A New Four–Stages High Algebraic Order Two–Step Method with Vanished Phase–Lag and its First, Second and Third Derivatives for the Numerical Solution of the Schrödinger Equation

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(Received June 29, 2016)

Abstract

A new high algebraic order four–stages symmetric two–step method is developed, for the first time in the literature, in the present paper. Requesting the elimination of the phase–lag and its first, second and third derivatives and requiring also the highest possible algebraic order, we determine the coefficients of the method. We study also the affection of the elimination of the phase–lag and its derivatives on the efficiency of the new proposed method. More specifically we will investigate the following:

\begin{itemize}
  \item the development of the method,
  \item the calculation of the local truncation error (LTE) of the new proposed method,
  \item the analysis of the method which consists of two stages: Stage 1: LTE analysis based on a test problem which is the radial Schrödinger equation. Stage 2: Stability and Interval
\end{itemize}
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order. Additionally, while the method obtained in [4] is of twelfth algebraic order and has eliminated the phase–lag and its first and second derivatives, the new method, which is first introduced in the literature, is of twelfth algebraic order and has eliminated the phase–lag and its first, second and third derivatives. Additionally, we give a new error control which is based on high order vanishing of the derivatives of the phase–lag.

The above mentioned problems which will be studied in this paper belong to the category of the special second order initial value problems with periodical and/or oscillating solution of the form:

\[ z''(x) = f(x, z), \ z(x_0) = z_0 \text{ and } z'(x_0) = z'_0. \quad (1) \]

More specifically, we will investigate the numerical solution of systems of ordinary differential equations of second order in the model of which the first derivative \( z' \) does not appear explicitly and additionally their solutions have with periodical and/or oscillating behavior.

Below we give some bibliography on the subject of the paper. We give the bibliography based on the categories of methods which developed the last decades:

1. In [43], [46], [55], [58]–[61], [52] [69], exponentially, trigonometrically and phase fitted Runge–Kutta and Runge–Kutta Nyström methods was developed.

2. Multistep exponentially, trigonometrically and phase fitted methods and multistep methods with minimal phase–lag developed in [1]–[4], [14]–[17], [21]–[24], [30], [34], [40], [44]–[45], [49], [54], [56]–[57], [63]–[64], [70]–[71].

3. Symplectic integrators in [38]–[39], [47], [50], [53], [61]–[62], [67].

4. Nonlinear methods developed in [48].

5. General methods are developed in [10]–[13], [18]–[20], [31]–[33], [36]–[37].

2. ANALYSIS OF SYMMETRIC 2m MULTISTEP METHODS

The analysis of symmetric multistep methods is based on the following algorithm:

1. Presentation of the general form of the 2m–step finite difference method for the numerical solution of the initial value problem (1):

\[
\sum_{i=-m}^{m} c_i z_{n+i} = h^2 \sum_{i=-m}^{m} b_i f(x_{n+i}, z_{n+i}). \quad (2)
\]
2. Definitions: (1) Space of integration which is known as integration interval and (2) stepsize (step length) of integration

3. Procedure for the numerical solution of the initial value problem (1) using the above determined $2m$–step method:
   
   • Let us consider the space $[a, b]$ as the integration interval for the approximate integration of the initial value problem (1).
   
   • Using the points $\{x_i\}_{i=-m}^{m} \in [a, b]$ we divide the above determined integration interval $[a, b]$ into $m$ equally spaced intervals.
   
   • Based on the above division of the integration area using the points $x_i, i = -m(1)m$, the quantity $h$ by $h = |x_{i+1} - x_i|, \ i = 1 - m(1)m - 1$ is determined. We call this quantity the stepsize of integration or the step length of integration.

4. Determination of a subclass of the general $2m$–step methods which is called symmetric $2m$–step methods.

   **Definition 1.** A method (2) is called symmetric if and only if $c_{-i} = c_i$ and $b_{-i} = b_i$, $i = 0(1)m$.

   **Remark 1.** The linear operator
   
   $$L(x) = \sum_{i=-m}^{m} c_i z(x + ih) - h^2 \sum_{i=-m}^{m} b_i z''(x + ih)$$

   where $z \in C^2$, is associated with the $2m$–step Method determined by (2).

5. Definition of the algebraic order $q$ of a $2m$–step Method presented by (2)

   **Definition 2.** [10] We call that a $2m$–step method given by (2) has algebraic of order $q$ if the associated linear operator $L$ given by (3) vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{q+1}$.

6. Introduction and Definition of the terms for a symmetric $2m$–step method: scalar test equation, difference equation and characteristic equation

   Application of the symmetric $2m$–step method (2) to the scalar test equation

   $$z'' = -\phi^2 z$$

   (4)
leads to the following difference equation:

\[ A_m(v) z_{n+m} + \cdots + A_1(v) z_{n+1} + A_0(v) z_n + A_1(v) z_{n-1} + \cdots + A_m(v) z_{n-m} = 0 \] (5)

and the associated characteristic equation

\[ A_m(v) \lambda^m + \cdots + A_1(v) \lambda + A_0(v) + A_1(v) \lambda^{-1} + \cdots + A_m(v) \lambda^{-m} = 0. \] (6)

where \( v = \phi h, h \) is the step length and \( A_j(v) j = 0(1)k \) are polynomials of \( v \) which are called stability polynomials of the symmetric \( 2m \)-step method (2).

7. Introduction and Definition of the terms for a symmetric \( 2m \)-step method: interval of periodicity, phase-lag, phase-fitted method

**Definition 3.** [11] We say that a symmetric \( 2m \)-step method with characteristic equation given by (6) has a non-zero interval of periodicity \((0, v_0^2)\) when, for all \( v \in (0, v_0^2) \), the roots \( \lambda_i, i = 1(1)2m \) of characteristic equation Eq. (6) satisfy:

\[ \lambda_1 = e^{i\theta(v)}, \quad \lambda_2 = e^{-i\theta(v)} \quad \text{and} \quad |\lambda_i| \leq 1, \quad i = 3(1)2m \] (7)

where \( \theta(v) \) is a real function of \( v \).

**Definition 4.** (see [11]) A symmetric \( 2m \)-step method is called P-stable method if its interval of periodicity is equal to \((0, \infty)\).

**Definition 5.** A symmetric \( 2m \)-step method is called singularly almost P-stable method if its interval of periodicity is equal to \((0, \infty) - S\) 2.

**Definition 6.** [12], [13] For any symmetric \( 2m \)-step method with a characteristic equation given by (6), the phase-lag is defined as the leading term in the expansion of

\[ t = v - \theta(v). \] (8)

In the above mentioned case if the quantity \( t = O(v^{s+1}) \) as \( v \to \infty \), then the order of the phase-lag is equal to \( s \).

**Definition 7.** [14] We call a symmetric \( 2m \)-step method phase-fitted if its phase-lag is equal to zero.

\(^2\)where \( S \) is a set of distinct points
8. Direct formula for the computation of the phase–lag for a symmetric $2m$–step method

**Theorem 1.** [12] A symmetric $2m$–step method with the characteristic equation given by (6) has phase–lag order $s$ and phase–lag constant $c$ given by

$$-cv^{s+2} + O(v^{s+4}) = \frac{2A_m(v) \cos(mv) + \cdots + 2A_1(v) \cos(v) + \cdots + A_0(v)}{2m^2 A_m(v) + \cdots + 2j^2 A_j(v) + \cdots + 2A_1(v)}. \quad (9)$$

**Remark 2.** The above formula (9) is a direct one for the computation of the phase–lag of any symmetric $2m$–step method.

**Remark 3.** For the specific case of a symmetric two–step method and for the calculation of its phase–lag, we will apply the above mentioned direct formula (9) with $m = 2$.

### 3. THE NEW TWELFTH ALGEBRAIC ORDER FOUR–STAGES SYMMETRIC TWO–STEP METHOD WITH VANISHED PHASE–LAG AND ITS FIRST, SECOND AND THIRD DERIVATIVES

We consider the family of methods

$$\hat{z}_n = z_n - a_0 h^2 \left( f_{n+1} - 2f_n + f_{n-1} \right) - 2a_1 h^2 f_n$$

$$\tilde{z}_n = z_n - a_2 h^2 \left( f_{n+1} - 2\hat{f}_n + f_{n-1} \right)$$

$$\bar{z}_n = z_n - a_3 h^2 \left( f_{n+1} - 2\tilde{f}_n + f_{n-1} \right)$$

$$z_{n+1} + a_4 z_n + z_{n-1} = h^2 \left[ b_1 \left( f_{n+1} + f_{n-1} \right) + b_0 \tilde{f}_n \right] \quad (10)$$

where $f_i = z''(x_i, z_i), i = -2(1)2, \hat{f}_n = z''(x_n, \hat{z}_n), \tilde{f}_n = z''(x_n, \tilde{z}_n), \bar{f}_n = z''(x_n, \bar{z}_n)$ and $a_j, j = 0(1)4$ and $b_i, i = 0, 1$ are parameters.

