremaine [35] and Jenkins [36], the error increases as the seventh power of G*
- *For the Classical Method of the Family (see [58] for more details) the error increases as the sixth power of G*
- *For the method produced by Alolyan and Simos [57], the error increases as the fourth power of G*
- *For the method produced by Alolyan and Simos [58], the error increases as the fourth power of G but with smaller coefficient than the method of Alolyan and Simos [57]*
- *For the method produced in paragraph 3.1 of the paper Alolyan and Simos [59], the error increases as the third power of G*
- *For the methods produced in paragraphs 3.2 and 3.3 of the paper Alolyan and Simos [59], the error increases as the third power of G*
- *For the method developed in paragraph 3.1 of this paper, the error increases as the third power of G*

- For the method developed in paragraph 3.2 of this paper, the error increases as the second power of G

So, for the numerical solution of the time independent radial Schrödinger equation the new methods produced in this paper have the smallest error, especially for large values of $|G| = |V_c - E|$, since they are of tenth algebraic order for which also the error increases as the second power of G .

5. STABILITY ANALYSIS

We apply two methods of the family of methods (8) developed in paragraphs 3.1 and 3.2 to the scalar test equation:

$$\psi'' = -t^2 \psi, \quad (47)$$

where $t \neq \omega$.

We thus obtain the following difference equation:

$$\begin{aligned} A_k(s) \psi_{n+k} + \dots + A_1(s) \psi_{n+1} + A_0(s) \psi_n + \\ + A_1(s) \psi_{n-1} + \dots + A_k(s) \psi_{n-k} = 0 \end{aligned} \quad (48)$$

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

The characteristic equation associated with (48) is given by:

$$A_k(s) \vartheta^k + \dots + A_1(s) \vartheta + A_0(s) + A_1(s) \vartheta^{-1} + \dots + A_k(s) \vartheta^{-k} = 0 \quad (49)$$

Definition 1. (see [34]) A symmetric $2k$ -step method with the characteristic equation given by (49) is said to have an interval of periodicity $(0, s_0^2)$ if, for all $s \in (0, s_0^2)$, the roots z_i , $i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i \zeta(th)}, \quad |z_i| \leq 1, \quad i = 3, 4 \quad (50)$$

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

Definition 2. (see [34]) 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 $(0, \infty) - S^4$ only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $v = s$.

In Figures 3, 4 we present the $s - v$ plane for the methods developed in the paragraphs 3.1 and 3.2 respectively. A shadowed area denotes the $s - v$ region where the method is stable, while a white area denotes the region where the method is unstable.

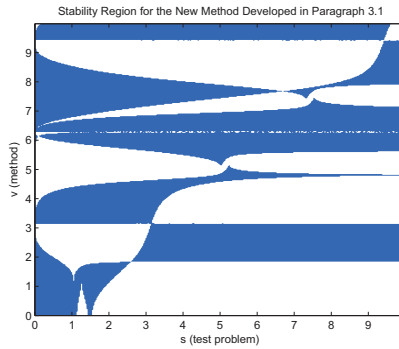


Figure 3: $s - v$ plane of the New Methods produced in section 3.1

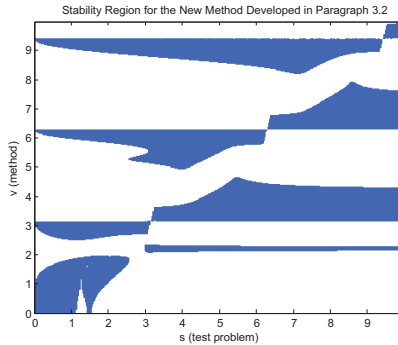


Figure 4: $s - v$ plane of the New Methods produced in section 3.2

In the case that the frequency of the scalar test equation is equal to the frequency of

⁴where S is a set of distinct points

phase fitting, i.e. in the case that $v = s$, and based on Figures 3, 4, it is easy to see that the interval of periodicity of the new methods is given by the following Table I

Table 1: Intervals of Periodicity for the New Developed Methods

<i>Method</i>	<i>Interval of Periodicity</i>
PLD1234	$(0, 3.3)$
PLD12345	$(0, 3.7)$

Remark 3. *For the solution of the Schrödinger equation the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to observe the surroundings of the first diagonal of the $s - v$ plane.*

From the above analysis we have the following theorem:

- Theorem 3.**
- *Method (8) with the coefficients (62) - (66) is of tenth algebraic order, has the phase-lag and its first, second, third and fourth derivatives equals to zero and has an interval of periodicity equals to: $(0, 3.3)$.*
 - *Method (8) with the coefficients (68) - (73) is of tenth algebraic order, has the phase-lag and its first, second, third, fourth and fifth derivatives equals to zero and has an interval of periodicity equals to: $(0, 3.7)$.*

Finally in Table II we present the characteristics of the methods developed and studied in this paper.

6. NUMERICAL RESULTS

6.1 Eigenvalue problem of the Schrödinger Equation

We shall illustrate the new developed methods on the computation of the eigenvalues of the radial time-independent Schrödinger equation. The Schrödinger equation (1) for $l = 0$ can be written in the form

$$-\frac{1}{2}y'' + V(x)y = Ey, \quad x \in [a, b], \quad y(a) = y(b) = 0 \quad (51)$$

Table 2: Basic Characteristics of the Methods Developed and Studied in this paper. We note that *AO* is the Algebraic Order, *CFAE* is the Coefficient of the Maximum Power of *G* in the Asymptotic Expansion and Order of *G* is the order of *G* in the Asymptotic Expansion of the Local Truncation Error. *IP* is the Interval of Periodicity

<i>Method</i>	<i>AO</i>	<i>Order of G</i>	<i>CFAE</i>	<i>IP</i>
QT9	8	5	-0.06306079145	$(0, 0.52)$
QT11	10	6	-0.05760622720	$(0, 0.17)$
QT13	12	7	-0.05609812676	$(0, 0.046)$
J9	8	5	0.06078510802	$(0, 0.2)$
JT11	10	6	0.05740847838	$(0, 0.058)$
JT13	12	7	0.05465633593	$(0, 0.003)$
CL	10	6	-0.001818188081	$(0, 1.3)$
PLD1	10	4	0.03090919738	$(0, 8.5264)$
PLD12	10	4	0.007272752325	$(0, 4.1)$
PLD123a	10	3	0.007272752325	$(0, 8.6)$
PLD123b	10	3	0.02181825697	$(0, 3.3)$
PLD123c	10	3	0.02181825697	$(0, 2.4)$
PLD1234	10	3	0.02909100930	$(0, 3.3)$
PLD12345	10	2	0.1745460558	$(0, 3.7)$

where E is the energy eigenvalue, $V(x)$ the potential, and $y(x)$ the wave function. The problems used are the harmonic oscillator, the doubly anharmonic oscillator and exponential potential. For all problems we use $w = \sqrt{B(x)}$.

For comparison purposes we use the following methods:

- The Numerov's method which is indicated as **Method I**
- The Exponentially-fitted two-step method developed by Raptis and Allison [82] which is indicated as **Method II**
- The Exponentially-fitted two-step P-stable method developed by Wang [95] which is indicated as **Method III**
- The Exponentially-fitted four-step method developed by Raptis [83] which is indicated as **Method IV**

- The eight-step eighth algebraic order method developed by Quinlan and Tremaine [35] which is indicated as **Method V**
- The ten-step tenth algebraic order method developed by Quinlan and Tremaine [35] which is indicated as **Method VI**
- The twelve-step twelfth algebraic order method developed by Quinlan and Tremaine [35] which is indicated as **Method VII**
- The classical eight-step method of the family of methods mentioned in Section 3 which is indicated as **Method VIII**
- The method produced by Alolyan and Simos [57] which is indicated as **Method IX**
- The method produced by Alolyan and Simos [58] which is indicated as **Method X**
- The method produced in paragraph 3.1 of the paper Alolyan and Simos [59] which is indicated as **Method XI**
- The method produced in paragraph 3.2 of the paper Alolyan and Simos [59] which is indicated as **Method XII**
- The method produced in paragraph 3.3 of the paper Alolyan and Simos [59] which is indicated as **Method XIII**
- The eight-step eighth algebraic order method developed by Jenkins [36] which is indicated as **Method XIV**
- The ten-step tenth algebraic order method developed by Jenkins [36] which is indicated as **Method XV**
- The twelve-step twelfth algebraic order method developed by Jenkins [36] which is indicated as **Method XVI**
- The method produced in paragraph 3.1 of this paper which is indicated as **Method XVII**
- The method produced in paragraph 3.2 of this paper which is indicated as **Method XVIII**

6.2 The Harmonic Oscillator

The potential of the one dimensional harmonic oscillator is

$$V(x) = \frac{1}{2}kx^2$$

we consider $k = 1$. The integration interval is $[-R, R]$.

The exact eigenvalues are given by

$$E_n = n + \frac{1}{2}, \quad n = 0, 1, 2, \dots$$

In Figures 5, 6 and 7 we present the maximum absolute error $\log_{10}(\text{Err})$ where

$$\text{Err} = |E_{\text{calculated}} - E_{\text{accurate}}| \quad (52)$$

for the eigenenergies E_{100} , E_{300} , E_{500} , for several values of NFE = Number of Function Evaluations.

The integration interval is presented in the following Table 3 for the above eigenenergies

Table 3: Integration Interval R for several eigenvalues E_n

<i>Eigenvalue</i>	<i>Integration Interval</i>
E_{100}	16
E_{300}	26
E_{500}	33

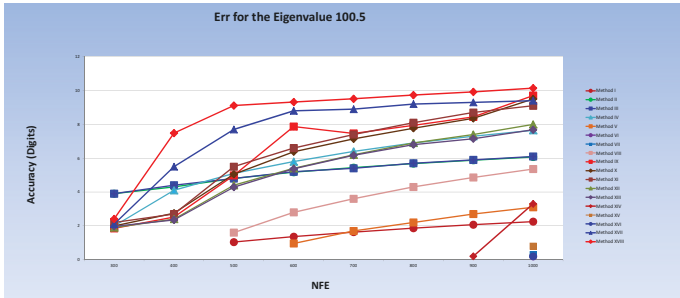


Figure 5: Accuracy (Digits) for several values of NFE for the eigenvalue E_{100} for the Harmonic Oscillator. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0

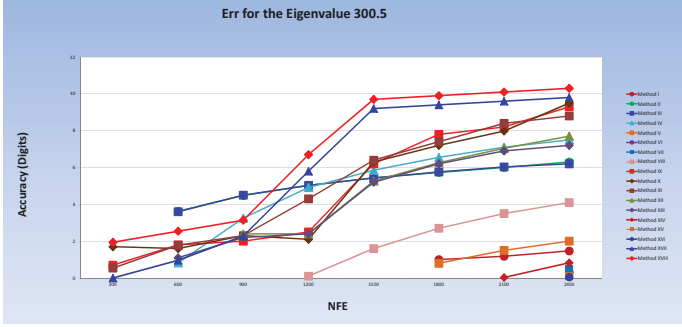


Figure 6: Accuracy (Digits) for several values of NFE for the eigenvalue E_{300} for the Harmonic Oscillator. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE , Accuracy (Digits) is less than 0

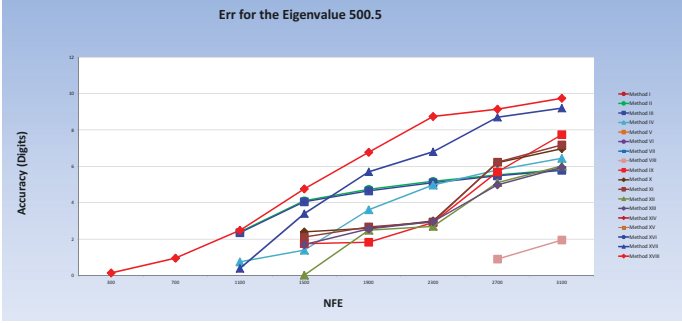


Figure 7: Accuracy (Digits) for several values of NFE for the eigenvalue E_{500} for the Harmonic Oscillator. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE , Accuracy (Digits) is less than 0

6.3 The Resonance Problem of the Schrödinger Equation

As second problem for the illustration of the new methods obtained in Section 3 we chose the application to the radial time independent Schrödinger equation.

Since our new methods are frequency dependent, in order to be applied to the radial Schrödinger equation the value of parameter v is needed. For every problem of the radial Schrödinger equation given by (1) the parameter v is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \quad (53)$$

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

6.4 Woods-Saxon potential

We use the well known Woods-Saxon potential given by

$$V(x) = \frac{u_0}{1 + z} - \frac{u_0 z}{a \left(1 + z\right)^2} \quad (54)$$

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

The behavior of Woods-Saxon potential is shown in the Figure 8.

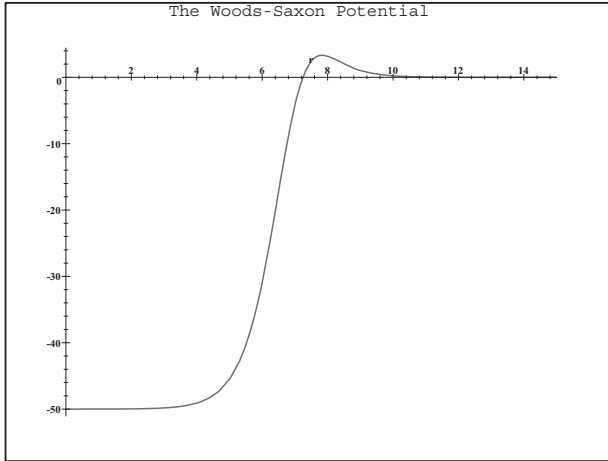


Figure 8: The Woods-Saxon potential.

It is well known that for some potentials, such as the Woods-Saxon potential, the definition of parameter v is not given as a function of x but it is based on some critical points which have been defined from the investigation of the appropriate potential (see for details [84]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [84]):

$$v = \begin{cases} \sqrt{-50 + E}, & \text{for } x \in [0, 6.5 - 2h], \\ \sqrt{-37.5 + E}, & \text{for } x = 6.5 - h \\ \sqrt{-25 + E}, & \text{for } x = 6.5 \\ \sqrt{-12.5 + E}, & \text{for } x = 6.5 + h \\ \sqrt{E}, & \text{for } x \in [6.5 + 2h, 15] \end{cases} \quad (55)$$

6.5 The Resonance Problem

In this section we present the results from the application of well known methods in the literature to the numerical solution of the radial time independent Schrödinger equation (1) in the case of the Woods-Saxon potential (54). The numerical solution of this problem is based on the approximation of the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $x \in [0, 15]$. We consider 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 dies away faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2} \right) y(x) = 0 \quad (56)$$

for x greater than some value X .

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

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC \left[\sin \left(kx - \frac{l\pi}{2} \right) + \tan \delta_l \cos \left(kx - \frac{l\pi}{2} \right) \right] \end{aligned} \quad (57)$$

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

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \quad (58)$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need $y_0, y_i, i = 1(1)8$ before starting an eight-step method. From the initial condition we obtain y_0 . The other values can be obtained using the Runge-Kutta-Nyström methods of

Dormand et. al. (see [8]). With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l .

