

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

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Abstract

In this paper we obtain, for the first time in the literature, a new twelfth algebraic order four–stages symmetric two–step method. The method is produced, i.e. its coefficients are determined, by requiring the vanishing of the phase–lag and its first, second, third and fourth derivatives and by requesting additionally the highest possible algebraic order. The result of the elimination of the phase–lag and its derivatives on the effectiveness of the new obtained method is also studied. The following are investigated:

- the construction of the method,
- the computation of the local truncation error (LTE) of the new obtained method,
- the full analysis of the method which consists: (1) LTE analysis which is based on the radial Schrödinger equation and (2) Stability and Interval of Periodicity Analysis which is based on a scalar test equation with frequency not equal with the frequency of the scalar test equation used for the phase–lag analysis,

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- the determination of two embedding techniques for the error estimation: (i) one is based on the algebraic order of the methods and (ii) one is based on the order of the vanished derivative of the phase-lag,
- the examination of the effectiveness of the new produced method by applying it into two problems: (i) the resonance problem of the Schrödinger equation and (ii) the coupled differential equations of the Schrödinger type.

The above analysis lead to the conclusion that the new developed method is very efficient for the approximate solution of the Schrödinger equation and related initial-value or boundary-value problems with solutions of periodic and /or oscillating behaviour. The new presented and analyzed method is an improvement of the recent developed methods in [1], [2], [3], [4] and [5].

1. Introduction

In the present paper, for the first time in the literature, we propose a high algebraic four-stages symmetric two-step method for the efficient numerical solution of problems of the form of the Schrödinger equation. We will examine the effectiveness of the new obtained method with an application to the numerical solution of the following problems:

- the radial time independent Schrödinger equation and
- the coupled differential equation arising from the Schrödinger equation.

In Computational Chemistry (see [6] and references therein) the effective solution of the above mentioned problems is very important. It is known (see [6] and references therein) that an important part of the quantum chemical calculations contains the Schrödinger equation. We note here that for more than one particle we can have approximate solution of the Schrödinger's equation. The efficient approximate solution of the Schrödinger equation gives us the following:

1. calculation of significant molecular properties (such as vibrational energy levels and wave functions of systems) and
2. supply us an substantial presentation of the molecule's electronic structure (see for more details in [7–10]).

The method obtained in this paper will improve the methods proposed for the first time in the literature in [1], [2], [4] and [5]. More specifically:

1. The methods produced in [1] and [2] are of tenth algebraic order, while the new developed method is of twelfth algebraic order.
2. The method obtained in [4] is of twelfth algebraic order and has vanished the phase-lag and its first and second derivatives
3. The method developed in [5] is of twelfth algebraic order and has vanished the phase-lag and its first, second and third derivatives.
4. The method developed in this paper and first introduced in the literature, is of twelfth algebraic order and has vanished the phase-lag and its first, second, third and fourth derivatives.

We also present in this paper a new error control. This error control is based on the order of the vanished derivatives of the phase-lag.

The above presented problems belong to the family of the special second order initial or boundary value problems with solution which behaves periodically and/or oscillatory and they have the general form:

$$q''(x) = f(x, q), \quad q(x_0) = q_0 \quad \text{and} \quad q'(x_0) = q'_0. \quad (1)$$

The last decades much research was done on the subject of this paper. The research created bibliography, some parts of which are given below:

- Exponentially, trigonometrically and phase fitted Runge–Kutta and Runge–Kutta Nyström methods: [44], [47], [56], [59]–[62], [53] [71].
- Multistep exponentially, trigonometrically and phase fitted methods and multistep methods with minimal phase-lag: [1]–[4], [15]–[18], [22]–[25], [31], [35], [41], [45]–[46], [50], [55], [57]–[58], [64]–[66], [72]–[75].
- Symplectic integrators: [39]–[40], [48], [51], [54], [62]–[63], [69].
- Nonlinear methods: [49].
- General methods: [11]–[14], [19]–[21], [32]–[34], [37]–[38].

2. Phase-lag and stability analysis of $2m$ symmetric multistep methods

The problem (1) can be solved numerically using the $2m$ -step method presented below at (2), if we discretize the integration interval $[a, b]$. The discretization can be done using a stepsize h . We note that x_n presents the n -th point of the discretized area, while h is determined as $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$ and is defined as the stepsize or the step length of the integration. Finally, q_n presents the approximated (computed using the $2m$ -step method (2)) value of the function $q(x)$ at the point x_n .

We consider the $2m$ -Step methods of the form:

$$\sum_{i=-m}^m c_i q_{n+i} = h^2 \sum_{i=-m}^m b_i f(x_{n+i}, q_{n+i}) \tag{2}$$

for the approximate integration of the initial value problem (1) on the interval $[a, b]$.

Definition 1. *The method (2) is called symmetric $2m$ -step method if the following conditions are hold:*

$$c_{-i} = c_i, i = 0(1)m$$

$$b_{-i} = b_i, i = 0(1)m$$

Remark 1. *The linear operator:*

$$L(x) = \sum_{i=-m}^m c_i q(x + ih) - h^2 \sum_{i=-m}^m b_i q''(x + ih) \tag{3}$$

where $q \in \mathbb{C}^2$, is associated with the method (2).

Definition 2. [11] The multistep method (2) is called of algebraic order p , if the associated linear operator L (3) vanishes for any linear combination of the linearly independent functions $1, x, x^2, \dots, x^{p+1}$.

If we apply the symmetric $2m$ -step method to the scalar test equation

$$q'' = -\phi^2 q \tag{4}$$

we obtain the following difference equation:

$$\begin{aligned}
 &A_m(v) q_{n+m} + \dots + A_1(v) q_{n+1} + A_0(v) q_n \\
 &+ A_1(v) q_{n-1} + \dots + A_m(v) q_{n-m} = 0
 \end{aligned} \tag{5}$$

where $v = \phi h$, h is the stepsize or step length and $A_j(v)$, $j = 0(1)m$ are polynomials of v .

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

$$\begin{aligned}
 &A_m(v) \lambda^m + \dots + A_1(v) \lambda + A_0(v) \\
 &+ A_1(v) \lambda^{-1} + \dots + A_m(v) \lambda^{-m} = 0.
 \end{aligned} \tag{6}$$

Definition 3. [12] A symmetric $2m$ -step method with characteristic equation given by (6) is said to have an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots λ_i , $i = 1(1)2m$ of Eq. (6) satisfy:

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

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

Definition 4. (see [12]) A multistep method is called P -stable if its interval of periodicity is equal to $(0, \infty)$. The necessary and sufficient conditions for the P -stability of a symmetric method are:

$$|\lambda_1| = |\lambda_2| = 1 \tag{8}$$

$$|\lambda_j| \leq 1, j = 3(1)2m, \forall v. \tag{9}$$

Definition 5. A multistep method is called singularly P -stable if its interval of periodicity is equal to $(0, \infty) \setminus S$ with S a finite set of points.

Definition 6. [13], [14] The phase-lag is the leading term in the expansion of

$$t = v - \theta(v). \tag{10}$$

for any symmetric multistep method which is associated to the characteristic equation (6). If $t = O(v^{t+1})$ as $v \rightarrow \infty$ then the order of phase-lag is t .

Definition 7. [15] A method is called **phase-fitted** if its phase-lag is equal to zero.

Theorem 1. [13] *The symmetric 2m-step method with associated characteristic equation given by (6) has phase-lag order t and phase-lag constant c given by*

$$-cv^{t+2} + O(v^{t+4}) = \frac{2 A_m(v) \cos(mv) + \dots + 2 A_j(v) \cos(jv) + \dots + A_0(v)}{2 m^2 A_m(v) + \dots + 2 j^2 A_j(v) + \dots + 2 A_1(v)} \quad (11)$$

Remark 2. *For the methods studied in this paper (symmetric two-step methods), the phase-lag of order t with phase-lag constant c are given by:*

$$-cv^{t+2} + O(v^{t+4}) = \frac{2 A_1(v) \cos(v) + A_0(v)}{2 A_1(v)} \quad (12)$$

considering that their characteristic polynomials are $A_j(v)$ $j = 0, 1$,

3. The new high order four-stages symmetric two-step method with vanished phase-lag and its first, second, third and fourth derivatives

Let us consider the methods

$$\begin{aligned} \widehat{q}_n &= q_n - a_0 h^2 (f_{n+1} - 2 f_n + f_{n-1}) - 2 a_1 h^2 f_n \\ \widetilde{q}_n &= q_n - a_2 h^2 (f_{n+1} - 2 \widehat{f}_n + f_{n-1}) \\ \bar{q}_n &= q_n - a_3 h^2 (f_{n+1} - 2 \widetilde{f}_n + f_{n-1}) \\ q_{n+1} + a_4 q_n + q_{n-1} &= h^2 \left[b_1 (f_{n+1} + f_{n-1}) + b_0 \bar{f}_n \right] \end{aligned} \quad (13)$$

where $f_{n+i} = q''(x_{n+i}, q_{n+i}), i = -1(1)1, \widehat{f}_n = q''(x_n, \widehat{q}_n), \widetilde{f}_n = z''(x_n, \widetilde{q}_n), \bar{f}_n = z''(x_n, \bar{q}_n)$ and $a_j, j = 0(1)4$ and $b_i, i = 0, 1$ are parameters.

We will investigate the case of the above noted methods (13):

$$a_0 = -\frac{27}{3200}, a_1 = \frac{3}{32}. \quad (14)$$

Requesting for the above symmetric two-step method (13), with the parameters given by (14), the vanishing of the phase-lag and its first, second, third and fourth derivatives, we obtain the following system of equations:

$$\text{Phase - Lag(PL)} = \frac{T_0}{T_{denom}} = 0 \quad (15)$$

$$\text{First Derivative of the Phase - Lag} = \frac{T_1}{T_{denom}^2} = 0 \quad (16)$$

$$\text{Second Derivative of the Phase - Lag} = \frac{T_2}{T_{denom}^3} = 0 \tag{17}$$

$$\text{Third Derivative of the Phase - Lag} = \frac{T_3}{T_{denom}^4} = 0 \tag{18}$$

$$\text{Fourth Derivative of the Phase - Lag} = \frac{T_4}{T_{denom}^5} = 0 \tag{19}$$

where $T_j, j = 0(1)4$ and T_{denom} are given in the Appendix A.

Solving the system of equations (15)–(19), we determine the rest of the parameters of the new method (13):

$$a_4 = -2 \frac{T_5}{T_{denom1}} \quad , \quad a_3 = \frac{1}{8} \frac{T_6}{T_{denom2}} \quad , \quad a_2 = \frac{T_7}{T_{denom3}}$$

$$b_0 = 48 \frac{T_8}{v^2 T_{denom1}} \quad , \quad b_1 = -24 \frac{T_9}{v^2 T_{denom1}} \tag{20}$$

where $T_j, j = 5(1)9, T_{denom1}, T_{denom2}$ and T_{denom3} are given in the Appendix B.

The truncated Taylor series expansions of the above mentioned coefficients (20) are presented the Appendix C. These formulae are provided in order to avoid cases of heavy cancelations or non definition (for example when the denominators of the formulae of the coefficients, given by (20), are equal to zero for some values of $|v|$)

In Figure 1 we present the behavior of the coefficients.

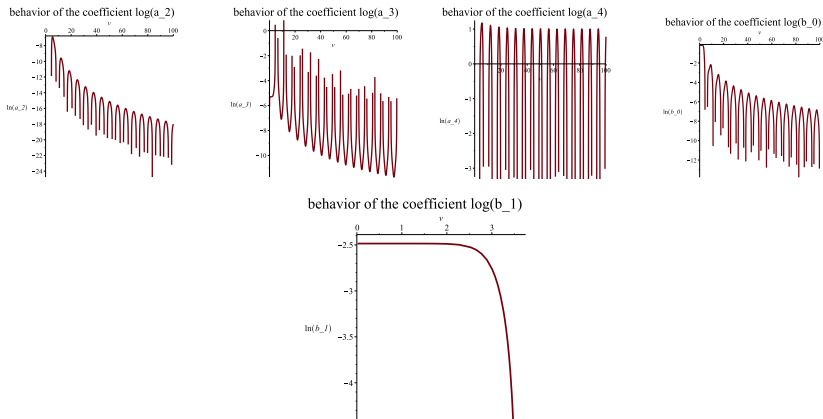


Figure 1. Behavior of the free parameters of the new proposed method (13) given by (20) for several values of $v = \phi h$.

The local truncation error of the new obtained method (13) with the coefficients given

by (14) and (20), which is indicated as *NM4SH4DV*, is given by:

$$LTE_{NM4SH4DV} = \frac{307}{186810624000} h^{14} \left(q_n^{(14)} + 35 \phi^6 z_n^{(8)} + 105 \phi^8 q_n^{(6)} + 126 \phi^{10} q_n^{(4)} + 70 \phi^{12} q_n^{(2)} \right) + O(h^{16}). \quad (21)$$

4. Error and stability analysis of the new developed method

4.1. Comparative error analysis

For the the local truncation error analysis we will use as test problem the radial time independent Schrödinger equation with potential $V(x)$:

$$q''(x) = (V(x) - V_c + G) q(x) \quad (22)$$

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
- E is the energy.

The following methods are studied:

4.1.1. Classical method (i.e., method (13) with constant coefficients)

$$LTE_{CL} = \frac{307}{186810624000} h^{14} q_n^{(14)} + O(h^{16}). \quad (23)$$

4.1.2. Method with vanished phase-lag and its first and second derivatives developed in [4]

$$LTE_{NM4SH2DV} = \frac{307}{186810624000} h^{14} \left(q_n^{(14)} - 15 \phi^8 q_n^{(6)} - 24 \phi^{10} q_n^{(4)} - 10 \phi^{12} q_n^{(2)} \right) + O(h^{16}). \quad (24)$$

4.1.3. Method with vanished phase-lag and its first, second and third derivatives developed in [5]

$$\begin{aligned}
 LTE_{NM4SH3DV} = & \frac{307}{186810624000} h^{14} \left(q_n^{(14)} - 35 \phi^8 q_n^{(6)} \right. \\
 & \left. - 84 \phi^{10} q_n^{(4)} - 70 \phi^{12} q_n^{(2)} \right) + O(h^{16}). \quad (25)
 \end{aligned}$$

4.1.4. Method with vanished phase-lag and its first, second, third and fourth derivatives developed in Section 3.

$$\begin{aligned}
 LTE_{NM4SH4DV} = & \frac{307}{186810624000} h^{14} \left(q_n^{(14)} + 35 \phi^6 z_n^{(8)} \right. \\
 & \left. + 105 \phi^8 q_n^{(6)} + 126 \phi^{10} q_n^{(4)} + 70 \phi^{12} q_n^{(2)} \right) + O(h^{16}). \quad (26)
 \end{aligned}$$

We follow the procedure:

- The new formulae of the Local Truncation Errors (LTEs), which are produced using the radial time independent Schrödinger equation (22), are calculated.
- The above is achieved by computing the derivatives of the function q , which are requested in the formulae of LTEs mentioned above (23), (24), (25) and (26), using (22).
- Some of the expressions of the derivatives of the function q are presented in the Appendix D.
- The new formulae of LTEs obtained from the above steps include the quantity G and the energy E .
- We investigate two cases for the parameter G :

1. The Energy and the Potential are closed each other.

Since the energy and the potential are closed each other, we obtain:

$$G = V_c - E \approx 0 \Rightarrow G^i \approx 0, i = 1, 2, \dots \quad (27)$$

Based on the above, new formulae of the LTEs are produced, the general form of which is given by:

$$LTE = h^{14} \sum_{j=0}^k Q_j G^j \quad (28)$$

where Q_j are: (1) constant numbers (classical case) or (2) formulae of v and $G = V_c - E$ (frequency dependent cases - eliminated phase-lag and its derivatives).

Remark 3. *In the case $G = V_c - E \approx 0$, we have:*

$$LTE_{G=0} = h^{14} Q_0 \quad (29)$$

where Q_0 is equal for all the above formulae (23), (24), (25) and (26).

Consequently, for $G = V_c - E \approx 0$ we obtain:

$$LTE_{CL} = LTE_{NM4SH2DV} = LTE_{NM4SH3DV} = LTE_{NM4SH4DV} = h^{14} Q_0 \quad (30)$$

where Q_0 is given in the Appendix E at every point $x = x_n$.

Theorem 2. *From (27) 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, the local truncation error for the method with eliminated phase-lag and its first, second and third derivatives and the local truncation error for the method with eliminated phase-lag and its first, second, third and fourth derivatives are the same and equal to $h^{14} Q_0$, where Q_0 is given in the Appendix E and therefore for $G = 0$ the methods are of comparable accuracy.*

2. **The Energy and the Potential are far from each other.** Consequently, $G \gg 0$ or $G \ll 0$ and the value of $|G|$ is a large number. Therefore, the method with asymptotic form of LTE which includes the minimum power of G is the most accurate one.

- Based on the above analysis the following asymptotic expressions of the LTEs are obtained.

4.1.5. Classical method

$$LTE_{CL} = \frac{307}{186810624000} h^{14} \left(q(x) G^7 + \dots \right) + O(h^{16}). \quad (31)$$

4.1.6. Method with vanished phase-lag and its first and second derivatives developed in [4]

$$LTE_{NM4SH2DV} = \frac{307}{2335132800} h^{14} \left(\left(\frac{d^2}{dx^2} g(x) \right) q(x) G^5 + \dots \right) + O(h^{16}). \quad (32)$$

4.1.7. Method with vanished phase-lag and its first, second and third derivatives developed in [5]

$$\begin{aligned} LTE_{NM4SH3DV} = & \frac{307}{6671808000} h^{14} \left[\left(15 \left(\frac{d}{dx} g(x) \right)^2 q(x) \right. \right. \\ & + 20 g(x) q(x) \frac{d^2}{dx^2} g(x) + 27 \left(\frac{d^4}{dx^4} g(x) \right) q(x) \\ & \left. \left. + 10 \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} q(x) \right) G^4 + \dots \right] + O(h^{16}). \quad (33) \end{aligned}$$

4.1.8. Method with vanished phase-lag and its first, second, third and fourth derivatives developed in Section 3.

$$LTE_{NM4SH4DV} = \frac{307}{555984000} h^{14} \left[\left(\frac{d^4}{dx^4} g(x) q(x) \right) G^4 + \dots \right] + O(h^{16}). \quad (34)$$

The analysis leads to the following theorem:

Theorem 3.