We give attention to the following case of the above noted family of methods (10):

$$a_0 = -\frac{27}{3200}, a_1 = \frac{3}{32}, a_2 = -\frac{10}{693}. \quad (11)$$

The requirement the above symmetric two-step method (10) with the newly defined free parameters (11) to have eliminated the phase–lag and its first, second and third derivatives leads to the following system of equations:

$$\text{Phase – Lag(PL)} = \frac{T_0}{T_{\text{denom}}} = 0 \quad (12)$$
First Derivative of the Phase $-\text{Lag} = \frac{T_1}{T_{\text{denom}}^2} = 0$ (13)

Second Derivative of the Phase $-\text{Lag} = \frac{T_2}{T_{\text{denom}}^3} = 0$ (14)

Third Derivative of the Phase $-\text{Lag} = \frac{T_3}{T_{\text{denom}}^4} = 0$ (15)

where $T_j, j = 0(1)3$ and $T_{\text{denom}}$ are given in the Appendix A.

In order to obtain the free parameters of the new proposed method (10) we solve the system of equations (12)–(15):

$$a_4 = \frac{T_4}{T_{\text{denom}1}}, \quad a_3 = 2310 \frac{T_5}{T_{\text{denom}2}},$$
$$b_0 = \frac{1}{81} \frac{T_6}{T_{\text{denom}3}}, \quad b_1 = \frac{1}{81} \frac{T_7}{T_{\text{denom}3}}$$

where $T_j, j = 4(1)7$, $T_{\text{denom}1}$, $T_{\text{denom}2}$ and $T_{\text{denom}3}$ are given in the Appendix B.

We use the Taylor series expansions given in the Appendix C in the cases of heavy cancelations for some values of $|v|$ of the above mentioned formulae given by (16).

The behavior of the coefficients is given in the Figure 1.

We indicate the new proposed method (10) with the coefficients given by (11) and (16) and their Taylor series expansions given in Appendix C with the symbol: $NM4SH3DV$.

For this method, the local truncation error is equal to:

$$LTE_{NM4SH3DV} = \frac{307}{186810624000} h^{14} \left( z^{(14)}_n - 35 \phi^8 z^{(6)}_n - 84 \phi^{10} z^{(4)}_n - 70 \phi^{12} z^{(2)}_n \right) + O \left( h^{16} \right).$$

(17)

4. ANALYSIS OF THE NEW OBTAINED METHOD

4.1. Comparative Local Truncation Error (LTE) Analysis

The following test problem is used for the local truncation error analysis:

$$z''(x) = (V(x) - V_c + G) z(x)$$

(18)

where

- $V(x)$ is a potential function,
- $V_c$ a constant approximation of the potential on the specific point $x$,
- $G = V_c - E$ and
Figure 1. Behavior of the free parameters of the new proposed method (10) given by (16) for several values of $v = \phi h$.

- $E$ is the energy.

Remark 4. The Eq. (18) is the radial time independent Schrödinger equation with potential $V(x)$.

We will investigate the following methods:

4.1.1. Classical Method (i.e., Method (10) with Constant Coefficients)

$$L T E_{CL} = \frac{307}{186810624000} h^{14} z_n^{(14)} + O \left(h^{16}\right).$$  (19)
4.1.2. Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in [4]

\[\text{LTE}_{NM4SH2DV} = \frac{307}{186810624000} \cdot h^{14} \left( z^{(14)}_n - 15 \phi^8 z^{(6)}_n \right) - 24 \phi^{10} z^{(4)}_n - 10 \phi^{12} z^{(2)}_n + O(h^{16}). \]  \hspace{1cm} (20)

4.1.3. Method with Vanished Phase–Lag and Its First, Second and Third Derivatives Developed in Section 3.

\[\text{LTE}_{NM4SH3DV} = \frac{307}{186810624000} \cdot h^{14} \left( z^{(14)}_n - 35 \phi^8 z^{(6)}_n \right) - 84 \phi^{10} z^{(4)}_n - 70 \phi^{12} z^{(2)}_n + O(h^{16}). \]  \hspace{1cm} (21)

The following scheme is followed

- We calculate the new formulae of the Local Truncation Errors (LTEs) which are based on the test problem (18)

- In order to achieve the above we have to compute the derivatives of the function \(z\) which are included in the formulae of LTEs mentioned above (19), (20) and (21).

- In order to satisfy the above step we use expressions of the derivatives of the function \(z\). Some of the requested expressions for the derivative of the function \(z\) are given in the Appendix D.

- Using the above achieved new formulae of the derivatives of the approximation of the function \(z\) to the point \(x_n\) and substitute them into the formulae of LTEs (19), (20) and (21), we obtain the new formulae of LTEs produced from the test equation (18).

- The new formulae of LTEs produced above are dependent from the quantity \(G\) and the energy \(E\).

- We study two cases for the parameter \(G\):
1. The Potential and the Energy are closed each other.

Consequently we have

\[ G = V_c - E \approx 0 \Rightarrow G^i = 0, \quad i = 1, 2, \ldots. \quad (22) \]

The general form of the LTEs is given by:

\[ LTE = h^{14} \sum_{k=0}^{j} B_k G^k \quad (23) \]

where \( B_k \) are constant numbers (classical case) or formulae of \( v \) and \( G = V_c - E \) (frequency dependent cases).

**Remark 5.** In the case \( G = V_c - E \approx 0 \), we have:

\[ LTE_{G=0} = h^{14} B_0 \quad (24) \]

where \( B_0 \) is equal for all the above formulae (19), (20) and (21).

Therefore, for \( G = V_c - E \approx 0 \) we have that:

\[ LTE_{CL} = LTE_{NM4SH2DV} = LTE_{NM4SH3DV} = h^{14} B_0 \quad (25) \]

where \( B_0 \) is given in the Appendix E at every point \( x = x_n \).

**Theorem 2.** From (22) it is easy to see that for \( G = V_c - E \approx 0 \) the local truncation error for the classical method (constant coefficients), the local truncation error for the method with eliminated phase–lag and its first and second derivatives and the local truncation error for the method with eliminated phase–lag and its first, second and third derivatives are the same and equal to \( h^{14} B_0 \), where \( B_0 \) is given in the Appendix E and consequently for \( G = 0 \) the methods are of comparable accuracy.

2. The Potential and the Energy are far from each other. Therefore, \( G >> 0 \) or \( G << 0 \) and the value of \( |G| \) is a large number. For these cases the most accurate method is the method with asymptotic form of LTE which has the minimum power of \( G \).

- Finally we compute, based on the above, the asymptotic expressions of the LTEs.
4.1.4. Classical Method

\[ LTE_{CL} = \frac{307}{18681062400} h^{14} \left( z(x) G^7 + \cdots \right) + O(h^{16}). \]  

(26)

4.1.5. Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in [4]

\[ LTE_{NM^{4}SH^{2}DV} = \frac{307}{2335132800} h^{14} \left( \left( \frac{d^2}{dx^2} g(x) \right) z(x) G^5 + \cdots \right) + O(h^{16}). \]  

(27)

4.1.6. Method with Vanished Phase–Lag and Its First, Second and Third Derivatives Developed in Section 3.

\[ LTE_{NM^{4}SH^{3}DV} = \frac{307}{6671808000} h^{14} \left[ 15 \left( \frac{d}{dx} g(x) \right)^2 z(x) + 20 g(x) z(x) \frac{d^2}{dx^2} g(x) + 27 \left( \frac{d^4}{dx^4} g(x) \right) z(x) + 10 \left( \frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} z(x) \right] G^4 + \cdots + O(h^{16}). \]  

(28)

From the above mentioned analysis we have the following theorem:

**Theorem 3.**  

- **Classical Method** (i.e., the method (10) with constant coefficients): For this method the error increases as the seventh power of \( G \).

- **High Algebraic Order Two–Step Method with Vanished Phase–lag and its First and Second Derivatives developed in [4]**: For this method the error increases as the fifth power of \( G \).

- **Twelfth Algebraic Order Two–Step Method with Eliminated Phase–lag and its First, Second and Third Derivatives developed in Section 3**: For this method the error increases as the fourth power of \( G \).

So, for the numerical solution of the time independent radial Schrödinger equation the New Proposed Twelfth Algebraic Order Method with vanished phase–lag and its first, second and third derivatives is the most accurate one, especially for large values of \( |G| = |V_c - E| \).
4.2. Stability and Interval of Periodicity Analysis

The following test problem is used for the stability and interval of periodicity analysis of the new proposed method:

$$z'' = -\omega^2 z.$$  \hspace{1cm} (29)

Remark 6. If we compare the test equations (4) and (29) we arrive to the remark that the frequencies of these test problems are not equal, i.e. $\omega \neq \phi$.

The application of the new proposed four–stages symmetric two–step method to the scalar test equation (29) leads to the difference equation:

$$A_1 (s, v) (z_{n+1} + z_{n-1}) + A_0 (s, v) z_n = 0$$ \hspace{1cm} (30)

which is associated to the characteristic equation:

$$A_1 (s, v) (\lambda^2 + 1) + A_0 (s, v) \lambda = 0$$ \hspace{1cm} (31)

where

$$A_1 (s, v) = 1 + b_1 s^2 + a_3 b_0 s^4 - 2 a_2 a_3 b_0 s^6 + 4 a_0 a_2 a_3 b_0 s^8$$

$$A_0 (s, v) = a_4 + b_0 s^2 - 2 a_3 b_0 s^4 + 4 a_2 a_3 b_0 s^6 + 8 a_2 a_3 b_0 (a_1 - a_0) s^8$$ \hspace{1cm} (32)

where $s = \omega h$ and $v = \phi h$.