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

The boundary conditions for this problem are:

$$y(0) = 0, \quad y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \quad (59)$$

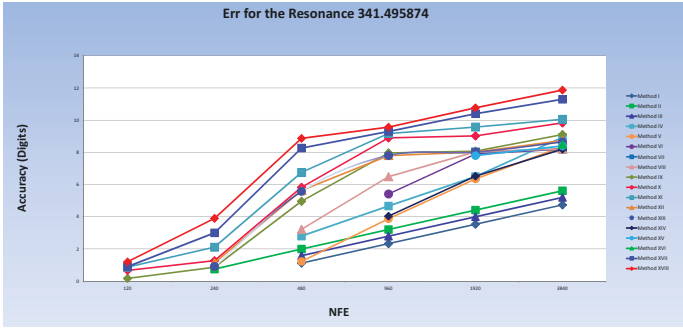


Figure 9: Accuracy (Digits) for several values of NFE for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE , Accuracy (Digits) is less than 0

We compute the approximate positive eigenenergies of the Woods-Saxon resonance problem using the eighteen methods mentioned in section 6.1

The computed eigenenergies are compared with exact ones. In Figure 9 we present the maximum absolute error $\log_{10}\left(Err\right)$ where

$$Err = |E_{calculated} - E_{accurate}| \quad (60)$$

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

$$Err = |E_{calculated} - E_{accurate}| \quad (61)$$

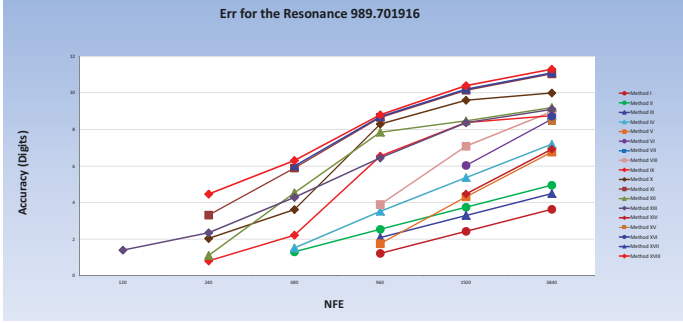


Figure 10: Accuracy (Digits) for several values of NFE for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE , Accuracy (Digits) is less than 0

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

7. CONCLUSIONS

In the present paper

1. we have developed two eight-step methods of tenth algebraic order with phase-lag and its derivatives equal to zero.
2. we have analyzed all the well known eight-step methods, well known ten-step methods and well known twelve-step methods together with some well known methods of fourth and sixth algebraic order

We have applied the above mentioned methods to the

- eigenvalue problem of the one-dimensional Schrödinger equation and
- resonance problem of the radial Schrödinger equation.

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

- *For the eigenvalue problem:* The Exponentially-fitted two-step method developed by Raptis and Allison [82] (denoted as Method II) is more efficient than the Numerov's Method (indicated as Method I) and has exactly the same behavior with the

Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III). *For the resonance problem:* The Exponentially-fitted two-step method developed by Raptis and Allison [82] (denoted as Method II) is more efficient than the Numerov's Method (indicated as Method I) and the Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III).

- *For both problems:* The Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III) is more efficient than the Numerov's method (indicated as Method I).
- *For the eigenvalue problem:* The Exponentially-fitted four-step method developed by Raptis [83] (indicated as Method IV) is more efficient than the Numerov' Method (indicated Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [82] (indicated as Method II), the Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III), the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V), the ten-step method developed by Quinlan and Tremaine [35] (indicated as Method VI), the twelve-step method developed by Quinlan and Tremaine [35] (indicated as Method VII), the eight-step method developed by Jenkins [36] (indicated as Method XIV), the ten-step method developed by Jenkins [36] (indicated as Method XV) and the twelve-step method developed by Jenkins [36] (indicated as Method XVI). *For the resonance problem:* The Exponentially-fitted four-step method developed by Raptis [83] (indicated as Method IV) is more efficient than the Numerov' Method (indicated Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [82] (indicated as Method II), the Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III), the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V) and the eight-step method developed by Jenkins [36] (indicated as Method XIV).
- *For the eigenvalue problem:* The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [35] (indicated as Method VI) is less efficient than the Numerov' Method (indicated Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [82] (indicated as Method II), the Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III),

the Exponentially-fitted four-step method developed by Raptis [83] (indicated as Method IV), the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V) and the eight-step method developed by Jenkins [36] (indicated as Method XIV). *For the resonance problem:* The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [35] (indicated as Method VI) is more efficient than the Numerov' Method (indicated Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [82] (indicated as Method II), the Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III), the Exponentially-fitted four-step method developed by Raptis [83] (indicated as Method IV), the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V) and the eight-step method developed by Jenkins [36] (indicated as Method XIV).

- *For the eigenvalue problem:* The twelve-step method developed by Quinlan and Tremaine [35] (indicated as Method VII) is less efficient than the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V) and has the same behavior with the ten-step method developed by Quinlan and Tremaine [35] (indicated as Method VI). *For the resonance problem:* The twelve-step method developed by Quinlan and Tremaine [35] (indicated as Method VII) gives for the two bigger numbers of function evaluations the same approximately results with the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V) and the ten-step method developed by Quinlan and Tremaine [35] (indicated as Method VI).
- *For the eigenvalue problem:* The classical eight-step method of the family of methods mentioned in paragraph 3 (indicated as Method VIII) is more efficient than the Numerov' Method (indicated as Method I), the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V), the ten-step method developed by Quinlan and Tremaine [35] (indicated as Method VI), the twelve-step method developed by Quinlan and Tremaine [35] (indicated as Method VII), the eight-step method developed by Jenkins [36] (indicated as Method XIV), the ten-step method developed by Jenkins [36] (indicated as Method XV) and the twelve-step method developed by Jenkins [36] (indicated as Method XVI). *For the resonance problem:* The classical eight-step method of the family of methods mentioned in paragraph 3

(indicated as Method VIII) is more efficient than the Numerov' Method (indicated as Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [82] (indicated as Method II), the Exponentially-fitted two-step P-stable method developed by Wang [95] (indicated as Method III), the Exponentially-fitted four-step method developed by Raptis [83] (indicated as Method IV), the eight-step method developed by Quinlan and Tremaine [35] (indicated as Method V), the ten-step method developed by Quinlan and Tremaine [35] (indicated as Method VI) and the twelve-step method developed by Quinlan and Tremaine [35] (indicated as Method VII).

- *For both problems:* The method produced by Alolyan and Simos [57] (indicated as Method IX) is more efficient than all the above methods indicated as Methods I - VIII
- *For both problems:* The method produced by Alolyan and Simos [58] (indicated as Method X) is more efficient than all the above methods indicated as Methods I - VIII. *For the eigenvalue problem:* The method produced by Alolyan and Simos [58] (indicated as Method X) has approximately the same behavior than the method developed in [57] (indicated as Method IX). *For the resonance problem:* The method produced by Alolyan and Simos [58] (indicated as Method X) is more efficient than the method developed in [57] (indicated as Method IX)
- *For both problems:* The methods developed in paragraphs 3.2 and 3.3 of the paper Alolyan and Simos [59] (indicated as Methods XII and XIII respectively) have very slow convergence and for this reason they more badly behaves than the Methods X and XI especially for high number of function evaluations.
- *For the eigenvalue problem:* (1) *Energies E_{100} and E_{300} :* The method developed in paragraph 3.1 of the paper Alolyan and Simos [59] (indicated as Method XI) is more efficient than all the above methods indicated as Methods I - IX and the other methods developed in [59] (indicated as Method XII and Method XIII). (2) *Energy E_{500} :* The method developed in paragraph 3.1 of the paper Alolyan and Simos [59] (indicated as Method XI) is more efficient than all the above methods indicated as Methods I - IX and the other methods developed in [59] (indicated as Method XII and Method XIII) only for big number of function evaluations. *For the*

resonance problem: The method developed in paragraph 3.1 of the paper Alolyan and Simos [59] (indicated as Method XI) is more efficient than all the above methods indicated as Methods I - IX and the other methods developed in [59] (indicated as Method XII and Method XIII).

- *For the resonance problem:* The ten-step method developed by Jenkins [36] (indicated as Method XV) and the twelve-step method developed by Jenkins [36] (indicated as Method XVI) give for the bigger numbers of function evaluations the same approximately results with the method developed in paragraph 3.3 of the paper Alolyan and Simos [59]. We note that for the eigenvalue problem we have given our conclusions for these methods above.
- *For both problems:* The method produced in paragraph 3.1 of this paper which is indicated as Method XVII, is more efficient than all the above methods indicated as Methods I - XVI
- *For both problems:* The method produced in paragraph 3.2 of this paper which is indicated as Method XVIII, is more efficient than all the above methods indicated as Methods I - XVII

8. GENERAL COMMENTS AND OPEN PROBLEMS

From the analysis presented above (comparative error analysis and comparative stability analysis) and from the numerical results presented above, the following summaries for the numerical methods used for the approximate solution of the radial Schrödinger Equation are excluded:

- Remark 4.**
- *The methods with phase-lag and its derivatives equal to zero are very efficient for the numerical solution of the radial Schrödinger Equation*
 - *The methods with constant coefficients cannot be so efficient like the above mentioned methods*
 - *The multistep methods with constant coefficients and with big number of steps are not efficient for the numerical solution of the radial Schrödinger Equation*

- *We must continue the research on the implicit multistep methods (with number of steps $k \geq 5$). The direction must be on the vanishing of phase-lag and its derivatives and the stability region*

Based on the above remark we have the following open problems for the construction of efficient multistep methods for the numerical solution of the radial Schrödinger Equation:

1. development of multistep methods with large interval of periodicity.
2. development of multistep methods with very good convergence properties.

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

Appendix A

$$\begin{aligned} b_0 = & -\frac{1}{48} \left[720 v - 7176 \sin(v) \cos(v)^6 v^2 + 14232 \sin(v) \cos(v)^4 v^2 \right. \\ & - 2304 \sin(v) \cos(v)^8 v^2 - 7200 \sin(v) \cos(v)^7 v^2 + 585 \sin(v) \cos(v)^2 v^2 \\ & - 2196 \sin(v) \cos(v)^3 v^2 - 3924 \cos(v) v^2 \sin(v) + 15432 \sin(v) \cos(v)^5 v^2 \\ & - 2112 \sin(v) \cos(v)^9 v^2 - 72 \cos(v) v + 960 \sin(v) \cos(v)^4 \\ & + 5760 \sin(v) \cos(v)^7 + 480 \sin(v) \cos(v)^6 - 13920 \sin(v) \cos(v)^5 \\ & + 3600 \sin(v) \cos(v)^3 + 3840 \sin(v) \cos(v)^9 - 1260 \sin(v) \cos(v)^2 \\ & + 720 \cos(v) \sin(v) - 4608 \cos(v)^{10} v + 512 \cos(v)^9 v^3 - 3072 \cos(v)^9 v \\ & + 384 \cos(v)^{10} v^3 - 8448 \cos(v)^8 v - 612 v^2 \sin(v) + 2577 \cos(v) v^3 \\ & + 1408 \cos(v)^8 v^3 + 1872 \cos(v)^7 v^3 - 4032 \cos(v)^7 v - 1008 \cos(v)^2 v \\ & + 1668 \cos(v)^2 v^3 - 592 \cos(v)^4 v^3 - 19488 \cos(v)^4 v + 1982 \cos(v)^3 v^3 \\ & - 4152 \cos(v)^3 v - 2832 \cos(v)^6 v^3 + 32832 \cos(v)^6 v - 5368 \cos(v)^5 v^3 \\ & \left. + 11328 \cos(v)^5 v - 180 \sin(v) - 36 v^3 \right] / \left(v^6 (\cos(v) + 1) \sin(v)^5 \right) \end{aligned} \quad (62)$$

$$\begin{aligned}
 b_1 = \frac{1}{12} & \left[36 v + 432 \sin(v) \cos(v)^6 v^2 + 2748 \sin(v) \cos(v)^4 v^2 - 1344 \sin(v) \cos(v)^8 \right. \\
 & v^2 - 1440 \sin(v) \cos(v)^7 v^2 - 1701 \sin(v) \cos(v)^2 v^2 + 2229 \sin(v) \cos(v)^3 v^2 \\
 & - 432 \cos(v) v^2 \sin(v) + 588 \sin(v) \cos(v)^5 v^2 + 576 \cos(v) v - 1200 \sin(v) \cos(v)^4 \\
 & - 1440 \sin(v) \cos(v)^6 + 240 \sin(v) \cos(v)^5 - 60 \sin(v) \cos(v)^3 + 720 \sin(v) \cos(v)^2 \\
 & - 180 \cos(v) \sin(v) + 256 \cos(v)^9 v^3 - 2688 \cos(v)^9 v - 1536 \cos(v)^8 v \\
 & - 135 v^2 \sin(v) + 75 \cos(v) v^3 + 352 \cos(v)^8 v^3 - 32 \cos(v)^7 v^3 + 3360 \cos(v)^7 v \\
 & - 576 \cos(v)^2 v + 1035 \cos(v)^2 v^3 - 975 \cos(v)^4 v^3 + 684 \cos(v)^4 v + 425 \cos(v)^3 v^3 \\
 & - 3504 \cos(v)^3 v - 196 \cos(v)^6 v^3 + 1392 \cos(v)^6 v - 724 \cos(v)^5 v^3 \\
 & + 2256 \cos(v)^5 v + 1920 \sin(v) \cos(v)^8 + 12 v^4 \sin(v) + 12 \sin(v) v^4 \cos(v)^5 \\
 & - 24 \sin(v) v^4 \cos(v)^3 + 12 \sin(v) \cos(v)^4 v^4 + 12 \sin(v) v^4 \cos(v) \\
 & \left. - 24 \sin(v) \cos(v)^2 v^4 + 99 v^3 \right] / \left(v^6 (\cos(v) + 1) \sin(v)^5 \right) \quad (63)
 \end{aligned}$$

$$\begin{aligned}
 b_2 = -\frac{1}{24} & \left[240 v - 2592 \sin(v) \cos(v)^6 v^2 + 3294 \sin(v) \cos(v)^4 v^2 - 2736 \sin(v) \right. \\
 & \cos(v)^7 v^2 + 435 \sin(v) \cos(v)^2 v^2 - 72 \sin(v) \cos(v)^3 v^2 - 1176 \cos(v) v^2 \sin(v) \\
 & + 3984 \sin(v) \cos(v)^5 v^2 - 72 \cos(v) v + 360 \sin(v) \cos(v)^4 + 2880 \sin(v) \cos(v)^7 \\
 & - 3840 \sin(v) \cos(v)^5 + 720 \sin(v) \cos(v)^3 - 300 \sin(v) \cos(v)^2 + 240 \cos(v) \sin(v) \\
 & - 4608 \cos(v)^8 v - 192 v^2 \sin(v) + 723 \cos(v) v^3 + 576 \cos(v)^8 v^3 + 864 \cos(v)^7 v^3 \\
 & - 2304 \cos(v)^7 v - 624 \cos(v)^2 v + 560 \cos(v)^2 v^3 - 284 \cos(v)^4 v^3 - 4416 \cos(v)^4 v \\
 & + 404 \cos(v)^3 v^3 - 984 \cos(v)^3 v - 800 \cos(v)^6 v^3 + 9408 \cos(v)^6 v \\
 & - 1676 \cos(v)^5 v^3 + 3360 \cos(v)^5 v + 48 v^4 \sin(v) + 48 \sin(v) v^4 \cos(v)^5 \\
 & - 96 \sin(v) v^4 \cos(v)^3 + 48 \sin(v) \cos(v)^4 v^4 + 48 \sin(v) v^4 \cos(v) \\
 & \left. - 96 \sin(v) \cos(v)^2 v^4 - 60 \sin(v) - 52 v^3 \right] / \left(v^6 (\cos(v) + 1) \sin(v)^5 \right) \quad (64)
 \end{aligned}$$

$$\begin{aligned}
 b_3 = \frac{1}{12} & \left[12 v - 624 \sin(v) \cos(v)^6 v^2 + 1152 \sin(v) \cos(v)^4 v^2 - 483 \sin(v) \cos(v)^2 v^2 \right. \\
 & + 759 \sin(v) \cos(v)^3 v^2 - 120 \cos(v) v^2 \sin(v) - 504 \sin(v) \cos(v)^5 v^2 + 192 \cos(v) v \\
 & \left. - 720 \sin(v) \cos(v)^4 + 480 \sin(v) \cos(v)^6 + 60 \sin(v) \cos(v)^3 + 240 \sin(v) \cos(v)^2 \right]
 \end{aligned}$$

$$\begin{aligned}
 & -60 \cos(v) \sin(v) - 45 v^2 \sin(v) - 23 \cos(v) v^3 + 192 \cos(v)^7 v^3 - 864 \cos(v)^7 v \\
 & -240 \cos(v)^2 v + 325 \cos(v)^2 v^3 - 537 \cos(v)^4 v^3 + 612 \cos(v)^4 v + 255 \cos(v)^3 v^3 \\
 & -1296 \cos(v)^3 v + 232 \cos(v)^6 v^3 - 384 \cos(v)^6 v - 424 \cos(v)^5 v^3 + 1968 \cos(v)^5 v \\
 & +24 v^4 \sin(v) + 24 \sin(v) v^4 \cos(v)^5 - 48 \sin(v) v^4 \cos(v)^3 + 24 \sin(v) \cos(v)^4 v^4 \\
 & +24 \sin(v) v^4 \cos(v) - 48 \sin(v) \cos(v)^2 v^4 + 25 v^3 \Big] / \left(v^6 (\cos(v) + 1) \sin(v)^5 \right) \quad (65)
 \end{aligned}$$

$$\begin{aligned}
 b_4 = & -\frac{1}{96} \Big[240 v - 576 \sin(v) \cos(v)^4 v^2 + 867 \sin(v) \cos(v)^2 v^2 + 1620 \sin(v) \\
 & \cos(v)^3 v^2 - 780 \cos(v) v^2 \sin(v) - 840 \sin(v) \cos(v)^5 v^2 - 216 \cos(v) v \\
 & +480 \sin(v) \cos(v)^5 - 720 \sin(v) \cos(v)^3 + 60 \sin(v) \cos(v)^2 + 240 \cos(v) \sin(v) \\
 & -156 v^2 \sin(v) + 507 \cos(v) v^3 - 1488 \cos(v)^2 v + 764 \cos(v)^2 v^3 - 992 \cos(v)^4 v^3 \\
 & +2208 \cos(v)^4 v - 814 \cos(v)^3 v^3 + 600 \cos(v)^3 v + 400 \cos(v)^6 v^3 - 960 \cos(v)^6 v \\
 & +352 \cos(v)^5 v^3 - 384 \cos(v)^5 v + 96 v^4 \sin(v) + 96 \sin(v) v^4 \cos(v)^5 \\
 & -192 \sin(v) v^4 \cos(v)^3 + 96 \sin(v) \cos(v)^4 v^4 + 96 \sin(v) v^4 \cos(v) \\
 & -192 \sin(v) \cos(v)^2 v^4 - 60 \sin(v) - 172 v^3 \Big] / \left(v^6 (\cos(v) + 1) \sin(v)^5 \right) \quad (66)
 \end{aligned}$$