- *Classical Method (i.e., the method (13) with constant coefficients): For this method the error increases as the seventh power of G.*

- *Twelfth 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 [5]: For this method the error increases as the fourth power of G .*
- *Twelfth Algebraic Order Two-Step Method with Eliminated Phase-lag and its First, Second, Third and Fourth Derivatives developed in Section 3: For this method the error increases as the fourth power of G but its coefficient is much smaller compared with the method developed in [5].*

Consequently, for the approximate solution of the time independent radial Schrödinger equation the New Obtained Twelfth Algebraic Order Method with vanished phase-lag and its first, second, third and fourth derivatives is the most accurate one, especially in the case of large values of $|G| = |V_c - E|$.

4.2. Stability analysis

For the stability and interval of periodicity analysis we will use the test equation:

$$q'' = -\omega^2 q. \quad (35)$$

with frequency ω different than the frequency ϕ of the test problem used for the phase-lag analysis, i.e. $\omega \neq \phi$.

Applying the new developed method to the scalar test problem (35) we obtain the difference equation:

$$A_1(s, v) (q_{n+1} + q_{n-1}) + A_0(s, v) q_n = 0 \quad (36)$$

and its associated characteristic equation:

$$A_1(s, v) (\lambda^2 + 1) + A_0(s, v) \lambda = 0 \quad (37)$$

where

$$\begin{aligned}
 A_1(s, v) &= 1 + b_1 s^2 + a_3 b_0 s^4 - 2 a_2 a_3 b_0 s^6 + 4 a_0 a_2 a_3 b_0 s^8 \\
 A_0(s, v) &= a_4 + b_0 s^2 - 2 a_3 b_0 s^4 + 4 a_2 a_3 b_0 s^6 + 8 a_2 a_3 b_0 (a_1 - a_0) s^8 \quad (38)
 \end{aligned}$$

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

Substituting the coefficients a_j , $j = 0, 1$ from (14) and the coefficients b_i , $j = 0, 1$ and a_k , $k = 2, 3, 4$ from (20) into the formulae (38) we obtain:

$$A_1(s, v) = -\frac{T_{10}}{T_{denom4}} \quad , \quad A_0(s, v) = 2 \frac{T_{11}}{T_{denom4}} \quad (39)$$

where

$$\begin{aligned}
 T_{10} &= 1310400 \cos(v) v^6 - 345600 v^5 \sin(v) - 619200 (\cos(v))^3 v^6 \\
 &+ 273600 (\cos(v))^2 v^6 + 158010 s^4 v^4 + 216000 s^4 v^2 - 1080000 s^2 v^4 \\
 &+ 108 s^8 v^4 - 7848 s^4 v^8 + 15264 s^2 v^{10} \\
 &- 162 s^8 v^2 + 6400 s^6 v^4 - 101604 s^4 v^6 \\
 &+ 108624 s^2 v^8 - 9600 s^6 v^2 - 346056 s^2 v^6 \\
 &- 81 (\cos(v))^3 v^{12} + 1881 (\cos(v))^2 v^{12} \\
 &+ 9821 (\cos(v))^3 v^{10} - 1134 \cos(v) v^{12} \\
 &- 6156 \sin(v) v^{11} + 81691 (\cos(v))^2 v^{10} \\
 &- 243 (\cos(v))^3 s^8 + 79545 (\cos(v))^3 v^8 \\
 &- 4454 \cos(v) v^{10} - 178620 \sin(v) v^9 \\
 &+ 243 (\cos(v))^2 s^8 + 654975 (\cos(v))^2 v^8 - 14400 (\cos(v))^3 s^6 \\
 &+ 243 \cos(v) s^8 + 377415 \cos(v) v^8 - 1603680 \sin(v) v^7 + 14400 (\cos(v))^2 s^6 \\
 &+ 14400 \cos(v) s^6 - 964800 v^6 \\
 &+ 81 \sin(v) (\cos(v))^2 s^8 v^3 - 1782 \sin(v) (\cos(v))^2 s^4 v^7 \\
 &+ 3240 \sin(v) (\cos(v))^2 s^2 v^9 + 81 \sin(v) \cos(v) s^8 v^3 \\
 &- 21582 \sin(v) \cos(v) s^4 v^7 + 21240 \sin(v) \cos(v) s^2 v^9 \\
 &+ 486 \sin(v) (\cos(v))^2 s^8 v + 4800 \sin(v) (\cos(v))^2 s^6 v^3 \\
 &- 40404 \sin(v) (\cos(v))^2 s^4 v^5 + 38544 \sin(v) (\cos(v))^2 s^2 v^7 \\
 &+ 486 \sin(v) \cos(v) s^8 v + 4800 \sin(v) \cos(v) s^6 v^3
 \end{aligned}$$

$$\begin{aligned}
& - 116004 \sin(v) \cos(v) s^4 v^5 + 475152 \sin(v) \cos(v) s^2 v^7 \\
& + 28800 \sin(v) (\cos(v))^2 s^6 v - 144000 \sin(v) (\cos(v))^2 s^4 v^3 \\
& - 83232 \sin(v) (\cos(v))^2 s^2 v^5 + 28800 \sin(v) \cos(v) s^6 v \\
& - 144000 \sin(v) \cos(v) s^4 v^3 + 1376064 \sin(v) \cos(v) s^2 v^5 \\
& - 576000 \sin(v) (\cos(v))^2 s^2 v^3 + 1152000 \sin(v) \cos(v) s^2 v^3 \\
& + 691200 \cos(v) v^5 \sin(v) \\
& - 345600 (\cos(v))^2 \sin(v) v^5 + 27 (\cos(v))^3 s^8 v^4 - 162 (\cos(v))^3 s^4 v^8 \\
& + 216 (\cos(v))^3 s^2 v^{10} - 1539 \sin(v) (\cos(v))^2 v^{11} - 27 (\cos(v))^2 s^8 v^4 \\
& + 1962 (\cos(v))^2 s^4 v^8 - 3816 (\cos(v))^2 s^2 v^{10} + 261 \sin(v) \cos(v) v^{11} \\
& + 81 (\cos(v))^3 s^8 v^2 + 1600 (\cos(v))^3 s^6 v^4 - 1398 (\cos(v))^3 s^4 v^6 \\
& - 10104 (\cos(v))^3 s^2 v^8 + 378 \cos(v) s^8 v^4 - 2268 \cos(v) s^4 v^8 \\
& + 3024 \cos(v) s^2 v^{10} + 17310 \sin(v) (\cos(v))^2 v^9 \\
& + 324 \sin(v) s^8 v^3 - 7128 \sin(v) s^4 v^7 + 12960 \sin(v) s^2 v^9 \\
& - 81 (\cos(v))^2 s^8 v^2 - 1600 (\cos(v))^2 s^6 v^4 - 36402 (\cos(v))^2 s^4 v^6 \\
& - 130008 (\cos(v))^2 s^2 v^8 + 179310 \sin(v) \cos(v) v^9 + 4800 (\cos(v))^3 s^6 v^2 \\
& + 41010 (\cos(v))^3 s^4 v^4 - 218424 (\cos(v))^3 s^2 v^6 + 162 \cos(v) s^8 v^2 \\
& + 22400 \cos(v) s^6 v^4 - 60396 \cos(v) s^4 v^6 + 42288 \cos(v) s^2 v^8 \\
& + 412320 \sin(v) (\cos(v))^2 v^7 - 972 \sin(v) s^8 v \\
& + 19200 \sin(v) s^6 v^3 - 120792 \sin(v) s^4 v^5 + 407904 \sin(v) s^2 v^7 \\
& - 4800 (\cos(v))^2 s^6 v^2 - 230010 (\cos(v))^2 s^4 v^4 - 334008 (\cos(v))^2 s^2 v^6 \\
& + 1191360 \sin(v) \cos(v) v^7 + 216000 (\cos(v))^3 s^4 v^2 - 504000 (\cos(v))^3 s^2 v^4 \\
& + 9600 \cos(v) s^6 v^2 + 30990 \cos(v) s^4 v^4 \\
& + 898488 \cos(v) s^2 v^6 - 57600 \sin(v) s^6 v \\
& + 288000 \sin(v) s^4 v^3 - 1292832 \sin(v) s^2 v^5 - 216000 (\cos(v))^2 s^4 v^2 \\
& - 72000 (\cos(v))^2 s^2 v^4 - 216000 \cos(v) s^4 v^2 \\
& + 1656000 \cos(v) s^2 v^4 - 576000 \sin(v) s^2 v^3 \\
& - 1111935 v^8 - 7524 v^{12} - 186058 v^{10} - 243 s^8 - 14400 s^6 \\
T_{11} = & -417600 \cos(v) v^6 - 273600 (\cos(v))^3 v^6 + 1310400 (\cos(v))^2 v^6
\end{aligned}$$

$$\begin{aligned} &+ 158010 s^4 v^4 + 216000 s^4 v^2 + 72000 s^2 v^4 \\ &+ 1308 s^8 v^4 - 7848 s^4 v^8 + 10464 s^2 v^{10} \\ &- 1962 s^8 v^2 + 6400 s^6 v^4 - 101604 s^4 v^6 \\ &+ 128496 s^2 v^8 - 9600 s^6 v^2 + 1057608 s^2 v^6 \\ &+ 819 (\cos(v))^3 v^{12} + 981 (\cos(v))^2 v^{12} - 145591 (\cos(v))^3 v^{10} \\ &+ 11466 \cos(v) v^{12} - 81756 \sin(v) v^{11} \\ &- 84881 (\cos(v))^2 v^{10} - 2943 (\cos(v))^3 s^8 \\ &- 290475 (\cos(v))^3 v^8 + 165394 \cos(v) v^{10} \\ &- 772620 \sin(v) v^9 + 2943 (\cos(v))^2 s^8 \\ &+ 1535715 (\cos(v))^2 v^8 - 14400 (\cos(v))^3 s^6 \\ &+ 2943 \cos(v) s^8 + 35115 \cos(v) v^8 \\ &- 748800 \sin(v) v^7 + 14400 (\cos(v))^2 s^6 + 14400 \cos(v) s^6 \\ &- 273600 v^6 + 981 \sin(v) (\cos(v))^2 s^8 v^3 \\ &- 1782 \sin(v) (\cos(v))^2 s^4 v^7 + 21240 \sin(v) (\cos(v))^2 s^2 v^9 \\ &+ 981 \sin(v) \cos(v) s^8 v^3 - 21582 \sin(v) \cos(v) s^4 v^7 \\ &+ 39240 \sin(v) \cos(v) s^2 v^9 + 5886 \sin(v) (\cos(v))^2 s^8 v \\ &+ 4800 \sin(v) (\cos(v))^2 s^6 v^3 - 40404 \sin(v) (\cos(v))^2 s^4 v^5 \\ &+ 259152 \sin(v) (\cos(v))^2 s^2 v^7 + 5886 \sin(v) \cos(v) s^8 v \\ &+ 4800 \sin(v) \cos(v) s^6 v^3 - 116004 \sin(v) \cos(v) s^4 v^5 \\ &- 244272 \sin(v) \cos(v) s^2 v^7 + 28800 \sin(v) (\cos(v))^2 s^6 v \\ &- 144000 \sin(v) (\cos(v))^2 s^4 v^3 + 1376064 \sin(v) (\cos(v))^2 s^2 v^5 \\ &+ 28800 \sin(v) \cos(v) s^6 v - 144000 \sin(v) \cos(v) s^4 v^3 \\ &- 2070432 \sin(v) \cos(v) s^2 v^5 + 1152000 \sin(v) (\cos(v))^2 s^2 v^3 \\ &- 576000 \sin(v) \cos(v) s^2 v^3 \\ &- 345600 \cos(v) v^5 \sin(v) + 691200 (\cos(v))^2 \sin(v) v^5 \\ &+ 327 (\cos(v))^3 s^8 v^4 - 162 (\cos(v))^3 s^4 v^8 \\ &- 984 (\cos(v))^3 s^2 v^{10} - 20439 \sin(v) (\cos(v))^2 v^{11} \\ &- 327 (\cos(v))^2 s^8 v^4 + 1962 (\cos(v))^2 s^4 v^8 - 2616 (\cos(v))^2 s^2 v^{10} \end{aligned}$$

$$\begin{aligned}
& - 18639 \sin(v) \cos(v) v^{11} + 981 (\cos(v))^3 s^8 v^2 + 1600 (\cos(v))^3 s^6 v^4 \\
& - 1398 (\cos(v))^3 s^4 v^6 + 58008 (\cos(v))^3 s^2 v^8 + 4578 \cos(v) s^8 v^4 \\
& - 2268 \cos(v) s^4 v^8 - 13776 \cos(v) s^2 v^{10} + 314310 \sin(v) (\cos(v))^2 v^9 \\
& + 3924 \sin(v) s^8 v^3 - 7128 \sin(v) s^4 v^7 \\
& + 84960 \sin(v) s^2 v^9 - 981 (\cos(v))^2 s^8 v^2 - 1600 (\cos(v))^2 s^6 v^4 \\
& - 36402 (\cos(v))^2 s^4 v^6 + 123864 (\cos(v))^2 s^2 v^8 + 476310 \sin(v) \cos(v) v^9 \\
& + 4800 (\cos(v))^3 s^6 v^2 + 41010 (\cos(v))^3 s^4 v^4 + 334008 (\cos(v))^3 s^2 v^6 \\
& + 1962 \cos(v) s^8 v^2 + 22400 \cos(v) s^6 v^4 \\
& - 60396 \cos(v) s^4 v^6 - 302160 \cos(v) s^2 v^8 \\
& + 1191360 \sin(v) (\cos(v))^2 v^7 - 11772 \sin(v) s^8 v \\
& + 19200 \sin(v) s^6 v^3 - 120792 \sin(v) s^4 v^5 \\
& + 885984 \sin(v) s^2 v^7 - 4800 (\cos(v))^2 s^6 v^2 - 230010 (\cos(v))^2 s^4 v^4 \\
& + 12888 (\cos(v))^2 s^2 v^6 - 480480 \sin(v) \cos(v) v^7 + 216000 (\cos(v))^3 s^4 v^2 \\
& + 72000 (\cos(v))^3 s^2 v^4 + 9600 \cos(v) s^6 v^2 \\
& + 30990 \cos(v) s^4 v^4 - 1388472 \cos(v) s^2 v^6 \\
& - 57600 \sin(v) s^6 v + 288000 \sin(v) s^4 v^3 \\
& + 518400 \sin(v) s^2 v^5 - 216000 (\cos(v))^2 s^4 v^2 \\
& + 1656000 (\cos(v))^2 s^2 v^4 - 216000 \cos(v) s^4 v^2 - 1224000 \cos(v) s^2 v^4 \\
& - 1203075 v^8 - 3924 v^{12} - 31330 v^{10} \\
& - 2943 s^8 - 14400 s^6 + 37920 (\cos(v))^3 \sin(v) v^7 \\
& - 345600 (\cos(v))^3 \sin(v) v^5 - 576000 (\cos(v))^3 \sin(v) s^2 v^3 \\
& + 20736 (\cos(v))^3 \sin(v) s^2 v^7 \\
& + 175968 (\cos(v))^3 \sin(v) s^2 v^5 - 16032 (\cos(v))^4 s^2 v^6 \\
& - 576000 (\cos(v))^4 s^2 v^4 + 2592 (\cos(v))^4 s^2 v^8 \\
& - 2592 (\cos(v))^4 v^{10} - 77280 (\cos(v))^4 v^8 - 345600 (\cos(v))^4 v^6 \\
T_{denom4} & = v^5 \left(964800 v + 6156 v^6 \sin(v) + 178620 v^4 \sin(v) \right. \\
& - 691200 \cos(v) \sin(v) - 377415 \cos(v) v^3 \\
& \left. - 1310400 v \cos(v) + 1603680 v^2 \sin(v) \right)
\end{aligned}$$

$$\begin{aligned}
 &+ 4454 v^5 \cos(v) - 654975 (\cos(v))^2 v^3 \\
 &+ 619200 (\cos(v))^3 v + 345600 (\cos(v))^2 \sin(v) - 273600 (\cos(v))^2 v \\
 &+ 81 (\cos(v))^3 v^7 - 1881 (\cos(v))^2 v^7 \\
 &- 9821 (\cos(v))^3 v^5 - 81691 (\cos(v))^2 v^5 \\
 &- 79545 (\cos(v))^3 v^3 + 1134 \cos(v) v^7 \\
 &+ 345600 \sin(v) + 7524 v^7 + 186058 v^5 \\
 &+ 1111935 v^3 - 412320 (\cos(v))^2 \sin(v) v^2 \\
 &- 1191360 \cos(v) v^2 \sin(v) - 179310 \cos(v) v^4 \sin(v) \\
 &- 17310 (\cos(v))^2 \sin(v) v^4 + 1539 (\cos(v))^2 \sin(v) v^6 \\
 &- 261 \cos(v) v^6 \sin(v).
 \end{aligned}$$

Remark 4. *The terms P-stable and singularly almost P-stable method are properties of a method which are related with problems where we have the condition $\omega = \phi$.*

If the roots of the characteristic equation (37) satisfy $|\lambda_{1,2}| = 1$, then the method (13) is called that has an non zero interval of periodicity. In order to obtain the $s - v$ plane, we find the roots of the characteristic equation (37) for several values of s and v . If the roots satisfy $|\lambda_{1,2}| = 1$, then the corresponding point (s, v) is defined.