Taken the coefficients $a_j, j = 0(1)2$ from (11) and the coefficients $b_i, j = 0, 1$ and $a_k, k = 3, 4$ from (16) and substituted them into the formulae (32) we have that:

$$A_1 (s, v) = \frac{T_8}{T_{\text{denom}4}}, \quad A_0 (s, v) = 2 \frac{T_9}{T_{\text{denom}4}}$$ \hspace{1cm} (33)

where

$$T_8 = 54 s^8 v^2 - 216 s^6 v^6 + 3200 s^6 v^2$$

$$- 7332 s^2 v^6 + 110880 s^4 v^2 - 149760 s^2 v^4$$

$$+ 997920 s^2 v^2 + 81 (\cos (v))^2 v^{10}$$

$$+ 81 (\cos (v))^2 s^8 - 3037 (\cos (v))^2 v^8$$

$$+ 7848 \sin (v) v^9 + 7848 \cos (v) v^8$$

$$+ 4800 (\cos (v))^2 s^6 - 88560 (\cos (v))^2 v^6$$

$$+ 136920 \sin (v) v^7 - 19200 \cos (v) v^6$$
\[ T_9 = 654 s^8 v^2 - 2616 s^2 v^8 + 3200 s^6 v^2 - 92004 s^2 v^6 \\
+ 110880 s^4 v^2 - 341760 s^2 v^4 \\
- 332640 s^2 v^2 + 981 (\cos (v))^2 v^{10} \\
+ 981 (\cos (v))^2 s^8 - 72337 (\cos (v))^2 v^8 \\
+ 3888 \sin (v) v^9 - 1296 \cos (v) v^8 + 4800 (\cos (v))^2 s^6 \\
- 88560 (\cos (v))^2 v^6 \\
+ 115200 \sin (v) v^7 + 38400 \cos (v) v^6 + 166320 (\cos (v))^2 s^4 \\
- 1164240 (\cos (v))^2 s^2 v^4 \\
+ 1330560 \sin (v) v^5 + 1330560 \cos (v) v^4 + 235680 v^6 + 498960 v^4 \\
+ 15696 \cos (v) \sin (v) s^2 v^7 + 93336 \cos (v) \sin (v) s^2 v^5 \\
+ 539520 \cos (v) \sin (v) s^2 v^3 + 665280 \cos (v) \sin (v) s^2 v \\
- 166320 s^4 + 327 (\cos (v))^2 s^8 v^2 \\
- 1308 (\cos (v))^2 s^2 v^8 - 15696 \cos (v) \sin (v) v^9 \\
+ 1600 (\cos (v))^2 s^6 v^2 + 22668 (\cos (v))^2 s^2 v^6 \\
\]
\[ \begin{align*}
- & \quad 3888 \sin(v) s^2 v^7 + 79320 \cos(v) \sin(v) v^7 \\
+ & \quad 9072 \cos(v) s^2 v^6 + 55440 (\cos(v))^2 s^4 v^2 \\
- & \quad 86880 (\cos(v))^2 s^2 v^4 - 115200 \sin(v) s^2 v^5 \\
- & \quad 270720 \cos(v) \sin(v) v^5 + 192000 \cos(v) s^2 v^4 \\
- & \quad 332640 (\cos(v))^2 s^2 v^2 - 1330560 \sin(v) s^2 v^3 \\
+ & \quad 665280 \cos(v) \sin(v) v^3 + 1330560 \cos(v) s^2 v^2 + 1962 v^{10} \\
- & \quad 981 s^8 + 89785 v^8 - 4800 s^6 - 648 (\cos(v))^2 \sin(v) v^9 \\
- & \quad 28920 (\cos(v))^2 \sin(v) v^7 \\
- & \quad 394560 (\cos(v))^2 \sin(v) v^5 \\
- & \quad 665280 (\cos(v))^2 \sin(v) v^3 \\
+ & \quad 648 (\cos(v))^2 \sin(v) s^2 v^7 \\
+ & \quad 14664 (\cos(v))^2 \sin(v) s^2 v^5 \\
+ & \quad 125760 (\cos(v))^2 \sin(v) s^2 v^3 \\
- & \quad 665280 (\cos(v))^2 \sin(v) s^2 v \\
- & \quad 4536 (\cos(v))^3 s^2 v^6 - 96000 (\cos(v))^3 s^2 v^4 \\
- & \quad 665280 (\cos(v))^3 s^2 v^2 + 648 (\cos(v))^3 v^8 \\
- & \quad 19200 (\cos(v))^3 v^6 - 665280 (\cos(v))^3 v^4 \\
T_{\text{denom}4} & = v^3 \left( 81 (\cos(v))^2 v^7 + 1296 \cos(v) \sin(v) v^6 \\
- & \quad 3037 (\cos(v))^2 v^5 + 7848 v^6 \sin(v) \\
+ & \quad 162 v^7 + 28680 \cos(v) \sin(v) v^4 + 7848 \cos(v) v^5 \\
- & \quad 88560 (\cos(v))^2 v^3 + 136920 v^4 \sin(v) + 11989 v^5 \\
+ & \quad 270720 \cos(v) \sin(v) v^2 - 19200 \cos(v) v^3 \\
- & \quad 1164240 (\cos(v))^2 v + 394560 v^2 \sin(v) + 274080 v^3 \\
- & \quad 665280 \cos(v) \sin(v) - 665280 \cos(v) v + 665280 \sin(v) + 1829520 v \right). 
\end{align*} \]

**Remark 7.** The term $P$–stable and singularly almost $P$-stable method are on the problems where we have the condition $\omega = \phi$.

In Figure 2 we present the plot of the $s-v$ plane for the new proposed method.
Remark 8. Observing the above mentioned plane we arrive to the following remarks:

1. the shadowed area is the stable space of the method,
2. the white area is the unstable space of the method.

Remark 9. The conclusions from the observation of the $s - v$ plane of the method are depended on the problems on which the specific new proposed method will be applied:

1. Problems for which $\phi \neq \omega$. For the problems of this case, the study of the $s - v$ plane must be done in all the space excluding the area around the first diagonal.

2. Problems for which $\phi = \omega$ (as an example we refer the Schrödinger equation and related problems). For the problems of this case, the study of the $s - v$ plane must be done around the first diagonal of the $s - v$ plane.

If we substitute on the stability polynomials, given by (33), $s = v$, then we will study the second case of the above mentioned problems in which the Schrödinger equation and related problems are belonged. Observing the space around the first diagonal of the plot $s - v$ we conclude that the interval of periodicity of the new proposed method is equal to $(0, \infty)$.

In Table 1 we present the interval of periodicity of similar methods:
Table in which the interval of periodicity of the new method is given together with
the intervals of periodicity of similar methods.

**Table 1.** Comparative Intervals of Periodicity for symmetric two–step methods of
the same form

<table>
<thead>
<tr>
<th>Method</th>
<th>Interval of Periodicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method developed in [4]</td>
<td>(0, 29)</td>
</tr>
<tr>
<td>Method developed in Section 3</td>
<td>(0, ∞)</td>
</tr>
</tbody>
</table>

The above developments lead to the following theorem:

**Theorem 4.** The method developed in section 3:

• *is of four stages*

• *is of twelfth algebraic order;*

• *has eliminated the phase–lag and its first, second and third derivatives*

• *has an interval of periodicity equals to: (0, ∞).*

5. NUMERICAL RESULTS

Our numerical experiments will be based on the application of the new obtained
method on two problems:

• the approximate solution of the radial time–independent Schrödinger equation and

• the approximate solution of coupled differential equations arising from the
  Schrödinger equation

5.1. Radial Time–Independent Schrödinger Equation

We will study the numerical solution of the radial time independent Schrödinger equa-
tion which is given by:

\[ z''(r) = [l(l+1)/r^2 + V(r) − k^2] z(r), \tag{34} \]

where

• we call the effective potential the function \( W(r) = l(l+1)/r^2 + V(r) \). This function
  satisfies the relation: \( W(x) \to 0 \) as \( x \to \infty \),
we call the energy the quantity \( k^2 \in \mathbb{R} \),
• we call angular momentum the quantity \( l \in \mathbb{Z} \),
• we call potential the function \( V \).

Since the problem (34)) is a boundary value one, we have to determine the boundary condition. The initial condition is defined from the value of the function \( z \) on the initial point of the integration area:

\[
z(0) = 0
\]
The final condition is defined at the end point of the integration space and is determined for large values of \( r \) from the physical conditions of the specific problem.

The numerical results from the numerical solution of the problem (34) are produced taking into account that the new developed method is a frequency dependent method. Consequently, the frequency \( \phi \) (which is required from the coefficients of the new method) for the radial Schrödinger equation (for the case \( l = 0 \)) is determined by:

\[
\phi = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|}
\]
where \( V(r) \) is the potential and \( E \) is the energy.