For small values of $|v|$ the formulae given by (62)-(66) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned}
 b_0 = & \frac{17273}{72576} + \frac{290305}{456192} v^2 - \frac{5146457}{20756736} v^4 + \frac{7920822209}{125536739328} v^6 - \frac{9148045993}{776045297664} v^8 \\
 & + \frac{685438436621}{360429927137280} v^{10} - \frac{861866236422343}{6744004366665646080} v^{12} \\
 & + \frac{12600569860102927}{620448401733239439360} v^{14} + \frac{8921092027353637}{9776762693978318438400} v^{16} + \dots \\
 b_1 = & \frac{280997}{181440} - \frac{58061}{114048} v^2 + \frac{4155299}{23063040} v^4 - \frac{6171445871}{156920924160} v^6 \\
 & + \frac{579822819683}{106706228428800} v^8 - \frac{1422920786503}{6758061133824000} v^{10} + \frac{699661076305589}{12969239166664704000} v^{12} \\
 & + \frac{132022490052283}{20736911822635008000} v^{14} + \frac{164232944944655369}{122209533674728980480000} v^{16} + \dots
 \end{aligned}$$

$$\begin{aligned}
 b_2 = & -\frac{33961}{181440} + \frac{58061}{228096} v^2 - \frac{2172983}{34594560} v^4 + \frac{2064563873}{313841848320} v^6 \\
 & + \frac{2724781733}{15243746918400} v^8 + \frac{214673377381}{1930874609664000} v^{10} + \frac{462572594947933}{21075013645830144000} v^{12} \\
 & + \frac{4746565597278053}{1107943574523641856000} v^{14} + \frac{1041226049632616773}{1344304870422018785280000} v^{16} + \dots \\
 b_3 = & \frac{173531}{181440} - \frac{58061}{798336} v^2 + \frac{7205971}{1452971520} v^4 + \frac{139440391}{156920924160} v^6 + \frac{2163203479}{9700566220800} v^8 \\
 & + \frac{742343452211}{15768809312256000} v^{10} + \frac{1536752835474911}{168600109166641152000} v^{12} \\
 & + \frac{6413588385252487}{3877802510832746496000} v^{14} + \frac{2683426764236251339}{9410134092954131496960000} v^{16} + \dots \\
 b_4 = & \frac{45767}{725760} + \frac{58061}{6386688} v^2 + \frac{800491}{484323840} v^4 + \frac{393677303}{1255367393280} v^6 \\
 & + \frac{24946527743}{426824913715200} v^8 + \frac{3984093755203}{378451423494144000} v^{10} + \frac{32443259855269}{17747379912278016000} v^{12} \\
 & + \frac{1358692009638011}{4431774298094567424000} v^{14} + \frac{1874552699488763323}{37640536371816525987840000} v^{16} + \dots \quad (67)
 \end{aligned}$$

Appendix B

$$\begin{aligned} b_0 = & \frac{1}{48} \Big(-10800 + 832512 \sin(v) \cos(v)^8 v^5 - 606720 \sin(v) \cos(v)^8 v^3 \\ & + 3317760 \sin(v) \cos(v)^{10} v + 829440 \sin(v) \cos(v)^{10} v^3 + 400578 \sin(v) \cos(v)^3 v^5 \\ & - 694848 \sin(v) \cos(v)^6 v^5 - 438912 \sin(v) \cos(v)^2 v^5 + 223680 \sin(v) \cos(v)^6 v^3 \\ & - 780480 \sin(v) \cos(v)^4 v^3 - 233280 \sin(v) \cos(v)^2 v + 488160 \sin(v) \cos(v)^2 v^3 \\ & - 122880 \sin(v) \cos(v)^{12} v^3 + 253440 \sin(v) \cos(v)^{11} v + 125280 \sin(v) \cos(v) v \\ & + 289920 \sin(v) \cos(v)^7 v^3 + 43200 \sin(v) \cos(v)^4 v - 449280 \sin(v) \cos(v)^9 v^3 \\ & - 12288 \sin(v) \cos(v)^{14} v^5 - 7392 \sin(v) \cos(v)^7 v^5 + 19776 \sin(v) \cos(v)^{11} v^5 \\ & - 55296 \sin(v) \cos(v)^{10} v^5 - 61440 \sin(v) \cos(v)^{14} v^3 - 129480 \sin(v) \cos(v)^3 v^3 \\ & - 76032 \sin(v) \cos(v)^9 v^5 + 96000 \sin(v) \cos(v)^{11} v^3 - 5137920 \sin(v) \cos(v)^8 v \\ & - 51480 \sin(v) \cos(v) v^3 - 24576 \sin(v) \cos(v)^{12} v^5 + 244320 \sin(v) \cos(v)^5 v^3 \\ & - 368640 \sin(v) \cos(v)^{12} v + 2537280 \sin(v) \cos(v)^6 v + 1422720 \sin(v) \cos(v)^7 v \\ & - 1140480 \sin(v) \cos(v)^9 v + 2880 \sin(v) \cos(v)^4 v^5 - 348480 \sin(v) \cos(v)^3 v \\ & - 184320 \sin(v) \cos(v)^{14} v - 312480 \sin(v) \cos(v)^5 v - 125952 \sin(v) \cos(v)^5 v^5 \\ & - 12528 \sin(v) \cos(v) v^5 + 30240 \sin(v) v^3 + 25920 \sin(v) v + 50328 v^5 \sin(v) \\ & + 100608 v^4 \cos(v)^{13} + 276480 v^2 \cos(v)^{13} + 27648 \cos(v)^{13} v^6 + 14592 \cos(v)^{15} v^4 \\ & + 3072 \cos(v)^{15} v^6 + 512 \cos(v)^{14} v^6 + 46080 \cos(v)^{14} v^2 + 11904 \cos(v)^{14} v^4 \\ & + 74880 \cos(v)^{12} v^2 - 138240 \cos(v)^{11} v^6 - 1935360 \cos(v)^{11} v^2 \\ & - 1055808 \cos(v)^{11} v^4 - 630720 \cos(v)^{10} v^2 + 4078080 \cos(v)^9 v^2 \\ & + 915120 \cos(v)^8 v^2 - 2661120 \cos(v)^7 v^2 - 652680 \cos(v)^6 v^2 - 825120 \cos(v)^5 v^2 \\ & + 419040 \cos(v)^4 v^2 + 1339200 \cos(v)^3 v^2 - 158760 \cos(v)^2 v^2 - 272160 \cos(v) v^2 \\ & + 43344 \cos(v)^{12} v^4 + 5824 \cos(v)^{12} v^6 - 13536 \cos(v)^{10} v^6 - 71400 \cos(v)^{10} v^4 \\ & + 46080 \cos(v)^9 v^6 + 2659200 \cos(v)^9 v^4 - 678930 \cos(v)^8 v^4 - 54680 \cos(v)^8 v^6 \\ & + 71280 \cos(v)^7 v^6 - 1975740 \cos(v)^7 v^4 + 38780 \cos(v)^6 v^6 + 1035765 \cos(v)^6 v^4 \\ & + 241488 \cos(v)^5 v^6 + 642348 \cos(v)^5 v^4 - 561759 \cos(v)^4 v^4 + 85398 \cos(v)^4 v^6 \\ & - 308028 \cos(v)^3 v^6 - 608328 \cos(v)^3 v^4 + 271476 \cos(v)^2 v^4 - 30339 \cos(v)^2 v^6 \\ & + 223128 \cos(v) v^4 + 25920 \cos(v) + 314640 \cos(v)^4 + 60480 \cos(v)^3 \\ & + 92160 \cos(v)^{14} + 1116 v^6 - 23760 \cos(v)^2 + 184320 \cos(v)^{13} - 80640 \cos(v)^{12} \end{aligned}$$

$$\begin{aligned}
 & -12960 v^2 - 50400 v^4 - 184320 \cos(v)^{15} + 967680 \cos(v)^{11} - 489600 \cos(v)^{10} \\
 & -2304000 \cos(v)^9 + 1087200 \cos(v)^8 + 2001600 \cos(v)^7 - 889200 \cos(v)^6 \\
 & -751680 \cos(v)^5 \Big) / \Big[v^5 \sin(v)^5 \Big(8 \cos(v)^6 v^4 + 120 \cos(v)^6 v^2 + 720 \cos(v)^6 \\
 & -1800 \cos(v)^4 v^4 - 420 \cos(v)^4 v^2 - 60 \cos(v)^4 v^4 - 120 \sin(v) \cos(v)^3 v^3 \\
 & -600 \sin(v) \cos(v)^3 v + 126 \cos(v)^2 v^4 - 60 \cos(v)^2 v^2 + 1440 \cos(v)^2 \\
 & +435 \sin(v) \cos(v) v^3 + 600 \sin(v) \cos(v) v - 360 + 31 v^4 + 360 v^2 \Big) \Big] \quad (68)
 \end{aligned}$$

$$\begin{aligned}
 b_1 = \frac{1}{12} \Big(& 9216 \cos(v)^{13} v^5 \sin(v) - 3372 \cos(v)^4 \sin(v) v^7 + 768 \cos(v)^2 \sin(v) v^7 \\
 & +3048 \cos(v)^6 \sin(v) v^7 - 1734 \cos(v) v^6 + 372 \sin(v) v^7 \\
 & +138240 \cos(v)^{13} \sin(v) v - 912 \cos(v)^8 \sin(v) v^7 + 46080 \cos(v)^{13} \sin(v) v^3 \\
 & +96 \cos(v)^{10} \sin(v) v^7 - 10848 \sin(v) \cos(v)^8 v^5 + 68880 \sin(v) \cos(v)^8 v^3 \\
 & +48960 \sin(v) \cos(v)^{10} v + 13440 \sin(v) \cos(v)^{10} v^3 - 98352 \sin(v) \cos(v)^3 v^5 \\
 & +91524 \sin(v) \cos(v)^6 v^5 + 16146 \sin(v) \cos(v)^2 v^5 - 96600 \sin(v) \cos(v)^6 v^3 \\
 & -9540 \sin(v) \cos(v)^4 v^3 - 29160 \sin(v) \cos(v)^2 v + 29880 \sin(v) \cos(v)^2 v^3 \\
 & -7680 \sin(v) \cos(v)^{12} v^3 - 380160 \sin(v) \cos(v)^{11} v - 12960 \sin(v) \cos(v) v \\
 & -211680 \sin(v) \cos(v)^7 v^3 + 210600 \sin(v) \cos(v)^4 v + 103680 \sin(v) \cos(v)^9 v^3 \\
 & -381024 \sin(v) \cos(v)^7 v^5 - 25344 \sin(v) \cos(v)^{11} v^5 + 4704 \sin(v) \cos(v)^{10} v^5 \\
 & -96480 \sin(v) \cos(v)^3 v^3 + 89856 \sin(v) \cos(v)^9 v^5 - 126720 \sin(v) \cos(v)^{11} v^3 \\
 & +107280 \sin(v) \cos(v)^8 v - 36720 \sin(v) \cos(v) v^3 - 1536 \sin(v) \cos(v)^{12} v^5 \\
 & +321840 \sin(v) \cos(v)^5 v^3 - 23040 \sin(v) \cos(v)^{12} v - 309240 \sin(v) \cos(v)^6 v \\
 & +635040 \sin(v) \cos(v)^7 v + 51840 \sin(v) \cos(v)^9 v - 129555 \sin(v) \cos(v)^4 v^5 \\
 & +177120 \sin(v) \cos(v)^3 v - 609120 \sin(v) \cos(v)^5 v + 423792 \sin(v) \cos(v)^5 v^5 \\
 & +49896 \sin(v) \cos(v) v^5 + 1620 \sin(v) v^3 - 5400 \sin(v) v - 10125 v^5 \sin(v) \\
 & -10752 v^4 \cos(v)^{13} - 34560 v^2 \cos(v)^{13} - 768 \cos(v)^{13} v^6 - 4096 \cos(v)^{14} v^6 \\
 & -23040 \cos(v)^{14} v^2 - 16896 \cos(v)^{14} v^4 + 74880 \cos(v)^{12} v^2 + 1952 \cos(v)^{11} v^6 \\
 & +102240 \cos(v)^{11} v^2 + 26880 \cos(v)^{11} v^4 + 198720 \cos(v)^{10} v^2 - 99000 \cos(v)^9 v^2 \\
 & -977040 \cos(v)^8 v^2 + 68580 \cos(v)^7 v^2 + 1231920 \cos(v)^6 v^2 - 62820 \cos(v)^5 v^2 \\
 & -550800 \cos(v)^4 v^2 + 12060 \cos(v)^3 v^2 + 32400 \cos(v)^2 v^2 + 13500 \cos(v) v^2 \\
 & +54912 \cos(v)^{12} v^4 + 13312 \cos(v)^{12} v^6 - 15360 \cos(v)^{10} v^6 + 75456 \cos(v)^{10} v^4 \\
 & -3512 \cos(v)^9 v^6 - 35952 \cos(v)^9 v^4 - 473712 \cos(v)^8 v^4 + 85504 \cos(v)^8 v^6 \\
 & +29616 \cos(v)^7 v^6 + 188376 \cos(v)^7 v^4 - 196288 \cos(v)^6 v^6 + 389760 \cos(v)^6 v^4
 \end{aligned}$$

$$\begin{aligned}
& -45158 \cos(v)^5 v^6 - 245886 \cos(v)^5 v^4 - 252 \cos(v)^4 v^4 + 145008 \cos(v)^4 v^6 \\
& + 12989 \cos(v)^3 v^6 + 95379 \cos(v)^3 v^4 - 24948 \cos(v)^2 v^4 - 27648 \cos(v)^2 v^6 \\
& - 18045 \cos(v) v^4 + 10800 \cos(v) + 112320 \cos(v)^4 - 48240 \cos(v)^3 \\
& + 92160 \cos(v)^{14} + 10908 v^6 - 25920 \cos(v)^2 - 46080 \cos(v)^{13} - 299520 \cos(v)^{12} \\
& + 12960 v^2 - 4320 v^4 + 144000 \cos(v)^{11} + 311040 \cos(v)^{10} - 139680 \cos(v)^9 \\
& - 31680 \cos(v)^8 + 5040 \cos(v)^7 - 158400 \cos(v)^6 + 74160 \cos(v)^5) / \\
& \left[v^5 \left(900 \sin(v) \cos(v)^6 v^2 - 660 \sin(v) \cos(v)^8 v^2 + 8 \sin(v) \cos(v)^{10} v^4 \right. \right. \\
& + 64 \sin(v) \cos(v)^2 v^4 + 435 \cos(v) v^3 + 600 v \cos(v) + 360 v^2 \sin(v) + 31 v^4 \sin(v) \\
& + 120 \cos(v)^9 v^3 - 795 \cos(v)^7 v^3 + 1665 \cos(v)^5 v^3 - 1425 \cos(v)^3 v^3 \\
& + 600 \cos(v)^9 v - 2400 \cos(v)^7 v + 3600 \cos(v)^5 v - 2400 \cos(v)^3 v \\
& - 5040 \sin(v) \cos(v)^4 + 720 \sin(v) \cos(v)^{10} - 3240 \sin(v) \cos(v)^8 \\
& + 5760 \sin(v) \cos(v)^6 + 2160 \sin(v) \cos(v)^2 + 254 \sin(v) \cos(v)^6 v^4 \\
& - 780 \sin(v) \cos(v)^2 v^2 - 281 \sin(v) \cos(v)^4 v^4 + 60 \sin(v) \cos(v)^4 v^2 \\
& \left. \left. - 76 \sin(v) \cos(v)^8 v^4 + 120 \sin(v) \cos(v)^{10} v^2 - 360 \sin(v) \right) \right] \quad (69)
\end{aligned}$$