The $s - v$ plane for the new developed method is shown in Figure 2.

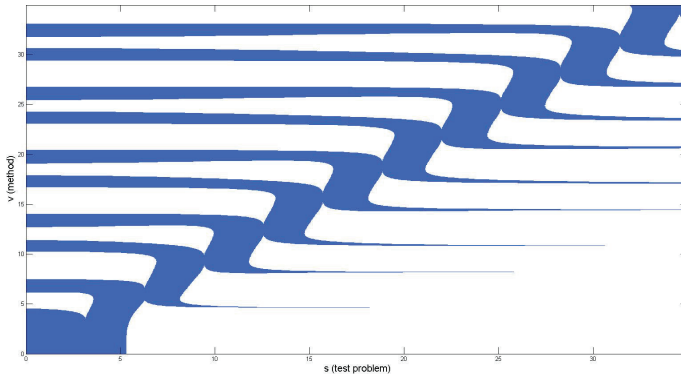


Figure 2. The plot of $s - v$ plane of the new proposed symmetric four-stages implicit twelfth algebraic order method with vanished phase-lag and its first, second, third and fourth derivatives.

Remark 5. Giving attention on the $s-v$ presented in the Figure 2, we obtain the following remarks :

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

Remark 6. In order to evaluate the application plain of the a numerical method, we have to observe the $s-v$ plane of the specific method and to arrive to conclusions based on the problems on which the specific numerical method will be applied:

1. **Problems for which $\omega \neq \phi$.** For these kind of problems, we have to give attention on all the area of the $s-v$ plane **excluding** the area around the first diagonal.
2. **Problems for which $\omega = \phi$** (see the Schrödinger equation and related problems). For these kind of problems we have to give attention on the area around the first diagonal of the $s-v$ plane.

Substituting $s = v$ in the stability polynomials given by (39)and giving attention the area around the first diagonal of the plot $s-v$, we conclude that the interval of periodicity of the new proposed method is equal to $(0, \infty)$. The interval of periodicity is a property regarding problems in which $s = v$ like the Schrödinger equation and related problems

The intervals of periodicity of similar methods are presented In Table 1.

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

Method	Interval of Periodicity
Method developed in [4]	$(0, 29)$
Method developed in [5]	$(0, \infty)$
Method developed in Section 3	$(0, \infty)$

The above achievements lead to the following theorem:

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

- is of four stages
- is of twelfth algebraic order,
- has vanished the phase-lag and its first, second, third and fourth derivatives and

- has an interval of periodicity equals to: $(0, \infty)$.

5. Numerical results

We will apply the new developed method on the following problems:

- the numerical solution of the radial (one dimensional) time-independent Schrödinger equation and
- the numerical solution of coupled differential equations of the Schrödinger type.

5.1. One dimensional (radial) time-independent Schrödinger equation

The approximate solution of the following Schrödinger equation is studied:

$$q''(r) = [l(l+1)/r^2 + V(r) - k^2] q(r), \quad (40)$$

where

- the function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. For this function we have: $W(x) \rightarrow 0$ as $x \rightarrow \infty$,
- the quantity $k^2 \in \mathbb{R}$ is called *the energy*,
- the quantity $l \in \mathbb{Z}$ is called *angular momentum*,
- the function V is called *potential*.

The above problem (40) is a boundary value one and therefore we have following boundary conditions:

$$q(0) = 0$$

and the end point condition which is defined for large values of r from the physical considerations of the problem.

Since the obtained method is a frequency dependent one, in order to be applied for the solution of the problem (40), the determination of the frequency ϕ is necessary. For the above mentioned problem and for the case $l = 0$ we have:

$$\phi = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|}$$

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

5.1.1. Woods–Saxon potential

In order to solve numerically the problem (40) we have also to determine the potential $V(r)$. For our numerical tests we use the Wood–Saxon potential:

$$V(r) = \frac{u_0}{1+y} - \frac{u_0 y}{a(1+y)^2} \tag{41}$$

with $y = \exp\left[\frac{r-X_0}{a}\right]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

In Figure 3 we present the behavior of the Woods–Saxon potential.

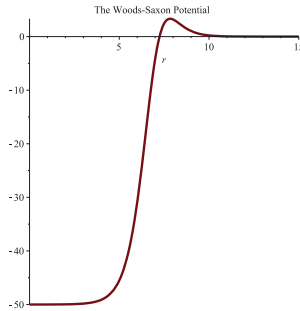


Figure 3. Behavior of the Woods–Saxon potential.

The value of the parameter ϕ is defined as follows ([17], [18]):

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

For the above definition we used the methodology introduced by Ixaru et al. ([16] [18]). Based on this methodology the values of the parameter ϕ are chosen from some approximate values of the Woods-Saxon potential on some critical points within the integration interval.

Based on the above methodology we give some examples for the determination of the values of ϕ : (1) On the point of the integration area $r = 6.5 - h$, the value of ϕ is equal to: $\sqrt{-37.5 + E}$. Consequently, $v = \phi h = \sqrt{-37.5 + E} h$. (2) On the point of the integration area $r = 6.5 - 3h$, the value of ϕ is equal to: $\sqrt{-50 + E}$, etc.

5.1.2. The resonance problem of the radial Schrödinger equation

The radial time independent Schrödinger equation (40) will be solved numerically for $l = 0$, with Woods-Saxon potential (41) and the new obtained method.

Since the integration interval for this problem is $(0, \infty)$, we have to approximate it with a finite interval. For our numerical tests we approximated the infinite interval by the finite one $r \in [0, 15]$. The new obtained method will be applied on a large space of energies: $E \in [1, 1000]$.

Since for positive energies, $E = k^2$ the potential vanished faster than the term $\frac{l(l+1)}{x^2}$ for $x \rightarrow \infty$, consequently, the radial Schrödinger equation can be written as:

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2} \right) q(r) = 0 \tag{42}$$

The above form of the 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. Then, the asymptotic form of the solution of equation (40) (in the case of $r \rightarrow \infty$) can be written as:

$$\begin{aligned} q(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC \left[\sin \left(kr - \frac{l\pi}{2} \right) + \tan \delta_l \cos \left(kr - \frac{l\pi}{2} \right) \right] \end{aligned}$$

where δ_l is the phase shift. For the computation of the phase shift we use the following direct formula:

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

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 $C(r) = -kr n_l(kr)$. We consider the specific problem as an initial-value problem (as we have mentioned previously). Therefore, we have to know the value of q_j , $j = 0, 1$ in order to be possible the application of a two-step method. The value q_0 is known from the initial condition. The value q_1 is computed using the high order Runge-Kutta-Nyström methods (see [19] and [20]). After determination of the values q_i , $i = 0, 1$, it is possible to compute the phase shift δ_l at r_2 of the asymptotic region.

The above described problem will be solved for positive energies. For this problem:

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

We chosen to solve the latter problem, which is known as **the resonance problem**.

For this problem the boundary conditions are:

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

For our numerical tests and for comparison purposes the positive eigenenergies of the resonance problem with the Woods-Saxon potential will be computed using the following methods:

- **Method QT8**: the eighth order multi-step method developed by Quinlan and Tremaine [21];
- **Method QT10**: the tenth order multi-step method developed by Quinlan and Tremaine [21];
- **Method QT12**: the twelfth order multi-step method developed by Quinlan and Tremaine [21];
- **Method MCR4**: the fourth algebraic order method of Chawla and Rao with minimal phase-lag [22];
- **Method RA**: the exponentially-fitted method of Raptis and Allison [23];
- **Method MCR6**: the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [24];
- **Method NMPF1**: the Phase-Fitted Method (Case 1) developed in [11];
- **Method NMPF2**: the Phase-Fitted Method (Case 2) developed in [11];
- **Method NMC2**: the Method developed in [25] (Case 2);
- **Method NMC1**: the method developed in [25] (Case 1);
- **Method NM2SH2DV**: the Two-Step Hybrid Method developed in [1];
- **Method NM4SH2DV**: the Four Stages Symmetric Two-Step method with vanished phase-lag and its first and second derivatives developed in [4];

- **Method NM4SH3DV**: the Four Stages Symmetric Two-Step method with vanished phase-lag and its first, second and third derivatives developed [5];
- **Method NM4SH4DV**: the Four Stages Symmetric Two-Step method with vanished phase-lag and its first, second, third and fourth derivatives developed in Section 3.

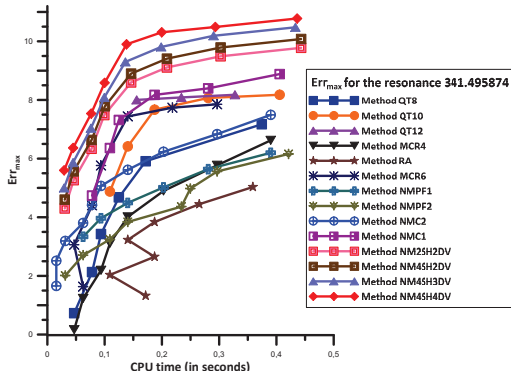


Figure 4. Accuracy (Digits) for several values of *CPU* Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of *CPU*, Accuracy (Digits) is less than 0.

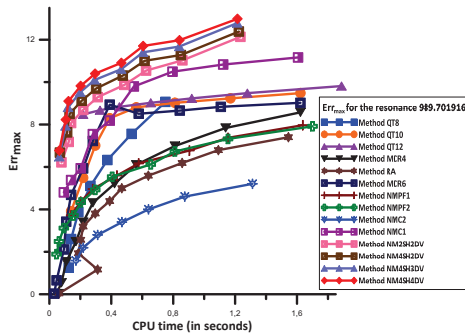


Figure 5. Accuracy (Digits) for several values of *CPU* Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of *CPU*, Accuracy (Digits) is less than 0.

The maximum absolute error $Err_{max} = |\log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}|$$

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ is presented in Figures 4 and 5, respectively, for several values of CPU time (in seconds).

As reference values, which in our experiments are mentioned as $E_{accurate}$, we take the results produced by the well known two-step method of Chawla and Rao [24]. In order to determine the value of Err , we compute the eigenenergies by each numerical method. These values are mentioned as $E_{calculated}$.

5.1.3 Conclusions on the produced numerical results for the radial Schrödinger equation

From our numerical experiments we obtain 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 more efficient than all the other methods mentioned above.

10. **Method NM4SH4DV**, is the most efficient one.

5.2. Error estimation

In order to solve numerically the coupled Schrödinger equations we will apply a variable-step technique.

Definition 8. *A numerical technique is called of variable-step type, if during the integration the step length of the method is changed based on a local truncation error estimation (LTEE) procedure.*

The last decades a lot of research has been done on the production of methods with constant or variable step length for the approximate solution of the coupled differential equations of the the Schrödinger type and related problems (see for example [11]– [75]).

As we mentioned above, for the approximate solution of the coupled differential equations arising from the Schrödinger equation embedded pairs will be used which will be based on an LTEE procedure. Our embedded pairs are based on the fact that the numerical solution of problems which have oscillatory and/or periodical solutions is more efficient if we use numerical methods with maximal possible algebraic order and/or with vanished phase-lag and its highest possible order derivatives.

For the estimation of the local truncation error in y_{n+1}^L we use the formula:

$$LTE = | y_{n+1}^H - y_{n+1}^L | \tag{43}$$

where y_{n+1}^L and y_{n+1}^H are determined using two techniques:

1. **Technique based on algebraic order of the methods.** In this technique y_{n+1}^L defines the lower algebraic order solution and is computed using the tenth algebraic order method developed in [3] and y_{n+1}^H defines the higher order solution which is computed using the four-stages symmetric two-step method of twelfth algebraic order with vanished phase-lag and its first, second, third and fourth derivatives developed in Section 3.
2. **Technique based on the highest possible order of the vanished derivative of the phase-lag.** In this technique y_{n+1}^L defines the solution which is computed

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 [5] and y_{n+1}^H defines the solution which is computed using the four–stages symmetric two–step method of twelfth algebraic order with vanished phase-lag and its first, second, third and fourth derivatives developed in Section 3.

We reduced the changes of the step sizes on duplication of step sizes. Consequently, we follow the procedure:

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

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

Remark 7. The local extrapolation procedure is also used, i.e. the higher order solution y_{n+1}^H is used at each integration point although the local error estimation technique is computed based on the lower order solution y_{n+1}^L .

5.3. Coupled differential equations

Coupled differential equations of the Schrödinger type are presented in many problems of quantum chemistry, material science, theoretical physics, quantum physics atomic physics, physical chemistry and chemical physics, quantum chemistry, and elsewhere.

The close-coupling differential equations arising from the Schrödinger equation can be written as:

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

for $1 \leq i \leq N$ and $m \neq i$.

For open channels problem the following boundary conditions are (see for details [26]):

$$y_{ij} = 0 \text{ at } x = 0$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x) \delta_{ij} + \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x) \quad (44)$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively.

Remark 8. We note that the schemes developed in this paper can be applied effectively to the case of close channels problem.

We follow the detailed analysis given in [26]. Based on this analysis and determining matrix K' and diagonal matrices M , N by:

$$\begin{aligned} K'_{ij} &= \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} \\ M_{ij} &= k_i x j l_i(k_i x) \delta_{ij} \\ N_{ij} &= k_i x n l_i(k_i x) \delta_{ij} \end{aligned}$$

we have the new forms of the asymptotic condition (44):

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N} \mathbf{K}'.$$

In this paper we will study the rotational excitation of a diatomic molecule by neutral particle impact which is a real problem can be observed in several areas like quantum chemistry, theoretical chemistry, theoretical physics, quantum physics, material science, atomic physics, molecular physics etc. The above mentioned problem is expressed via close-coupling differential equations arising from the Schrödinger equation. For the model of this problem we make the following notes: (1) the quantum numbers (j, l) present the entrance channel (see for details in [26]), (2) the quantum numbers (j', l') present the exit channels and (3) $J = j + l = j' + l'$ presents the total angular momentum. Then we have

$$\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2} \right] y_{j'l'}^{j'l}(x) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l'; J | V | j''l''; J \rangle y_{j''l''}^{j'l}(x)$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2} \left[E + \frac{\hbar^2}{2I} \{j(j+1) - j'(j'+1)\} \right].$$

and 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 μ denotes the reduced mass of the system.

Based on the details presented in [26] we use the following potential V :

$$V(x, \hat{\mathbf{k}}_{j'j} \hat{\mathbf{k}}_{jj}) = V_0(x) P_0(\hat{\mathbf{k}}_{j'j} \hat{\mathbf{k}}_{jj}) + V_2(x) P_2(\hat{\mathbf{k}}_{j'j} \hat{\mathbf{k}}_{jj})$$

and therefore, the element of the coupling matrix is given by:

$$\langle j'l'; J | V | j''l''; J \rangle = \delta_{j'j''} \delta_{l'l''} V_0(x) + f_2(j'l', j''l''; J) V_2(x)$$

where the f_2 coefficients are obtained from formulas given by Bernstein et al. [27] and $\hat{\mathbf{k}}_{j'j}$ is a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and P_i , $i = 0, 2$ are Legendre polynomials (see for details [28]). The boundary conditions are given by:

$$y_{j'l'}^{Jj'l}(x) = 0 \text{ at } x = 0 \quad (45)$$

$$y_{j'l'}^{Jj'l}(x) \sim \delta_{jj'}\delta_{ll'} \exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp[i(k_{j'j}x - 1/2l'\pi)]$$

where S matrix and for K matrix of (44) the following relation is hold:

$$\mathbf{S} = (\mathbf{I} + i\mathbf{K})(\mathbf{I} - i\mathbf{K})^{-1}.$$

The approximate solution of the above described problem an algorithm fully described in [26] is used. This algorithm contains the new schemes presented above for the integration from the starting value to matching points.

The \mathbf{S} matrix used for our numerical experiments has the following parameters

$$\frac{2\mu}{\hbar^2} = 1000.0 \quad ; \quad \frac{\mu}{I} = 2.351 \quad ; \quad E = 1.1$$

$$V_0(x) = \frac{1}{x^{12}} - 2\frac{1}{x^6} \quad ; \quad V_2(x) = 0.2283V_0(x).$$

For our numerical tests we take the value $J = 6$ (see for full details in [26]) and excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 is considered. The results of the above values are sets of **four, nine and sixteen coupled differential equations**, respectively. We consider the potential infinite for values of x less than some x_0 (see for full details in [28] and in [26]). Based on the above, the boundary condition (45) are given by as

$$y_{j'l'}^{Jj'l}(x_0) = 0.$$

The above described problem solved numerically using the following methods:

- the Iterative Numerov method of Allison [26] which is indicated as **Method I²**,
- the variable-step method of Raptis and Cash [29] which is indicated as **Method II**,

²We note here that Iterative Numerov method developed by Allison [26] is one of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation

- the embedded Runge–Kutta Dormand and Prince method 5(4) [20] which is indicated as **Method III**,
- the embedded Runge–Kutta method ERK4(2) developed in Simos [30] 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 embedded two–step method developed in [4] which is indicated as **Method VIII**.
- the embedded two–step method with error control based on the order of the eliminated derivative of the phase-lag of the method developed in [5] which is indicated as **Method IX**.
- the embedded two–step method with error control based on the algebraic order of the method developed in [5] which is indicated as **Method X**.
- 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 XI**.
- 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 XII**.

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.

