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Three–Stages Tenth Algebraic Order Two–Step Method with Vanished Phase–Lag and its First, Second, Third and Fourth Derivatives

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Abstract

A new three–stages symmetric two–step method of high algebraic order is obtained in this paper. For this new method we require the elimination of the phase–lag and its first, second, third and fourth derivatives. The affect of the elimination of the phase–lag and its first, second, third and fourth derivatives of the new developed multistage symmetric two-step method on the efficiency of the produced method is studied in this paper. We will investigate the following: (1) the development of the method, (2) the definition of the local truncation error (LTE) of the new method and the analysis of the LTE when the obtained method is applied to a test problem (which is the radial Schrödinger equation, (3) the comparison of the asymptotic formula of the LTE produced by the application of the new developed method to the test equation with the asymptotic formulae of the LTEs of other similar methods in the literature (comparative local truncation error analysis), (4) the stability (interval of periodicity) of the new produced method. It is noted that for the study of the stability of the new obtained method we will use

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a scalar test equation with frequency different than the frequency of the scalar test equation used for the phase–lag analysis (stability analysis), (5) the examination of the efficiency of the new proposed method applying it to two problems of the literature: (i) the resonance problem of the Schrödinger equation and (ii) the coupled differential equations arising from the Schrödinger equation. Finally, it will proved that this category of methods are very efficient for the approximate solution of the Schrödinger equation and related initial-value or boundary-value problems with periodical and /or oscillating solutions . We mention here that the proposed method is an improvement of the recent developed methods in [1] and [2]. .

1 Introduction

The maximization of the efficiency of a family of low computational cost tenth algebraic order symmetric two–step methods for the numerical solution of the Schrödinger equation and related problems is studied in the present paper . The efficiency of the new obtained scheme will be tested on the approximate solution of both (1) the radial time independent Schrödinger equation and (2) the coupled differential equation arising from the Schrödinger equation. It is noted that the efficient numerical solution of this kind of problems is very important on Computational Chemistry (see [3] and references therein). The most of the quantum chemical calculations contain as a very critical part the Schrödinger equation. It is mentioned here that the Schrödinger's equation can be solved only numerically for more than one particle. Solving efficiently the Schrödinger equation we can (1) compute important molecular properties (for example vibrational energy levels and wave functions of systems) and (2) give a substantial presentation of the molecule's electronic structure (see for more details in [4–7]).

More specifically in this paper we optimized the methods developed for the first time in the literature in [1] and [2]. In more details we have optimized the number of derivatives of the phase–lag which will be vanished. In [1] we had vanished phase–lag and its first and second derivatives. In [2] we had vanished phase–lag and its first, second and third derivatives. In the present paper we will have vanished phase–lag and its first, second, third and fourth derivatives. As we will prove in the analysis of the new obtained method, this optimization improves the efficiency of the method (accuracy and computational efficiency). The method retains the benefits of the methods obtained in [1] and [2], i.e., we have a tenth algebraic order symmetric two–step method of only three stages.

We will investigate the approximate solution of special second order initial value problems with solution of periodical and/or oscillatory behavior of the form:

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

More specifically, we will investigate the systems of ordinary differential equations of second order in which the first derivative q' does not appear explicitly and which they have periodic and/or oscillating solutions .

2 Phase–lag analysis of symmetric $2\,m$ multistep methods

The phase–lag analysis of symmetric multistep methods is based on the following stages:

- Definition of the multistep finite difference method for the the numerical solution of the initial value problem (1). The method has the general form

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

- Definition of the area of integration, the integration interval and the stepsize of integration

  The above mentioned multistep method can be used for the numerical integration of the initial value problem (1) following the procedure: (1) Consider that the integration of the initial value problem (1) is taken place within the interval $[a, b]$. (2) The interval of integration $[a, b]$ is divided into m equally spaced intervals i.e., $\{x_i\}_{i=-m}^{m} \in [a, b]$. (3) Based on (2) we define the quantity h by $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$. This quantity is called **the stepsize of integration**.

- Definition of $2\,m$-step method and symmetric $2\,m$-step method,

  Remark 1. *For the multistep method given by (2), the number of steps is equal to* $2\,m$.

  Remark 2. *We call the method (2) symmetric if and only if* $c_{-i} = c_i$ *and* $b_{-i} = b_i$, $i = 0(1)m$.

- Definition of the algebraic order p of a Multistep Method (2)

Remark 3. *The Multistep Method (2) is associated with the following 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 $q \in C^2$.

Definition 1. [8] The multistep method (2) is called algebraic of order p if the associated linear operator L given by (3) vanishes for any linear combination of the linearly independent functions $1, \, x, \, x^2, \, \ldots, \, x^{p+1}$.