5.1.1. Woods–Saxon Potential

Another quantity which is requested for the numerical integration of the radial Schrödinger equation by the new method is the potential \( V(r) \). For our numerical experiments we use the Wood–Saxon potential:

\[
V(r) = \frac{u_0}{1 + q} - \frac{u_0 q}{a (1 + q)^2}
\]
with \( q = \exp \left[ \frac{r - X_0}{a} \right] \), \( u_0 = -50 \), \( a = 0.6 \), and \( X_0 = 7.0 \).

The plot of the Woods–Saxon potential is given in Figure 3.

Using the methodology proposed by Ixaru et al. ([15] [17]), we use for the Woods–Saxon potential approximate values in some critical points (within the integration area). Based on these approximate values, the value of the parameter \( \phi \) is defined.

Based on the above, the parameter \( \phi \) is chosen as follows (see for details [16] and [17]):

\[
\phi = \begin{cases} 
\sqrt{-50 + E} & \text{for } r \in [0, 6.5 - 2h] \\
\sqrt{-37.5 + E} & \text{for } r = 6.5 - h \\
\sqrt{-25 + E} & \text{for } r = 6.5 \\
\sqrt{-12.5 + E} & \text{for } r = 6.5 + h \\
\sqrt{E} & \text{for } r \in [6.5 + 2h, 15]. 
\end{cases}
\]
From the above we observe that, for example, on the point of the integration area $r = 6.5 - h$, the value of $\phi$ is equal to: $\sqrt{-37.5 + E}$. Consequently, $v = \phi h = \sqrt{-37.5 + E} h$.

On the point of the integration area $r = 6.5 - 3h$, the value of $\phi$ is equal to: $\sqrt{-50 + E}$, etc.

### 5.1.2. The Radial Schrödinger Equation and the Resonance Problem

We will solve numerically the radial time independent Schrödinger equation (34) using as potential the Woods-Saxon potential (35) and the new developed method.

The area of integration of the above mentioned problem is $(0, \infty)$. Consequently, we have to approximate the infinite interval of integration with a finite one. This is necessary in order to be possible to apply a numerical methods for the solution of (34). For our experiments we will approximate the infinite space of integration by the finite space $r \in [0, 15]$. For our numerical example, we will apply the new propose method to a large domain of energies: $E \in [1, 1000]$.

We observe that for positive energies, $E = k^2$, the potential vanished for $x \to \infty$ faster than the term $\frac{l(l+1)}{x^2}$. Therefore and in this case the form of the radial Schrödinger equation is leaded to:

$$ z''(r) + \left( k^2 - \frac{l(l+1)}{r^2} \right) z(r) = 0 \quad (36) $$

The mathematical model (36) of the Schrödinger equation has linearly independent solutions $kr j_l(kr)$ and $kr n_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Consequently, the asymptotic form of the solution of equation (34) (when $r \to \infty$) is given by:

$$ z(r) \approx Akr j_l(kr) - Bkr n_l(kr) $$
\[
\approx AC \left[ \sin \left( kr - \frac{l\pi}{2} \right) + \tan \delta_l \cos \left( kr - \frac{l\pi}{2} \right) \right]
\]

where \( \delta_l \) is the phase shift. The direct formula for the computation of the phase shift is given by:

\[
\tan \delta_l = \frac{p(r_2) S(r_1) - p(r_1) S(r_2)}{p(r_1) C(r_1) - p(r_2) C(r_2)}
\]

where \( r_1 \) and \( r_2 \) are distinct points in the asymptotic region (we selected as \( r_1 \) the right hand end point of the interval of integration (i.e. \( r_1 = 15 \)) and \( r_2 = r_1 - h \)) with \( S(r) = kr j_l(kr) \) and \( C(r) = -kr n_l(kr) \). The problem is considered as an initial–value problem (as we have mentioned previously), and consequently we need the value of \( z_j, j = 0, 1 \) in order to apply a two–step method for the solution of the above described problem. The value \( z_0 \) is computed from the initial condition. The value \( z_1 \) is obtained by using high order Runge–Kutta–Nyström methods (see [18] and [19]). Based on the starting (initial) values \( z_i, i = 0, 1 \), we can compute at \( r_2 \) of the asymptotic region the phase shift \( \delta_l \).

We will solve the above described problem for positive energies. This problem has two types:

- we can find the phase-shift \( \delta_l \) or
- we can find those \( E \), for \( E \in [1, 1000] \), at which \( \delta_l = \frac{\pi}{2} \).

We selected to solve the latter problem, known as the resonance problem. The boundary conditions are give by:

\[
z(0) = 0, \quad z(r) = \cos \left( \sqrt{E} r \right) \text{ for large } r.
\]

For comparison purposes we compute the positive eigenenergies of the resonance problem with the Woods-Saxon potential using the following methods:

- **Method QT8**: the eighth order multi-step method developed by Quinlan and Tremaine [20];
- **Method QT10**: the tenth order multi-step method developed by Quinlan and Tremaine [20];
- **Method QT12**: the twelfth order multi-step method developed by Quinlan and Tremaine [20];
- **Method MCR4**: the fourth algebraic order method of Chawla and Rao with minimal phase–lag [21];
• **Method RA**: the exponentially-fitted method of Raptis and Allison [22];

• **Method MCR6**: the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [23];

• **Method NMPF1**: the Phase-Fitted Method (Case 1) developed in [10];

• **Method NMPF2**: the Phase-Fitted Method (Case 2) developed in [10];

• **Method NMC2**: the Method developed in [24] (Case 2);

• **Method NMC1**: the method developed in [24] (Case 1);

• **Method NM2SH2DV**: the Two-Step Hybrid Method developed in [1];

• **Method NM4SH2DV**: the Four Stages Symmetric Two–Step method with eliminated phase-lag and its first and second derivatives developed in [4];

• **Method NM4SH3DV**: the Four Stages Symmetric Two–Step method with eliminated phase-lag and its first, second and third derivatives developed in Section 3.

![Graph showing accuracy (digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.](image)

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

In Figures 4 and 5, we present the maximum absolute error $Err_{max} = |\log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}|$$
Figure 5. Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of CPU time (in seconds). The computational cost for each method is calculated via the CPU time (in seconds).

In order to compute the above mentioned absolute error we need references values which are mentioned as $E_{\text{accurate}}$. For our numerical experiments we use the well known two-step method of Chawla and Rao [23] with small step size of integration, in order to determine the reference values. Now the procedure for computation of the absolute errors mentioned above is the following: For each method we compute the eigenenergies, which are mentioned as $E_{\text{calculated}}$, and we compare the numerically computed eigenenergies with the reference values.

5.1.3 Remarks and Conclusions on the Numerical Results for the Radial Schrödinger Equation

The achieved numerical results lead us to the following conclusions:

1. **Method QT10** is more efficient than **Method MCR4** and **Method QT8**.

2. **Method QT10** is more efficient than **Method MCR6** for large CPU time and less efficient than **Method MCR6** for small CPU time.

3. **Method QT12** is more efficient than **Method QT10**

4. **Method NMPF1** is more efficient than **Method RA** and **Method NMPF2**
5. Method NMC2 is more efficient than Method RA, Method NMPF2 and Method NMPF1

6. Method NMC1, is more efficient than all the other methods mentioned above.

7. Method NM2SH2DV, is more efficient than all the other methods mentioned above.

8. Method NM4SH2DV, is more efficient than all the other methods mentioned above.

9. Method NM4SH3DV, is the most efficient one.

5.2. Error Estimation

For the numerical solution of the couple differential equations of the Schrödinger type variable–step methods will be applied. We call a method variable–step when during the integration procedure changes the stepsize of integration using a local truncation error estimation (LTEE) technique. Much research has been done the last decades on the development of numerical methods with constant or variable stepsize for the numerical solution of coupled differential equations arising from the Schrödinger equation and related problems (see for example [10]–[71]).

For our numerical experiments we will use an embedded pair and an error estimation procedure. Our methodology is based on the fact that for problems which have solutions with oscillatory and/or periodical behavior, the approximation is better using numerical methods with maximal algebraic order and/or with eliminated phase–lag and its derivatives of the highest possible order.

The local truncation error in \( y_{n+1}^L \) is estimated by

\[
LTE = | z_{n+1}^H - z_{n+1}^L |
\]

(37)

where \( z_{n+1}^L \) and \( z_{n+1}^H \) are determined with two methodologies

1. **Methodology based on algebraic order of the numerical methods.** In this methodology \( z_{n+1}^L \) defines the lower algebraic order solution and is achieved using the tenth algebraic order method developed in [2] and \( z_{n+1}^H \) defines the higher order solution which is achieved using the four–stages symmetric two–step method of twelfth algebraic order with vanished phase-lag and its first, second and third derivatives developed in Section 3.
2. **Methodology based on the higher order of the eliminated derivative of the phase-lag.** In this methodology \( z^L_{n+1} \) defines the solution which is achieved using the four-stages symmetric two-step method of twelfth algebraic order with eliminated phase-lag and its first and second derivatives developed in [4] and \( z^H_{n+1} \) defines the solution which is achieved using the four-stages symmetric two-step method of twelfth algebraic order with vanished phase-lag and its first, second and third derivatives developed in Section 3.