$$\begin{aligned}
b_2 = & \frac{1}{24} \left(-3600 + 140376 \cos(v)^4 \sin(v) v^7 + 26712 \cos(v)^7 \sin(v) v^7 \right. \\
& - 79152 \cos(v)^2 \sin(v) v^7 - 16560 \cos(v) \sin(v) v^7 - 8208 \cos(v)^9 \sin(v) v^7 \\
& + 4608 \cos(v)^{12} \sin(v) v^7 - 142464 \cos(v)^6 \sin(v) v^7 + 45768 \cos(v) v^6 \\
& + 19416 \sin(v) v^7 - 49968 \cos(v)^5 \sin(v) v^7 + 87936 \cos(v)^8 \sin(v) v^7 \\
& + 46872 \cos(v)^3 \sin(v) v^7 - 30720 \cos(v)^{10} \sin(v) v^7 - 143568 \sin(v) \cos(v)^8 v^5 \\
& - 334080 \sin(v) \cos(v)^8 v^3 + 1036800 \sin(v) \cos(v)^{10} v + 299520 \sin(v) \cos(v)^{10} v^3 \\
& + 222522 \sin(v) \cos(v)^3 v^5 + 402192 \sin(v) \cos(v)^6 v^5 + 50976 \sin(v) \cos(v)^2 v^5 \\
& + 377280 \sin(v) \cos(v)^6 v^3 - 457920 \sin(v) \cos(v)^4 v^3 - 77760 \sin(v) \cos(v)^2 v \\
& + 205920 \sin(v) \cos(v)^2 v^3 - 92160 \sin(v) \cos(v)^{12} v^3 + 69120 \sin(v) \cos(v)^{11} v \\
& + 34560 \sin(v) \cos(v) v + 322800 \sin(v) \cos(v)^7 v^3 + 95040 \sin(v) \cos(v)^4 v \\
& - 241440 \sin(v) \cos(v)^9 v^3 + 194340 \sin(v) \cos(v)^7 v^5 + 19008 \sin(v) \cos(v)^{11} v^5 \\
& + 80640 \sin(v) \cos(v)^{10} v^5 + 131880 \sin(v) \cos(v)^3 v^3 - 99912 \sin(v) \cos(v)^9 v^5 \\
& + 57600 \sin(v) \cos(v)^{11} v^3 - 1278720 \sin(v) \cos(v)^8 v - 50760 \sin(v) \cos(v) v^3 \\
& - 24192 \sin(v) \cos(v)^{12} v^5 - 220080 \sin(v) \cos(v)^5 v^3 - 276480 \sin(v) \cos(v)^{12} v \\
& + 492480 \sin(v) \cos(v)^6 v + 266400 \sin(v) \cos(v)^7 v - 262080 \sin(v) \cos(v)^9 v \\
& \left. - 417744 \sin(v) \cos(v)^4 v^5 - 119520 \sin(v) \cos(v)^3 v + 11520 \sin(v) \cos(v)^5 v \right)
\end{aligned}$$

$$\begin{aligned}
& -271572 \sin(v) \cos(v)^5 v^5 - 24696 \sin(v) \cos(v) v^5 + 1440 \sin(v) v^3 \\
& + 8640 \sin(v) v - 16344 v^5 \sin(v) + 68544 v^4 \cos(v)^{13} + 138240 v^2 \cos(v)^{13} \\
& + 24192 \cos(v)^{13} v^6 + 34560 \cos(v)^{12} v^2 - 140096 \cos(v)^{11} v^6 - 737280 \cos(v)^{11} v^2 \\
& - 366432 \cos(v)^{11} v^4 - 82080 \cos(v)^{10} v^2 + 1307520 \cos(v)^9 v^2 + 27360 \cos(v)^8 v^2 \\
& - 708480 \cos(v)^7 v^2 + 12600 \cos(v)^6 v^2 - 329760 \cos(v)^5 v^2 + 47520 \cos(v)^4 v^2 \\
& + 411840 \cos(v)^3 v^2 - 39240 \cos(v)^2 v^2 - 82080 \cos(v) v^2 + 26208 \cos(v)^{12} v^4 \\
& + 576 \cos(v)^{12} v^6 + 7464 \cos(v)^{10} v^6 - 83748 \cos(v)^{10} v^4 + 349808 \cos(v)^9 v^6 \\
& + 650472 \cos(v)^9 v^4 + 116364 \cos(v)^8 v^4 - 57944 \cos(v)^8 v^6 - 586248 \cos(v)^7 v^6 \\
& - 350460 \cos(v)^7 v^4 + 128708 \cos(v)^6 v^6 - 262479 \cos(v)^6 v^4 + 641024 \cos(v)^5 v^6 \\
& + 102228 \cos(v)^5 v^4 + 304923 \cos(v)^4 v^4 - 151308 \cos(v)^4 v^6 - 345788 \cos(v)^3 v^6 \\
& - 171528 \cos(v)^3 v^4 - 121188 \cos(v)^2 v^4 + 104867 \cos(v)^2 v^6 + 67176 \cos(v) v^4 \\
& + 8640 \cos(v) + 72720 \cos(v)^4 + 2880 \cos(v)^3 - 25748 v^6 - 720 \cos(v)^2 \\
& - 138240 \cos(v)^{13} + 69120 \cos(v)^{12} - 720 v^2 + 19920 v^4 + 529920 \cos(v)^{11} \\
& - 256320 \cos(v)^{10} - 789120 \cos(v)^9 + 365760 \cos(v)^8 + 561600 \cos(v)^7 \\
& - 246960 \cos(v)^6 - 175680 \cos(v)^5 + 1152 \cos(v)^{11} \sin(v) v^7) / \\
& \left[v^5 \left(900 \sin(v) \cos(v)^6 v^2 - 660 \sin(v) \cos(v)^8 v^2 + 8 \sin(v) \cos(v)^{10} v^4 \right. \right. \\
& + 64 \sin(v) \cos(v)^2 v^4 + 435 \cos(v) v^3 + 600 v \cos(v) + 360 v^2 \sin(v) + 31 v^4 \sin(v) \\
& + 120 \cos(v)^9 v^3 - 795 \cos(v)^7 v^3 + 1665 \cos(v)^5 v^3 - 1425 \cos(v)^3 v^3 \\
& + 600 \cos(v)^9 v - 2400 \cos(v)^7 v + 3600 \cos(v)^5 v - 2400 \cos(v)^3 v \\
& - 5040 \sin(v) \cos(v)^4 + 720 \sin(v) \cos(v)^{10} - 3240 \sin(v) \cos(v)^8 \\
& + 5760 \sin(v) \cos(v)^6 + 2160 \sin(v) \cos(v)^2 + 254 \sin(v) \cos(v)^6 v^4 \\
& - 780 \sin(v) \cos(v)^2 v^2 - 281 \sin(v) \cos(v)^4 v^4 + 60 \sin(v) \cos(v)^4 v^2 \\
& \left. \left. - 76 \sin(v) \cos(v)^8 v^4 + 120 \sin(v) \cos(v)^{10} v^2 - 360 \sin(v) \right) \right] \quad (70)
\end{aligned}$$

$$\begin{aligned}
b_3 = \frac{1}{12} & \left(-6744 \cos(v)^4 \sin(v) v^7 + 1536 \cos(v)^2 \sin(v) v^7 + 6096 \cos(v)^6 \sin(v) v^7 \right. \\
& + 1362 \cos(v) v^6 + 744 \sin(v) v^7 - 1824 \cos(v)^8 \sin(v) v^7 + 192 \cos(v)^{10} \sin(v) v^7 \\
& - 16944 \sin(v) \cos(v)^8 v^5 + 43440 \sin(v) \cos(v)^8 v^3 - 17280 \sin(v) \cos(v)^{10} v \\
& - 11520 \sin(v) \cos(v)^{10} v^3 - 92208 \sin(v) \cos(v)^3 v^5 + 50256 \sin(v) \cos(v)^6 v^5 \\
& + 12882 \sin(v) \cos(v)^2 v^5 - 50040 \sin(v) \cos(v)^6 v^3 + 23700 \sin(v) \cos(v)^4 v^3 \\
& - 2520 \sin(v) \cos(v)^2 v - 10920 \sin(v) \cos(v)^2 v^3 + 57600 \sin(v) \cos(v)^{11} v \\
& \left. - 4320 \sin(v) \cos(v) v - 171360 \sin(v) \cos(v)^7 v^3 + 45720 \sin(v) \cos(v)^4 v \right)
\end{aligned}$$

$$\begin{aligned}
& +55680 \sin(v) \cos(v)^9 v^3 - 260064 \sin(v) \cos(v)^7 v^5 - 19200 \sin(v) \cos(v)^{11} v^5 \\
& +1728 \sin(v) \cos(v)^{10} v^5 - 54240 \sin(v) \cos(v)^3 v^3 + 117120 \sin(v) \cos(v)^9 v^5 \\
& -3840 \sin(v) \cos(v)^{11} v^3 + 69840 \sin(v) \cos(v)^8 v - 6480 \sin(v) \cos(v)^3 v^3 \\
& +180240 \sin(v) \cos(v)^5 v^3 - 93960 \sin(v) \cos(v)^6 v + 332640 \sin(v) \cos(v)^7 v \\
& -230400 \sin(v) \cos(v)^9 v - 48297 \sin(v) \cos(v)^4 v^5 + 53280 \sin(v) \cos(v)^3 v \\
& -208800 \sin(v) \cos(v)^5 v + 235920 \sin(v) \cos(v)^5 v^5 + 28152 \sin(v) \cos(v)^5 v^5 \\
& +5340 \sin(v) v^3 - 1800 \sin(v) v - 5295 v^5 \sin(v) - 51840 \cos(v)^{12} v^2 \\
& +704 \cos(v)^{11} v^6 + 2880 \cos(v)^{11} v^2 + 10752 \cos(v)^{11} v^4 + 276480 \cos(v)^{10} v^2 \\
& -29880 \cos(v)^9 v^2 - 555120 \cos(v)^8 v^2 + 82620 \cos(v)^7 v^2 + 507600 \cos(v)^6 v^2 \\
& -89820 \cos(v)^5 v^2 - 192240 \cos(v)^4 v^2 + 36900 \cos(v)^3 v^2 + 10800 \cos(v)^2 v^2 \\
& -2700 \cos(v) v^2 - 34944 \cos(v)^{12} v^4 + 3072 \cos(v)^{12} v^6 - 27648 \cos(v)^{10} v^6 \\
& +174336 \cos(v)^{10} v^4 - 3416 \cos(v)^9 v^6 - 63504 \cos(v)^9 v^4 - 325008 \cos(v)^8 v^4 \\
& +96768 \cos(v)^8 v^6 + 3036 \cos(v)^7 v^6 + 139200 \cos(v)^7 v^4 - 147456 \cos(v)^6 v^6 \\
& +269808 \cos(v)^6 v^4 + 5302 \cos(v)^5 v^6 - 125286 \cos(v)^5 v^4 - 123396 \cos(v)^4 v^4 \\
& +104976 \cos(v)^4 v^6 - 7933 \cos(v)^3 v^6 + 46773 \cos(v)^3 v^4 + 52164 \cos(v)^2 v^4 \\
& -38448 \cos(v)^2 v^6 - 7935 \cos(v) v^4 + 3600 \cos(v) + 48960 \cos(v)^4 \\
& -20880 \cos(v)^3 + 10356 v^6 - 8640 \cos(v)^2 + 23040 \cos(v)^{12} + 4320 v^2 - 12960 v^4 \\
& -11520 \cos(v)^{11} - 92160 \cos(v)^{10} + 44640 \cos(v)^9 + 146880 \cos(v)^8 \\
& -68400 \cos(v)^7 - 118080 \cos(v)^6 + 52560 \cos(v)^5) / \\
& \left[v^5 \left(900 \sin(v) \cos(v)^6 v^2 - 660 \sin(v) \cos(v)^8 v^2 \right. \right. \\
& \quad + 8 \sin(v) \cos(v)^{10} v^4 + 64 \sin(v) \cos(v)^2 v^4 + 435 \cos(v) v^3 \\
& \quad + 600 v \cos(v) + 360 v^2 \sin(v) + 31 v^4 \sin(v) + 120 \cos(v)^9 v^3 - 795 \cos(v)^7 v^3 \\
& \quad + 1665 \cos(v)^5 v^3 - 1425 \cos(v)^3 v^3 + 600 \cos(v)^9 v - 2400 \cos(v)^7 v \\
& \quad + 3600 \cos(v)^5 v - 2400 \cos(v)^3 v - 5040 \sin(v) \cos(v)^4 + 720 \sin(v) \cos(v)^{10} \\
& \quad - 3240 \sin(v) \cos(v)^8 + 5760 \sin(v) \cos(v)^6 + 2160 \sin(v) \cos(v)^2 \\
& \quad + 254 \sin(v) \cos(v)^6 v^4 - 780 \sin(v) \cos(v)^2 v^2 - 281 \sin(v) \cos(v)^4 v^4 \\
& \quad \left. \left. + 60 \sin(v) \cos(v)^4 v^2 - 76 \sin(v) \cos(v)^8 v^4 + 120 \sin(v) \cos(v)^{10} v^2 - 360 \sin(v) \right) \right] \quad (71)
\end{aligned}$$

$$\begin{aligned}
b_4 = & -\frac{1}{96} \left(3600 - 26976 \cos(v)^4 \sin(v) v^7 + 6144 \cos(v)^2 \sin(v) v^7 \right. \\
& + 24384 \cos(v)^6 \sin(v) v^7 + 35808 \cos(v) v^6 + 2976 \sin(v) v^7 \\
& \left. - 7296 \cos(v)^8 \sin(v) v^7 + 768 \cos(v)^{10} \sin(v) v^7 - 9792 \sin(v) \cos(v)^8 v^5 \right)
\end{aligned}$$