- Definition of the scalar test equation, difference equation, characteristic equation of a symmetric $2\,m$-step method

If we apply the symmetric $2\,m$-step method, $(i = -m(1)m)$, to the scalar test equation

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

we have the following difference equation:

$$A_m(v) \, q_{n+m} + \cdots + A_1(v) \, q_{n+1} + A_0(v) \, q_n + A_1(v) \, q_{n-1} + \cdots + A_m(v) \, q_{n-m} = 0 \tag{5}$$

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

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

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

- Definition of the interval of periodicity, the phase–lag, the term phase-fitted for a symmetric $2\,m$-step method

Definition 2. [9] *A symmetric* $2\,m$*-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* $\lambda_i, i = 1(1)2\,m$ *of Eq. (6) satisfy:*

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

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

Definition 3. [10], [11] *For any method corresponding to the characteristic equation (6), the phase–lag is defined as the leading term in the expansion of*

$$t = v - \theta(v)\,. \tag{8}$$

Then if the quantity $t = O(v^{s+1})$ *as* $v \to \infty$*, the order of the phase–lag is* s*.*

Definition 4. [12] *A method is called* **phase-fitted** *if its phase–lag is equal to zero.*

- Direct formula for the computation of the phase–lag for a symmetric $2\,m$-step method

Theorem 1. [10] *The symmetric* $2\,m$*-step method with characteristic equation given by (6) has phase–lag order* s *and phase–lag constant* c *given by*

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

Remark 4. *The direct calculation of the the phase–lag of any symmetric* $2\,m$*-step method can be done using the above mentioned formula .*

Remark 5. *A symmetric two-step method has phase–lag order* s *and phase–lag constant* c *given by:*

$$-cv^{s+2} + O(v^{s+4}) = \frac{2\,A_1(v)\,\cos(v) + A_0(v)}{2\,A_1(v)}\,. \tag{10}$$

3 The new high algebraic order three–stages symmetric two–step method with vanished phase–lag and its first, second, third and fourth derivatives

Let us consider the family of methods

$$\widehat{q}_n = q_n - a_0\,h^2\left(f_{n+1} - 2\,f_n + f_{n-1}\right) - 2\,a_1\,h^2\,f_n$$

$$\widetilde{q}_n = q_n - a_2\, h^2 \left(f_{n+1} - 2\, \widehat{f}_n + f_{n-1} \right)$$
$$q_{n+1} + a_3\, q_n + q_{n-1} = h^2 \left[b_1 \, \left(f_{n+1} + f_{n-1} \right) + b_0 \, \widetilde{f}_n \right] \tag{11}$$

where $f_i = q''\left(x_i, q_i\right), i = -2(1)2$ and $a_j,\ j = 0(1)3$ and $b_i,\ i = 0, 1$ are free parameters.

3.1 Development of the method

We will investigate in this paper the above mentioned family of methods (11), with:

$$b_1 \; = \; \frac{1}{12}\,. \tag{12}$$

We require the above symmetric multistage two-step method (11) with coefficient (12) to have vanished phase–lag and its first, second, third and fourth derivatives. This request leads to the following equations:

$$\text{Phase}--\text{Lag(PL)} \; = \; \frac{1}{2}\, \frac{T_0}{1 + v^2 \left(\frac{1}{12} + b_0\, a_2\, v^2 \left(-2\, a_0\, v^2 + 1 \right) \right)} = 0 \tag{13}$$

$$\text{First Derivative of the Phase}--\text{Lag} \; = \; \frac{T_1}{\left(24\, v^6\, a_0\, a_2\, b_0 - 12\, v^4\, a_2\, b_0 - v^2 - 12\right)^2} = 0 \tag{14}$$

$$\text{Second Derivative of the Phase}--\text{Lag} \; = \; \frac{T_2}{\left(24\, v^6\, a_0\, a_2\, b_0 - 12\, v^4\, a_2\, b_0 - v^2 - 12\right)^3} = 0 \tag{15}$$

$$\text{Third Derivative of the Phase}--\text{Lag} \; = \; \frac{T_3}{\left(24\, v^6\, a_0\, a_2\, b_0 - 12\, v^4\, a_2\, b_0 - v^2 - 12\right)^4} = 0 \tag{16}$$

$$\text{Fourth Derivative of the Phase}--\text{Lag} \; = \; \frac{T_4}{\left(24\, v^6\, a_0\, a_2\, b_0 - 12\, v^4\, a_2\, b_0 - v^2 - 12\right)^5} = 0 \tag{17}$$

where $T_j,\ j = 0(1)4$ are given in the Appendix A.