In our numerical experiments we reduce the changes of the step sizes on duplication of step sizes. We use the following procedure:

- if \( LTE < acc \) then the step size is duplicated, i.e. \( h_{n+1} = 2h_n \).
- if \( acc \leq LTE \leq 100 acc \) then the step size remains stable, i.e. \( h_{n+1} = h_n \).
- if \( 100 acc < LTE \) then the step size is halved and the step is repeated, i.e. \( h_{n+1} = \frac{1}{2} h_n \).

where \( h_n \) is the step length used for the \( n^{th} \) step of the integration and \( acc \) is the requested accuracy of the local truncation error \( LTE \).

**Remark 10.** In our numerical test we use also the well known technique of the **local extrapolation.** Based on this technique we accept at each point of integration the higher order solution \( z^H_{n+1} \) while for the error estimation less than \( acc \) the lower order solution \( z^L_{n+1} \) is used.

### 6.3. Coupled Differential Equations

Problems which are expressed via coupled differential equations arising from the Schrödinger equation can be observed in many areas of sciences like: quantum chemistry, material science, theoretical physics, quantum physics atomic physics, physical chemistry and chemical physics, quantum chemistry, etc.

The mathematical model of the close-coupling differential equations of the Schrödinger is given by:

\[
\left[ \frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i + 1)}{x^2} - V_{ii} \right] z_{ij} = \sum_{m=1}^{N} V_{im} z_{mj}
\]

for \( 1 \leq i \leq N \) and \( m \neq i \).  

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The following boundary conditions are hold, since we study the case in which all channels are open (see for details [25]):

\[
z_{ij} = 0 \text{ at } x = 0
\]

\[
z_{ij} \sim k_i x j_i (k_i x) \delta_{ij} + \left( \frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_i (k_i x) \tag{38}
\]

where \(j_i(x)\) and \(n_i(x)\) are the spherical Bessel and Neumann functions, respectively.

**Remark 11.** *In the case of close channels the proposed method can be applied also efficiently.*

Based on the detailed analysis presented in [25] and defining a matrix \(K'\) and diagonal matrices \(M\), \(N\) by:

\[
K'_{ij} = \left( \frac{k_i}{k_j} \right)^{1/2} K_{ij}
\]

\[
M_{ij} = k_i x j_i (k_i x) \delta_{ij}
\]

\[
N_{ij} = k_i x n_i (k_i x) \delta_{ij}
\]

we achieve that the asymptotic condition (38) is given now by:

\[
\mathbf{z} \sim \mathbf{M} + \mathbf{N} \mathbf{K}'.
\]

The rotational excitation of a diatomic molecule by neutral particle impact is a real problem which can be found in several scientific areas like quantum chemistry, theoretical chemistry, theoretical physics, quantum physics, material science, atomic physics, molecular physics etc. The model of this problem can be expressed via close–coupling differential equations of the Schrödinger type. In this model we have the following notations:

- the quantum numbers \((j, l)\) present the entrance channel (see for details in [25]),
- the quantum numbers \((j', l')\) present the exit channels and
- \(J = j + l = j' + l'\) presents the total angular momentum.

The above lead to

\[
\left[ \frac{d^2}{dx^2} + k_{j,j}^2 - \frac{l'(l' + 1)}{x^2} \right] z_{jj'}^{j'l'}(x) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} < j' l'; J \mid V \mid j'' l''; J > z_{jj'}^{j'l'}(x)
\]

where

\[
k_{j',j} = \frac{2\mu}{\hbar^2} \left[ E + \frac{\hbar^2}{2I} \{ j(j + 1) - j'(j' + 1) \} \right].
\]
\( E \) denotes the kinetic energy of the incident particle in the center-of-mass system, \( I \) denotes the moment of inertia of the rotator, and \( \mu \) denotes the reduced mass of the system.

The potential \( V \) is given by (see for details [25]):
\[
V(x, \hat{k}_j, \hat{k}_j) = V_0(x)P_0(\hat{k}_j, \hat{k}_j) + V_2(x)P_2(\hat{k}_j, \hat{k}_j)
\]
and consequently, the element of the coupling matrix can be written as
\[
< j' l'; J | V | j'' l''; J > = \delta_{j'j''} \delta_{l'l''} V_0(x) + f_2(j' l', j'' l''; J) V_2(x)
\]
where the \( f_2 \) coefficients are determined from formulas given by Bernstein et al. [26] and \( \hat{k}_j \) is a unit vector parallel to the wave vector \( k_j \) and \( P_i, i = 0, 2 \) are Legendre polynomials (see for details [27]). The boundary conditions can be written as:
\[
z_{jl}(x) = 0 \text{ at } x = 0
\]
\[
z_{jl}(x) \sim \delta_{jj'} \delta_{ll'} \exp[-i(k_{jj}x - 1/2l\pi)] - \left( \frac{k_i}{k_j} \right)^{1/2} S^l(jl; j'l') \exp[i(k_{jj}x - 1/2l'\pi)]
\]
where \( S \) matrix and \( K \) matrix of (38) satisfy the relation:
\[
S = (I + iK)(I - iK)^{-1}.
\]

For the numerical solution of the above mentioned problem and the computation of the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles, an algorithm is used. This algorithm contains a numerical method for the step-by-step integration from the initial value to matching points. For our numerical experiments an analogous algorithm with the algorithm developed for the numerical tests of [25] is used.

For our numerical tests we choose the \( S \) matrix with the following parameters
\[
\frac{2\mu}{\hbar^2} = 1000.0 \quad ; \quad \frac{\mu}{I} = 2.351 \quad ; \quad E = 1.1
\]
\[
V_0(x) = \frac{1}{x^{12}} - 2 \frac{1}{x^6} \quad ; \quad V_2(x) = 0.2283V_0(x).
\]

Based on the description given in full details in [25], we take the value \( J = 6 \) and we consider excitation of the rotator from the \( j = 0 \) state to levels up to \( j' = 2, 4 \) and 6 which has as result sets of four, nine and sixteen coupled differential equations, respectively. Based on the methodology given by Bernstein [27] and Allison [25], we consider the potential infinite for values of \( x \) less than some \( x_0 \). Consequently, the wave
functions tends to zero in this region and the boundary condition (39) effectively are given by as

\[ z_{j,l}^{(1)}(x_0) = 0. \]

For the approximate solution of the above presented problem we have used the following methods:

- the Iterative Numerov method of Allison [25] which is indicated as Method I\(^3\),
- the variable–step method of Raptis and Cash [28] which is indicated as Method II,
- the embedded Runge–Kutta Dormand and Prince method 5(4) [19] which is indicated as Method III,
- the embedded Runge–Kutta method ERK4(2) developed in Simos [29] which is indicated as Method IV,
- the embedded two–step method developed in [1] which is indicated as Method V,
- the embedded two–step method developed in [2] which is indicated as Method VI,
- the embedded two–step method developed in [3] which is indicated as Method VII,
- the new developed embedded two–step method developed in [4] which is indicated as Method VIII.
- the new developed embedded two–step method with error control based on the order of the eliminated derivative of the phase-lag of the method developed in this paper which is indicated as Method IX.
- the new developed embedded two–step method with error control based on the algebraic order of the method developed in this paper which is indicated as Method X.

In Table 2 we present the real time of computation requested by the numerical methods I-X mentioned above in order to calculate the square of the modulus of the \( S \) matrix for the sets of 4, 9 and 16 coupled differential equations respectively. In the same table we also present the maximum error in the calculation of the square of the modulus of the \( S \) matrix.

\(^3\)We note here that Iterative Numerov method developed by Allison [25] is one of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation.
Table 2. Coupled Differential Equations. Real time of computation (in seconds) (RTC) and maximum absolute error (MErr) to calculate $|S|^2$ for the variable-step methods Method I - Method VII. $acc=10^{-6}$. Note that hmax is the maximum stepsize. N indicates the number of equations of the set of coupled differential equations.

<table>
<thead>
<tr>
<th>Method</th>
<th>N</th>
<th>hmax</th>
<th>RTC</th>
<th>MErr</th>
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<td>9</td>
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<td>8.43</td>
<td>$7.4 \times 10^{-3}$</td>
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<td></td>
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<tr>
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</tr>
<tr>
<td></td>
<td>16</td>
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6. CONCLUSIONS

In this paper we develop, for the first time in the literature, a four-stages twelfth algebraic order symmetric two-step methods with eliminated phase-lag and its first, second and third derivatives. For this new proposed method we investigated:

- the development of the method,
- the computation of the local truncation error and the comparison of the asymptotic form of the local truncation error (based on the radial Schrödinger equation) with the asymptotic forms of the local truncation error of similar methods,
- the stability and the interval of periodicity analysis and
- the computational effectiveness of the new proposed method. This analysis was based on the numerical experiments produced by the application of the new method, well known methods of the literature and recently obtained methods on the radial Schrödinger equation and on the coupled differential equations arising from the Schrödinger equation (which are of high importance for chemistry).