$$\begin{aligned}
& +368640 \sin(v) \cos(v)^8 v^3 + 69120 \sin(v) \cos(v)^{10} v - 69120 \sin(v) \cos(v)^{10} v^3 \\
& -870 \sin(v) \cos(v)^3 v^5 + 76032 \sin(v) \cos(v)^6 v^5 + 152064 \sin(v) \cos(v)^2 v^5 \\
& -751680 \sin(v) \cos(v)^6 v^3 + 694080 \sin(v) \cos(v)^4 v^3 + 77760 \sin(v) \cos(v)^2 v \\
& -266400 \sin(v) \cos(v)^2 v^3 - 12960 \sin(v) \cos(v) v - 32640 \sin(v) \cos(v)^7 v^3 \\
& -267840 \sin(v) \cos(v)^4 v + 3840 \sin(v) \cos(v)^9 v^3 - 9696 \sin(v) \cos(v)^7 v^5 \\
& -1152 \sin(v) \cos(v)^{10} v^5 - 100200 \sin(v) \cos(v)^3 v^3 + 1344 \sin(v) \cos(v)^9 v^5 \\
& -276480 \sin(v) \cos(v)^8 v + 36360 \sin(v) \cos(v) v^3 + 92640 \sin(v) \cos(v)^5 v^3 \\
& +406080 \sin(v) \cos(v)^6 v + 92160 \sin(v) \cos(v)^7 v - 23040 \sin(v) \cos(v)^9 v \\
& -184896 \sin(v) \cos(v)^4 v^5 + 72000 \sin(v) \cos(v)^3 v - 128160 \sin(v) \cos(v)^5 v \\
& +20976 \sin(v) \cos(v)^5 v^5 - 17424 \sin(v) \cos(v) v^5 + 24480 \sin(v) v^3 \\
& -8640 \sin(v) v - 22536 v^5 \sin(v) + 3968 \cos(v)^{11} v^6 - 92160 \cos(v)^{11} v^2 \\
& +28896 \cos(v)^{11} v^4 + 17280 \cos(v)^{10} v^2 + 472320 \cos(v)^9 v^2 - 98640 \cos(v)^8 v^2 \\
& -933120 \cos(v)^7 v^2 + 209880 \cos(v)^6 v^2 + 874080 \cos(v)^5 v^2 - 203040 \cos(v)^4 v^2 \\
& -377280 \cos(v)^3 v^2 + 84600 \cos(v)^2 v^2 + 56160 \cos(v) v^2 - 192 \cos(v)^{10} v^6 \\
& +2352 \cos(v)^{10} v^4 - 26624 \cos(v)^9 v^6 - 193344 \cos(v)^9 v^4 - 10074 \cos(v)^8 v^4 \\
& +2168 \cos(v)^8 v^6 + 58992 \cos(v)^7 v^6 + 528372 \cos(v)^7 v^4 - 7916 \cos(v)^6 v^6 \\
& +4305 \cos(v)^6 v^4 - 26096 \cos(v)^5 v^6 - 730212 \cos(v)^5 v^4 + 39669 \cos(v)^4 v^4 \\
& +7974 \cos(v)^4 v^6 - 44428 \cos(v)^3 v^6 + 480984 \cos(v)^3 v^4 - 50172 \cos(v)^2 v^4 \\
& +2353 \cos(v)^2 v^6 - 114696 \cos(v) v^4 - 8640 \cos(v) + 52560 \cos(v)^4 \\
& +48960 \cos(v)^3 - 5332 v^6 - 20880 \cos(v)^2 - 10080 v^2 + 13920 v^4 \\
& +23040 \cos(v)^{11} - 11520 \cos(v)^{10} - 92160 \cos(v)^9 + 44640 \cos(v)^8 \\
& +146880 \cos(v)^7 - 68400 \cos(v)^6 - 118080 \cos(v)^5 \Big) / \Big[v^5 \Big(900 \sin(v) \cos(v)^6 v^2 \\
& -660 \sin(v) \cos(v)^8 v^2 + 8 \sin(v) \cos(v)^{10} v^4 + 64 \sin(v) \cos(v)^2 v^4 + 435 \cos(v) v^3 \\
& +600 v \cos(v) + 360 v^2 \sin(v) + 31 v^4 \sin(v) + 120 \cos(v)^9 v^3 - 795 \cos(v)^7 v^3 \\
& +1665 \cos(v)^5 v^3 - 1425 \cos(v)^3 v^3 + 600 \cos(v)^9 v - 2400 \cos(v)^7 v \\
& +3600 \cos(v)^5 v - 2400 \cos(v)^3 v - 5040 \sin(v) \cos(v)^4 + 720 \sin(v) \cos(v)^{10} \\
& -3240 \sin(v) \cos(v)^8 + 5760 \sin(v) \cos(v)^6 + 2160 \sin(v) \cos(v)^2 \\
& +254 \sin(v) \cos(v)^6 v^4 - 780 \sin(v) \cos(v)^2 v^2 - 281 \sin(v) \cos(v)^4 v^4 \\
& +60 \sin(v) \cos(v)^4 v^2 - 76 \sin(v) \cos(v)^8 v^4 + 120 \sin(v) \cos(v)^{10} v^2 - 360 \sin(v) \Big) \Big] \quad (72)
\end{aligned}$$

$$\begin{aligned}
 a_2 = & - \left(360 - 120 \sin(v) \cos(v)^6 v^3 + 405 \sin(v) \cos(v)^4 v^3 - 7200 \sin(v) \cos(v)^2 v \right. \\
 & - 90 \sin(v) \cos(v)^2 v^3 - 4200 \sin(v) \cos(v) v - 1200 \sin(v) \cos(v)^7 v^3 \\
 & + 8100 \sin(v) \cos(v)^4 v - 6690 \sin(v) \cos(v)^3 v^3 + 3525 \sin(v) \cos(v) v^3 \\
 & + 4680 \sin(v) \cos(v)^5 v^3 - 2400 \sin(v) \cos(v)^6 v + 4800 \sin(v) \cos(v)^7 v \\
 & + 13800 \sin(v) \cos(v)^3 v - 14400 \sin(v) \cos(v)^5 v - 1140 \sin(v) v^3 + 1500 \sin(v) v \\
 & - 3360 \cos(v)^8 v^2 + 480 \cos(v)^7 v^2 + 13440 \cos(v)^6 v^2 - 2700 \cos(v)^5 v^2 \\
 & - 19140 \cos(v)^4 v^2 + 5580 \cos(v)^3 v^2 + 10860 \cos(v)^2 v^2 - 3360 \cos(v) v^2 \\
 & + 192 \cos(v)^8 v^4 + 48 \cos(v)^7 v^4 - 896 \cos(v)^6 v^4 - 246 \cos(v)^5 v^4 + 1680 \cos(v)^4 v^4 \\
 & + 573 \cos(v)^3 v^4 - 1680 \cos(v)^2 v^4 - 690 \cos(v) v^4 + 1800 \cos(v) + 9000 \cos(v)^4 \\
 & - 6480 \cos(v)^3 - 3600 \cos(v)^2 - 1800 v^2 + 809 v^4 + 2880 \cos(v)^8 - 2880 \cos(v)^7 \\
 & \left. - 8640 \cos(v)^6 + 7560 \cos(v)^5 \right) / \\
 & \left(8 \cos(v)^6 v^4 + 120 \cos(v)^6 v^2 + 720 \cos(v)^6 \right. \\
 & - 1800 \cos(v)^4 - 420 \cos(v)^4 v^2 - 60 \cos(v)^4 v^4 - 120 \sin(v) \cos(v)^3 v^3 \\
 & - 600 \sin(v) \cos(v)^3 v + 126 \cos(v)^2 v^4 - 60 \cos(v)^2 v^2 + 1440 \cos(v)^2 \\
 & \left. + 435 \sin(v) \cos(v) v^3 + 600 \sin(v) \cos(v) v - 360 + 31 v^4 + 360 v^2 \right) \quad (73)
 \end{aligned}$$

For small values of $|v|$ the formulae given by (68)-(73) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned}
 b_0 = & \frac{17273}{72576} + \frac{58061}{76032} v^2 - \frac{928762181}{2490808320} v^4 + \frac{5566793867}{44834549760} v^6 - \frac{196859105291}{6097498767360} v^8 \\
 & + \frac{70799714119243}{8109673360588800} v^{10} - \frac{176491684172663863}{96342919523794944000} v^{12} \\
 & + \frac{4913676130972033213}{31022420086661971968000} v^{14} - \frac{39589661903200572089}{1240896803466478878720000} v^{16} + \dots \\
 b_1 = & \frac{280997}{181440} - \frac{58061}{95040} v^2 + \frac{1687695937}{6227020800} v^4 - \frac{1078024163}{14010796800} v^6 + \frac{16440524041}{1172595916800} v^8 \\
 & + \frac{148316364059}{405483668029440} v^{10} - \frac{6827282630651881}{12676699937341440000} v^{12} \\
 & + \frac{169060768980582727}{2769858936309104640000} v^{14} - \frac{60477846614652841307}{3102242008666197196800000} v^{16} + \dots \\
 b_2 = & -\frac{33961}{181440} + \frac{58061}{190080} v^2 - \frac{589105331}{6227020800} v^4 + \frac{1363181447}{112086374400} v^6 + \frac{20552199571}{15243746918400} v^8 \\
 & + \frac{10794171699811}{20274183401472000} v^{10} + \frac{12863028425460287}{240857298809487360000} v^{12} \\
 & + \frac{1833852717523296121}{77556050216654929920000} v^{14} + \frac{76765303497434207}{2169400060602777600000} v^{16} + \dots
 \end{aligned}$$

$$\begin{aligned}
 b_3 = & \frac{173531}{181440} - \frac{58061}{665280} v^2 + \frac{47009791}{6227020800} v^4 + \frac{29800801}{14010796800} v^6 + \frac{6264867143}{9700566220800} v^8 \\
 & + \frac{1662548783477}{10137091700736000} v^{10} + \frac{9930639794620043}{240857298809487360000} v^{12} \\
 & + \frac{181124896891621531}{19389012554163732480000} v^{14} + \frac{42359250984577014973}{217156940606633803776000000} v^{16} + \dots \\
 b_4 = & \frac{45767}{725760} + \frac{58061}{5322240} v^2 + \frac{61409317}{24908083200} v^4 + \frac{256452461}{448345497600} v^6 \\
 & + \frac{54602191981}{426824913715200} v^8 + \frac{88336917061}{3243869344235520} v^{10} + \frac{5123418702332951}{963429195237949440000} v^{12} \\
 & + \frac{280280526557119531}{310224200866619719680000} v^{14} + \frac{9830407697358330991}{86862776242653521510400000} v^{16} + \dots \\
 a_2 = & 2 - \frac{58061}{63866880} v^{12} - \frac{2399921}{87178291200} v^{14} - \frac{3552859}{99632332800} v^{16} + \dots \quad (74)
 \end{aligned}$$

Appendix C

The eight-step ninth algebraic order method developed by Jenkins [36]

$$\begin{aligned}
 \text{LTE}_{J9} = & h^{10} \left[\frac{31511}{518400} G^5 y(x) + \frac{31511}{103680} G^4 g(x) y(x) \right. \\
 & + G^3 \left[\frac{31511}{25920} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} y(x) + \frac{31511}{10368} \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \frac{31511}{51840} (g(x))^2 y(x) \right] \\
 & + G^2 \left[\frac{31511}{3456} g(x) y(x) \frac{d^2}{dx^2} g(x) + \frac{31511}{6480} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) \right. \\
 & \quad + \frac{31511}{8640} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + \frac{31511}{51840} (g(x))^3 y(x) \\
 & \quad + \frac{31511}{5184} \left(\frac{d}{dx} g(x) \right)^2 y(x) + \frac{1354973}{259200} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \left. \right] + G \\
 & \left[\frac{6648821}{518400} \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) + \frac{31511}{3456} (g(x))^2 y(x) \frac{d^2}{dx^2} g(x) \right. \\
 & \quad + \frac{5325359}{259200} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^3}{dx^3} g(x) + \frac{31511}{2592} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
 & \quad + \frac{31511}{1620} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x) + \frac{976841}{259200} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} y(x) \\
 & \quad + \frac{31511}{3240} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{31511}{8640} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) \\
 & \quad + \frac{913819}{518400} \left(\frac{d^6}{dx^6} g(x) \right) y(x) + \frac{1354973}{129600} g(x) y(x) \frac{d^4}{dx^4} g(x) \\
 & \quad \left. + \frac{31511}{103680} (g(x))^4 y(x) \right] \\
 & + \frac{31511}{6480} \left(\frac{d}{dx} g(x) \right)^3 \frac{d}{dx} y(x) + \frac{31511}{518400} \left(\frac{d^8}{dx^8} g(x) \right) y(x) \\
 & + \frac{31511}{64800} \left(\frac{d^7}{dx^7} g(x) \right) \frac{d}{dx} y(x) + \frac{31511}{5184} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
 & + \frac{220577}{12960} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{976841}{259200} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) \\
 & + \frac{5325359}{259200} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} g(x) + \frac{220577}{64800} \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) \\
 & + \frac{913819}{64800} \left(\frac{d}{dx} g(x) \right)^2 y(x) \frac{d^2}{dx^2} g(x) + \frac{31511}{1620} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d}{dx} g(x) +
 \end{aligned}$$

$$\begin{aligned} & + \frac{31511}{518400} (g(x))^5 y(x) + \frac{6648821}{518400} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 \\ & + \frac{31511}{6480} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{31511}{25920} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) \\ & + \frac{31511}{10368} (g(x))^3 y(x) \frac{d^2}{dx^2} g(x) + \frac{913819}{518400} g(x) y(x) \frac{d^6}{dx^6} g(x) \\ & + \frac{1354973}{259200} (g(x))^2 y(x) \frac{d^4}{dx^4} g(x) + \frac{1544039}{259200} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^4}{dx^4} g(x) \\ & + \frac{31511}{2880} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) + \frac{31511}{8100} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) \end{aligned} \quad (75)$$

The ten-step eleventh algebraic order method developed by Jenkins [36]

$$\begin{aligned}
 \text{LTE}_{J11} = & h^{12} \left[\frac{3055417}{53222400} G^6 y(x) + \frac{3055417}{8870400} G^5 g(x) y(x) \right. \\
 & + G^4 \left[\frac{58052923}{10644480} \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \frac{3055417}{1774080} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} y(x) \right. \\
 & \quad \left. \left. + \frac{3055417}{3548160} (g(x))^2 y(x) \right] \right. \\
 & + G^3 \left[\frac{3055417}{443520} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + \frac{3055417}{266112} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) \right. \\
 & \quad + \frac{113050429}{6652800} \left(\frac{d^4}{dx^4} g(x) \right) y(x) + \frac{39720421}{2661120} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
 & \quad \left. + \frac{3055417}{2661120} (g(x))^3 y(x) + \frac{58052923}{2661120} g(x) y(x) \frac{d^2}{dx^2} g(x) \right] \\
 & + G^2 \left[\frac{3055417}{88704} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{479700469}{26611200} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} y(x) \right. \\
 & \quad + \frac{3055417}{3548160} (g(x))^4 y(x) + \frac{3055417}{44352} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x) \\
 & \quad + \frac{3055417}{295680} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + \frac{3669555817}{53222400} \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) \\
 & \quad + \frac{730244663}{53222400} \left(\frac{d^6}{dx^6} g(x) \right) y(x) + \frac{956345521}{8870400} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^3}{dx^3} g(x) \\
 & \quad + \frac{39720421}{887040} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 + \frac{113050429}{2217600} g(x) y(x) \frac{d^4}{dx^4} g(x) \\
 & \quad \left. + \frac{58052923}{1774080} (g(x))^2 y(x) \frac{d^2}{dx^2} g(x) \right] + G \\
 & \quad \left[\frac{3055417}{88704} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \right. \\
 & \quad + \frac{479700469}{13305600} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) + \frac{730244663}{26611200} g(x) y(x) \frac{d^6}{dx^6} g(x) \\
 & \quad + \frac{131382931}{1663200} \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) + \frac{70274591}{26611200} \left(\frac{d^8}{dx^8} g(x) \right) y(x) \\
 & \quad + \frac{3055417}{22176} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d}{dx} g(x) + \\
 & \quad + \frac{223045441}{1330560} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\
 & \quad \left. + \frac{3055417}{88704} \left(\frac{d}{dx} g(x) \right)^3 \frac{d}{dx} y(x) + \frac{3055417}{415800} \left(\frac{d^7}{dx^7} g(x) \right) \frac{d}{dx} y(x) \right]
 \end{aligned}$$

$$\begin{aligned}
& + \frac{3055417}{8870400} (g(x))^5 y(x) + \frac{39720421}{302400} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^4}{dx^4} g(x) \\
& + \frac{3669555817}{26611200} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 + \frac{113050429}{2217600} (g(x))^2 y(x) \frac{d^4}{dx^4} g(x) \\
& + \frac{70274591}{665280} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) + \frac{956345521}{4435200} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} g(x) \\
& \quad + \frac{3055417}{443520} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) \\
& + \frac{39720421}{887040} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 + \frac{58052923}{2661120} (g(x))^3 y(x) \frac{d^2}{dx^2} g(x) \\
& \quad + \frac{2270174831}{13305600} \left(\frac{d}{dx} g(x) \right)^2 y(x) \frac{d^2}{dx^2} g(x) \\
& \quad + \frac{986899691}{13305600} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) \Big] \\
& \quad + \frac{39720421}{2661120} (g(x))^3 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{3055417}{88704} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 + \frac{3055417}{1774080} (g(x))^4 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) \\
& \quad + \frac{2270174831}{13305600} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& \quad \frac{d^2}{dx^2} g(x) + \frac{3055417}{44352} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& \quad \frac{d^2}{dx^2} g(x) + \frac{956345521}{8870400} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right) \\
& \quad \frac{d^3}{dx^3} g(x) + \frac{3669555817}{53222400} (g(x))^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 \\
& \quad + \frac{3055417}{266112} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\
& + \frac{39720421}{5322240} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^7}{dx^7} g(x) + \frac{94717927}{4435200} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) \\
& \quad + \frac{58052923}{985600} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) + \\
& \quad + \frac{51942089}{3548160} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^6}{dx^6} g(x) + \frac{3055417}{42240} \left(\frac{d}{dx} g(x) \right)^2 y(x) \frac{d^4}{dx^4} g(x) \\
& + \frac{21387919}{760320} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^6}{dx^6} g(x) + \frac{3055417}{36960} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) \\
& \quad + \frac{94717927}{591360} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right)^2 \\
& \quad + \frac{333040453}{2661120} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\
& + \frac{3055417}{190080} \left(\frac{d}{dx} g(x) \right)^4 y(x) + \frac{70274591}{26611200} g(x) y(x) \frac{d^8}{dx^8} g(x)
\end{aligned}$$

$$\begin{aligned} & + \frac{58052923}{10644480} (g(x))^4 y(x) \frac{d^2}{dx^2} g(x) + \frac{730244663}{53222400} (g(x))^2 y(x) \frac{d^6}{dx^6} g(x) \\ & + \frac{131382931}{1663200} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 + \frac{479700469}{26611200} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) \\ & + \frac{3055417}{415800} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^7}{dx^7} g(x) \\ & + \frac{113050429}{6652800} (g(x))^3 y(x) \frac{d^4}{dx^4} g(x) + \frac{70274591}{665280} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \frac{d}{dx} g(x) \\ & + \frac{223045441}{1330560} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \frac{d^2}{dx^2} g(x) \\ & + \frac{986899691}{13305600} g(x) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} g(x) \\ & + \frac{39720421}{302400} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \frac{d^2}{dx^2} g(x) \\ & + \frac{3055417}{53222400} \left(\frac{d^{10}}{dx^{10}} g(x) \right) y(x) + \frac{3055417}{5322240} \left(\frac{d^9}{dx^9} g(x) \right) \frac{d}{dx} y(x) \\ & + \frac{3055417}{78848} \left(\frac{d^2}{dx^2} g(x) \right)^3 y(x) + \frac{3055417}{253440} \left(\frac{d^4}{dx^4} g(x) \right)^2 y(x) \\ & + \frac{1078562201}{5322240} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \\ & \left. \frac{d^2}{dx^2} g(x) + \frac{3055417}{53222400} (g(x))^6 y(x) \right] (76) \end{aligned}$$