Solving the above mentioned system of equations (13)–(17), we produce the coefficients of the new proposed two–stage symmetric two–step method :

$$a_0 = \frac{1}{4}\, \frac{T_5}{T_6} \quad , \quad a_1 = -\frac{1}{12}\, \frac{T_7}{T_6}$$
$$a_2 = -\frac{T_8}{T_9} \quad , \quad a_3 = -\frac{1}{9}\, \frac{T_{10}}{T_{11}}$$
$$b_0 = \frac{1}{6}\, \frac{T_{12}}{v\, T_{11}} \tag{18}$$

where

$$T_5 \; = \; \left(\cos\left(v\right)\right)^2 v^7 + 5\, \cos\left(v\right) \sin\left(v\right) v^6 + 35\, \left(\cos\left(v\right)\right)^2 v^5 - 4\, v^7$$

$$
\begin{aligned}
& + \quad 62\,\cos(v)\sin(v)\,v^4 + 8\,v^5\cos(v) + 639\,(\cos(v))^2\,v^3 \\
& + \quad 16\,\sin(v)\,v^4 - 154\,v^5 - 792\,\cos(v)\sin(v)\,v^2 \\
& + \quad 168\,\cos(v)\,v^3 + 1080\,(\cos(v))^2\,v - 648\,\sin(v)\,v^2 + 273\,v^3 \\
& - \quad 1440\,\cos(v)\sin(v) - 1440\,\cos(v)\,v + 1440\,\sin(v) + 360\,v \\
T_6 & = \quad v^3\Big((\cos(v))^2\,v^6 + 11\,\cos(v)\sin(v)\,v^5 + (\cos(v))^2\,v^4 \\
& - \quad 4\,v^6 + 210\,\cos(v)\sin(v)\,v^3 + 315\,(\cos(v))^2\,v^2 - 106\,v^4 \\
& + \quad 1260\,\cos(v)\sin(v)\,v + 3150\,(\cos(v))^2 + 1575\,v^2 - 3150\Big) \\
T_7 & = \quad -8100\,v - (\cos(v))^2\,v^7 - 207\,(\cos(v))^2\,v^5 + 630\,v^5\cos(v) \\
& - \quad 2007\,(\cos(v))^2\,v^3 + 2292\,\sin(v)\,v^4 + 261\,\cos(v)\,v^3 - 540\,(\cos(v))^2\,v \\
& - \quad 4536\,\sin(v)\,v^2 + 8640\,\cos(v)\sin(v) + 12420\,\cos(v)\,v + (\cos(v))^3\,v^7 \\
& + \quad 14\,\cos(v)\,v^7 - 57\,(\cos(v))^3\,v^5 - 945\,(\cos(v))^3\,v^3 - 3780\,(\cos(v))^3\,v \\
& + \quad 60\,\sin(v)\,v^6 - 4320\,(\cos(v))^2\sin(v) + 4\,v^7 - 4320\,\sin(v) \\
& + \quad 282\,v^5 + 2691\,v^3 + 15\,\cos(v)\sin(v)\,v^6 + 4536\,\cos(v)\sin(v)\,v^2 \\
& - \quad 30\,\cos(v)\sin(v)\,v^4 + 114\,(\cos(v))^2\sin(v)\,v^4 + 15\,(\cos(v))^2\sin(v)\,v^6 \\
T_8 & = \quad (\cos(v))^2\,v^6 + 11\,\cos(v)\sin(v)\,v^5 + (\cos(v))^2\,v^4 \\
& - \quad 4\,v^6 + 210\,\cos(v)\sin(v)\,v^3 + 315\,(\cos(v))^2\,v^2 - 106\,v^4 \\
& + \quad 1260\,\cos(v)\sin(v)\,v + 3150\,(\cos(v))^2 + 1575\,v^2 - 3150 \\
T_9 & = \quad v^2\Big(11340 - 2\,(\cos(v))^2\,v^6 - 58\,(\cos(v))^2\,v^4 - 1782\,(\cos(v))^2\,v^2 \\
& + \quad (\cos(v))^3\,v^6 + 14\,\cos(v)\,v^6 + 670\,\cos(v)\,v^4 + 3873\,\cos(v)\,v^2 \\
& + \quad 63\,(\cos(v))^3\,v^4 + 12\,\sin(v)\,v^5 + 1467\,(\cos(v))^3\,v^2 + 108\,\sin(v)\,v^3 \\
& - \quad 5040\,\sin(v)\,v - 11340\,\cos(v) + 8\,v^6 - 11340\,(\cos(v))^2 + 180\,v^4 \\
& - \quad 3558\,v^2 + 11340\,(\cos(v))^3 - 14\,\cos(v)\sin(v)\,v^5 - 204\,\cos(v)\sin(v)\,v^3 \\
& + \quad 1680\,\cos(v)\sin(v)\,v + 126\,(\cos(v))^2\sin(v)\,v^3 + 3360\,(\cos(v))^2\sin(v)\,v \\
& + \quad 3\,(\cos(v))^2\sin(v)\,v^5\Big) \\
T_{10} & = \quad 11070\,v - (\cos(v))^2\,v^7 - 33\,(\cos(v))^2\,v^5 + 534\,v^5\cos(v) \\
& - \quad 531\,(\cos(v))^2\,v^3 - 1008\,\sin(v)\,v^4 - 1269\,\cos(v)\,v^3 + 1458\,(\cos(v))^2\,v \\
& - \quad 4320\,\sin(v)\,v^2 + 15120\,\cos(v)\sin(v) - 16740\,\cos(v)\,v + (\cos(v))^3\,v^7 \\
& + \quad 14\,\cos(v)\,v^7 + 51\,(\cos(v))^3\,v^5 + 441\,(\cos(v))^3\,v^3
\end{aligned}
$$