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

Method	N	hmax	RTC	MErr
Method I	4	0.014	3.25	1.2×10^{-3}
	9	0.014	23.51	5.7×10^{-2}
	16	0.014	99.15	6.8×10^{-1}
Method II	4	0.056	1.55	8.9×10^{-4}
	9	0.056	8.43	7.4×10^{-3}
	16	0.056	43.32	8.6×10^{-2}
Method III	4	0.007	45.15	9.0×10^0
	9			
	16			
Method IV	4	0.112	0.39	1.1×10^{-5}
	9	0.112	3.48	2.8×10^{-4}
	16	0.112	19.31	1.3×10^{-3}
Method V	4	0.448	0.20	1.1×10^{-6}
	9	0.448	2.07	5.7×10^{-6}
	16	0.448	11.18	8.7×10^{-6}
Method VI	4	0.448	0.15	3.2×10^{-7}
	9	0.448	1.40	4.3×10^{-7}
	16	0.448	10.13	5.6×10^{-7}
Method VII	4	0.448	0.10	2.5×10^{-7}
	9	0.448	1.10	3.9×10^{-7}
	16	0.448	9.43	4.2×10^{-7}
Method VIII	4	0.448	0.08	6.4×10^{-8}
	9	0.448	1.04	7.6×10^{-8}
	16	0.448	9.12	8.5×10^{-8}
Method IX	4	0.896	0.05	4.2×10^{-8}
	9	0.896	1.00	6.3×10^{-8}
	16	0.896	8.57	7.2×10^{-8}
Method X	4	0.896	0.04	4.0×10^{-8}
	9	0.896	0.58	5.9×10^{-8}
	16	0.896	8.55	7.0×10^{-8}
Method XI	4	0.896	0.04	3.7×10^{-8}
	9	0.896	0.56	5.8×10^{-8}
	16	0.896	8.42	6.8×10^{-8}
Method XII	4	0.896	0.03	3.5×10^{-8}
	9	0.896	0.51	5.4×10^{-8}
	16	0.896	8.24	6.3×10^{-8}

6. Conclusions

A four–stages twelfth algebraic order symmetric two–step methods with vanished phase–lag and its first, second, third and fourth derivatives was obtained, for the first time in the literature, in this paper. More specifically:

- We presented the construction of the method ,
- We studied the determination of the local truncation error (LTE) and we investigated the comparison of the asymptotic form of the LTE, which was produced using the radial time independent Schrödinger equation, with the asymptotic forms of the LTE of similar methods,
- We presented the stability and the interval of periodicity analysis and
- We studied the computational efficiency of the new proposed method.

The theoretical and numerical results obtained in this paper, proved that the new developed method is much more effective than the other well known and recently developed methods of the literature for the approximate solution of the radial Schrödinger equation and of the coupled differential equations of the Schrödinger type.

All computations were carried out on a x86-64 compatible PC using double-precision arithmetic data type (64 bits) according to IEEE[©] Standard 754 for double precision.

Appendix A: Formulae for the T_i , $i = 0(1)4$ and T_{denom}

$$\begin{aligned}
 T_0 &= 27 \cos(v) v^8 b_0 a_3 a_2 - 327 v^8 a_2 a_3 b_0 + 1600 \cos(v) b_0 a_3 v^6 a_2 \\
 &- 1600 v^6 a_2 a_3 b_0 - 800 \cos(v) v^4 a_3 b_0 + 800 v^4 a_3 b_0 \\
 &- 800 \cos(v) v^2 b_1 - 400 v^2 b_0 - 800 \cos(v) - 400 a_4 \\
 T_1 &= -640000 \sin(v) + 2092800 v^7 b_0 a_3 a_2 + 7680000 b_0 a_3 v^5 a_2 \\
 &- 1280000 \sin(v) v^4 a_3 b_0 - 960000 v^{13} a_2^2 a_3^2 b_0^2 \\
 &+ 960000 v^{11} a_2 a_3^2 b_0^2 + 64800 v^9 a_2 a_3 b_0^2 \\
 &+ 2560000 v^7 a_2 a_3 b_0^2 - 1280000 v^5 a_3 b_0 b_1 - 1280000 v^3 a_3 a_4 b_0 \\
 &- 640000 \sin(v) v^8 a_3^2 b_0^2 + 43200 \sin(v) v^8 a_2 a_3 b_0
 \end{aligned}$$

$$\begin{aligned}
 & - 86400 \sin(v) v^{14} a_2^2 a_3^2 b_0^2 + 1569600 v^9 a_2 a_3 b_0 b_1 \\
 & + 2560000 \sin(v) b_0 a_3 v^6 a_2 - 2560000 \sin(v) v^{12} a_2^2 a_3^2 b_0^2 \\
 & - 729 \sin(v) v^{16} a_2^2 a_3^2 b_0^2 + 3840000 v^5 a_2 a_3 a_4 b_0 \\
 & + 2560000 \sin(v) v^{10} a_2 a_3^2 b_0^2 - 1280000 \sin(v) v^6 a_3 b_0 b_1 \\
 & + 43200 \sin(v) v^{12} a_2 a_3^2 b_0^2 + 86400 v^7 a_2 a_3 a_4 b_0 \\
 & + 5120000 v^7 a_2 a_3 b_0 b_1 + 640000 v b_0 - 2560000 v^3 a_3 b_0 \\
 & - 640000 v a_4 b_1 - 640000 v^5 a_3 b_0^2 - 640000 \sin(v) v^4 b_1^2 \\
 & - 1280000 \sin(v) v^2 b_1 + 43200 \sin(v) v^{10} a_2 a_3 b_0 b_1 \\
 & + 2560000 \sin(v) v^8 a_2 a_3 b_0 b_1 \\
 T_2 = & 6144000000 v^2 a_3 b_0 + 1536000000 \cos(v) v^2 b_1 + 512000000 \cos(v) \\
 & + 512000000 a_4 b_1 + 512000000 \cos(v) v^6 b_1^3 + 1536000000 v^2 b_0 b_1 \\
 & - 1536000000 v^2 a_4 b_1^2 + 6144000000 v^4 a_3 b_0^2 + 1536000000 \cos(v) v^4 b_1^2 \\
 & - 1296000000 v^{18} a_2^2 a_3^3 b_0^3 - 1536000000 v^{18} a_2^3 a_3^3 b_0^3 \\
 & - 10240000000 v^6 a_3^2 b_0^2 - 1536000000 v^8 a_3^2 b_0^3 \\
 & + 1536000000 \cos(v) v^8 a_3^2 b_0^2 + 3072000000 v^2 a_3 a_4 b_0 \\
 & + 512000000 \cos(v) v^{12} a_3^3 b_0^3 + 3072000000 v^4 a_3 b_0 b_1 \\
 & + 1024000000 v^6 a_3 b_0 b_1^2 - 51840000 \cos(v) v^8 b_0 a_3 a_2 \\
 & - 3072000000 \cos(v) b_0 a_3 v^6 a_2 - 20995200 v^{14} a_2^2 a_3^2 a_4 b_0^2 \\
 & + 55296000000 v^8 a_2 a_3^2 b_0^2 - 3072000000 v^8 a_3^2 b_0^2 b_1 \\
 & - 103680000 \cos(v) v^{12} a_2 a_3^2 b_0^2 + 77760000 v^{20} a_2^3 a_3^3 b_0^3 \\
 & - 296654400 v^{16} a_2^2 a_3^2 b_0^2 b_1 + 9216000000 v^{10} a_2 a_3^2 b_0^3 \\
 & - 1866240000 v^{14} a_2^2 a_3^2 b_0^2 b_1 - 1831680000 v^{12} a_2^2 a_3^2 a_4 b_0^2 \\
 & - 16323840000 v^8 a_2 a_3 b_0 b_1 + 2304000000 v^{16} a_2^2 a_3^3 b_0^3 \\
 & + 1749600 \cos(v) v^{16} a_2^2 a_3^2 b_0^2 + 207360000 \cos(v) v^{14} a_2^2 a_3^2 b_0^2 \\
 & - 725760000 v^8 a_2 a_3 b_0^2 - 6144000000 v^8 a_2 a_3 b_0^2 b_1 \\
 & + 27648000000 v^8 a_2 a_3^2 a_4 b_0^2 + 512000000 v^6 a_3 b_0^2 b_1 \\
 & - 5120000000 v^6 a_3^2 a_4 b_0^2 - 25600000000 v^6 a_2 a_3 b_0^2 \\
 & - 30720000000 v^4 a_2 a_3 b_0 - 15360000000 v^4 a_2 a_3 a_4 b_0
 \end{aligned}$$

$$\begin{aligned}
 & - 12288000000 v^8 a_2 a_3 b_0 b_1^2 - 34816000000 v^6 a_2 a_3 b_0 b_1 \\
 & - 512000000 b_0 - 11719680000 b_0 a_3 v^6 a_2 + 1536000000 \cos(v) v^4 a_3 b_0 \\
 & - 508550400 v^{14} a_2^2 a_3^2 b_0^2 - 9039360000 v^{12} a_2^2 a_3^2 b_0^2 \\
 & - 5875200000 v^{10} a_2 a_3^2 b_0^2 - 12247200 v^{16} a_2^2 a_3^2 b_0^3 \\
 & - 933120000 v^{14} a_2^2 a_3^2 b_0^3 - 2304000000 v^{14} a_2 a_3^3 b_0^3 \\
 & - 2048000000 v^{12} a_2^2 a_3^2 b_0^3 + 138240000 v^{12} a_2 a_3^2 b_0^3 \\
 & - 8601600000 v^{10} a_2^2 a_3^2 b_0^2 - 483840000 v^6 a_2 a_3 a_4 b_0 \\
 & - 43008000000 v^{10} a_2^2 a_3^2 a_4 b_0^2 - 6251520000 v^{12} a_2 a_3^2 b_0^2 b_1 \\
 & + 6144000000 \cos(v) v^{12} a_2^2 a_3^2 b_0^2 - 4096000000 \cos(v) v^{18} a_2^3 a_3^3 b_0^3 \\
 & - 4608000000 v^4 a_3 a_4 b_0 b_1 - 19683 \cos(v) v^{24} a_2^3 a_3^3 b_0^3 \\
 & - 3499200 \cos(v) v^{22} a_2^3 a_3^3 b_0^3 - 4096000000 v^{12} a_2^2 a_3^2 b_0^2 b_1 \\
 & + 207360000 \cos(v) v^{18} a_2^2 a_3^3 b_0^3 - 207360000 \cos(v) v^{20} a_2^3 a_3^3 b_0^3 \\
 & + 1749600 \cos(v) v^{20} a_2^2 a_3^3 b_0^3 - 6144000000 \cos(v) v^{10} a_2 a_3^2 b_0^2 \\
 & + 1536000000 \cos(v) v^{10} a_3^2 b_0^2 b_1 + 1536000000 \cos(v) v^8 a_3 b_0 b_1^2 \\
 & + 3072000000 \cos(v) v^6 a_3 b_0 b_1 + 6144000000 \cos(v) v^{16} a_2^2 a_3^3 b_0^3 \\
 & - 51840000 \cos(v) v^{16} a_2 a_3^3 b_0^3 - 3072000000 \cos(v) v^{14} a_2 a_3^3 b_0^3 \\
 & + 518400000 v^{10} a_2 a_3^2 a_4 b_0^2 + 18432000000 v^{10} a_2 a_3^2 b_0^2 b_1 \\
 & - 259200000 v^{10} a_2 a_3 b_0^2 b_1 - 6278400000 v^{10} a_2 a_3 b_0 b_1^2 \\
 & - 6144000000 \cos(v) v^8 a_2 a_3 b_0 b_1 - 3072000000 \cos(v) v^{10} a_2 a_3 b_0 b_1^2 \\
 & - 103680000 \cos(v) v^{10} a_2 a_3 b_0 b_1 - 6144000000 \cos(v) v^{12} a_2 a_3^2 b_0^2 b_1 \\
 & - 51840000 \cos(v) v^{12} a_2 a_3 b_0 b_1^2 + 1749600 \cos(v) v^{18} a_2^2 a_3^2 b_0^2 b_1 \\
 & + 207360000 \cos(v) v^{16} a_2^2 a_3^2 b_0^2 b_1 + 6144000000 \cos(v) v^{14} a_2^2 a_3^2 b_0^2 b_1 \\
 & - 103680000 \cos(v) v^{14} a_2 a_3^2 b_0^2 b_1 + 51840000 v^8 a_2 a_3 a_4 b_0 b_1 \\
 & + 8192000000 v^6 a_2 a_3 a_4 b_0 b_1 \\
 T_3 = & 409600000000 \sin(v) + 5668704000 v^{21} a_2^3 a_3^3 a_4 b_0^3 \\
 & - 3317760000000 v^{17} a_2^2 a_3^3 b_0^4 + 3686400000000 v^{17} a_2 a_3^4 b_0^4 \\
 & + 39321600000000 v^7 a_2 a_3 a_4 b_0 b_1^2 + 20995200000 v^{25} a_2^3 a_3^4 b_0^4 \\
 & - 13107200000000 \sin(v) v^{20} a_2^3 a_3^3 b_0^3 b_1 + 497664000000 v^{25} a_2^4 a_3^4 b_0^4
 \end{aligned}$$

$$\begin{aligned} & - 6967296000000 v^{11} a_2 a_3^2 b_0^3 - 9830400000000 v a_3 b_0 \\ & + 2457600000000 \sin(v) v^4 b_1^2 - 9830400000000 v^{11} a_3^3 b_0^3 b_1 \\ & + 328384512000000 v^{11} a_2^2 a_3^2 b_0^2 + 562544640000000 b_0 a_3 v^5 a_2 \\ & + 1638400000000 \sin(v) v^4 a_3 b_0 + 98304000000000 v^9 a_2 a_3^2 a_4 b_0^2 b_1 \\ & + 9830400000000 v^9 a_2 a_3 b_0^2 b_1^2 + 4915200000000 v^9 a_3^2 b_0^3 b_1 \\ & - 663552000000 \sin(v) v^{22} a_2^3 a_3^3 b_0^3 b_1 + 727833600000 v^{19} a_2^3 a_3^3 a_4 b_0^3 \\ & + 76345344000000 v^9 a_2 a_3 b_0 b_1^2 + 11391528960000 v^{13} a_2^2 a_3^2 b_0^2 \\ & + 4976640000000 v^7 a_2 a_3 b_0^2 + 2457600000000 \sin(v) v^8 a_3^2 b_0^2 \\ & + 9830400000000 b_0 a_3 v^3 a_2 - 8398080000 v^{27} a_2^4 a_3^4 b_0^4 \\ & - 165888000000 \sin(v) v^{10} a_2 a_3 b_0 b_1 - 983040000000 \sin(v) v^8 a_2 a_3 b_0 b_1 \\ & - 1966080000000 v^5 a_3 a_4 b_0 b_1^2 + 1638400000000 \sin(v) v^2 b_1 \\ & + 7864320000000 v^7 a_2 a_3 b_0 b_1^2 + 5598720000 \sin(v) v^{22} a_2^2 a_3^3 b_0^3 b_1 \\ & + 2949120000000 v^3 a_3 a_4 b_0 b_1 + 4915200000000 v^5 a_3^2 a_4 b_0^2 \\ & - 334233600000000 v^9 a_2 a_3^2 b_0^3 - 24576000000000 v^9 a_3^3 a_4 b_0^3 \\ & + 137625600000000 v^9 a_2^2 a_3^2 b_0^2 + 9830400000000 v^9 a_3^2 b_0^2 b_1^2 \\ & - 12902400000000 v^9 a_2 a_3^2 b_0^2 - 663552000000 v^7 a_2 a_3 a_4 b_0 b_1 \\ & + 39960576000000 v^{19} a_2^3 a_3^3 b_0^3 b_1 + 582266880000 v^{21} a_2^3 a_3^3 b_0^3 b_1 \\ & - 11197440000 \sin(v) v^{26} a_2^3 a_3^4 b_0^4 - 353894400000000 v^7 a_2 a_3^2 a_4 b_0^2 \\ & + 4900746240000 v^{17} a_2^2 a_3^3 b_0^3 + 39321600000000 v^7 a_3^2 b_0^2 b_1 \\ & + 125971200 \sin(v) v^{30} a_2^4 a_3^4 b_0^4 - 471859200000000 v^9 a_2 a_3^2 b_0^2 b_1 \\ & + 2138112000000 v^{13} a_2 a_3^3 b_0^3 + 68812800000000 v^{11} a_2^2 a_3^2 b_0^3 \\ & + 39321600000000 v^{13} a_2 a_3^3 b_0^4 + 34504704000000 v^{13} a_2^2 a_3^2 b_0^3 \\ & + 663552000000 v^{15} a_2 a_3^3 b_0^4 + 470292480000 v^{15} a_2^2 a_3^2 b_0^3 \\ & - 1022361600000000 v^{13} a_2^2 a_3^3 b_0^3 + 1101004800000000 v^{15} a_2^3 a_3^3 b_0^3 \\ & - 117964800000000 v^{15} a_2^2 a_3^3 b_0^4 + 21823488000000 v^{15} a_2^2 a_3^3 b_0^3 \\ & + 3981312000000 v^{13} a_2^2 a_3^2 a_4 b_0^2 b_1 \\ & - 29491200000000 v^7 a_3^2 a_4 b_0^2 b_1 + 98304000000000 v^5 a_3^2 b_0^2 \\ & - 24576000000000 v^3 a_3 b_0^2 - 4915200000000 v^3 a_4 b_1^3 \end{aligned}$$