The twelve-step thirteenth algebraic order method developed by Jenkins [36]

$$\begin{aligned}
 \text{LTE}_{\text{J13}} = & h^{14} \left[\frac{12995034463}{237758976000} G^7 y(x) + \frac{12995034463}{33965568000} G^6 g(x) y(x) \right. \\
 & + G^5 \left[\frac{12995034463}{5660928000} \left(\frac{d}{dx} g(x) \right) \frac{d}{dx} y(x) + \frac{298885792649}{33965568000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \right. \\
 & \left. + \frac{12995034463}{11321856000} (g(x))^2 y(x) \right] + G^4 \left[\frac{298885792649}{6793113600} g(x) y(x) \frac{d^2}{dx^2} g(x) \right. \\
 & + \frac{1468438894319}{33965568000} \left(\frac{d^4}{dx^4} g(x) \right) y(x) + \frac{12995034463}{424569600} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
 & + \frac{12995034463}{1132185600} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + \frac{12995034463}{566092800} \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) \\
 & + \frac{12995034463}{6793113600} (g(x))^3 y(x) \left. \right] + G^3 \left[\frac{298885792649}{3396556800} (g(x))^2 y(x) \frac{d^2}{dx^2} g(x) \right. \\
 & + \frac{12995034463}{106142400} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 + \frac{12995034463}{566092800} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \\
 & \frac{d}{dx} g(x) + \frac{12995034463}{6793113600} (g(x))^4 y(x) + \frac{12995034463}{70761600} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x) \\
 & + \frac{922647446873}{2426112000} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^3}{dx^3} g(x) + \frac{8355807159709}{33965568000} \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) \\
 & + \frac{15113225080469}{237758976000} \left(\frac{d^6}{dx^6} g(x) \right) y(x) + \frac{12995034463}{141523200} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\
 & + \frac{1026607722577}{16982784000} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} y(x) + \frac{1468438894319}{8491392000} g(x) y(x) \frac{d^4}{dx^4} g(x) \left. \right] \\
 & + G^2 \left[\frac{33124342846187}{59439744000} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) + \frac{298885792649}{3396556800} (g(x))^3 y(x) \frac{d^2}{dx^2} g(x) \right. \\
 & + \frac{12995034463}{70761600} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 + \frac{922647446873}{808704000} g(x) y(x) \left(\frac{d}{dx} g(x) \right) \\
 & \frac{d^3}{dx^3} g(x) + \frac{122504189882701}{118879488000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^4}{dx^4} g(x) + \frac{8355807159709}{11321856000} \\
 & g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 + \frac{12995034463}{94348800} \left(\frac{d}{dx} g(x) \right)^3 \frac{d}{dx} y(x) \\
 & + \frac{12995034463}{566092800} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + \frac{8173876677227}{8491392000} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
 & \left. \frac{d^2}{dx^2} g(x) + \frac{1026607722577}{5660928000} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) + \frac{12995034463}{11321856000} (g(x))^5 y(x) \right]
 \end{aligned}$$

$$\begin{aligned}
& + \frac{12995034463}{23587200} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^2}{dx^2} g(x) + \frac{15113225080469}{79252992000} g(x) y(x) \frac{d^6}{dx^6} \\
& \quad g(x) + \frac{12995034463}{15163200} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{7030313644483}{237758976000} \\
& \quad \left(\frac{d^8}{dx^8} g(x) \right) y(x) + \frac{12995034463}{94348800} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{298885792649}{5943974400} \\
& \quad \left(\frac{d^7}{dx^7} g(x) \right) \frac{d}{dx} y(x) + \frac{1468438894319}{5660928000} (g(x))^2 y(x) \frac{d^4}{dx^4} g(x) + \frac{6224621507777}{9906624000} \\
& \quad \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) + \frac{4535267027587}{8491392000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) \Bigg] \\
& + G \left[\frac{37412704218977}{79252992000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^6}{dx^6} g(x) + \frac{6224621507777}{4953312000} g(x) \right. \\
& \quad y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 + \frac{3521654339473}{7925299200} \left(\frac{d^4}{dx^4} g(x) \right)^2 y(x) + \frac{870667309021}{237758976000} \\
& \quad \left(\frac{d^{10}}{dx^{10}} g(x) \right) y(x) + \frac{298885792649}{23775897600} \left(\frac{d^9}{dx^9} g(x) \right) \frac{d}{dx} y(x) + \frac{12995034463}{106142400} (g(x))^3 \\
& \quad y(x) \left(\frac{d}{dx} g(x) \right)^2 + \frac{12995034463}{47174400} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 + \frac{12995034463}{1132185600} \\
& \quad (g(x))^4 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + \frac{8173876677227}{4245696000} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \frac{d^2}{dx^2} g(x) \\
& \quad + \frac{12995034463}{23587200} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^2}{dx^2} g(x) + \frac{4769177647921}{5660928000} \\
& \quad \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) + \frac{63246832731421}{79252992000} \left(\frac{d^2}{dx^2} g(x) \right)^3 y(x) \\
& \quad + \frac{922647446873}{808704000} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x) + \frac{402846068353}{314496000} \\
& \quad \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{12995034463}{65318400} \left(\frac{d}{dx} g(x) \right)^4 y(x) \\
& \quad + \frac{1026607722577}{849139200} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) + \frac{1338488549689}{808704000} \\
& \quad \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right)^2 + \frac{24313709480273}{118879488000} \left(\frac{d}{dx} g(x) \right) y(x) \\
& \quad \frac{d^7}{dx^7} g(x) + \frac{12995034463}{141523200} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{7030313644483}{118879488000} \\
& \quad g(x) y(x) \frac{d^8}{dx^8} g(x) + \frac{1468438894319}{8491392000} (g(x))^3 y(x) \frac{d^4}{dx^4} g(x) \\
& \quad + \frac{8355807159709}{11321856000} (g(x))^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 + \frac{15113225080469}{79252992000} (g(x))^2 y(x) \\
& \quad \frac{d^6}{dx^6} g(x) + \frac{122504189882701}{59439744000} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^4}{dx^4} g(x) \\
& \quad + \frac{33124342846187}{29719872000} g(x) y(x) \left(\frac{d}{dx} g(x) \right) \frac{d^5}{dx^5} g(x) + \frac{298885792649}{2971987200}
\end{aligned}$$

$$\begin{aligned} & g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^7}{dx^7} g(x) + \frac{298885792649}{6793113600} (g(x))^4 y(x) \frac{d^2}{dx^2} g(x) + \frac{1026607722577}{5660928000} \\ & \quad (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) + \frac{12995034463}{10160640} \left(\frac{d}{dx} g(x) \right)^2 y(x) \frac{d^4}{dx^4} g(x) \\ & \quad + \frac{45235714965703}{59439744000} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) + \frac{6614472541667}{16982784000} \left(\frac{d}{dx} g(x) \right) \\ & \quad \left(\frac{d}{dx} y(x) \right) \frac{d^6}{dx^6} g(x) + \frac{153510342111419}{39626496000} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \frac{d^2}{dx^2} g(x) \\ & \quad + \frac{12995034463}{7581600} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^3}{dx^3} g(x) + \frac{4535267027587}{4245696000} g(x) \\ & \quad \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^4}{dx^4} g(x) + \frac{12995034463}{33965568000} (g(x))^6 y(x) \Bigg] + \\ & \quad \frac{12995034463}{5616000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \frac{d^2}{dx^2} g(x) + \frac{610766619761}{619164000} \\ & \quad \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \frac{d^2}{dx^2} g(x) + \frac{4769177647921}{5660928000} g(x) \\ & \quad \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \frac{d^2}{dx^2} g(x) + \frac{1026607722577}{849139200} g(x) \left(\frac{d}{dx} y(x) \right) \\ & \quad \left(\frac{d^4}{dx^4} g(x) \right) \frac{d^3}{dx^3} g(x) + \frac{24313709480273}{118879488000} g(x) y(x) \left(\frac{d^7}{dx^7} g(x) \right) \frac{d}{dx} g(x) \\ & \quad + \frac{12995034463}{424569600} (g(x))^4 y(x) \left(\frac{d}{dx} g(x) \right)^2 + \frac{12995034463}{65318400} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^4 \\ & \quad + \frac{12995034463}{94348800} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 + \frac{12995034463}{5660928000} (g(x))^5 \left(\frac{d}{dx} y(x) \right) \\ & \quad \frac{d}{dx} g(x) + \frac{142945379093}{80870400} \left(\frac{d^2}{dx^2} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) + \frac{142945379093}{377395200} \\ & \quad \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) + \frac{298885792649}{23775897600} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^9}{dx^9} g(x) \\ & \quad + \frac{63246832731421}{79252992000} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^3 + \frac{8355807159709}{33965568000} (g(x))^3 y(x) \\ & \quad \left(\frac{d^2}{dx^2} g(x) \right)^2 + \frac{298885792649}{5943974400} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^7}{dx^7} g(x) + \frac{122504189882701}{118879488000} \\ & \quad (g(x))^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^4}{dx^4} g(x) + \frac{33124342846187}{59439744000} (g(x))^2 y(x) \\ & \quad \left(\frac{d}{dx} g(x) \right) \frac{d^5}{dx^5} g(x) + \frac{6614472541667}{16982784000} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^6}{dx^6} g(x) \right) \frac{d}{dx} g(x) \\ & \quad + \frac{1026607722577}{16982784000} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) + \frac{153510342111419}{39626496000} g(x) \\ & \quad y(x) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^3}{dx^3} g(x) + \frac{10668923294123}{7925299200} \left(\frac{d}{dx} g(x) \right) \end{aligned}$$

$$\begin{aligned} & y(x) \left(\frac{d^4}{dx^4} g(x) \right) \frac{d^3}{dx^3} g(x) + \frac{12995034463}{70761600} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \\ & \left(\frac{d}{dx} g(x) \right) \frac{d^2}{dx^2} g(x) + \frac{922647446873}{2426112000} (g(x))^3 y(x) \left(\frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x) \\ & + \frac{12995034463}{18289152} \left(\frac{d}{dx} g(x) \right)^3 y(x) \frac{d^3}{dx^3} g(x) + \frac{5211008819663}{19813248000} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\ & \frac{d^6}{dx^6} g(x) + \frac{2430071444581}{8491392000} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^6}{dx^6} g(x) + \frac{1468438894319}{33965568000} \\ & (g(x))^4 y(x) \frac{d^4}{dx^4} g(x) + \frac{3521654339473}{7925299200} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right)^2 \\ & + \frac{6224621507777}{9906624000} (g(x))^2 y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 + \frac{870667309021}{237758976000} g(x) y(x) \frac{d^{10}}{dx^{10}} g(x) \\ & + \frac{142945379093}{3302208000} \left(\frac{d^5}{dx^5} g(x) \right)^2 y(x) + \frac{1572399170023}{9906624000} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\ & \frac{d^7}{dx^7} g(x) + \frac{142945379093}{163296000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 + \frac{3287743719139}{59439744000} \\ & \left(\frac{d^3}{dx^3} g(x) \right) y(x) \frac{d^7}{dx^7} g(x) + \frac{142945379093}{176904000} \left(\frac{d}{dx} g(x) \right)^3 \left(\frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x) \\ & + \frac{12995034463}{237758976000} \left(\frac{d^{12}}{dx^{12}} g(x) \right) y(x) + \frac{12995034463}{19813248000} \left(\frac{d^{11}}{dx^{11}} g(x) \right) \frac{d}{dx} y(x) \\ & + \frac{376855999427}{29719872000} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^9}{dx^9} g(x) + \frac{25353312237313}{19813248000} \left(\frac{d}{dx} g(x) \right)^2 \\ & y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 + \frac{298885792649}{471744000} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) \\ & + \frac{2430071444581}{79252992000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^8}{dx^8} g(x) + \frac{298885792649}{33965568000} (g(x))^5 y(x) \frac{d^2}{dx^2} g(x) \\ & + \frac{5938730749591}{4245696000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right)^2 + \frac{60180004598153}{79252992000} \\ & \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) \frac{d^4}{dx^4} g(x) + \frac{12995034463}{10160640} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \frac{d^4}{dx^4} g(x) \\ & + \frac{12995034463}{15163200} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^3}{dx^3} g(x) + \frac{4535267027587}{8491392000} \\ & (g(x))^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^4}{dx^4} g(x) + \frac{1338488549689}{808704000} g(x) \left(\frac{d}{dx} y(x) \right) \\ & \left(\frac{d}{dx} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right)^2 + \frac{402846068353}{314496000} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^2 \\ & \frac{d^3}{dx^3} g(x) + \frac{37412704218977}{79252992000} g(x) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \frac{d^2}{dx^2} g(x) + \frac{45235714965703}{59439744000} \\ & g(x) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \frac{d^3}{dx^3} g(x) + \frac{8173876677227}{8491392000} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\ & \frac{d^2}{dx^2} g(x) + \frac{6146651300999}{79252992000} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \frac{d^6}{dx^6} g(x) + \frac{792697102243}{13208832000} \left(\frac{d}{dx} g(x) \right) \end{aligned}$$

$$\begin{aligned} & \left(\frac{d}{dx} y(x) \right) \frac{d^8}{dx^8} g(x) + \frac{12995034463}{566092800} (g(x))^4 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\ & + \frac{7030313644483}{237758976000} (g(x))^2 y(x) \frac{d^8}{dx^8} g(x) + \frac{15113225080469}{237758976000} \\ & \left. (g(x))^3 y(x) \frac{d^6}{dx^6} g(x) + \frac{12995034463}{237758976000} (g(x))^7 y(x) \right] \end{aligned} \quad (77)$$