$$
\begin{aligned}
&+ && 4212\,(\cos(v))^3\,v - 12\,\sin(v)\,v^6 - 15120\,(\cos(v))^2\sin(v)\\
&+ && 4\,v^7 + 42\,v^5 - 2367\,v^3 - 3\,\cos(v)\sin(v)\,v^6 + 2916\,\cos(v)\sin(v)\,v^2\\
&+ && 54\,\cos(v)\sin(v)\,v^4 - 252\,(\cos(v))^2\sin(v)\,v^4\\
&- && 3\,(\cos(v))^2\sin(v)\,v^6 - 3024\,(\cos(v))^2\sin(v)\,v^2\\
T_{11} &= && (\cos(v))^2\,v^5 + 17\,\cos(v)\sin(v)\,v^4 - 93\,(\cos(v))^2\,v^3\\
&- && 4\,v^5 - 102\,\cos(v)\sin(v)\,v^2 - 8\,\cos(v)\,v^3 - 381\,(\cos(v))^2\,v - 144\,\sin(v)\,v^2\\
&- && 106\,v^3 - 840\,\cos(v)\sin(v) + 696\,\cos(v)\,v + 840\,\sin(v) - 315\,v\\
T_{12} &= && 11340 - 2\,(\cos(v))^2\,v^6 - 58\,(\cos(v))^2\,v^4 - 1782\,(\cos(v))^2\,v^2\\
&+ && (\cos(v))^3\,v^6 + 14\,\cos(v)\,v^6 + 670\,\cos(v)\,v^4 + 3873\,\cos(v)\,v^2\\
&+ && 63\,(\cos(v))^3\,v^4 + 12\,\sin(v)\,v^5 + 1467\,(\cos(v))^3\,v^2 + 108\,\sin(v)\,v^3\\
&- && 5040\,\sin(v)\,v - 11340\,\cos(v) + 8\,v^6 - 11340\,(\cos(v))^2 + 180\,v^4\\
&- && 3558\,v^2 + 11340\,(\cos(v))^3 - 14\,\cos(v)\sin(v)\,v^5 - 204\,\cos(v)\sin(v)\,v^3\\
&+ && 1680\,\cos(v)\sin(v)\,v + 126\,(\cos(v))^2\sin(v)\,v^3 + 3360\,(\cos(v))^2\sin(v)\,v\\
&+ && 3\,(\cos(v))^2\sin(v)\,v^5.
\end{aligned}
$$

For the above mentioned formulae given by (18) and in the case of heavy cancelations for some values of $|v|$, the following Taylor series expansions should be used :