$$\begin{aligned}
& + 4915200000000 v^3 b_0 b_1^2 + 4096000000000 \sin(v) v^8 b_1^4 \\
& + 1638400000000 \sin(v) v^6 b_1^3 \\
& + 196608000000000 v^{17} a_2^3 a_3^3 b_0^4 - 8294400000000 v^9 a_2 a_3^2 a_4 b_0^2 \\
& + 11197440000 \sin(v) v^{28} a_2^4 a_3^4 b_0^4 + 9830400000000 \sin(v) v^{20} a_2^2 a_3^4 b_0^4 \\
& + 2322432000000 v^9 a_2 a_3 b_0^2 b_1 + 19660800000000 v^9 a_2 a_3 b_0 b_1^3 \\
& - 11197440000 \sin(v) v^{22} a_2^3 a_3^3 b_0^3 + 6553600000000 \sin(v) v^{24} a_2^4 a_3^4 b_0^4 \\
& - 19660800000000 v^{11} a_2^2 a_3^2 a_4 b_0^2 b_1 \\
& + 2322432000000 v^5 a_2 a_3 a_4 b_0 + 104472576000000 v^7 a_2 a_3 b_0 b_1 \\
& - 3276800000000 \sin(v) b_0 a_3 v^6 a_2 - 78643200000000 v^5 a_2 a_3 a_4 b_0 b_1 \\
& - 707788800000000 v^7 a_2 a_3^2 b_0^2 + 33841152000000 v^{17} a_2^3 a_3^3 a_4 b_0^3 \\
& + 373555200000000 v^{11} a_2 a_3^3 b_0^3 + 2457600000000 \sin(v) v^{12} a_2^3 b_0^2 b_1^2 \\
& - 55296000000 \sin(v) v^8 a_2 a_3 b_0 + 1638400000000 \sin(v) v^{14} a_3^3 b_0^3 b_1 \\
& - 9830400000000 \sin(v) v^{14} a_2 a_3^3 b_0^3 + 4423680000000 \sin(v) v^{26} a_2^4 a_3^4 b_0^4 \\
& - 62985600 \sin(v) v^{28} a_2^3 a_3^4 b_0^4 + 1638400000000 \sin(v) v^{12} a_3^3 b_0^3 \\
& + 4096000000000 \sin(v) v^{16} a_3^4 b_0^4 + 19660800000000 v^5 a_3 b_0^2 b_1 \\
& + 137625600000000 v^5 a_2 a_3 b_0^2 + 20090880000000 v^{11} a_2 a_3 b_0 b_1^3 \\
& + 995328000000 v^{11} a_2 a_3^2 a_4 b_0^2 b_1 + 8294400000000 v^9 a_2 a_3 a_4 b_0 b_1^2 \\
& - 49152000000000 v^9 a_3^3 b_0^3 + 49152000000000 v^7 a_3^2 b_0^3 \\
& - 4915200000000 v^{11} a_3^3 b_0^4 - 11197440000 \sin(v) v^{24} a_2^3 a_3^3 b_0^3 b_1 \\
& - 117964800000000 v^{11} a_2 a_3^2 b_0^2 b_1^2 + 9830400000000 v^3 a_3 b_0 b_1 \\
& - 58982400000000 v^{11} a_2 a_3^2 b_0^3 b_1 - 4915200000000 v a_3 a_4 b_0 \\
& + 64077350400 v^{23} a_2^3 a_3^3 b_0^3 b_1 + 4218946560000 v^{19} a_2^2 a_3^3 b_0^3 b_1 \\
& + 2799360000 \sin(v) v^{24} a_2^2 a_3^4 b_0^4 - 663552000000 \sin(v) v^{24} a_2^3 a_3^4 b_0^4 \\
& - 62985600 \sin(v) v^{26} a_2^3 a_3^3 b_0^3 b_1 + 4915200000000 v^3 a_2 a_3 a_4 b_0 \\
& - 9830400000000 \sin(v) v^{10} a_2 a_3 b_0 b_1^2 + 137308608000 v^{21} a_2^3 a_3^3 b_0^3 \\
& + 4939315200000 v^{19} a_2^3 a_3^3 b_0^3 + 141410304000000 v^{17} a_2^3 a_3^3 b_0^3 \\
& + 4915200000000 \sin(v) v^8 a_3 b_0 b_1^2 + 1638400000000 \sin(v) v^{10} a_3 b_0 b_1^3 \\
& + 4915200000000 \sin(v) v^{10} a_3^2 b_0^2 b_1 + 331776000000 \sin(v) v^{22} a_2^2 a_3^4 b_0^4
\end{aligned}$$

$$\begin{aligned} & - 1310720000000 \sin(v) v^{22} a_2^3 a_3^4 b_0^4 - 62985600 \sin(v) v^{24} a_2^3 a_3^3 b_0^3 \\ & + 829440000000 v^{11} a_2 a_3 b_0^2 b_1^2 + 24920064000000 v^{11} a_2 a_3^2 b_0^2 b_1 \\ & + 4915200000000 \sin(v) v^6 a_3 b_0 b_1 - 9830400000000 \sin(v) v^{10} a_2 a_3^2 b_0^2 \\ & - 165888000000 \sin(v) v^{12} a_2 a_3^2 b_0^2 + 9830400000000 \sin(v) v^{12} a_2^2 a_3^2 b_0^2 \\ & + 117964800000000 v^5 a_2 a_3 b_0 b_1 + 331776000000 \sin(v) v^{14} a_2^2 a_3^2 b_0^2 \\ & + 2799360000 \sin(v) v^{16} a_2^2 a_3^2 b_0^2 + 531441 \sin(v) v^{32} a_2^4 a_3^4 b_0^4 \\ & + 68812800000000 v^9 a_2^2 a_3^2 a_4 b_0^2 + 1336934400000000 v^{11} a_2^2 a_3^2 b_0^2 b_1 \\ & + 35168256000000 v^{11} a_2^2 a_3^2 a_4 b_0^2 + 186777600000000 v^{11} a_2 a_3^3 a_4 b_0^3 \\ & + 663552000000 \sin(v) v^{20} a_2^2 a_3^3 b_0^3 b_1 - 165888000000 \sin(v) v^{16} a_2 a_3^3 b_0^3 \\ & + 19660800000000 \sin(v) v^{16} a_2^2 a_3^3 b_0^3 + 663552000000 \sin(v) v^{18} a_2^2 a_3^3 b_0^3 b_1 \\ & + 2799360000 \sin(v) v^{20} a_2^2 a_3^2 b_0^2 b_1^2 - 3276800000000 \sin(v) v^{18} a_2 a_3^4 b_0^4 \\ & - 13107200000000 \sin(v) v^{18} a_2^3 a_3^3 b_0^3 + 5598720000 \sin(v) v^{20} a_2^2 a_3^3 b_0^3 \\ & - 55296000000 \sin(v) v^{20} a_2 a_3^4 b_0^4 - 663552000000 \sin(v) v^{20} a_2^3 a_3^3 b_0^3 \\ & - 5598720000 v^{19} a_2^2 a_3^3 b_0^4 + 7372800000000 v^{19} a_2^2 a_3^4 b_0^4 \\ & + 12607488000000 v^{19} a_2^3 a_3^3 b_0^4 + 1244160000000 v^{21} a_2^2 a_3^4 b_0^4 \\ & + 291133440000 v^{21} a_2^3 a_3^3 b_0^4 + 2645395200 v^{23} a_2^3 a_3^3 b_0^4 \\ & - 995328000000 v^{23} a_2^3 a_3^4 b_0^4 + 19464192000000 v^{13} a_2 a_3^2 b_0^2 b_1^2 \\ & - 1327104000000 v^{13} a_2 a_3^2 b_0^3 b_1 + 97615872000000 v^{15} a_2^2 a_3^2 b_0^2 b_1^2 \\ & + 11943936000000 v^{15} a_2^2 a_3^2 b_0^3 b_1 - 235929600000000 v^{15} a_2^2 a_3^3 b_0^3 b_1 \\ & + 342392832000000 v^{13} a_2^2 a_3^2 b_0^2 b_1 + 470292480000 v^{13} a_2^2 a_3^2 a_4 b_0^2 \\ & + 78643200000000 v^{13} a_2 a_3^3 b_0^3 b_1 - 18579456000000 v^{15} a_2^2 a_3^3 a_4 b_0^3 \\ & + 550502400000000 v^{15} a_2^3 a_3^3 a_4 b_0^3 + 3317760000000 v^{13} a_2 a_3^3 a_4 b_0^3 \\ & + 39321600000000 v^{13} a_2^2 a_3^2 b_0^2 b_1^2 + 196608000000000 v^{13} a_2^2 a_3^2 b_0^3 b_1 \\ & + 4746470400000 v^{17} a_2^2 a_3^2 b_0^2 b_1^2 + 195955200000 v^{17} a_2^2 a_3^2 b_0^3 b_1 \\ & - 511180800000000 v^{13} a_2^2 a_3^3 a_4 b_0^3 + 14103797760000 v^{15} a_2^2 a_3^2 b_0^2 b_1 \\ & + 16072704000000 v^{15} a_2 a_3^3 b_0^3 b_1 + 37601280000000 v^{17} a_2^2 a_3^3 b_0^3 b_1 \\ & - 162362880000 v^{17} a_2^2 a_3^3 a_4 b_0^3 + 39321600000000 v^{17} a_2^3 a_3^3 b_0^3 b_1 \\ & + 111974400000 v^{15} a_2^2 a_3^2 a_4 b_0^2 b_1 - 165888000000 \sin(v) v^{12} a_2 a_3 b_0 b_1^2 \end{aligned}$$

$$\begin{aligned}
 & - 327680000000 \sin(v) v^{12} a_2 a_3 b_0 b_1^3 - 1966080000000 \sin(v) v^{12} a_2 a_3^2 b_0^2 b_1 \\
 & - 4915200000000 v b_0 b_1 + 4915200000000 v a_4 b_1^2 \\
 & - 55296000000 \sin(v) v^{14} a_2 a_3 b_0 b_1^3 \\
 & - 331776000000 \sin(v) v^{14} a_2 a_3^2 b_0^2 b_1 - 9830400000000 \sin(v) v^{14} a_2 a_3^2 b_0^2 b_1^2 \\
 & + 19660800000000 \sin(v) v^{14} a_2^2 a_3^2 b_0^2 b_1 - 165888000000 \sin(v) v^{16} a_2 a_3^2 b_0^2 b_1^2 \\
 & + 663552000000 \sin(v) v^{16} a_2^2 a_3^2 b_0^2 b_1 - 9830400000000 \sin(v) v^{16} a_2 a_3^3 b_0^3 b_1 \\
 & + 9830400000000 \sin(v) v^{16} a_2^2 a_3^2 b_0^2 b_1^2 + 5598720000 \sin(v) v^{18} a_2^2 a_3^2 b_0^2 b_1 \\
 & - 165888000000 \sin(v) v^{18} a_2 a_3^3 b_0^3 b_1 + 331776000000 \sin(v) v^{18} a_2^2 a_3^2 b_0^2 b_1^2 \\
 & + 19660800000000 \sin(v) v^{18} a_2^2 a_3^3 b_0^3 b_1 \\
 T_4 = & - 32768000000000 \cos(v) - 199065600000000 v^{28} a_2^4 a_3^5 b_0^5 \\
 & - 90699264000000 v^{28} a_2^4 a_3^4 b_0^5 - 520680960000000 v^{28} a_2^3 a_3^5 b_0^5 \\
 & - 5822668800000000 v^{26} a_2^4 a_3^4 b_0^5 - 2985984000000000 v^{26} a_2^3 a_3^5 b_0^5 \\
 & + 251942400000 \cos(v) v^{26} a_2^3 a_3^3 b_0^3 b_1 \\
 & + 2013265920000000000 v^{10} a_2^2 a_3^2 a_4 b_0^2 b_1 \\
 & - 58982400000000000 v^{24} a_2^3 a_3^5 b_0^5 - 111106598400000 v^{24} a_2^3 a_3^3 b_0^4 b_1 \\
 & - 180486144000000000 v^{24} a_2^4 a_3^4 b_0^5 - 12849062400000 v^{26} a_2^3 a_3^4 b_0^5 \\
 & + 8487659520000000 v^{16} a_2^2 a_3^3 a_4 b_0^3 - 366280704000000000 v^{12} a_2 a_3^3 b_0^3 \\
 & - 4617625190400000000 v^{18} a_2^3 a_3^3 b_0^3 + 6942412800000000 v^{18} a_2^2 a_3^3 a_4 b_0^3 b_1 \\
 & + 1133740800000 v^{34} a_2^5 a_3^5 b_0^5 \\
 & - 2125764000 \cos(v) v^{36} a_2^4 a_3^5 b_0^5 + 1966080000000000000 v^{16} a_2 a_3^4 b_0^5 \\
 & + 221184000000000 \cos(v) v^{10} a_2 a_3 b_0 b_1 \\
 & + 13107200000000000 \cos(v) v^8 a_2 a_3 b_0 b_1 \\
 & - 62373888000000000 v^{14} a_2^2 a_3^2 a_4 b_0^2 b_1^2 - 90243072000000000 v^{16} a_2^2 a_3^2 b_0^3 b_1^2 \\
 & - 23589273600000000 v^{26} a_2^4 a_3^4 b_0^4 b_1 + 511180800000000000 v^6 a_2 a_3 b_0^2 b_1 \\
 & - 264539520000000 v^{22} a_2^3 a_3^3 b_0^4 - 1022361600000000000 v^{16} a_2^2 a_3^4 b_0^4 \\
 & - 16986931200000000000 v^{16} a_2^3 a_3^3 b_0^4 + 44117913600000000 v^{18} a_2^2 a_3^3 b_0^4 \\
 & + 33177600000000000 v^{18} a_2 a_3^4 b_0^5 - 312980889600000000 v^{16} a_2^2 a_3^3 b_0^3 \\
 & - 642831033600 v^{30} a_2^4 a_3^4 b_0^5 - 4789370880000000000 v^{24} a_2^4 a_3^4 b_0^4 b_1
 \end{aligned}$$

$$\begin{aligned} & - 976748544000000000 v^{16} a_2^2 a_3^2 b_0^2 b_1^3 \\ & + 8626176000000000 v^{14} a_2 a_3^2 b_0^3 b_1^2 - 5898240000000000 v^{22} a_2^2 a_3^5 b_0^5 \\ & + 2621440000000000 \cos(v) v^{18} a_2^3 a_3^3 b_0^3 \\ & + 3185049600000000 v^{16} a_2^2 a_3^3 a_4 b_0^3 b_1 \\ & - 7864320000000000 v^{18} a_2^2 a_3^4 b_0^5 - 118908518400000000 v^{18} a_2^3 a_3^3 b_0^4 \\ & - 1343692800000000 v^{32} a_2^5 a_3^5 b_0^5 - 27072921600000000 v^{20} a_2^2 a_3^4 b_0^5 \\ & + 97085030400000000 v^{20} a_2^3 a_3^4 b_0^4 + 154140672000000000 v^{20} a_2^3 a_3^4 b_0^5 \\ & - 102236160000000000 v^{14} a_2^2 a_3^2 b_0^3 b_1^2 \\ & - 2949120000000000 v^{20} a_2 a_3^5 b_0^5 - 11197440000000 \cos(v) v^{26} a_2^2 a_3^4 b_0^4 b_1 \\ & - 1966080000000000 v^{14} a_3^4 b_0^5 - 1585446912000000000 v^{20} a_2^4 a_3^4 b_0^4 \\ & - 37158912000000000 v^{16} a_2^2 a_3^3 b_0^3 b_1 - 9953280000000000 v^{16} a_2 a_3^3 b_0^4 b_1 \\ & + 1887436800000000000 v^{18} a_2^3 a_3^4 b_0^4 - 9437184000000000000 v^{12} a_2^2 a_3^2 b_0^2 b_1^2 \\ & + 61046784000000000 v^{22} a_2^3 a_3^4 b_0^5 \\ & - 2089156608000000000 v^{22} a_2^4 a_3^4 b_0^4 - 2202009600000000000 v^{22} a_2^4 a_3^4 b_0^5 \\ & - 6469632000000000 v^{24} a_2^2 a_3^5 b_0^5 + 2239488000000000 v^{24} a_2^3 a_3^4 b_0^5 \\ & + 10616832000000000 v^{14} a_2 a_3^3 a_4 b_0^3 b_1 \\ & - 4423680000000000 \cos(v) v^{26} a_2^2 a_3^5 b_0^5 \\ & - 26214400000000000 \cos(v) v^{28} a_2^4 a_3^5 b_0^5 \\ & - 27869184000000000 v^6 a_2 a_3 b_0^2 - 1683605088000 v^{28} a_2^4 a_3^4 a_4 b_0^4 \\ & - 6740858880000000 v^{16} a_2^2 a_3^2 b_0^3 b_1 - 29364166656000000 v^{20} a_2^3 a_3^3 b_0^4 \\ & - 116785152000000000 v^{12} a_2 a_3^3 a_4 b_0^3 - 975175680000000000 v^{18} a_2^3 a_3^3 b_0^3 b_1^2 \\ & - 2911334400000000 v^{22} a_2^2 a_3^4 b_0^5 \\ & - 49397760000000000 v^{16} a_2 a_3^3 b_0^3 b_1^2 - 9608232960000000000 v^{16} a_2^3 a_3^3 b_0^3 \\ & - 15570796147200 v^{30} a_2^4 a_3^4 b_0^4 b_1 - 1881169920000000 v^{18} a_2^2 a_3^2 b_0^3 b_1^2 \\ & - 45566115840000000 v^{18} a_2^2 a_3^2 b_0^2 b_1^3 + 13107200000000000 \cos(v) v^{10} a_2 a_3^2 b_0^2 \\ & + 796262400000000 v^{30} a_2^5 a_3^5 b_0^5 + 349360128000000 v^{30} a_2^4 a_3^5 b_0^5 \\ & + 535530700800000000 v^{10} a_2 a_3^2 b_0^2 b_1 - 110350771200000 v^{22} a_2^3 a_3^3 a_4 b_0^3 b_1 \\ & + 22394880000000 \cos(v) v^{26} a_2^3 a_3^3 b_0^3 b_1^2 \end{aligned}$$