The theoretical developments and the numerical achievements obtained above, lead us to the conclusion that the new proposed method is much more efficient than the other methods of the literature for the numerical solution of the radial Schrödinger equation and of the coupled differential equations arising from the Schrödinger equation.

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

Acknowledgments: The authors wish to thank the anonymous reviewers for their fruitful comments and suggestions.

Appendix A: Formulae for the $T_i$, $i = 0(1)3$ and $T_{\text{denom}}$

\[
T_0 = \left(27 v^8 a_3 b_0 + 1600 v^6 a_3 b_0 + 55440 v^4 a_3 b_0 + 55440 v^2 b_1 + 27720 v^4 a_3 b_0 + 27720 v^2 b_1 \right) \cos (v) - 327 v^8 a_3 b_0 - 1600 v^6 a_3 b_0 - 55440 v^4 a_3 b_0 + 27720 v^2 b_1
\]

\[
T_1 = \frac{729 \left(v^8 a_3 b_0 \right)}{27} + \frac{1600 v^6 a_3 b_0}{3} + \frac{6160 v^4 a_3 b_0}{3} + \frac{6160 v^2 b_1}{3}
\]
\[ T_2 = -19683 \left( v^{a_3 b_0} + \frac{1600 v^6 a_3 b_0}{27} + \frac{6160 v^4 a_3 b_0}{3} + \frac{6160 v^2 b_1}{3} \right) + \frac{6160}{3} \cos(v) + 777600000 v^{20 a_3^3 b_0^3} + \frac{74452800000 v^{18 a_3^3 b_0^3}}{1596672000000 b_0^2 a_3^2 \left( a_3 - \frac{1701}{3200000} \right) b_0} - \frac{20601 b_1}{160000} v^{16} - 1106493696000000 b_0^2 a_3^2 \left( a_3 - \frac{9}{1540} \right) b_0 - \frac{81 a_4}{616000} - \frac{9 b_1}{770} - \frac{981}{308000} v^{14} + 20831602176000 b_0^2 \left( a_3 - \frac{11755 a_4}{117422} \right) b_0 + \frac{586153 b_1}{58711} + \frac{17655}{58711} a_3^2 v^{12} + 442597478400000 b_0 a_3 \left( a_3 - \frac{320}{11947} \right) b_0 - \frac{109 b_1^2}{160} v^{10} + 511200087552000 \left( a_3 - \frac{20 a_4}{77} + 2 b_1 + \frac{40}{77} a_3 \right) b_0 a_3 v^8 - \frac{40 b_1}{693} - \frac{3}{440} b_0 + \frac{3 b_1}{6160} \left( a_3 - \frac{6400 b_1}{27} - \frac{2834}{9} \right) b_0 a_3 v^8 + \frac{17040002918400000 b_0 a_3 \left( a_3 - \frac{1}{10} b_1 - \frac{50}{693} \right) b_0 - \frac{1}{5} b_1^2}{16 a_4 - \frac{68}{693} - \frac{109}{3300}} v^6 - \frac{20448003502080000 b_0 a_3 \left( -3/4 a_4 + 1/2 \right) b_1 + \frac{25 a_4}{693} + \frac{50}{693} a_3}{20448003502080000 a_3} v^4 - \frac{1}{10} b_1^2 + \frac{20448003502080000 a_4 b_1^2}{511200087552000 b_1} v^2 - \frac{17040002918400000 a_4 b_1^2}{511200087552000 b_1} v^2 + \frac{531441 \left( v^{a_3 b_0} + \frac{1600 v^6 a_3 b_0}{27} + \frac{6160 v^4 a_3 b_0}{3} + \frac{6160 v^2 b_1}{3} \right) + \frac{6160}{3} \sin(v) - 83980800000 v^{v^{26 a_3^3 b_0^4}} + \frac{12311 v^{22 a_3^3 b_0^4}}{108} b_0^3 a_3^3 v_{22} + \frac{24640 b_0^3 a_3^3 v_{22}}{3} \left( a_3 - \frac{1701}{640000} \right) b_0 - \frac{20601 b_1}{320000} \right)
\[-711480 \left( \frac{a_3 - 13}{3850} \right) b_0 - \frac{81 a_4}{123200} \]
\[-13 b_1 - \frac{981 a_4}{1925616000} b_0 a_3^3 b_0^2 a_3 v^{20} - \frac{37945600 v^{18} a_3^3 b_0^3}{9} \left( a_3 \right) \]
\[-\frac{626711}{24640000} b_0 - \frac{351 a_4}{246400} + \frac{54777001 b_1}{110880000} - \frac{1191}{123200} \]
\[+ 146090560 b_0^2 a_3^2 \left( \frac{a_3^2 + 34711 a_3}{1440747} \right) b_0^2 + \left( \frac{724873 a_4}{284592000} \right) \]
\[-\frac{180058 b_1}{1440747} - \frac{6144947}{548860000} a_3 - \frac{27 b_1}{35200} b_0 - \frac{327 b_1^2}{17600} v^{16} \]
\[+ \frac{4218981536 b_0^2 a_3^2 v^{14}}{45} \left( b_0^2 a_3 + \left( \frac{1068440 a_4}{6604389} + \frac{183074 b_1}{22237} \right) \right) \]
\[-\frac{239120}{6604389} a_3 - \frac{1620 b_1}{22237} - \frac{5103}{1778960} b_0 - \frac{243 b_1}{355792} a_4 \]
\[+ \frac{211840 b_1}{221760} + \frac{566 b_1^2}{45} \right) + \frac{4674897920 v^{12} a_3^2 b_0^2}{3} \left( b_0^2 a_3 \right) \]
\[+ \left( \frac{60311 a_4}{221760} + 2 b_1 + \frac{101891}{110880} a_3 - \frac{58711 b_1}{554400} \right) \]
\[-\frac{39}{3080} b_0 + \frac{48607 b_1^2}{138600} + \left( -\frac{9 a_4}{6160} - \frac{387}{3080} \right) b_1 \]
\[-\frac{243 a_4}{1408000} - \frac{2943}{704000} \right) + 13498767744 b_0 a_3 \left( b_0^3 a_3^2 + \frac{380 b_0^2 a_3}{693} \right) \left( a_4 \right) \]
\[+ \frac{693 b_1 + 2}{190} a_3 - \frac{6 b_1}{19} - \frac{136133}{1504800} + \left( \frac{-80 b_1^2}{231} \right) \]
\[+ \frac{72133 a_4}{19209960} + \frac{79351}{4802490} b_1 - \frac{53 a_4}{35574} \]
\[-\frac{2227}{160083} a_3 + \frac{3 b_1^2}{1232} b_0 + \frac{109 b_1^3}{1848} v^{10} \]
\[+ 67493838720 b_0 a_3 \left( a_3 \right) \left( a_4 + 2 \right) a_3 - \frac{136}{693} b_0^2 + \left( -\frac{2}{5} b_1^2 \right) \]
\[+ \left( \frac{40 a_4}{693} - \frac{64}{231} \right) b_1 - \frac{839 a_4}{78408} - \frac{5279}{274428} a_3 + \frac{4 b_1^2}{693} \]
\[+ \frac{3 b_1}{2200} b_0 + \frac{3 b_1^2}{6160} a_3 \left( a_4 + \frac{640 b_1}{27} + \frac{4144}{45} \right) \right) v^8 \]
\[-\frac{134987677440 \left( b_0^2 a_3 + \left( -\frac{9}{6160} + \left( -\frac{3}{5} a_4 \right) \right) \right) b_0 a_3 v^6 \]
\[\left( a_4 + 2 \right) b_1 - \frac{27 a_4}{1600} + \frac{4251}{1600} \right) b_0 a_3 v^6 \]
\[-\frac{134987677440 b_0 a_3 \left( \left( a_4 + 2 \right) a_3 + \frac{2}{5} b_1 \right) b_0^2 a_3 \left( a_4 + 2 \right) a_3 + \frac{2}{5} b_1 \]
\[\left( \frac{4}{99} b_0 - \frac{2}{5} a_4 b_1^2 + \frac{16 a_4}{693} \right) b_0 - \frac{8 a_4}{231} b_1 - \frac{109 b_1^3}{6600} v^4 + \left( 67493838720 b_0^2 a_3 \right) \]
\[ T_{\text{denom}} = 27 v^8 a_3 b_0 + 1600 v^6 a_3 b_0 + 55440 v^4 a_3 b_0 + 55440 v^2 b_1 + 55440. \]