The new proposed method developed in paragraph 3.1 (see in Appendix B for details)

$$\begin{aligned}
 \text{LTE}_{\text{PLD1234}} = & h^{12} \left[G^3 \left(-\frac{58061}{1995840} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \right) + G^2 \left(-\frac{58061}{71280} \left(\frac{d}{dx} g(x) \right) \right. \right. \\
 & y(x) \frac{d^3}{dx^3} g(x) - \frac{58061}{399168} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x) - \frac{58061}{532224} g(x) y(x) \\
 & \left(\frac{d}{dx} g(x) \right)^2 - \frac{58061}{798336} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) - \frac{2728867}{7983360} g(x) y(x) \frac{d^4}{dx^4} g(x) \\
 & - \frac{58061}{798336} (g(x))^2 y(x) \frac{d^2}{dx^2} g(x) - \frac{58061}{498960} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} y(x) - \frac{2148257}{3991680} \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) \\
 & - \frac{754793}{3991680} \left(\frac{d^6}{dx^6} g(x) \right) y(x) \left. \right) + G \left(-\frac{290305}{199584} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^2}{dx^2} g(x) \right. \\
 & - \frac{59977013}{15966720} g(x) y(x) \left(\frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x) - \frac{1103159}{399168} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\
 & - \frac{52196839}{15966720} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^4}{dx^4} g(x) - \frac{8767211}{2661120} \left(\frac{d}{dx} g(x) \right)^2 y(x) \frac{d^2}{dx^2} g(x) \\
 & - \frac{2728867}{1596672} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) - \frac{174183}{98560} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) \\
 & - \frac{754793}{3193344} (g(x))^3 y(x) \frac{d^2}{dx^2} g(x) - \frac{3077233}{5322240} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) - \frac{58061}{114048} (g(x))^2 y \\
 & (x) \left(\frac{d}{dx} g(x) \right)^2 - \frac{26069389}{10644480} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 - \frac{13295969}{15966720} (g(x))^2 y(x) \frac{d^4}{dx^4} g(x) \\
 & - \frac{58061}{1596672} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) - \frac{2148257}{3548160} g(x) y(x) \frac{d^6}{dx^6} g(x) \\
 & - \frac{290305}{798336} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) - \frac{58061}{31933440} (g(x))^5 y(x) \\
 & - \frac{58061}{362880} \left(\frac{d^7}{dx^7} g(x) \right) \frac{d}{dx} y(x) - \frac{7954357}{3991680} \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) \\
 & - \frac{290305}{798336} \left(\frac{d}{dx} g(x) \right)^3 \frac{d}{dx} y(x) - \frac{2380501}{31933440} \left(\frac{d^8}{dx^8} g(x) \right) y(x) \left. \right) \\
 & - \frac{43139323}{7983360} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
 & \frac{d^2}{dx^2} g(x) - \frac{290305}{133056} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)
 \end{aligned}$$

$$\begin{aligned}
& \frac{d^2}{dx^2}g(x) - \frac{1103159}{6386688}(g(x))^4y(x)\frac{d^2}{dx^2}g(x) \\
& - \frac{9115577}{15966720}(g(x))^2\left(\frac{d}{dx}y(x)\right)\frac{d^5}{dx^5}g(x) \\
& - \frac{69731261}{31933440}(g(x))^2y(x)\left(\frac{d^2}{dx^2}g(x)\right)^2 \\
& - \frac{58061}{249480}g(x)\left(\frac{d}{dx}y(x)\right)\frac{d^7}{dx^7}g(x) - \frac{1335403}{15966720}g(x)y(x)\frac{d^8}{dx^8}g(x) \\
& - \frac{2496623}{997920}g(x)y(x)\left(\frac{d^3}{dx^3}g(x)\right)^2 - \frac{13876579}{31933440}(g(x))^2y(x)\frac{d^6}{dx^6}g(x) \\
& - \frac{2148257}{3991680}(g(x))^3y(x)\frac{d^4}{dx^4}g(x) - \frac{1103159}{591360}\left(\frac{d^2}{dx^2}g(x)\right)\left(\frac{d}{dx}y(x)\right)\frac{d^5}{dx^5}g(x) \\
& - \frac{987037}{2128896}\left(\frac{d^2}{dx^2}g(x)\right)y(x)\frac{d^6}{dx^6}g(x) - \frac{754793}{3193344}\left(\frac{d}{dx}g(x)\right)y(x)\frac{d^7}{dx^7}g(x) \\
& - \frac{6328649}{1596672}\left(\frac{d}{dx}g(x)\right)^2\left(\frac{d}{dx}y(x)\right)\frac{d^3}{dx^3}g(x) \\
& - \frac{406427}{456192}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}y(x)\right)\frac{d^6}{dx^6}g(x) - \frac{58061}{22176}\left(\frac{d^3}{dx^3}g(x)\right)\left(\frac{d}{dx}y(x)\right)\frac{d^4}{dx^4}g(x) \\
& - \frac{58061}{25344}\left(\frac{d}{dx}g(x)\right)^2y(x)\frac{d^4}{dx^4}g(x) - \frac{1799891}{354816}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}y(x)\right)\left(\frac{d^2}{dx^2}g(x)\right)^2 \\
& - \frac{1799891}{2661120}\left(\frac{d^3}{dx^3}g(x)\right)y(x)\frac{d^5}{dx^5}g(x) - \frac{290305}{266112}g(x)\left(\frac{d}{dx}y(x)\right)\left(\frac{d}{dx}g(x)\right)^3 \\
& - \frac{58061}{1064448}(g(x))^4\left(\frac{d}{dx}y(x)\right)\frac{d}{dx}g(x) - \frac{754793}{1596672}(g(x))^3y(x)\left(\frac{d}{dx}g(x)\right)^2 \\
& - \frac{290305}{236544}\left(\frac{d^2}{dx^2}g(x)\right)^3y(x) - \frac{58061}{152064}\left(\frac{d^4}{dx^4}g(x)\right)^2y(x) \\
& - \frac{58061}{114048}\left(\frac{d}{dx}g(x)\right)^4y(x) - \frac{20495533}{3193344}\left(\frac{d}{dx}g(x)\right)y(x)\left(\frac{d^3}{dx^3}g(x)\right) \\
& \frac{d^2}{dx^2}g(x) - \frac{18173093}{5322240}(g(x))^2y(x)\left(\frac{d}{dx}g(x)\right) \\
& \frac{d^3}{dx^3}g(x) - \frac{1335403}{399168}g(x)\left(\frac{d}{dx}y(x)\right)\left(\frac{d^4}{dx^4}g(x)\right)\frac{d}{dx}g(x) \\
& - \frac{4238453}{798336}g(x)\left(\frac{d}{dx}y(x)\right)\left(\frac{d^3}{dx^3}g(x)\right)\frac{d^2}{dx^2}g(x) \\
& - \frac{18753703}{7983360}g(x)y(x)\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}g(x) \\
& - \frac{754793}{181440}g(x)y(x)\left(\frac{d^4}{dx^4}g(x)\right)\frac{d^2}{dx^2}g(x) - \frac{58061}{31933440}(g(x))^6y(x) \\
& - \frac{58061}{31933440}\left(\frac{d^{10}}{dx^{10}}g(x)\right)y(x) - \frac{58061}{3193344}\left(\frac{d^9}{dx^9}g(x)\right)\frac{d}{dx}y(x) \\
& - \frac{290305}{798336}(g(x))^3\left(\frac{d}{dx}y(x)\right)\frac{d^3}{dx^3}g(x) \Big] (78)
\end{aligned}$$

The new proposed method developed in paragraph 3.2

$$\begin{aligned}
 \text{LTE}_{\text{PLD12345}} = h^{12} & \left[G^2 \left[-\frac{58061}{133056} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^3}{dx^3} g(x) - \frac{58061}{332640} g(x) \right. \right. \\
 & y(x) \frac{d^4}{dx^4} g(x) - \frac{58061}{399168} \left(\frac{d^6}{dx^6} g(x) \right) y(x) - \frac{58061}{997920} \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} y(x) \\
 & \left. - \frac{58061}{199584} \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) \right] + G \left[-\frac{1799891}{798336} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \right. \\
 & - \frac{58061}{66528} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^2}{dx^2} g(x) - \frac{58061}{18480} g(x) y(x) \left(\frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x) \\
 & - \frac{4586819}{1596672} \left(\frac{d}{dx} g(x) \right)^2 y(x) \frac{d^2}{dx^2} g(x) - \frac{1103159}{798336} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) \\
 & - \frac{58061}{177408} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 - \frac{13179847}{7983360} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) \\
 & - \frac{4935185}{1596672} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^4}{dx^4} g(x) - \frac{58061}{399168} (g(x))^3 y(x) \frac{d^2}{dx^2} g(x) - \frac{1799891}{2661120} \\
 & (g(x))^2 y(x) \frac{d^4}{dx^4} g(x) - \frac{58061}{266112} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) - \frac{1103159}{1995840} g(x) y(x) \\
 & \frac{d^6}{dx^6} g(x) - \frac{58061}{124740} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) - \frac{4122331}{1995840} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 \\
 & - \frac{58061}{266112} \left(\frac{d}{dx} g(x) \right)^3 \frac{d}{dx} y(x) - \frac{58061}{798336} \left(\frac{d^8}{dx^8} g(x) \right) y(x) - \frac{754793}{399168} \\
 & \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) - \frac{58061}{399168} \left(\frac{d^7}{dx^7} g(x) \right) \frac{d}{dx} y(x) \left. \right] - \frac{20495533}{3193344} \left(\frac{d}{dx} g(x) \right) \\
 & y(x) \left(\frac{d^3}{dx^3} g(x) \right) \frac{d^2}{dx^2} g(x) - \frac{754793}{1596672} (g(x))^3 y(x) \left(\frac{d}{dx} g(x) \right)^2 - \frac{290305}{266112} g(x) \\
 & \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 - \frac{58061}{1064448} (g(x))^4 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) - \frac{18753703}{7983360} g(x) \\
 & y(x) \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} g(x) - \frac{754793}{181440} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \frac{d^2}{dx^2} g(x) - \frac{43139323}{7983360} \\
 & g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \frac{d^2}{dx^2} g(x) - \frac{290305}{133056} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
 & \frac{d^2}{dx^2} g(x) - \frac{18173093}{5322240} (g(x))^2 y(x) \left(\frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x) - \frac{1335403}{399168} g(x) \\
 & \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \frac{d}{dx} g(x) - \frac{4238453}{798336} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \frac{d^2}{dx^2} g(x) \\
 & - \frac{6328649}{1596672} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) - \frac{58061}{114048} \left(\frac{d}{dx} g(x) \right)^4 y(x) \\
 & - \frac{2496623}{997920} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 - \frac{1103159}{6386688} (g(x))^4 y(x) \frac{d^2}{dx^2} g(x)
 \end{aligned}$$

$$\begin{aligned}
& -\frac{1335403}{15966720} g(x) y(x) \frac{d^8}{dx^8} g(x) - \frac{69731261}{31933440} (g(x))^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 \\
& -\frac{987037}{2128896} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^6}{dx^6} g(x) - \frac{58061}{31933440} \left(\frac{d^{10}}{dx^{10}} g(x) \right) y(x) \\
& -\frac{58061}{3193344} \left(\frac{d^9}{dx^9} g(x) \right) \frac{d}{dx} y(x) - \frac{290305}{236544} \left(\frac{d^2}{dx^2} g(x) \right)^3 y(x) \\
& -\frac{58061}{152064} \left(\frac{d^4}{dx^4} g(x) \right)^2 y(x) - \frac{290305}{798336} (g(x))^3 \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\
& -\frac{2148257}{3991680} (g(x))^3 y(x) \frac{d^4}{dx^4} g(x) - \frac{13876579}{31933440} (g(x))^2 y(x) \frac{d^6}{dx^6} g(x) \\
& -\frac{9115577}{15966720} (g(x))^2 \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) \\
& -\frac{58061}{249480} g(x) \left(\frac{d}{dx} y(x) \right) \frac{d^7}{dx^7} g(x) - \frac{1799891}{354816} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right)^2 \\
& -\frac{58061}{25344} \left(\frac{d}{dx} g(x) \right)^2 y(x) \frac{d^4}{dx^4} g(x) - \frac{406427}{456192} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^6}{dx^6} g(x) \\
& -\frac{58061}{22176} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^4}{dx^4} g(x) - \frac{1103159}{591360} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) \\
& -\frac{1799891}{2661120} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \frac{d^5}{dx^5} g(x) - \frac{754793}{3193344} \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^7}{dx^7} g(x) \\
& -\frac{58061}{31933440} (g(x))^6 y(x) \Big] (79)
\end{aligned}$$

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] I. Prigogine, Stuart Rice (Eds.), *New Methods in Computational Quantum Mechanics*, Wiley, New York, 1997.
- [4] G. Herzberg, *Spectra of Diatomic Molecules*, Van Nostrand, Toronto, 1950.
- [5] T. E. Simos, Atomic structure computations in chemical modelling: Applications and theory, in: A. Hinchliffe (Ed.), *Chemical Modelling: Applications and Theory*, Roy. Soc. Chem., Cambridge, 2000, pp. 38–142.
- [6] T. E. Simos, Numerical methods for 1D, 2D and 3D differential equations arising in chemical problems, in: A. Hinchliffe (Ed.), *Chemical Modelling: Applications and Theory*, Roy. Soc. Chem., Cambridge, 2002, pp. 170–270.

- [7] T. E. Simos, *Numerical Solution of Ordinary Differential Equations with Periodical Solution*, PhD Thesis, National Technical University of Athens, Greece, 1990 (in Greek).
- [8] J. R. Dormand, M. E. A. El-Mikkawy, P. J. Prince, Families of Runge–Kutta–Nyström formulae, *IMA J. Numer. Anal.* **7** (1987) 235–250.
- [9] J. R. Dormand, P. J. Prince, A family of embedded Runge–Kutta formulae, *J. Comput. Appl. Math.* **6** (1980) 19–26.
- [10] T. E. Simos, J. Vigo–Aguiar, A modified Runge–Kutta method with phase-lag of order infinity for the numerical solution of the of Schrödinger equation and related problems, *Comput. Chem.* **25** (2001) 275–281.
- [11] T. E. Simos, J. Vigo–Aguiar, A modified phase-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **30** (2001) 121–131.
- [12] T. E. Simos, P. S. Williams, A new Runge–Kutta–Nyström method with phase-lag of order infinity for the numerical solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **45** (2002) 123–137.
- [13] C. Tsitouras, T. E. Simos, Optimized Runge–Kutta pairs for problems with oscillating solutions, *J. Comp. Appl. Math.* **147** (2002) 397–409.
- [14] Z. A. Anastassi, T. E. Simos, Special optimized Runge–Kutta methods for IVPs with oscillating solutions, *Int. J. Mod. Phys. C* **15** (2004) 1–15.
- [15] Z. A. Anastassi, T. E. Simos, A dispersive-fitted and dissipative-fitted explicit Runge–Kutta method for the numerical solution of orbital problems, *New Astronomy* **10** (2004) 31–37.
- [16] K. Tselios, T. E. Simos, Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics, *J. Comp. Appl. Math.* **175** (2005) 173–181.
- [17] Z. A. Anastassi, T. E. Simos, An optimized Runge–Kutta method for the solution of orbital problems, *J. Comp. Appl. Math.* **175** (2005) 1–9.
- [18] K. Tselios, T. E. Simos, Optimized Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics, *Phys. Lett. A* **363** (2007) 38–47.
- [19] T. V. Triantafyllidis, Z. A. Anastassi, T. E. Simos, Two optimized Runge–Kutta methods for the solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 753–771.

- [20] D. F. Papadopoulos, Z. A. Anastassi, T. E. Simos, A phase-fitted Runge-Kutta-Nystrom method for the numerical solution of initial value problems with oscillating solutions, *Comput. Phys. Commun.* **180** (2009) 1839–1846.
- [21] A. A. Kosti, Z. A. Anastassi, T. E. Simos, An optimized explicit Runge-Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems, *J. Math. Chem.* **47** (2010) 315–330.
- [22] D. F. Papadopoulos, Z. A. Anastassi, T. E. Simos, A modified phase-fitted and amplification-fitted Runge-Kutta-Nyström method for the numerical solution of the radial Schrödinger equation, *J. Mol. Model.* **16** (2010) 1339–1346.
- [23] D. F. Papadopoulos, Z. A. Anastassi, T. E. Simos, The use of phase-Lag and amplification error derivatives in the numerical integration of ODES with oscillating solutions, *International Conference on Numerical Analysis and Applied Mathematics*, Rethymno, Greece, **1168** (2009) 547–549.
- [24] D. F. Papadopoulos, Z. A. Anastassi, T. E. Simos, A zero dispersion RKN method for the numerical integration of initial value problems with oscillating solutions, *International Conference on Numerical Analysis and Applied Mathematics*, Rethymno, Greece, **1168** (2009) 550–553.
- [25] T. Monovasilis, Z. Kalogiratu, T. E. Simos, A phase-fitted symplectic partitioned Runge-Kutta methods for the numerical solution of the Schrödinger equation, *International Conference on Numerical Analysis and Applied Mathematics*, Rethymno, Greece, **1168** (2009) 1595–1599.
- [26] D. F. Papadopoulos, Z. A. Anastassi, T. E. Simos, An optimized Runge-Kutta-Nyström method for the numerical solution of the Schrödinger equation and related problems, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 551–566.
- [27] D. F. Papadopoulos, Z. A. Anastassi, T. E. Simos, A modified zero dispersion and zero dissipation RKN method for the numerical solution of the radial Schrödinger equation, *International Conference on Numerical Analysis and Applied Mathematics*, Rethymno, Greece, **1168** (2009) 1604–1607.
- [28] Z. Kalogiratu, T. E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nyström methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order, *J. Math. Chem.* **31** (2002) 211–232.
- [29] Z. A. Anastassi, T. E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation *J. Math. Chem.* **37** (2005) 281–293.