$$\begin{aligned}
 &+ 2654208000000000 \cos(v) v^{26} a_2^3 a_3^4 b_0^4 b_1 \\
 &- 2621440000000000 \cos(v) v^{26} a_2^4 a_3^4 b_0^4 b_1 \\
 &- 267386880000000000 v^{16} a_2^3 a_3^3 a_4 b_0^3 b_1 - 50909036544000000 v^{20} a_2^2 a_3^3 b_0^3 b_1^2 \\
 &+ 133693440000000000 v^{14} a_2 a_3^4 a_4 b_0^4 - 231211008000000000 v^{14} a_2^3 a_3^3 a_4 b_0^3 \\
 &- 682721280000000000 v^{18} a_2^2 a_3^4 b_0^4 \\
 &+ 801570816000000000 v^{14} a_2^2 a_3^3 a_4 b_0^3 + 2359296000000000000 v^{14} a_2^2 a_3^3 b_0^3 b_1 \\
 &- 1310720000000000 \cos(v) v^{12} a_2^2 a_3^2 b_0^2 - 58445660160000000 v^{22} a_2^3 a_3^4 b_0^4 \\
 &- 594542592000000000 v^{12} a_2^2 a_3^2 b_0^3 - 8110080000000000 v^{18} a_2 a_3^4 b_0^4 b_1 \\
 &- 1769472000000000 \cos(v) v^{30} a_2^4 a_3^5 b_0^5 + 3932160000000000 v^4 a_3 b_0 b_1^2 \\
 &- 442633420800000000 v^{14} a_2^2 a_3^2 b_0^2 b_1^2 \\
 &- 1990656000000000 v^{12} a_2 a_3 b_0^2 b_1^3 - 157286400000000000 v^{18} a_2^2 a_3^4 b_0^4 b_1 \\
 &+ 573308928000000 v^{20} a_2^2 a_3^3 b_0^4 b_1 - 20525875200000000 v^{14} a_2 a_3^3 b_0^3 b_1 \\
 &- 4821811200000000 v^{12} a_2 a_3 b_0 b_1^4 - 9830400000000000 v^6 a_3 a_4 b_0 b_1^3 \\
 &+ 223948800000000 \cos(v) v^{30} a_2^3 a_3^5 b_0^5 - 383798476800000000 v^{20} a_2^3 a_3^3 b_0^4 b_1 \\
 &+ 251942400000 \cos(v) v^{30} a_2^3 a_3^4 b_0^4 b_1 - 44789760000000 \cos(v) v^{30} a_2^4 a_3^4 b_0^4 b_1 \\
 &+ 31703040000000000 v^{16} a_2 a_3^4 b_0^4 + 1218969600000000000 v^{14} a_2^2 a_3^3 b_0^4 \\
 &+ 267386880000000000 v^{14} a_2 a_3^4 b_0^4 + 480411648000000000 v^{16} a_2^2 a_3^3 b_0^4 \\
 &+ 121896960000000000 v^8 a_3^3 b_0^3 - 418568601600000000 v^{10} a_2^2 a_3^2 a_4 b_0^2 \\
 &- 1638400000000000 \cos(v) v^8 b_1^4 + 5242880000000000 \cos(v) v^{24} a_2^3 a_3^4 b_0^4 b_1 \\
 &+ 397148160000000000 v^{10} a_3^3 b_0^4 \\
 &+ 26214400000000000 \cos(v) v^{26} a_2^3 a_3^5 b_0^5 \\
 &- 442368000000000 \cos(v) v^{20} a_2^2 a_3^2 b_0^2 b_1^3 \\
 &- 542638080000000000 v^{12} a_2 a_3^3 b_0^3 b_1 \\
 &- 1959041433600000000 v^{20} a_2^3 a_3^3 b_0^3 b_1^2 \\
 &- 396809280000 v^{32} a_2^4 a_3^5 b_0^5 - 468320256000000000 v^{18} a_2^2 a_3^3 b_0^3 b_1^2 \\
 &+ 1966080000000000 v^4 b_0 b_1^3 - 1966080000000000 v^4 a_4 b_1^4 \\
 &+ 1327104000000000 \cos(v) v^{24} a_2^3 a_3^3 b_0^3 b_1^2 \\
 &- 1327104000000000 \cos(v) v^{24} a_2^2 a_3^4 b_0^4 b_1
 \end{aligned}$$

$$\begin{aligned} & - 179159040000000000 v^{18} a_2^2 a_3^4 a_4 b_0^4 \\ & - 39321600000000000 v^{14} a_3^4 b_0^4 b_1 - 69009408000000000 v^{14} a_2 a_3^3 b_0^4 \\ & - 137625600000000000 v^{12} a_3^4 a_4 b_0^4 - 3617587200000000000 v^{12} a_2 a_3^3 b_0^4 \\ & + 39321600000000000 v^{12} a_3^3 b_0^4 b_1 + 7864320000000000 v^{12} a_3^3 b_0^3 b_1^2 \\ & - 10239344640000000000 v^{10} a_2^2 a_3^2 b_0^3 + 4089446400000000000 v^{10} a_3^3 b_0^3 b_1 \\ & - 39321600000000000 v^{10} a_3^2 b_0^3 b_1^2 - 7864320000000000 v^{10} a_3^2 b_0^2 b_1^3 \\ & - 3696230400000000000 v^{12} a_2^2 a_3^2 b_0^3 b_1 \\ & + 609484800000000000 v^8 a_3^3 a_4 b_0^3 + 4443340800000000000 v^8 a_2 a_3^2 b_0^3 \\ & + 176947200000000000 v^8 a_3^2 b_0^3 b_1 - 39321600000000000 v^8 a_3^2 b_0^2 b_1^2 \\ & + 98304000000000000 v^6 a_3 b_0^2 b_1^2 - 25559040000000000 v^4 a_3^2 a_4 b_0^2 \\ & - 235929600000000000 v^4 a_3 b_0^2 b_1 + 39321600000000000 v^2 a_4 b_1^3 \\ & - 1638400000000000 \cos(v) v^{16} a_3^4 b_0^4 - 40780656576000 v^{28} a_2^4 a_3^4 b_0^4 \\ & - 4875878400000000000 v^{18} a_2^3 a_3^3 b_0^4 b_1 \\ & + 13271040000000000 \cos(v) v^{28} a_2^3 a_3^5 b_0^5 \\ & + 19660800000000000 \cos(v) v^{14} a_2 a_3^3 b_0^3 \\ & + 503884800000 \cos(v) v^{36} a_2^5 a_3^5 b_0^5 \\ & + 3538944000000000000 v^8 a_2 a_3^2 b_0^2 b_1 \\ & - 366752563200000000 v^{20} a_2^2 a_3^4 b_0^4 b_1 \\ & - 337084416000000000 v^{14} a_2^2 a_3^2 b_0^3 b_1 \\ & + 7864320000000000 a_3 b_0 - 1022361600000000000 v^{14} a_2 a_3^3 b_0^3 b_1^2 \\ & - 2125218124800000 v^{26} a_2^3 a_3^4 b_0^4 b_1 + 58982400000000000 v^2 a_3 b_0^2 \\ & - 78643200000000000 \cos(v) v^{18} a_2^2 a_3^3 b_0^3 b_1 \\ & - 511180800000000000 v^{14} a_2 a_3^3 b_0^4 b_1 - 19528335360000000 v^{24} a_2^4 a_3^4 a_4 b_0^4 \\ & + 943718400000000000 v^{18} a_2^3 a_3^4 a_4 b_0^4 \\ & - 35790999552000000 v^{20} a_2^2 a_3^4 b_0^4 + 1879572480000000000 v^{12} a_2^2 a_3^3 a_4 b_0^3 \\ & - 8150638970880000 v^{20} a_2^3 a_3^3 b_0^3 \\ & - 336494269440000 v^{20} a_2^3 a_3^3 a_4 b_0^3 - 11197440000000 \cos(v) v^{20} a_2^2 a_3^2 b_0^2 b_1^2 \\ & + 331776000000000 \cos(v) v^{20} a_2 a_3^3 b_0^3 b_1^2 \end{aligned}$$

$$\begin{aligned} &+ 18874368000000000 v^{10} a_2 a_3^2 b_0^3 b_1 \\ &- 9289728000000000 v^4 a_2 a_3 a_4 b_0 - 15728640000000000 v^{10} a_2 a_3 b_0 b_1^4 \\ &- 7864320000000000 v^{10} a_2 a_3 b_0^2 b_1^3 + 1981808640000000000 v^{10} a_2 a_3^2 b_0^2 b_1^2 \\ &+ 165298176000000000 v^{12} a_2 a_3^2 b_0^2 b_1^2 + 291962880000000000 v^{12} a_2 a_3^2 b_0^3 b_1 \\ &+ 25067520000000000 v^{14} a_2 a_3^2 b_0^2 b_1^3 - 6584094720000000 v^{12} a_2^2 a_3^2 a_4 b_0^2 \\ &+ 51118080000000000 v^4 a_2 a_3 a_4 b_0 b_1 - 192675840000000000 v^{10} a_3^3 a_4 b_0^3 b_1 \\ &- 5685903360000000000 v^{10} a_2 a_3^3 a_4 b_0^3 \\ &- 2044723200000000000 v^{14} a_2^2 a_3^2 b_0^2 b_1^3 \\ &- 11421388800000000 v^{16} a_2^2 a_3^2 a_4 b_0^2 b_1^2 \\ &+ 596164608000000000 v^8 a_2 a_3^2 b_0^2 - 4676891443200000000 v^{10} a_2^2 a_3^2 b_0^2 \\ &- 504299520000000000 v^{12} a_2^2 a_3^2 a_4 b_0^2 b_1 \\ &+ 39321600000000000 \cos(v) v^{12} a_2 a_3^2 b_0^2 b_1 \\ &+ 3317760000000000 \cos(v) v^{12} a_2 a_3 b_0 b_1^2 \\ &+ 19660800000000000 \cos(v) v^{10} a_2 a_3 b_0 b_1^2 \\ &- 13271040000000000 \cos(v) v^{16} a_2^2 a_3^2 b_0^2 b_1 \\ &- 39321600000000000 \cos(v) v^{14} a_2^2 a_3^2 b_0^2 b_1 \\ &+ 6635520000000000 \cos(v) v^{14} a_2 a_3^2 b_0^2 b_1 \\ &+ 9289728000000000 v^6 a_2 a_3 a_4 b_0 b_1 - 11197440000000 \cos(v) v^{18} a_2^2 a_3^2 b_0^2 b_1 \\ &- 39280619520000000 v^{18} a_2^3 a_3^3 a_4 b_0^3 + 14348907 \cos(v) v^{40} a_2^5 a_3^5 b_0^5 \\ &+ 255590400000000000 v^4 a_3 a_4 b_0 b_1^2 - 2211382425600000 v^{26} a_2^4 a_3^4 b_0^4 \\ &+ 393216000000000000 v^{12} a_2 a_3^2 b_0^2 b_1^3 - 282679372800000 v^{26} a_2^4 a_3^4 a_4 b_0^4 \\ &- 1572120576000000 v^{20} a_2^2 a_3^4 a_4 b_0^4 - 13005619200000000 v^{10} a_2 a_3 b_0^2 b_1^2 \\ &- 237876019200000000 v^{10} a_2 a_3 b_0 b_1^3 - 2776965120000000 v^{14} a_2^2 a_3^2 a_4 b_0^2 b_1 \\ &+ 4251528000 \cos(v) v^{38} a_2^5 a_3^5 b_0^5 \\ &- 8409710592000000000 v^{18} a_2^3 a_3^3 b_0^3 b_1 \\ &+ 90243072000000000 v^{18} a_2^2 a_3^3 b_0^4 b_1 + 3082813440000000000 v^{20} a_2^3 a_3^4 b_0^4 b_1 \\ &- 11371806720000000000 v^{10} a_2 a_3^3 b_0^3 - 1478062080000000 v^{28} a_2^4 a_3^4 b_0^4 b_1 \\ &+ 37591449600000000000 v^{12} a_2^2 a_3^3 b_0^3 \end{aligned}$$

$$\begin{aligned} & - 2654208000000000 \cos(v) v^{20} a_2^2 a_3^3 b_0^3 b_1 \\ & + 1310720000000000 \cos(v) v^{20} a_2 a_3^4 b_0^4 b_1 \\ & - 3932160000000000 \cos(v) v^{20} a_2^2 a_3^3 b_0^3 b_1^2 \\ & + 5242880000000000 \cos(v) v^{20} a_2^3 a_3^3 b_0^3 b_1 \\ & - 3732480000000 \cos(v) v^{22} a_2^2 a_3^2 b_0^2 b_1^3 \\ & - 22394880000000 \cos(v) v^{22} a_2^2 a_3^3 b_0^3 b_1 \\ & - 32768000000000 \cos(v) v^{20} a_3^5 b_0^5 \\ & - 3936522240000000 v^{24} a_2^3 a_3^4 b_0^4 b_1 \\ & + 663552000000000 \cos(v) v^{18} a_2 a_3^3 b_0^3 b_1 \\ & + 221184000000000 \cos(v) v^{18} a_2 a_3^2 b_0^2 b_1^3 \\ & - 1327104000000000 \cos(v) v^{18} a_2^2 a_3^2 b_0^2 b_1^2 \\ & + 43082150400000 v^{24} a_2^3 a_3^4 a_4 b_0^4 - 7864320000000000 v^4 a_2 a_3 b_0 b_1 \\ & - 3732480000000 \cos(v) v^{28} a_2^2 a_3^5 b_0^5 - 4624220160000000000 v^{14} a_2^3 a_3^3 b_0^3 \\ & + 10485760000000000 \cos(v) v^{30} a_2^5 a_3^5 b_0^5 + 125971200000 \cos(v) v^{32} a_2^3 a_3^5 b_0^5 \\ & + 58982400000000000 v^6 a_3^2 a_4 b_0^2 b_1 + 2673868800000000000 v^6 a_2 a_3^2 a_4 b_0^2 \\ & - 9830400000000000 v^2 a_3 a_4 b_0 b_1 - 13107200000000000 \cos(v) v^{18} a_2^2 a_3^2 b_0^2 b_1^3 \\ & + 19660800000000000 \cos(v) v^{18} a_2 a_3^3 b_0^3 b_1^2 \\ & - 1022361600000000000 v^{12} a_2^2 a_3^2 a_4 b_0^2 b_1^2 \\ & - 393216000000000000 v^{14} a_2^2 a_3^3 a_4 b_0^3 b_1 \\ & + 502706995200000000 v^{20} a_2^3 a_3^4 a_4 b_0^4 - 7927234560000000000 v^{20} a_2^4 a_3^4 a_4 b_0^4 \\ & - 30442106880000000 v^{22} a_2^2 a_3^4 b_0^4 b_1 - 44789760000000 \cos(v) v^{32} a_2^4 a_3^5 b_0^5 \\ & + 884736000000000 \cos(v) v^{32} a_2^5 a_3^5 b_0^5 - 7864320000000000 v^8 a_2 a_3 b_0 b_1^3 \\ & - 10402172928000000 v^{22} a_2^3 a_3^3 b_0^3 b_1^2 \\ & - 511180800000000000 v^{16} a_2^2 a_3^4 a_4 b_0^4 \\ & - 161906688000000000 v^{16} a_2^3 a_3^3 a_4 b_0^3 \\ & - 9830400000000000 \cos(v) v^{10} a_3^2 b_0^2 b_1 \\ & - 10704752640000000 v^{22} a_2^3 a_3^3 b_0^4 b_1 \\ & - 1645215744000000000 v^{10} a_2^2 a_3^2 b_0^2 b_1 \end{aligned}$$