$$
\begin{aligned}
a_0 &= && -\frac{1}{112} - \frac{5\,v^2}{9408} - \frac{284857\,v^4}{8475667200} - \frac{100705691\,v^6}{46989098956800}\\
&- && \frac{13116028349339\,v^8}{959536196337438720000} - \frac{29352616379577233\,v^{10}}{336912349258001483366400 0}\\
&- && \frac{673873194408043267991\,v^{12}}{1214097341786134145459159040000} - \frac{364872558618989244547201\,v^{14}}{103207986830555691437192191672320000}\\
&- && \frac{10316056266056756706696433999\,v^{16}}{4581626900597129220487042240924876800000}\\
&- && \frac{83775540772854161980354833782663\,v^{18}}{584212409348941141162743730224812890521600000} + \cdots\\
a_1 &= && \frac{1}{8} - \frac{15\,v^2}{2464} + \frac{192893\,v^4}{739939200} + \frac{88461\,v^6}{151934182400}\\
&+ && \frac{2279624625181\,v^8}{83769033013585920000} + \frac{877868361000271\,v^{10}}{5882596574346057646080 0}\\
&+ && \frac{1023258587664974750 29\,v^{12}}{1059926250765672666670694400000} + \frac{27647319584095207996 3039\,v^{14}}{45051105362544151024171194777600000}\\
&+ && \frac{3994811331119026974159088547\,v^{16}}{1022179546605885090637761628707225600000}\\
&+ && \frac{33963180701691321120766588 3\,v^{18}}{13646199507009295647481405812970094592 00} + \cdots\\
a_2 &= && \frac{1}{300} + \frac{v^2}{18480} - \frac{1361\,v^4}{945945000} - \frac{889297\,v^6}{3814050240000}
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{50979389033\, v^{8}}{2995555058496000000} - \frac{58277501501\, v^{10}}{817248867240960000000} \\
&- \frac{436295660980970093\, v^{12}}{1566224764112610201600000000} - \frac{62701608727182273971\, v^{14}}{665708173738423840088064000000000} \\
&- \frac{5384260332911863564 97\, v^{16}}{164469078217728242845286400000000000} \\
&- \frac{215309160711159284029369\, v^{18}}{1409171062169495584698413875200000000000} + \cdots
\end{aligned}
$$

$$
\begin{aligned}
a_3 = &= -2 + \frac{v^{12}}{47900160} + \frac{4751\, v^{14}}{4358914560000} \\
&+ \frac{67097\, v^{16}}{1098446469120000} + \frac{7165454749\, v^{18}}{258815957054054400000} + \cdots \\
b_0 &= \frac{5}{6} - \frac{v^{10}}{15966720} - \frac{1151\, v^{12}}{326918592000} - \frac{27187\, v^{14}}{137305808640000} \\
&- \frac{524737841\, v^{16}}{575146571231232000000} - \frac{2922867080249\, v^{18}}{826140534916541644800000000} + \cdots \qquad (19)
\end{aligned}
$$

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

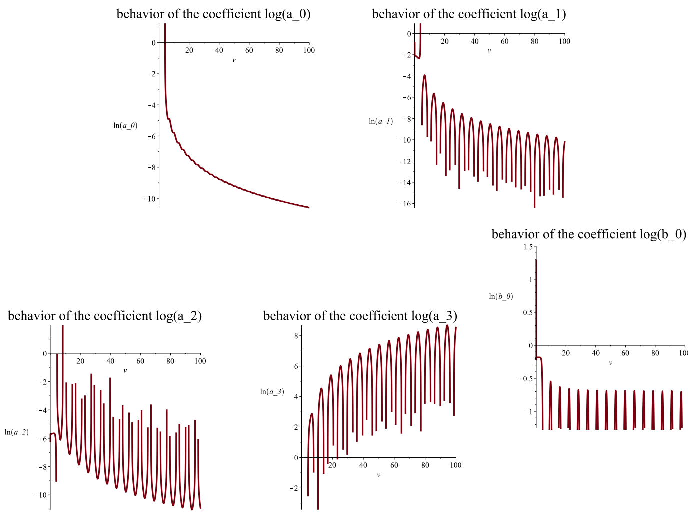

Figure 1: Behavior of the coefficients of the new proposed method given by (18) for several values of $v = \phi\, h$.

We present the new method (11) with the coefficients given by (18)–(19) with the symbol: $NM2SH4DV$. The local truncation error of this method is given by:

$$LTE_{NM2SH4DV} = -\frac{1}{47900160}\, h^{12} \left(2\, q_n^{(12)} + 9\, \phi^2\, q_n^{(10)} + 15\, \phi^4\, q_n^{(8)} + 10\phi^6\, q_n^{(6)} - 3\phi^{10}\, q_n^{(2)} - \phi^{12}\, q_n \right) + O\left(h^{14}\right). \quad (20)$$

4 Comparative error analysis

Our study on local truncation error analysis is based on the test problem:

$$q''(x) = \left(V(x) - V_c + G\right)\, q(x) \quad (21)$$

where

- $V(x)$ is a potential function,
- V_c a constant value approximation of the potential for the specific x,
- $G = V_c - E$ and
- E is the energy.

which is the radial Schrödinger equation with potential $V(x)$

We investigate the following methods :

4.1 Classical method (i.e., method (11) with constant coefficients)

$$LTE_{CL} = -\frac{1}{23950080}\, h^{12}\, q_n^{(12)} + O\left(h^{14}\right). \quad (22)$$