Appendix B: Formulae for the $T_j$, $j = 4(1)7$,

$T_{\text{denom}}$, $T_{\text{denom}2}$ and $T_{\text{denom}3}$

\[
T_4 = \left( -1296 v^5 + 38400 v^3 + 1330560 v \right) \left( \cos(v) \right)^3 \\
+ \left( -1296 v^6 + 57840 v^4 + 789120 v^2 + 1330560 \right) \sin(v) \\
- 1962 v^7 + 144674 v^5 + 177120 v^3 \\
+ 2328480 v \left( \cos(v) \right)^2 + \left( 31392 v^6 - 158640 v^4 \right) \\
+ 541440 v^2 - 1330560 \right) \sin(v) \\
+ 2592 v^5 - 76800 v^3 - 2661120 v \right) \cos(v) \\
+ \left( -7776 v^6 - 230400 v^4 - 2661120 v^2 \right) \sin(v) \\
- 3924 v^7 - 179570 v^5 - 471360 v^3 - 997920 v \]

\[
T_{\text{denom}1} = \left( 81 v^7 - 3037 v^5 - 88560 v^3 - 1164240 v \right) \left( \cos(v) \right)^2 \\
+ \left( -1296 v^6 + 28680 v^4 \right) \\
+ 270720 v^2 - 665280 \right) \sin(v) + 7848 v^5 \\
- 19200 v^3 - 665280 v \right) \cos(v) \\
+ \left( 7848 v^6 + 136920 v^4 + 394560 v^2 + 665280 \right) \sin(v) \\
+ 162 v^7 + 11989 v^5 + 274080 v^3 + 1829520 v \]

\[
T_5 = \left( \cos(v) \right)^2 v^2 + 3 \left( \cos(v) \right)^2 + 2 v^2 - 3 \]

\[
T_{\text{denom}2} = v \left( 27720 v + 109 \left( \cos(v) \right)^2 v^7 - 1889 \left( \cos(v) \right)^2 v^5 \right) \\
- 756 \cos(v) v^5 + 7240 \left( \cos(v) \right)^2 v^3 \\
+ 378 \left( \cos(v) \right)^3 v^5 + 324 v^6 \sin(v) + 9600 v^4 \sin(v) \]
\[-558-\]

\[-16000 \cos(v) v^3 + 110880 v^2 \sin(v) + 8000 \left(\cos(v)\right)^3 v^3 + 55440 \left(\cos(v)\right)^2 v + 27720 \left(\cos(v)\right)^2 v - 55440 \cos(v) \sin(v) - 110880 \cos(v) v + 7667 v^5 + 28480 v^3 + 218 v^7 - 10480 \left(\cos(v)\right)^2 \sin(v) v^2 - 1222 \left(\cos(v)\right)^2 \sin(v) v^4 - 1308 \cos(v) \sin(v) v^6 - 7778 \cos(v) \sin(v) v^4 - 44960 \cos(v) \sin(v) v^2 - 54 \left(\cos(v)\right)^2 \sin(v) v^6\]

\[T_6 = \left(9072 v^5 + 192000 v^3 + 1330560 v\right) \left(\cos(v)\right)^3 + \left(\left(-1296 v^6 - 29328 v^4 - 251520 v^2\right)\right) \sin(v) + 2616 v^7 - 45336 v^5 + 173760 v^3 + 665280 v\]

\[T_7 = \left(-108 v^7 - 2532 v^5 - 86880 v^3 - 332640 v\right) \left(\cos(v)\right)^2 + \left(\left(-1296 v^6 - 42936 v^4 - 539520 v^2 - 665280\right)\right) \sin(v) + 18144 v^5 - 384000 v^3 - 2661120 v\]

\[T_{\text{denom}} = v^2 \left(\left(v^7 - \frac{3037 v^5}{81} - \frac{3280 v^3}{3} - \frac{43120 v}{3}\right)\right) \left(\cos(v)\right)^2 + \left(\left(16 v^6 + \frac{9560 v^4}{27} + \frac{30080 v^2}{9} - \frac{24640}{3}\right)\right) \sin(v) + \frac{872 v^5}{9} - \frac{6400 v^3}{27} - \frac{24640 v}{3} \cos(v) + \left(\frac{872 v^6}{9} + \frac{45640 v^4}{27} + \frac{43840 v^2}{9} + \frac{24640}{3}\right) \sin(v) + 2 v^7 + \frac{11989 v^5}{81} + \frac{91360 v^3}{27} + \frac{67760 v}{3}\]
Appendix C: Taylor Series Expansion Formulae for the coefficients of the new obtained method given by (16)

\[ a_4 = -2 - \frac{307 v^{14}}{9340531200} - \frac{41 v^{16}}{53801459712} - \frac{1552351 v^{18}}{39614687304192000} + \cdots \]

\[ a_3 = \frac{1}{200} - \frac{307 v^{8}}{44478720000} + \frac{237023 v^{10}}{35026992000000} - \frac{330122394201600000 v^{14}}{1200862451441 v^{16}} - \frac{15932710316247588800 v^{18}}{40097184957786457 v^{18}} + \frac{20635569156169634108928000000 v^{20}}{20635569156169634108928000000} + \cdots \]

\[ b_0 = \frac{5}{6} - \frac{307 v^{10}}{1111968000} + \frac{739 v^{12}}{15015614353 v^{16}} + \frac{4424473 v^{14}}{175037669363 v^{18}} + \frac{10116006549984691200000 v^{20}}{199158878953094860800000 v^{20}} + \cdots \]

\[ b_1 = \frac{1}{12} + \frac{307 v^{10}}{2223936000} + \frac{67 v^{12}}{8302694400 v^{16}} + \frac{460087 v^{14}}{330908311609 v^{18}} + \frac{595059208823439360000 v^{20}}{199158878953094860800000 v^{20}} + \cdots \]

Appendix D: Expressions for the Derivatives of \( z_n \)

Expressions of the derivatives which are presented in the formulae of the Local Truncation Errors:

\[ z^{(2)} = (V(x) - V_c + G) z(x) \]

\[ z^{(3)} = \left( \frac{d}{dx} g(x) \right) z(x) + (g(x) + G) \frac{d}{dx} z(x) \]

\[ z^{(4)} = \left( \frac{d^2}{dx^2} g(x) \right) z(x) + 2 \left( \frac{d}{dx} g(x) \right) \frac{d}{dx} z(x) + (g(x) + G)^2 z(x) \]

\[ z^{(5)} = \left( \frac{d^3}{dx^3} g(x) \right) z(x) + 3 \left( \frac{d^2}{dx^2} g(x) \right) \frac{d}{dx} z(x) + 4 (g(x) + G) z(x) \frac{d}{dx} g(x) + (g(x) + G)^2 \frac{d}{dx} z(x) \]
\[ z^{(6)} = \left( \frac{d^4}{dx^4} g(x) \right) z(x) + 4 \left( \frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} z(x) \]

\[ + \quad 7 (g(x) + G) z(x) \frac{d^2}{dx^2} g(x) + 4 \left( \frac{d}{dx} g(x) \right)^2 z(x) \]

\[ + \quad 6 (g(x) + G) \left( \frac{d}{dx} z(x) \right) \frac{d}{dx} g(x) + (g(x) + G)^3 z(x) \]

\[ z^{(7)} = \left( \frac{d^5}{dx^5} g(x) \right) z(x) + 5 \left( \frac{d^4}{dx^4} g(x) \right) \frac{d}{dx} z(x) \]

\[ + \quad 11 (g(x) + G) z(x) \frac{d^3}{dx^3} g(x) + 15 \left( \frac{d}{dx} g(x) \right)^2 z(x) \]

\[ + \quad \frac{d^2}{dx^2} g(x) + 13 (g(x) + G) \left( \frac{d}{dx} z(x) \right) \frac{d^2}{dx^2} g(x) \]

\[ + \quad 10 \left( \frac{d}{dx} g(x) \right)^2 \frac{d}{dx} z(x) + 9 (g(x) + G)^2 z(x) \]

\[ + \quad \frac{d}{dx} g(x) + (g(x) + G)^3 \frac{d}{dx} z(x) \]

\[ z^{(8)} = \left( \frac{d^6}{dx^6} g(x) \right) z(x) + 6 \left( \frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} z(x) \]

\[ + \quad 16 (g(x) + G) z(x) \frac{d^4}{dx^4} g(x) + 26 \left( \frac{d}{dx} g(x) \right)^2 z(x) \]

\[ + \quad \frac{d^3}{dx^3} g(x) + 24 (g(x) + G) \left( \frac{d}{dx} z(x) \right) \frac{d^3}{dx^3} g(x) \]

\[ + \quad 15 \left( \frac{d^2}{dx^2} g(x) \right)^2 z(x) + 48 \left( \frac{d}{dx} g(x) \right) \]

\[ + \quad \left( \frac{d}{dx} z(x) \right) \frac{d^2}{dx^2} g(x) + 22 (g(x) + G)^2 z(x) \]

\[ + \quad \frac{d^2}{dx^2} g(x) + 28 (g(x) + G) z(x) \left( \frac{d}{dx} g(x) \right)^2 \]

\[ + \quad 12 (g(x) + G)^2 \left( \frac{d}{dx} z(x) \right) \frac{d}{dx} g(x) + (g(x) + G)^4 z(x) \]
We compute the $j$-th derivative of the function $z$ at the point $x_n$, i.e. $z_n^{(j)}$, substituting in the above formulae $x$ with $x_n$.