$$\begin{aligned}
 & - 39321600000000000000 v^{16} a_2^3 a_3^3 b_0^3 b_1 \\
 & + 23592960000000000000 v^{16} a_2^2 a_3^3 b_0^4 b_1 \\
 & + 47185920000000000000 v^{16} a_2^2 a_3^3 b_0^3 b_1^2 \\
 & - 9830400000000000 \cos(v) v^8 a_3 b_0 b_1^2 + 23224320000000000 v^{16} a_2 a_3^4 a_4 b_0^4 \\
 & + 8021606400000000000 v^{10} a_2 a_3^2 a_4 b_0^2 b_1^2 \\
 & - 299925504000000000 v^{10} a_2 a_3^2 a_4 b_0^2 b_1 \\
 & + 31850496000000000 v^{10} a_2 a_3 a_4 b_0 b_1^3 \\
 & - 2673868800000000000 v^8 a_2 a_3^2 a_4 b_0^2 b_1 \\
 & + 1966080000000000000 v^8 a_2 a_3 a_4 b_0 b_1^3 - 10616832000000000 v^8 a_2 a_3 a_4 b_0 b_1^2 \\
 & - 5898240000000000000 v^6 a_2 a_3 a_4 b_0 b_1^2 - 2125764000 \cos(v) v^{34} a_2^4 a_3^4 b_0^4 b_1 \\
 & - 503884800000 \cos(v) v^{32} a_2^4 a_3^4 b_0^4 b_1 - 4087480320000000000 v^{22} a_2^3 a_3^4 b_0^4 b_1 \\
 & - 23592960000000000000 v^8 a_2 a_3 b_0^2 b_1^2 - 1966080000000000000 v^8 a_3^2 a_4 b_0^2 b_1^2 \\
 & - 66060288000000000000 v^8 a_2^2 a_3^2 a_4 b_0^2 - 39321600000000000 a_4 b_1^2 \\
 & + 39321600000000000 b_0 b_1 + 8599633920000000 v^{22} a_2^3 a_3^4 a_4 b_0^4 \\
 & - 1572864000000000000 v^6 a_2 a_3 b_0 b_1^2 - 4404019200000000000 v^{22} a_2^4 a_3^4 b_0^4 b_1 \\
 & - 503884800000 \cos(v) v^{34} a_2^4 a_3^5 b_0^5 - 393216000000000000 \cos(v) v^{16} a_2^2 a_3^3 b_0^3 \\
 & + 29859840000000 \cos(v) v^{34} a_2^5 a_3^5 b_0^5 - 631701504000000000 v^{22} a_2^4 a_3^4 a_4 b_0^4 \\
 & - 2691248716800000 v^{24} a_2^3 a_3^3 b_0^3 b_1^2 + 39321600000000000 \cos(v) v^{16} a_2 a_3^3 b_0^3 b_1 \\
 & - 393216000000000000 \cos(v) v^{16} a_2^2 a_3^2 b_0^2 b_1^2 \\
 & - 1638400000000000 \cos(v) v^4 a_3 b_0 - 159481405440000000 v^{12} a_2^2 a_3^2 b_0^2 \\
 & - 2250178560000000000 v^4 a_2 a_3 b_0 - 235929600000000000 v^2 a_2 a_3 b_0 \\
 & - 190943723520000000 v^{16} a_2^2 a_3^2 b_0^2 b_1^2 \\
 & - 1179648000000000000 v^2 a_2 a_3 a_4 b_0 + 196608000000000000 v^{12} a_2 a_3^2 b_0^3 b_1^2 \\
 & - 6553600000000000 \cos(v) v^{10} a_3 b_0 b_1^3 - 1638400000000000 \cos(v) v^{12} a_3 b_0 b_1^4 \\
 & - 450035712000000000 v^6 a_2 a_3 b_0 b_1 + 393216000000000000 v^{16} a_2 a_3^4 b_0^4 b_1 \\
 & - 6553600000000000 \cos(v) v^6 a_3 b_0 b_1 - 39321600000000000 v^2 b_0 b_1^2 \\
 & + 39321600000000000 a_3 a_4 b_0 - 327680000000000 \cos(v) v^{10} b_1^5 \\
 & - 9830400000000000 \cos(v) v^{12} a_3^2 b_0^2 b_1^2
 \end{aligned}$$

$$\begin{aligned} & - 327680000000000 \cos(v) v^{14} a_3^2 b_0^2 b_1^3 \\ & - 655360000000000 \cos(v) v^{14} a_3^3 b_0^3 b_1 - 102259998720000000 v^{18} a_2^2 a_3^3 b_0^3 b_1 \\ & - 327680000000000 \cos(v) v^{16} a_3^3 b_0^3 b_1^2 - 466108416000000000 v^8 a_2 a_3 b_0 b_1^2 \\ & - 163840000000000 \cos(v) v^{18} a_3^4 b_0^4 b_1 \\ & + 1310720000000000 \cos(v) v^{18} a_2 a_3^4 b_0^4 \\ & - 1327104000000000 \cos(v) v^{18} a_2^2 a_3^3 b_0^3 \\ & + 221184000000000 \cos(v) v^{20} a_2 a_3^4 b_0^4 \\ & + 1327104000000000 \cos(v) v^{20} a_2^3 a_3^3 b_0^3 \\ & - 11197440000000 \cos(v) v^{20} a_2^2 a_3^3 b_0^3 \\ & - 1327104000000000 \cos(v) v^{22} a_2^2 a_3^4 b_0^4 \\ & + 22394880000000 \cos(v) v^{22} a_2^3 a_3^3 b_0^3 \\ & + 125971200000 \cos(v) v^{24} a_2^3 a_3^3 b_0^3 \\ & - 11197440000000 \cos(v) v^{24} a_2^2 a_3^4 b_0^4 \\ & - 431990267904000000 v^{20} a_2^3 a_3^3 b_0^3 b_1 \\ & - 3932160000000000 \cos(v) v^{20} a_2^2 a_3^4 b_0^4 \\ & - 8626176000000000 v^8 a_2 a_3 b_0^2 b_1 + 3276800000000000 \cos(v) v^{22} a_2 a_3^5 b_0^5 \\ & + 2654208000000000 \cos(v) v^{24} a_2^3 a_3^4 b_0^4 \\ & + 44789760000000 \cos(v) v^{26} a_2^3 a_3^4 b_0^4 \\ & - 1769472000000000 \cos(v) v^{26} a_2^4 a_3^4 b_0^4 \\ & + 251942400000 \cos(v) v^{28} a_2^3 a_3^4 b_0^4 \\ & - 44789760000000 \cos(v) v^{28} a_2^4 a_3^4 b_0^4 \\ & - 503884800000 \cos(v) v^{30} a_2^4 a_3^4 b_0^4 \\ & - 2125764000 \cos(v) v^{32} a_2^4 a_3^4 b_0^4 \\ & + 8427110400000000 v^8 a_2 a_3^2 a_4 b_0^2 \\ & - 9080675942400000 v^{22} a_2^3 a_3^3 b_0^3 b_1 \\ & + 5242880000000000 \cos(v) v^{22} a_2^3 a_3^4 b_0^4 \\ & + 55296000000000 \cos(v) v^{24} a_2 a_3^5 b_0^5 \\ & + 331776000000000 \cos(v) v^{16} a_2 a_3^3 b_0^3 \end{aligned}$$

$$\begin{aligned} &+ 22118400000000 \cos(v) v^{12} a_2 a_3^2 b_0^2 \\ &- 44236800000000 \cos(v) v^{14} a_2^2 a_3^2 b_0^2 \\ &+ 125971200000 \cos(v) v^{28} a_2^3 a_3^3 b_0^3 b_1^2 \\ &+ 44789760000000 \cos(v) v^{28} a_2^3 a_3^4 b_0^4 b_1 \\ &- 1769472000000000 \cos(v) v^{28} a_2^4 a_3^4 b_0^4 b_1 \\ &- 1310720000000000 \cos(v) v^{24} a_2^2 a_3^5 b_0^5 \\ &- 2621440000000000 \cos(v) v^{24} a_2^4 a_3^4 b_0^4 \\ &- 3732480000000 \cos(v) v^{16} a_2^2 a_3^2 b_0^2 \\ &+ 55296000000000 \cos(v) v^8 b_0 a_3 a_2 \\ &+ 3276800000000000 \cos(v) b_0 a_3 v^6 a_2 \\ &+ 16588800000000000 v^{12} a_2 a_3^2 a_4 b_0^2 b_1^2 \\ &- 302579712000000000 v^{18} a_2^3 a_3^3 a_4 b_0^3 b_1 \\ &+ 904396800000000000 v^{12} a_2 a_3^3 a_4 b_0^3 b_1 \\ &- 100597800960000000 v^{20} a_2^3 a_3^3 a_4 b_0^3 b_1 \\ &- 550502400000000000 v^4 a_2 a_3 b_0^2 \\ &+ 2211840000000000 \cos(v) v^{22} a_2 a_3^4 b_0^4 b_1 \\ &- 13271040000000000 \cos(v) v^{22} a_2^2 a_3^3 b_0^3 b_1^2 \\ &+ 26542080000000000 \cos(v) v^{22} a_2^3 a_3^3 b_0^3 b_1 \\ &- 39321600000000000 \cos(v) v^{22} a_2^2 a_3^4 b_0^4 b_1 \\ &+ 262144000000000000 \cos(v) v^{22} a_2^3 a_3^3 b_0^3 b_1^2 \\ &- 111974400000000 \cos(v) v^{24} a_2^2 a_3^3 b_0^3 b_1^2 \\ &+ 447897600000000 \cos(v) v^{24} a_2^3 a_3^3 b_0^3 b_1 \\ &+ 117964800000000000 v^6 a_3^2 b_0^2 b_1 \\ &- 3276800000000000 \cos(v) v^4 b_1^2 - 3276800000000000 \cos(v) v^6 b_1^3 \\ &+ 5347737600000000000 v^6 a_2 a_3^2 b_0^2 - 1638400000000000 \cos(v) v^2 b_1 \\ &- 13212057600000000000 v^8 a_2^2 a_3^2 b_0^2 \\ &+ 131072000000000000 \cos(v) v^{12} a_2 a_3 b_0 b_1^3 \\ &+ 2211840000000000 \cos(v) v^{14} a_2 a_3 b_0 b_1^3 \end{aligned}$$

$$\begin{aligned}
& + 327680000000000 \cos(v) v^{14} a_2 a_3 b_0 b_1^4 \\
& - 7864320000000000 v^2 a_3 b_0 b_1 - 106738974720000000 v^{24} a_2^4 a_3^4 b_0^4 \\
& + 39321600000000000 \cos(v) v^{14} a_2 a_3^2 b_0^2 b_1^2 \\
& + 55296000000000 \cos(v) v^{16} a_2 a_3 b_0 b_1^4 \\
& + 13107200000000000 \cos(v) v^{16} a_2 a_3^2 b_0^2 b_1^3 \\
& + 6635520000000000 \cos(v) v^{16} a_2 a_3^2 b_0^2 b_1^2 \\
& - 530841600000000000 v^6 a_3^2 b_0^3 - 275251200000000000 v^{12} a_3^4 b_0^4 \\
& - 2953940659200000 v^{24} a_2^3 a_3^4 b_0^4 + 116387020800000000 v^{10} a_2 a_3^2 b_0^3 \\
& - 3276800000000000 \cos(v) v^{12} a_3^3 b_0^3 - 3276800000000000 \cos(v) v^8 a_3^2 b_0^2 \\
& - 9002741760000000 v^{14} a_2^2 a_3^2 b_0^3 + 1839071232000000000 v^{14} a_2^2 a_3^3 b_0^3 \\
& - 285330677760000000 v^{14} a_2^2 a_3^2 b_0^2 b_1 - 7276658688000000000 v^{12} a_2^2 a_3^2 b_0^2 b_1 \\
& - 5111808000000000000 v^4 a_3^2 b_0^2 \\
T_{denom} & = 27 v^8 a_2 a_3 b_0 + 1600 v^6 a_2 a_3 b_0 - 800 v^4 a_3 b_0 - 800 v^2 b_1 - 800.
\end{aligned}$$

Appendix B: Formulae for the T_j , $j = 5(1)9$, T_{denom1} , T_{denom2} and T_{denom3}

$$\begin{aligned}
T_5 & = 273600 v + 81756 v^6 \sin(v) + 772620 v^4 \sin(v) + 345600 \cos(v) \sin(v) \\
& - 35115 \cos(v) v^3 + 417600 v \cos(v) + 748800 v^2 \sin(v) \\
& - 165394 v^5 \cos(v) - 1535715 \left(\cos(v)\right)^2 v^3 \\
& + 273600 \left(\cos(v)\right)^3 v - 691200 \left(\cos(v)\right)^2 \sin(v) - 1310400 \left(\cos(v)\right)^2 v \\
& + 345600 \left(\cos(v)\right)^3 \sin(v) - 819 \left(\cos(v)\right)^3 v^7 + 2592 \left(\cos(v)\right)^4 v^5 \\
& - 981 \left(\cos(v)\right)^2 v^7 + 145591 \left(\cos(v)\right)^3 v^5 + 77280 \left(\cos(v)\right)^4 v^3 \\
& + 84881 \left(\cos(v)\right)^2 v^5 + 290475 \left(\cos(v)\right)^3 v^3 + 345600 \left(\cos(v)\right)^4 v \\
& - 11466 \cos(v) v^7 + 3924 v^7 + 31330 v^5 \\
& + 1203075 v^3 - 37920 \left(\cos(v)\right)^3 \sin(v) v^2 \\
& - 1191360 \left(\cos(v)\right)^2 \sin(v) v^2 + 480480 \cos(v) v^2 \sin(v) \\
& - 476310 \cos(v) v^4 \sin(v) - 314310 \left(\cos(v)\right)^2 \sin(v) v^4
\end{aligned}$$

$$\begin{aligned} & + 20439 \left(\cos(v) \right)^2 \sin(v) v^6 + 18639 \cos(v) v^6 \sin(v) \\ T_6 = & -36000 + 10066 \cos(v) v^4 - 5165 \cos(v) v^2 + 378 \cos(v) v^6 \\ & + 1188 v^5 \sin(v) + 20132 v^3 \sin(v) - 48000 v \sin(v) \\ & - 6835 \left(\cos(v) \right)^3 v^2 + 38335 \left(\cos(v) \right)^2 v^2 \\ & + 27 \left(\cos(v) \right)^3 v^6 - 327 \left(\cos(v) \right)^2 v^6 \\ & + 233 \left(\cos(v) \right)^3 v^4 + 6067 \left(\cos(v) \right)^2 v^4 \\ & + 36000 \cos(v) + 16934 v^4 + 36000 \left(\cos(v) \right)^2 \\ & + 1308 v^6 - 26335 v^2 - 36000 \left(\cos(v) \right)^3 \\ & + 19334 \cos(v) v^3 \sin(v) + 24000 \left(\cos(v) \right)^2 \sin(v) v \\ & + 3597 \cos(v) v^5 \sin(v) + 297 \left(\cos(v) \right)^2 \sin(v) v^5 \\ & + 6734 \left(\cos(v) \right)^2 \sin(v) v^3 + 24000 \cos(v) v \sin(v) \\ T_7 = & 400 \left(\cos(v) \right)^3 v^4 + 1200 \left(\cos(v) \right)^2 \sin(v) v^3 - 400 \left(\cos(v) \right)^2 v^4 \\ & + 1200 \left(\cos(v) \right)^3 v^2 + 1200 \cos(v) v^3 \sin(v) \\ & + 5600 \cos(v) v^4 + 7200 \left(\cos(v) \right)^2 \sin(v) v \\ & - 1200 \left(\cos(v) \right)^2 v^2 + 4800 v^3 \sin(v) + 1600 v^4 \\ & - 3600 \left(\cos(v) \right)^3 + 7200 \cos(v) v \sin(v) \\ & + 2400 \cos(v) v^2 + 3600 \left(\cos(v) \right)^2 - 14400 v \sin(v) \\ & - 2400 v^2 + 3600 \cos(v) - 3600 \\ T_8 = & 3000 v + 3540 v^6 \sin(v) + 36916 v^4 \sin(v) \\ & - 24000 \cos(v) \sin(v) - 57853 \cos(v) v^3 \\ & - 51000 v \cos(v) + 21600 v^2 \sin(v) - 12590 v^5 \cos(v) \\ & + 537 \left(\cos(v) \right)^2 v^3 + 3000 \left(\cos(v) \right)^3 v \\ & + 48000 \left(\cos(v) \right)^2 \sin(v) + 69000 \left(\cos(v) \right)^2 v - 24000 \left(\cos(v) \right)^3 \sin(v) \\ & - 41 \left(\cos(v) \right)^3 v^7 + 108 \left(\cos(v) \right)^4 v^5 \\ & - 109 \left(\cos(v) \right)^2 v^7 + 2417 \left(\cos(v) \right)^3 v^5 \\ & - 668 \left(\cos(v) \right)^4 v^3 + 5161 \left(\cos(v) \right)^2 v^5 \end{aligned}$$

$$\begin{aligned}
 & + 13917 \left(\cos(v)\right)^3 v^3 - 24000 \left(\cos(v)\right)^4 v \\
 & - 574 \cos(v) v^7 + 436 v^7 + 5354 v^5 + 44067 v^3 \\
 & + 7332 \left(\cos(v)\right)^3 \sin(v) v^2 + 57336 \left(\cos(v)\right)^2 \sin(v) v^2 \\
 & - 86268 \cos(v) v^2 \sin(v) - 10178 \cos(v) v^4 \sin(v) \\
 & + 10798 \left(\cos(v)\right)^2 \sin(v) v^4 + 885 \left(\cos(v)\right)^2 \sin(v) v^6 \\
 & + 1635 \cos(v) v^6 \sin(v) + 864 \left(\cos(v)\right)^3 \sin(v) v^4 \\
 T_9 = & -45000 v + 540 v^6 \sin(v) + 16996 v^4 \sin(v) \\
 & + 48000 \cos(v) \sin(v) + 37437 \cos(v) v^3 \\
 & + 69000 v \cos(v) - 53868 v^2 \sin(v) + 1762 v^5 \cos(v) \\
 & - 13917 \left(\cos(v)\right)^2 v^3 - 21000 \left(\cos(v)\right)^3 v \\
 & - 24000 \left(\cos(v)\right)^2 \sin(v) - 3000 \left(\cos(v)\right)^2 v \\
 & + 9 \left(\cos(v)\right)^3 v^7 - 159 \left(\cos(v)\right)^2 v^7 \\
 & - 421 \left(\cos(v)\right)^3 v^5 - 5417 \left(\cos(v)\right)^2 v^5 \\
 & - 9101 \left(\cos(v)\right)^3 v^3 + 126 \cos(v) v^7 \\
 & - 24000 \sin(v) + 636 v^7 + 4526 v^5 - 14419 v^3 \\
 & - 3468 \left(\cos(v)\right)^2 \sin(v) v^2 + 57336 \cos(v) v^2 \sin(v) \\
 & + 19798 \cos(v) v^4 \sin(v) + 1606 \left(\cos(v)\right)^2 \sin(v) v^4 \\
 & + 135 \left(\cos(v)\right)^2 \sin(v) v^6 + 885 \cos(v) v^6 \sin(v) \\
 T_{denom1} = & 964800 v + 6156 v^6 \sin(v) + 178620 v^4 \sin(v) \\
 & - 691200 \cos(v) \sin(v) - 377415 \cos(v) v^3 \\
 & - 1310400 v \cos(v) + 1603680 v^2 \sin(v) \\
 & + 4454 v^5 \cos(v) - 654975 \left(\cos(v)\right)^2 v^3 \\
 & + 619200 \left(\cos(v)\right)^3 v + 345600 \left(\cos(v)\right)^2 \sin(v) \\
 & - 273600 \left(\cos(v)\right)^2 v + 81 \left(\cos(v)\right)^3 v^7 \\
 & - 1881 \left(\cos(v)\right)^2 v^7 - 9821 \left(\cos(v)\right)^3 v^5 - 81691 \left(\cos(v)\right)^2 v^5 \\
 & - 79545 \left(\cos(v)\right)^3 v^3 + 1134 \cos(v) v^7 \\
 & + 345600 \sin(v) + 7524 v^7 + 186058 v^5
 \end{aligned}$$