4.2 Method with vanished phase–lag and its first and second derivatives developed in [1]

$$LTE_{ExplTwoStepPC} = -\frac{1}{23950080}\, h^{12} \left(q_n^{(12)} + 3\, \phi^2\, q_n^{(10)} + 3\, \phi^4\, q_n^{(8)} + \phi^6\, q_n^{(6)} \right) + O\left(h^{14}\right). \quad (23)$$

4.3 Method with vanished phase–lag and its first, second and third derivatives developed in [2]

$$LTE_{NM2SH3DV} = -\frac{1}{95800320}\, h^{12} \left(4\, q_n^{(12)} + 15\, \phi^2\, q_n^{(10)} + 20\, \phi^4\, q_n^{(8)} - \phi^{10}\, q_n^{(2)} \right) + O\left(h^{14}\right). \tag{24}$$

4.4 Method with vanished phase–lag and its first, second, third and fourth derivatives developed in Section 3

$$\begin{aligned} LTE_{NM2SH4DV} &= -\frac{1}{47900160}\, h^{12} \Big(2\, q_n^{(12)} + 9\, \phi^2\, q_n^{(10)} + 15\, \phi^4\, q_n^{(8)} + 10\phi^6\, q_n^{(6)} \\ &- 3\phi^{10}\, q_n^{(2)} - \phi^{12}\, q_n \Big) + O\left(h^{14}\right). \end{aligned} \tag{25}$$

We use the following procedure

- Based on the formulae of the Local Truncation Errors given above and the test problem (21) which we use for our error analysis, it is necessary to compute the derivatives of the function described in the test problem . Some of the expressions of the above mentioned derivatives which are used in these calculations are presented in the Appendix B.
- The above calculated expressions of the derivatives (some of which are presented in the Appendix B), are substituted in the formulae of the Local Truncation Error. Consequently, the resulting formulae of the Local Truncation Errors are dependent from the quantity G and the energy E.
- We base our study on the two cases for the parameter G :
  1. **The Energy and the potential are closed each other.** Consequently $G = V_c - E \approx 0$ i.e., the value of the parameter G is approximately equal to zero. We note here that the general form of the Local Truncation Errors is given by:

$$LTE = h^{12} \sum_{k=0}^{j} B_k\, G^k \tag{26}$$

where B_k are constant numbers or polynomials of v and $G = V_c - E$.

Remark 6. *In the case $G = V_c - E \approx 0$, all the quantities in the expressions of the local truncation error with terms of several power of G are approximately equal to zero, i.e., $G^k = 0$, $k = 1, 2, 3, \cdots$.*

Remark 7. *In the case $G = V_c - E \approx 0$, only the terms of the expressions of the local truncation error for which the power to G is equal to zero (i.e., the terms of G^0) i.e., the terms which are free from G are considered. The reason is the previous remark.*

In the case $G = V_c - E \approx 0$ (free from G terms) the local truncation error for the classical method (constant coefficients), the local truncation error for the method with vanished the phase–lag and its first and second derivatives, the local truncation error for the method with vanished the phase–lag and its first, second and third derivatives and the local truncation error for the method with vanished the phase–lag and its first, second, third and fourth derivatives are the same since the expressions which are free from G in the local truncation errors in this case are the same. Therefore, for these values of G, the methods are of comparable accuracy.

2. **The Energy and the potential are far from each other.** Consequently $G >> 0$ or $G << 0$. Then $|G|$ is a large number. In these cases the best (more accurate) method is the method which has the minimum power of G in the expressions of the local truncation error.

- Finally the asymptotic expansions of the Local Truncation Errors are calculated.

The following asymptotic expansions of the Local Truncation Errors are produced, based on the above mentioned procedure :

4.5 Classical method

$$LTE_{CL} = -\frac{1}{23950080}\, h^{12} \left(q\left(x\right)\, G^6 + \cdots \right) + O\left(h^{14}\right). \tag{27}$$

4.6 Method with vanished phase–lag and its first and second derivatives developed in [1]

$$LTE_{ExplTwoStepPC} = -\frac{1}{5987520}\, h^{12} \left(\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g\left(x\right) \right) q\left(x\right)\, G^4 + \cdots \right) + O\left(h^{14}\right). \tag{28}$$

4.7 The new proposed method with vanished phase–lag and its first, second and third derivatives developed in [2]

$$LTE_{NM2SH3DV} = -\frac{1}{23950080}\, h^{12} \left[\left(15 \left(\frac{\mathrm{d}}{\mathrm{d}x} g\left(x\right) \right)^{2} q\left(x\right) + 20\, g\left(x\right)\, q\left(x\right)\, \frac{\mathrm{d}^2}{\mathrm{d}x^2} g\left(x\right) \right.\right.$$
$$\left.\left. +10 \left(\frac{\mathrm{d}^3}{\mathrm{d}x^3} g\left(x\right) \right) \frac{\mathrm{d}}{\mathrm{d}x} q\left(x\right) + 51 \left(\frac{\mathrm{d}^4}{\mathrm{d}x^4} g\left(x\right) \right) q\left(x\right) \right) G^3 + \cdots \right] + O\left(h^{14}\right). \quad (29)$$