**Appendix E: Formula for the quantity $B_0$**

\[
B_0 = \frac{107143 \ (g(x))^2 \ (\frac{d}{dx} y(x)) \ (\frac{d}{dx} g(x)) \ (\frac{d^4}{dx^4} g(x))}{6671808000} \\
+ \frac{307 \ g(x) \ y(x) \ (\frac{d}{dx} g(x))^2 \ \frac{d^4}{dx^4} g(x)}{7983360} \\
+ \frac{2149 \ (g(x))^2 \ (\frac{d}{dx} y(x)) \ (\frac{d^2}{dx^2} g(x)) \ (\frac{d^4}{dx^4} g(x))}{83397600} \\
+ \frac{221347 \ g(x) \ (\frac{d}{dx} y(x)) \ (\frac{d}{dx} g(x)) \ (\frac{d^2}{dx^2} g(x))^2}{4447872000} \\
+ \frac{9517 \ g(x) \ (\frac{d}{dx} y(x)) \ (\frac{d}{dx} g(x))^2 \ \frac{d^3}{dx^3} g(x)}{247104000} \\
+ \frac{34691 \ (g(x))^4 \ y(x) \ \frac{d^4}{dx^4} g(x)}{26687232000} \\
+ \frac{7061 \ (g(x))^2 \ (\frac{d}{dx} y(x)) \ (\frac{d^2}{dx^2} g(x))}{4670265600} \\
+ \frac{166087 \ (g(x))^2 \ y(x) \ \frac{d^4}{dx^4} g(x)}{186810624000} \\
+ \frac{1068667 \ g(x) \ y(x) \ (\frac{d^5}{dx^5} g(x)) \ (\frac{d^4}{dx^4} g(x))}{46702656000} \\
+ \frac{883853 \ g(x) \ y(x) \ (\frac{d^6}{dx^6} g(x)) \ (\frac{d^2}{dx^2} g(x))}{62270208000} \\
+ \frac{574397 \ g(x) \ y(x) \ (\frac{d^7}{dx^7} g(x)) \ \frac{d}{dx} g(x)}{93405312000} \\
+ \frac{112669 \ g(x) \ (\frac{d}{dx} y(x)) \ (\frac{d^5}{dx^5} g(x)) \ (\frac{d^2}{dx^2} g(x))}{4447872000} \\
+ \frac{24253 \ g(x) \ (\frac{d}{dx} y(x)) \ (\frac{d^4}{dx^4} g(x)) \ (\frac{d^3}{dx^3} g(x))}{6671808000} \\
+ \frac{156263 \ g(x) \ (\frac{d}{dx} y(x)) \ (\frac{d^5}{dx^5} g(x)) \ \frac{d}{dx} g(x)}{13343616000} \\
+ \frac{263099 \ (g(x))^2 \ y(x) \ (\frac{d^2}{dx^2} g(x)) \ (\frac{d^4}{dx^4} g(x))}{8491392000}
\]
\[
\begin{align*}
+ \quad & \frac{782543}{46702656000} (g(x))^2 y(x) \left( \frac{d}{dx} g(x) \right) \frac{d^5}{dx^5} g(x) \\
+ \quad & \frac{7061}{18681062400} g(x) \left( \frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x) \\
+ \quad & \frac{3626591}{31135104000} g(x) 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) \\
+ \quad & \frac{1494169}{62270208000} g(x) y(x) \left( \frac{d^2}{dx^2} g(x) \right)^3 \\
+ \quad & \frac{5219}{606528000} \left( \frac{d^3}{dx^3} g(x) \right) \left( \frac{d}{dx} y(x) \right) \frac{d^6}{dx^6} g(x) \\
+ \quad & \frac{18727}{10378368000} \left( \frac{d}{dx} g(x) \right) \left( \frac{d}{dx} y(x) \right) \frac{d^6}{dx^6} g(x) \\
+ \quad & \frac{598957}{15567552000} \left( \frac{d}{dx} g(x) \right)^2 y(x) \left( \frac{d^2}{dx^2} g(x) \right)^2 \\
+ \quad & \frac{2149}{40435200} \left( \frac{d^2}{dx^2} g(x) \right)^2 y(x) \frac{d^4}{dx^4} g(x) \\
+ \quad & \frac{129247}{5660928000} \left( \frac{d^2}{dx^2} g(x) \right)^2 y(x) \frac{d^4}{dx^4} g(x) \\
+ \quad & 307 \left( \frac{d}{dx} g(x) \right)^3 y(x) \frac{d^3}{dx^3} g(x) \\
+ \quad & \frac{5219}{14370048} \left( \frac{d^2}{dx^2} g(x) \right) y(x) \frac{d^8}{dx^8} g(x) \\
+ \quad & \frac{5660928000}{12245696000} \left( \frac{d}{dx} g(x) \right)^3 (g(x))^3 y(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) \frac{d^7}{dx^7} g(x) \\
+ \quad & \frac{307}{55598400} \left( \frac{d}{dx} g(x) \right)^3 (g(x))^3 y(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x) \\
+ \quad & \frac{155279}{13343616000} \left( \frac{d}{dx} g(x) \right)^3 (g(x))^3 y(x) \left( \frac{d}{dx} y(x) \right) \left( \frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x) \\
+ \quad & \frac{193103}{6671808000} \left( g(x) \right)^2 y(x) \left( \frac{d}{dx} g(x) \right)^2 \frac{d^2}{dx^2} g(x) \\
+ \quad & \frac{2149}{30888000} \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) \\
+ \quad & \frac{14429}{486486000} \left( \frac{d}{dx} g(x) \right) y(x) \left( \frac{d^4}{dx^4} g(x) \right) \frac{d^2}{dx^2} g(x) \\
+ \quad & \frac{252047}{62270208000} \left( \frac{d}{dx} g(x) \right) y(x) \left( \frac{d^4}{dx^4} g(x) \right) \frac{d^3}{dx^3} g(x) \\
+ \quad & \frac{307}{15567552000} \left( \frac{d^{11}}{dx^{11}} g(x) \right) \frac{d}{dx} y(x)
\end{align*}
\]
\[-563-\]

\[
\begin{align*}
&+ 307 \left( \frac{d^5}{dx^5} g(x) \right)^2 y(x) + \frac{307 \left( \frac{d^3}{dx^3} g(x) \right) y(x)}{235872000} \\
&+ \frac{3377 \left( \frac{d^2}{dx^2} g(x) \right) \left( \frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x)}{707616000} \\
&+ \frac{307 \left( \frac{d}{dx} g(x) \right)^3 \left( \frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x)}{12636000} \\
&+ \frac{8903 \left( \frac{d}{dx} g(x) \right) y(x) \frac{d^3}{dx^3} g(x)}{2351328000} \\
&+ \frac{140299 \left( \frac{d^2}{dx^2} g(x) \right) \left( \frac{d}{dx} y(x) \right) \left( \frac{d^3}{dx^3} g(x) \right)^2}{3335904000} \\
&+ \frac{307 \left( \frac{d^4}{dx^4} g(x) \right) \left( \frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x)}{26956800} \\
&+ \frac{20569 g(x) y(x) \frac{d^6}{dx^6} g(x)}{186810624000} \\
&+ \frac{307 (g(x))^4 \left( \frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x)}{444787200} \\
&+ \frac{123107 \left( \frac{d}{dx} g(x) \right)^2 y(x) \frac{d^6}{dx^6} g(x)}{15567552000} \\
&+ \frac{307 \left( \frac{d^2}{dx^2} g(x) \right) y(x) \left( \frac{d^3}{dx^3} g(x) \right)^2}{11664000} \\
&+ \frac{7061 \left( \frac{d^2}{dx^2} g(x) \right)^2 \left( \frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x)}{370656000} \\
&+ \frac{13201 \left( \frac{d^4}{dx^4} g(x) \right) y(x) \frac{d^6}{dx^6} g(x)}{5660928000} \\
&+ \frac{7061 (g(x))^5 y(x) \frac{d^2}{dx^2} g(x)}{26687232000} \\
&+ \frac{357041 (g(x))^3 y(x) \frac{d^6}{dx^6} g(x)}{186810624000} \\
&+ \frac{147053 (g(x))^2 y(x) \left( \frac{d^3}{dx^3} g(x) \right)^2}{7783776000} \\
&+ \frac{83197 g(x) y(x) \left( \frac{d^4}{dx^4} g(x) \right)^2}{6227020800} + \frac{197401 (g(x))^3 y(x) \left( \frac{d^2}{dx^2} g(x) \right)^2}{26687232000} \\
&+ \frac{307 (g(x))^5 \left( \frac{d}{dx} y(x) \right) \frac{d}{dx} g(x)}{4447872000} + \frac{24253 (g(x))^3 \left( \frac{d}{dx} y(x) \right) \frac{d^5}{dx^5} g(x)}{13343616000} \\
&+ \frac{307 (g(x))^7 y(x)}{186810624000} + \frac{307 (g(x))^4 y(x) \left( \frac{d}{dx} g(x) \right)^2}{333590400} \\
&+ \frac{307 g(x) y(x) \left( \frac{d}{dx} g(x) \right)^4}{51321600} + \frac{307 (g(x))^2 y(x) \left( \frac{d}{dx} g(x) \right)^3}{74131200}
\end{align*}
\]

at every point \(x = x_n\).
References