$$\begin{aligned}
 & + 1111935 v^3 - 412320 (\cos(v))^2 \sin(v) v^2 \\
 & - 1191360 \cos(v) v^2 \sin(v) - 179310 \cos(v) v^4 \sin(v) \\
 & - 17310 (\cos(v))^2 \sin(v) v^4 + 1539 (\cos(v))^2 \sin(v) v^6 \\
 & - 261 \cos(v) v^6 \sin(v) \\
 T_{denom2} = & v(3000 v + 3540 v^6 \sin(v) + 36916 v^4 \sin(v)) \\
 & - 24000 \cos(v) \sin(v) - 57853 \cos(v) v^3 - 51000 v \cos(v) \\
 & + 21600 v^2 \sin(v) - 12590 v^5 \cos(v) + 537 (\cos(v))^2 v^3 + 3000 (\cos(v))^3 v \\
 & + 48000 (\cos(v))^2 \sin(v) + 69000 (\cos(v))^2 v - 24000 (\cos(v))^3 \sin(v) \\
 & - 41 (\cos(v))^3 v^7 + 108 (\cos(v))^4 v^5 \\
 & - 109 (\cos(v))^2 v^7 + 2417 (\cos(v))^3 v^5 \\
 & - 668 (\cos(v))^4 v^3 + 5161 (\cos(v))^2 v^5 \\
 & + 13917 (\cos(v))^3 v^3 - 24000 (\cos(v))^4 v \\
 & - 574 \cos(v) v^7 + 436 v^7 + 5354 v^5 + 44067 v^3 \\
 & + 7332 (\cos(v))^3 \sin(v) v^2 + 57336 (\cos(v))^2 \sin(v) v^2 \\
 & - 86268 \cos(v) v^2 \sin(v) - 10178 \cos(v) v^4 \sin(v) \\
 & + 10798 (\cos(v))^2 \sin(v) v^4 + 885 (\cos(v))^2 \sin(v) v^6 \\
 & + 1635 \cos(v) v^6 \sin(v) + 864 (\cos(v))^3 \sin(v) v^4 \\
 T_{denom3} = & 3 v^2 (-36000 + 10066 \cos(v) v^4) \\
 & - 5165 \cos(v) v^2 + 378 \cos(v) v^6 + 1188 v^5 \sin(v) \\
 & + 20132 v^3 \sin(v) - 48000 v \sin(v) \\
 & - 6835 (\cos(v))^3 v^2 + 38335 (\cos(v))^2 v^2 \\
 & + 27 (\cos(v))^3 v^6 - 327 (\cos(v))^2 v^6 \\
 & + 233 (\cos(v))^3 v^4 + 6067 (\cos(v))^2 v^4 \\
 & + 36000 \cos(v) + 16934 v^4 + 36000 (\cos(v))^2 \\
 & + 1308 v^6 - 26335 v^2 - 36000 (\cos(v))^3 \\
 & + 19334 \cos(v) v^3 \sin(v) + 24000 (\cos(v))^2 \sin(v) v \\
 & + 3597 \cos(v) v^5 \sin(v) + 297 (\cos(v))^2 \sin(v) v^5
 \end{aligned}$$

$$+ 6734 \left(\cos(v) \right)^2 \sin(v) v^3 + 24000 \cos(v) v \sin(v) \Big).$$

Appendix C: Truncated Taylor series expansion formulae for the coefficients of the new obtained method given by (20)

$$\begin{aligned} a_4 &= -2 + \frac{307 v^{14}}{12454041600} + \frac{367 v^{16}}{355829760000} + \frac{923129 v^{18}}{1863124623360000} + \dots \\ a_3 &= \frac{1}{200} + \frac{307 v^8}{1482624000} - \frac{2417 v^{10}}{741312000000} \\ &+ \frac{1473239 v^{12}}{7763019264000000} - \frac{519798397381 v^{14}}{7805560609566720000000} \\ &+ \frac{634951433527 v^{16}}{98127047663124480000000} - \frac{3353222549436577 v^{18}}{8215196430356781465600000000} + \dots \\ a_2 &= -\frac{10}{693} + \frac{307 v^6}{61158240} + \frac{12871 v^8}{51372921600} \\ &+ \frac{3915281 v^{10}}{384269453568000} - \frac{490295749 v^{12}}{360761204643840000} \\ &- \frac{819052406254949 v^{14}}{5156821672316349235200000} - \frac{65485222444932977 v^{16}}{6099783349539910238208000000} \\ &+ \frac{19451811235875157 v^{18}}{988806985083311764930560000000} + \dots \\ b_0 &= \frac{5}{6} + \frac{307 v^{10}}{741312000} - \frac{13997 v^{12}}{160123392000} - \frac{8376059 v^{14}}{1834013301120000} \\ &- \frac{1647568883 v^{16}}{4460320348323840000} + \frac{829887639481 v^{18}}{26494302869043609600000} + \dots \\ b_1 &= \frac{1}{12} - \frac{307 v^{10}}{1482624000} - \frac{4423 v^{12}}{320246784000} - \frac{39301201 v^{14}}{58688425635840000} \\ &+ \frac{1060489 v^{16}}{23851980472320000} - \frac{7698503677 v^{18}}{6233953616245555200000} + \dots \end{aligned}$$

Appendix D: Expressions for the derivatives of z_n

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

$$q^{(2)} = (V(x) - V_c + G) q(x)$$

$$\begin{aligned}q^{(3)} &= \left(\frac{d}{dx}g(x)\right)q(x) + (g(x) + G)\frac{d}{dx}q(x) \\q^{(4)} &= \left(\frac{d^2}{dx^2}g(x)\right)q(x) + 2\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}q(x) + (g(x) + G)^2q(x) \\q^{(5)} &= \left(\frac{d^3}{dx^3}g(x)\right)q(x) + 3\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}q(x) \\&+ 4(g(x) + G)q(x)\frac{d}{dx}g(x) + (g(x) + G)^2\frac{d}{dx}q(x) \\q^{(6)} &= \left(\frac{d^4}{dx^4}g(x)\right)q(x) + 4\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}q(x) \\&+ 7(g(x) + G)q(x)\frac{d^2}{dx^2}g(x) + 4\left(\frac{d}{dx}g(x)\right)^2q(x) \\&+ 6(g(x) + G)\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}g(x) + (g(x) + G)^3q(x) \\q^{(7)} &= \left(\frac{d^5}{dx^5}g(x)\right)q(x) + 5\left(\frac{d^4}{dx^4}g(x)\right)\frac{d}{dx}q(x) \\&+ 11(g(x) + G)q(x)\frac{d^3}{dx^3}g(x) + 15\left(\frac{d}{dx}g(x)\right)q(x) \\&+ \frac{d^2}{dx^2}g(x) + 13(g(x) + G)\left(\frac{d}{dx}q(x)\right)\frac{d^2}{dx^2}g(x) \\&+ 10\left(\frac{d}{dx}g(x)\right)^2\frac{d}{dx}q(x) + 9(g(x) + G)^2q(x) \\&+ \frac{d}{dx}g(x) + (g(x) + G)^3\frac{d}{dx}q(x) \\q^{(8)} &= \left(\frac{d^6}{dx^6}g(x)\right)q(x) + 6\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}q(x) \\&+ 16(g(x) + G)q(x)\frac{d^4}{dx^4}g(x) + 26\left(\frac{d}{dx}g(x)\right)q(x) \\&+ \frac{d^3}{dx^3}g(x) + 24(g(x) + G)\left(\frac{d}{dx}q(x)\right)\frac{d^3}{dx^3}g(x)\end{aligned}$$

$$\begin{aligned}
 & + 15 \left(\frac{d^2}{dx^2} g(x) \right)^2 q(x) + 48 \left(\frac{d}{dx} g(x) \right) \\
 & + \left(\frac{d}{dx} q(x) \right) \frac{d^2}{dx^2} g(x) + 22 (g(x) + G)^2 q(x) \\
 & + \frac{d^2}{dx^2} g(x) + 28 (g(x) + G) q(x) \left(\frac{d}{dx} g(x) \right)^2 \\
 & + 12 (g(x) + G)^2 \left(\frac{d}{dx} q(x) \right) \frac{d}{dx} g(x) + (g(x) + G)^4 q(x) \\
 & \dots
 \end{aligned}$$

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 Q_0

$$\begin{aligned}
 Q_0 = & \frac{5219 \left(\frac{d^2}{dx^2} g(x) \right) q(x) \frac{d^8}{dx^8} g(x)}{5660928000} + \frac{8903 \left(\frac{d}{dx} g(x) \right) q(x) \frac{d^9}{dx^9} g(x)}{23351328000} \\
 & + \frac{5219 \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} q(x) \right) \frac{d^6}{dx^6} g(x)}{606528000} + \frac{166087 (g(x))^2 q(x) \frac{d^8}{dx^8} g(x)}{186810624000} \\
 & + \frac{307 \left(\frac{d^{12}}{dx^{12}} g(x) \right) q(x)}{186810624000} + \frac{107143 (g(x))^2 \left(\frac{d}{dx} q(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^4}{dx^4} g(x)}{6671808000} \\
 & + \frac{263099 (g(x))^2 q(x) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^4}{dx^4} g(x)}{8491392000} \\
 & + \frac{2149 (g(x))^2 \left(\frac{d}{dx} q(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^3}{dx^3} g(x)}{83397600} \\
 & + \frac{123107 \left(\frac{d}{dx} g(x) \right)^2 q(x) \frac{d^6}{dx^6} g(x)}{15567552000} + \frac{7061 \left(\frac{d^3}{dx^3} g(x) \right) q(x) \frac{d^7}{dx^7} g(x)}{4245696000} \\
 & + \frac{3377 \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} q(x) \right) \frac{d^7}{dx^7} g(x)}{707616000} + \frac{2149 \left(\frac{d^2}{dx^2} g(x) \right)^2 \left(\frac{d}{dx} q(x) \right) \frac{d^3}{dx^3} g(x)}{40435200} \\
 & + \frac{129247 \left(\frac{d^2}{dx^2} g(x) \right)^2 q(x) \frac{d^4}{dx^4} g(x)}{5660928000} + \frac{18727 \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} q(x) \right) \frac{d^8}{dx^8} g(x)}{10378368000} \\
 & + \frac{307 \left(\frac{d^{11}}{dx^{11}} g(x) \right) \frac{d}{dx} q(x)}{15567552000} + \frac{307 \left(\frac{d^5}{dx^5} g(x) \right)^2 q(x)}{235872000}
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{307 (g(x))^7 q(x)}{186810624000} + \frac{2149 \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} q(x)\right) \left(\frac{d^4}{dx^4} g(x)\right) \frac{d^2}{dx^2} g(x)}{30888000} \\
 & + \frac{221347 g(x) \left(\frac{d}{dx} q(x)\right) \left(\frac{d}{dx} g(x)\right) \left(\frac{d^2}{dx^2} g(x)\right)^2}{4447872000} \\
 & + \frac{9517 g(x) \left(\frac{d}{dx} q(x)\right) \left(\frac{d}{dx} g(x)\right)^2 \frac{d^3}{dx^3} g(x)}{247104000} \\
 & + \frac{307 \left(\frac{d}{dx} g(x)\right)^3 \left(\frac{d}{dx} q(x)\right) \frac{d^2}{dx^2} g(x)}{12636000} + \frac{34691 (g(x))^4 q(x) \frac{d^4}{dx^4} g(x)}{26687232000} \\
 & + \frac{20569 g(x) q(x) \frac{d^{10}}{dx^{10}} g(x)}{186810624000} + \frac{147053 (g(x))^2 q(x) \left(\frac{d^3}{dx^3} g(x)\right)^2}{7783776000} \\
 & + \frac{197401 (g(x))^3 q(x) \left(\frac{d^2}{dx^2} g(x)\right)^2}{26687232000} + \frac{1068667 g(x) q(x) \left(\frac{d^5}{dx^5} g(x)\right) \frac{d^3}{dx^3} g(x)}{46702656000} \\
 & + \frac{357041 (g(x))^3 q(x) \frac{d^6}{dx^6} g(x)}{186810624000} + \frac{7061 (g(x))^2 \left(\frac{d}{dx} q(x)\right) \frac{d^7}{dx^7} g(x)}{4670265600} \\
 & + \frac{83197 g(x) q(x) \left(\frac{d^4}{dx^4} g(x)\right)^2}{6227020800} + \frac{307 (g(x))^4 q(x) \left(\frac{d}{dx} g(x)\right)^2}{333590400} \\
 & + \frac{307 g(x) q(x) \left(\frac{d}{dx} g(x)\right)^2 \frac{d^4}{dx^4} g(x)}{7983360} + \frac{782543 (g(x))^2 q(x) \left(\frac{d}{dx} g(x)\right) \frac{d^5}{dx^5} g(x)}{46702656000} \\
 & + \frac{307 \left(\frac{d^2}{dx^2} g(x)\right) q(x) \left(\frac{d^3}{dx^3} g(x)\right)^2}{11664000} + \frac{7061 \left(\frac{d}{dx} g(x)\right)^2 \left(\frac{d}{dx} q(x)\right) \frac{d^5}{dx^5} g(x)}{370656000} \\
 & + \frac{307 \left(\frac{d^4}{dx^4} g(x)\right) \left(\frac{d}{dx} q(x)\right) \frac{d^5}{dx^5} g(x)}{26956800} + \frac{13201 \left(\frac{d^4}{dx^4} g(x)\right) q(x) \frac{d^6}{dx^6} g(x)}{5660928000} \\
 & + \frac{307 \left(\frac{d}{dx} g(x)\right)^3 q(x) \frac{d^3}{dx^3} g(x)}{14370048} + \frac{24253 (g(x))^3 \left(\frac{d}{dx} q(x)\right) \frac{d^5}{dx^5} g(x)}{13343616000} \\
 & + \frac{307 (g(x))^4 \left(\frac{d}{dx} q(x)\right) \frac{d^3}{dx^3} g(x)}{444787200} + \frac{7061 (g(x))^5 q(x) \frac{d^2}{dx^2} g(x)}{26687232000} \\
 & + \frac{140299 \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} q(x)\right) \left(\frac{d^3}{dx^3} g(x)\right)^2}{3335904000} \\
 & + \frac{598957 \left(\frac{d}{dx} g(x)\right)^2 q(x) \left(\frac{d^2}{dx^2} g(x)\right)^2}{15567552000} \\
 & + \frac{1494169 g(x) q(x) \left(\frac{d^2}{dx^2} g(x)\right)^3}{62270208000} + \frac{7061 g(x) \left(\frac{d}{dx} q(x)\right) \frac{d^9}{dx^9} g(x)}{18681062400} \\
 & + \frac{307 (g(x))^5 \left(\frac{d}{dx} q(x)\right) \frac{d}{dx} g(x)}{4447872000} + \frac{883853 g(x) q(x) \left(\frac{d^6}{dx^6} g(x)\right) \frac{d^2}{dx^2} g(x)}{62270208000} \\
 & + \frac{24253 g(x) \left(\frac{d}{dx} q(x)\right) \left(\frac{d^4}{dx^4} g(x)\right) \frac{d^3}{dx^3} g(x)}{667180800}
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{574397 g(x) q(x) \left(\frac{d^7}{dx^7} g(x) \right) \frac{d}{dx} g(x)}{93405312000} \\
 & + \frac{307 (g(x))^3 \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} g(x) \right) \frac{d^2}{dx^2} g(x)}{55598400} \\
 & + \frac{252047 \left(\frac{d}{dx} g(x) \right) q(x) \left(\frac{d^4}{dx^4} g(x) \right) \frac{d^3}{dx^3} g(x)}{6227020800} \\
 & + \frac{193103 (g(x))^2 q(x) \left(\frac{d}{dx} g(x) \right)^2 \frac{d^2}{dx^2} g(x)}{6671808000} \\
 & + \frac{112669 g(x) \left(\frac{d}{dx} q(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \frac{d^2}{dx^2} g(x)}{4447872000} \\
 & + \frac{156263 g(x) \left(\frac{d}{dx} q(x) \right) \left(\frac{d^6}{dx^6} g(x) \right) \frac{d}{dx} g(x)}{13343616000} \\
 & + \frac{14429 \left(\frac{d}{dx} g(x) \right) q(x) \left(\frac{d^5}{dx^5} g(x) \right) \frac{d^2}{dx^2} g(x)}{486486000} \\
 & + \frac{3626591 g(x) q(x) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \frac{d^3}{dx^3} g(x)}{31135104000} \\
 & + \frac{152579 (g(x))^3 q(x) \left(\frac{d}{dx} g(x) \right) \frac{d^3}{dx^3} g(x)}{13343616000} + \frac{307 g(x) q(x) \left(\frac{d}{dx} g(x) \right)^4}{51321600} \\
 & + \frac{307 (g(x))^2 \left(\frac{d}{dx} q(x) \right) \left(\frac{d}{dx} g(x) \right)^3}{74131200}
 \end{aligned}$$

at every point $x = x_n$.

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