4.8 The new proposed method with vanished phase–lag and its first, second, third and fourth derivatives developed in Section 3

$$LTE_{NM2SH4DV} = -\frac{1}{997920}\, h^{12} \left(\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4} g\left(x\right) q\left(x\right) \right) G^3 + \cdots \right) + O\left(h^{14}\right). \quad (30)$$

From the above mentioned analysis we have the following theorem:

Theorem 2.

- *Classical Method (i.e., the method (11) with constant coefficients): For this method the error increases as the sixth power of G.*
- *High Algebraic Order Two–Step Method with Vanished Phase–lag and its First and Second Derivatives developed in* [1]*: For this method the error increases as the fourth power of G.*
- *High Algebraic Order Two–Step Method with Vanished Phase–lag and its First, Second and Third Derivatives developed in* [2]*: For this method the error increases as the third power of G.*
- *High Algebraic Order Two–Step Method with Vanished Phase–lag and its First, Second, Third and Fourth Derivatives developed in Section 3: For this method the error increases as the third power of G but with much more simpler coefficient.*

So, for the approximate integration of the time independent radial Schrödinger equation the New Obtained High Algebraic Order Method with vanished phase–lag and its first, second, third and fourth derivatives is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

5 Stability analysis

In order to investigate the stability of the new developed method we use the scalar test equation:

$$q'' = -\omega^2 \, q \, . \tag{31}$$

Remark 8. *The frequency of the scalar test equation used for the stability analysis (ω) is different with the frequency of the scalar test equation of the phase–lag analysis (ϕ) – studied above – i.e., $\omega \neq \phi$.*

Application of the three stages symmetric two–step method developed in this paper to the scalar test equation (31) leads to the following difference equation:

$$A_1\,(s,v)\;\left(q_{n+1}+q_{n-1}\right)+A_0\,(s,v)\;q_n=0 \tag{32}$$

where

$$\begin{aligned} A_1\,(s,v) &= 1+b_1\,s^2+a_2\,b_0\,s^4-2\,a_0\,a_2\,b_0\,s^6 \\ A_0\,(s,v) &= -2+b_0\,s^2-2\,a_2\,b_0\,s^4+4\,a_2\,b_0\,s^6\;\left(a_0-a_1\right) \end{aligned} \tag{33}$$

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

Substituting the coefficients $b_1 = \frac{1}{12}$, a_i, $i = 0(1)3$ and b_0 given by (18) into the formulae (33) we obtain:

$$A_1\,(s,v)=\frac{1}{12}\,\frac{T_{13}}{T_{14}} \quad , \quad A_0\,(s,v) \;=\; -\frac{1}{18}\,\frac{T_{15}}{T_{14}} \tag{34}$$

where

$$\begin{aligned} T_{13} \;=\;& -4572\,\left(\cos\left(v\right)\right)^2 v^7+8352\,\cos\left(v\right)v^7+10080\,\sin\left(v\right)v^6 \\ -\;& 315\,s^2v^7+212\,s^4v^7-106\,s^2v^9-3150\,s^4v^5+6300\,s^4v^3-4\,s^6v^7+8\,s^4v^9 \\ -\;& 4\,s^2v^{11}-154\,s^6v^5+273\,s^6v^3+360\,s^6v+12\,\left(\cos\left(v\right)\right)^2 v^{11}-1116\,\left(\cos\left(v\right)\right)^2 v^9 \\ -\;& 96\,\cos\left(v\right)v^9-1728\,\sin\left(v\right)v^8+1440\,\sin\left(v\right)s^6-3780\,v^7+5\,\cos\left(v\right)\sin\left(v\right)s^6v^6 \\ -\;& 22\,\cos\left(v\right)\sin\left(v\right)s^4v^8+17\,\cos\left(v\right)\sin\left(v\right)s^2v^{10}+62\,\cos\left(v\right)\sin\left(v\right)s^6v^4 \\ -\;& 420\,\cos\left(v\right)\sin\left(v\right)s^4v^6-102\,\cos\left(v\right)\sin\left(v\right)s^2v^8-792\,\cos\left(v\right)\sin\left(v\right)s^6v^2 \\ -\;& 2520\,\cos\left(v\right)\sin\left(v\right)s^4v^4-840\,\cos\left(v\right)\sin\left(v\right)s^2v^6-10080\,\cos\left(v\right)\sin\left(v\right)v^6 \end{aligned}$$