- [30] Z. A. Anastassi, T. E. Simos, A family of exponentially-fitted Runge–Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **41** (2007) 79–100.
- [31] T. Monovasilis, Z. Kalogiratou, T. E. Simos, A family of trigonometrically fitted partitioned Runge–Kutta symplectic methods, *Appl. Math. Comput.* **209** (2009) 91–96.
- [32] Z. Kalogiratou, T. Monovasilis, T. E. Simos, Computation of the eigenvalues of the Schrödinger equation by exponentially-fitted Runge–Kutta–Nyström methods, *Comput. Phys. Commun.* **180** (2009) 167–176.
- [33] Z. Kalogiratou, T. Monovasilis, T. E. Simos, New modified Runge–Kutta–Nyström methods for the numerical integration of the Schrödinger equation, *Comput. Math. Appl.* **60** (2010) 1639–1647.
- [34] J. D. Lambert, I. A. Watson, Symmetric multistep methods for periodic initial values problems, *J. Inst. Math. Appl.* **18** (1976) 189–202.
- [35] G. D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits, *Astronom. J.* **100** (1990) 1694–1700.
- [36] <http://burtleburtle.net/bob/math/multistep.html>
- [37] T. E. Simos, P. S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation, *J. Comput. Appl. Math.* **79** (1997) 189–205.
- [38] G. Avdelas, A. Konguetsof, T. E. Simos, A family of hybrid eighth order methods with minimal phase-lag for the numerical solution of the Schrödinger equation and related problems, *Int. J. Mod. Phys. C* **11** (2000) 415–437.
- [39] G. Avdelas, T. E. Simos, Dissipative high phase-lag order Numerov-type methods for the numerical solution of the Schrödinger equation, *Phys. Rev. E* (2000) 1375–1381.
- [40] G. Avdelas, T. E. Simos, On variable-step methods for the numerical solution of Schrödinger equation and related problems, *Comput. Chem.* **25** (2001) 3–13.
- [41] T. E. Simos, P. S. Williams, New insights in the development of Numerov-type methods with minimal phase-lag for the numerical solution of the Schrödinger equation, *Comput. Chem.* **25** (2001) 77–82.
- [42] G. Avdelas, A. Konguetsof, T. E. Simos, A generator of hybrid explicit methods for the numerical solution of the Schrödinger equation and related problems, *Comput. Phys. Commun.* **136** (2001) 14–28.

- [43] T. E. Simos, J. Vigo-Aguiar, A symmetric high-order method with minimal phase-lag for the numerical solution of the Schrödinger equation, *Int. J. Mod. Phys. C* **12** (2001) 1035–1042.
- [44] T. E. Simos, J. Vigo-Aguiar, On the construction of efficient methods for second order IVPs with oscillating solution, *Int. J. Mod. Phys. C* **12** (2001) 1453–1476.
- [45] G. Avdelas, A. Konguetsof, T. E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method, *J. Math. Chem.* **29** (2001) 281–291.
- [46] G. Avdelas, A. Konguetsof, T. E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results, *J. Math. Chem.* **29** (2001) 293–305.
- [47] C. Tsitouras, T. E. Simos, High algebraic, high phase-lag order embedded Numerov-type methods for oscillatory problems, *Appl. Math. Comput.* **131** (2002) 201–211.
- [48] G. Avdelas, A. Konguetsof, T. E. Simos, A generator of dissipative methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.* **148** (2002) 59–73.
- [49] A. Konguetsof, T. E. Simos, P-stable eighth algebraic order methods for the numerical solution of the Schrödinger equation, *Comput. Chem.* **26** (2002) 105–111.
- [50] T. E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation *J. Math. Chem.* **31** (2002) 135–144.
- [51] A. Konguetsof, T. E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation, *J. Comput. Appl. Math.* **158** (2003) 93–106.
- [52] T. E. Simos, I. T. Famelis, C. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions, *Num. Algorithms* **34** (2003) 27–40.
- [53] D. P. Sakas, T. E. Simos, Multiderivative methods of eighth algebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation, *J. Comput. Appl. Math.* **175** (2005) 161–172.

- [54] D. P. Sakas, T. E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **37** (2005) 317–331.
- [55] G. A. Panopoulos, Z. A. Anastassi, T. E. Simos, Two new pttimized eight-step symmetric methods for the efficient solution of the Schrödinger equation and related problems, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 773–785.
- [56] T. E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **46** (2009) 981–1007.
- [57] I. Alolyan, T. E. Simos, High algebraic order methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **48** (2010) 925–958.
- [58] I. Alolyan, T. E. Simos, Multistep methods with vanished phase-lag and its first and second derivatives for the numerical integration of the Schrödinger equation, *J. Math. Chem.* **48** (2010) 1092–1143.
- [59] I. Alolyan, T. E. Simos, A family of eight-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation, *J. Math. Chem.*, to appear.
- [60] A. Konguetsof, A new two-step hybrid method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **47** (2010) 871–890.
- [61] K. Tselios, T. E. Simos, Symplectic methods for the numerical solution of the radial Shrodinger equation, *J. Math. Chem.* **34** (2003) 83–94.
- [62] K. Tselios, T. E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Shrodinger equation, *J. Math. Chem.* **35** (2004) 55–63.
- [63] T. Monovasilis, T. E. Simos, New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation, *J. Math. Chem.* **42** (2007) 535–545.
- [64] T. Monovasilis, Z. Kalogiratou, T. E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation *J. Math. Chem.* **37** (2005) 263–270.
- [65] T. Monovasilis, Z. Kalogiratou, T. E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation, *J. Math. Chem.* **40** (2006) 257–267.
- [66] Z. Kalogiratou, T. E. Simos, Newton–Cotes formulae for long-time integration, *J. Comput. Appl. Math.* **158** (2003) 75–82.

- [67] T. E. Simos, High order closed Newton–Cotes trigonometrically–fitted formulae for the numerical solution of the Schrödinger equation, *Appl. Math. Comput.* **209** (2009) 137–151.
- [68] T. E. Simos, Closed Newton–Cotes trigonometrically–fitted formulae for the solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 787–801.
- [69] T. E. Simos, Closed Newton–Cotes trigonometrically–fitted formulae of high order for the numerical integration of the Schrödinger equation, *J. Math. Chem.* **44** (2008) 483–499.
- [70] T. E. Simos, High–order closed Newton–Cotes trigonometrically–fitted formulae for long–time integration of orbital problems, *Comput. Phys. Commun.* **178** (2008) 199–207.
- [71] T. E. Simos, Closed Newton–Cotes trigonometrically–fitted formulae for numerical integration of the Schrödinger equation, *Comput. Lett.* **3** (2007) 45–57.
- [72] T. E. Simos, Closed Newton–Cotes trigonometrically–fitted formulae for long–time integration of orbital problems, *Rev. Mexic. Astron. Astrof.* **42** (2006) 167–177.
- [73] T. E. Simos, Closed Newton–Cotes trigonometrically–fitted formulae for long–time integration, *Int. J. Mod. Phys. C* **14** (2003) 1061–1074.
- [74] Z. Kalogiratu, T. Monovasilis, T. E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation, *J. Comput. Appl. Math.* **158** (2003) 83–92.
- [75] T. E. Simos, Closed Newton–Cotes trigonometrically–fitted formulae of high–order for long–time integration of orbital problems, *Appl. Math. Lett.* **22** (2009) 1616–1621.
- [76] Z. Kalogiratu, T. Monovasilis, T. E. Simos, A fifth–order symplectic trigonometrically fitted partitioned Runge–Kutta method, International Conference on Numerical Analysis and Applied Mathematics, SEP 16–20, 2007 Corfu, GREECE, Numerical Analysis and Applied Mathematics, *AIP Conference Proceedings* **936** (2007) 313–317.
- [77] T. Monovasilis, Z. Kalogiratu, T. E. Simos, Families of third and fourth algebraic order trigonometrically fitted symplectic methods for the numerical integration of Hamiltonian systems, *Comput. Phys. Commun.* **177** (2007) 757–763.

- [78] T. Monovasilis, T. E. Simos, Symplectic methods for the numerical integration of the Schrödinger equation, *Comput. Mater. Sci.* **38** (2007) 526–532.
- [79] T. Monovasilis, Z. Kalogiratou, T. E. Simos, Computation of the eigenvalues of the Schrödinger equation by symplectic and trigonometrically fitted symplectic partitioned Runge–Kutta methods, *Phys. Lett. A* **372** (2008) 569–573.
- [80] T. Monovasilis, Z. Kalogiratou, T. E. Simos, Symplectic partitioned Runge–Kutta methods with minimal phase-lag, *Comput. Phys. Commun.* **181** (2010) 1251–1254.
- [81] J. Vigo-Aguiar, T. E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **32** (2002) 257–270.
- [82] A. D. Raptis, A. C. Allison, Exponential – fitting methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.* **14** (1978) 1–5.
- [83] A. D. Raptis, Exponentially–fitted solutions of the eigenvalue Schrödinger equation with automatic error control, *Comput. Phys. Commun.* **28** (1983) 427–431.
- [84] L. G. Ixaru, M. Rizea, A Numerov–like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. *Comput. Phys. Commun.* **19** (1980) 23–27.
- [85] Z. Kalogiratou, T. E. Simos, A P–stable exponentially-fitted method for the numerical integration of the Schrödinger equation, *Appl. Math. Comput.* **112** (2000) 99–112.
- [86] G. Avdelas, E. Kefalidis, T. E. Simos, New P–stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation, *J. Math. Chem.* **31** (2002) 371–404.
- [87] T. E. Simos, A family of trigonometrically–fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems *J. Math. Chem.* **34** (2003) 39–58.
- [88] T. E. Simos, Exponentially – fitted multiderivative methods for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **36** (2004) 13–27.
- [89] T. E. Simos, A four–step exponentially fitted method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **40** (2006) 305–318.
- [90] T. E. Simos, A family of four–step trigonometrically–fitted methods and its application to the Schrödinger equation, *J. Math. Chem.* **44** (2009) 447–466.

- [91] T. E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation, *Acta Appl. Math.* **110** (2010) 1331–1352.
- [92] Z. A. Anastassi, T. E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution, *J. Math. Chem.* **45** (2009) 1102–1129.
- [93] G. Psihoyios, T. E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation, *J. Math. Chem.* **37** (2005) 295–316.
- [94] G. Psihoyios, T. E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order predictor-corrector methods, *J. Math. Chem.* **40** (2006) 269–293.
- [95] Z. Wang, P-stable linear symmetric multistep methods for periodic initial-value problems, *Comput. Phys. Commun.* **171** (2005) 162–174.
- [96] T. E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **27** (2000) 343–356.
- [97] Z. A. Anastassi, T. E. Simos, New trigonometrically fitted six-step symmetric methods for the efficient solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 733–752.
- [98] Z. A. Anastassi, T. E. Simos, A six-step P-stable trigonometrically-fitted method for the numerical integration of the radial Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 803–830.
- [99] Z. A. Anastassi, T. E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution, *J. Math. Chem.* **45** (2009) 1102–1129.
- [100] T. E. Simos, Stabilization of a four-step exponentially-fitted method and its application to the Schrödinger equation, *Int. J. Mod. Phys C* **18** (2007) 315–328.
- [101] T. E. Simos, P-stability, trigonometric-fitting and the numerical solution of the radial Schrödinger equation, *Comput. Phys. Commun.* **180** (2009) 1072–1085.
- [102] G. A. Panopoulos, Z.A. Anastassi, T. E. Simos, Two optimized symmetric eight-step implicit methods for initial-value problems with oscillating solutions, *J. Math. Chem.* **46** (2009) 604–620.

- [103] G. Psihoyios, T. E. Simos, Trigonometrically fitted predictor–corrector methods for IVPs with oscillating solutions, *J. Comput. Appl. Math.* **158** (2003) 135–144.
- [104] D. P. Sakas, T. E. Simos, Trigonometrically–fitted multiderivative methods for the numerical solution of the radial Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 299–320.
- [105] G. Psihoyios, T. E. Simos, A family of fifth algebraic order trigonometrically fitted P–C schemes for the numerical solution of the radial Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 321–344.
- [106] T. E. Simos, Multiderivative methods for the numerical solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 7–26.
- [107] H. Van de Vyver, Efficient one–step methods for the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 711–732.
- [108] T. E. Simos, Dissipative trigonometrically–fitted methods for linear second–order IVPs with oscillating solution, *Appl. Math. Lett.* **17** (2004) 601–607.
- [109] S. Stavroyiannis, T. E. Simos, Optimization as a function of the phase–lag order of nonlinear explicit two–step P–stable method for linear periodic IVPs, *Appl. Numer. Math.* **59** (2009) 2467–2474.
- [110] S. Stavroyiannis, T. E. Simos, A nonlinear explicit two–step fourth algebraic order method of order infinity for linear periodic initial value problems, *Comput. Phys. Commun.* **181** (2010) 1362–1368.
- [111] Z. A. Anastassi, T. E. Simos, Numerical multistep methods for the efficient solution of quantum mechanics and related problems, *Phys. Rep.* **482** (2009) 1–240.
- [112] R. Vujasin, M. Senćanski, J. Radić–Perić, M. Perić, A comparison of various variational approaches for solving the one–dimensional vibrational Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 363–378.
- [113] T. E. Simos, P. S. Williams, On finite difference methods for the solution of the Schrödinger equation, *Comput. Chem.* **23** (2009) 513–554.
- [114] L. G. Ixaru, M. Rizea, Comparison of some four–step methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.* **38** (1985) 329–337.
- [115] J. Vigo–Aguiar, T. E. Simos, Review of multistep methods for the numerical solution of the radial Schrödinger equation, *Int. J. Quantum Chem.* **103** (2005) 278–290.

- [116] T. E. Simos, A. D. Zdetsis, G. Psihoyios, Z. A. Anastassi, Special Issue on Mathematical Chemistry based on papers presented within ICCMSE 2005 Preface, *J. Math. Chem.* **46** (2009) 727–728.
- [117] T. E. Simos, G. Psihoyios, Z. Anastassi, Preface, Proceedings of the International Conference of Computational Methods in Sciences and Engineering 2005, *Math. Comput. Model.* **51** (2010) 137–137.
- [118] T. E. Simos, G. Psihoyios, Special issue: The International Conference on Computational Methods in Sciences and Engineering 2004 – Preface, *J. Comput. Appl. Math.* **191** (2006) 165–165.
- [119] T. E. Simos, G. Psihoyios, Special issue – Selected papers of the International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003) Kastoria, Greece, 12-16 September 2003 – Preface, *J. Comput. Appl. Math.* **175** (2005) IX–IX.
- [120] T. E. Simos, J. Vigo-Aguiar, Special Issue – Selected Papers from the Conference on Computational and Mathematical Methods for Science and Engineering (CMMSE-2002) – Alicante University, Spain, 20-25 September 2002 – Preface, *J. Comput. Appl. Math.* **158** (2003) IX–IX.
- [121] T. E. Simos, C. Tsitouras, I. Gutman, Preface for the special issue – Numerical Methods in Chemistry, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 695–696.
- [122] T. E. Simos, I. Gutman, Papers presented on the International Conference on Computational Methods in Sciences and Engineering (Castoria, Greece, September 12-16, 2003), *MATCH Commun. Math. Comput. Chem.* **53** (2005) 3–4.