$$
\begin{aligned}
& - && 1272\,v^9 - 48\,v^{11} + (\cos(v))^2\,s^6v^7 - 2\,(\cos(v))^2\,s^4v^9 + (\cos(v))^2\,s^2v^{11} \\
& + && 35\,(\cos(v))^2\,s^6v^5 - 2\,(\cos(v))^2\,s^4v^7 \\
& - && 93\,(\cos(v))^2\,s^2v^9 + 204\,\cos(v)\sin(v)\,v^{10} \\
& + && 8\,\cos(v)\,s^6v^5 - 8\,\cos(v)\,s^2v^9 + 639\,(\cos(v))^2\,s^6v^3 - 630\,(\cos(v))^2\,s^4v^5 \\
& - && 381\,(\cos(v))^2\,s^2v^7 + 16\,\sin(v)\,s^6v^4 - 144\,\sin(v)\,s^2v^8 - 1224\,\cos(v)\sin(v)\,v^8 \\
& + && 168\,\cos(v)\,s^6v^3 + 696\,\cos(v)\,s^2v^7 + 1080\,(\cos(v))^2\,s^6v - 6300\,(\cos(v))^2\,s^4v^3 \\
& - && 648\,\sin(v)\,s^6v^2 + 840\,\sin(v)\,s^2v^6 - 1440\,\cos(v)\sin(v)\,s^6 - 1440\,\cos(v)\,s^6v \\
T_{14} & = && v^6\Big((\cos(v))^2\,v^5 + 17\,\cos(v)\sin(v)\,v^4 \\
& - && 93\,(\cos(v))^2\,v^3 - 4\,v^5 - 102\,\cos(v)\sin(v)\,v^2 \\
& - && 8\,\cos(v)\,v^3 - 381\,(\cos(v))^2\,v - 144\,\sin(v)\,v^2 - 106\,v^3 \\
& - && 840\,\cos(v)\sin(v) + 696\,\cos(v)\,v + 840\,\sin(v) - 315\,v\Big) \\
T_{15} & = && 2916\,(\cos(v))^2\,v^7 + 8424\,(\cos(v))^3\,v^7 - 33480\,\cos(v)\,v^7 \\
& + && 10674\,s^2v^7 + 636\,s^4v^7 - 540\,s^2v^9 - 9450\,s^4v^5 + 18900\,s^4v^3 - 8\,s^6v^7 + 24\,s^4v^9 \\
& - && 24\,s^2v^{11} - 180\,s^6v^5 + 3510\,s^6v^3 - 7020\,s^6v - 66\,(\cos(v))^2\,v^{11} - 1062\,(\cos(v))^2\,v^9 \\
& - && 2538\,\cos(v)\,v^9 - 8640\,\sin(v)\,v^8 + 22140\,v^7 + 30\,\cos(v)\sin(v)\,s^6v^6 \\
& - && 66\,\cos(v)\sin(v)\,s^4v^8 + 42\,\cos(v)\sin(v)\,s^2v^{10} + 156\,\cos(v)\sin(v)\,s^6v^4 \\
& - && 1260\,\cos(v)\sin(v)\,s^4v^6 + 612\,\cos(v)\sin(v)\,s^2v^8 \\
& + && 2160\,\cos(v)\sin(v)\,s^6v^2 - 7560\,\cos(v)\sin(v)\,s^4v^4 \\
& - && 5040\,\cos(v)\sin(v)\,s^2v^6 + 30240\,\cos(v)\sin(v)\,v^6 \\
& - && 30240\,(\cos(v))^2\sin(v)\,v^6 - 4734\,v^9 + 84\,v^{11} + 2\,(\cos(v))^2\,s^6v^7 \\
& - && 6\,(\cos(v))^2\,s^4v^9 + 6\,(\cos(v))^2\,s^2v^{11} - 102\,(\cos(v))^2\,s^6v^5 \\
& - && 6\,(\cos(v))^2\,s^4v^7 + 174\,(\cos(v))^2\,s^2v^9 \\
& + && 108\,\cos(v)\sin(v)\,v^{10} + 654\,\cos(v)\,s^6v^5 - 2010\,\cos(v)\,s^2v^9 - 90\,(\cos(v))^2\,s^6v^3 \\
& - && 1890\,(\cos(v))^2\,s^4v^5 + 5346\,(\cos(v))^2\,s^2v^7 + 2340\,\sin(v)\,s^6v^4 - 324\,\sin(v)\,s^2v^8 \\
& + && 5832\,\cos(v)\sin(v)\,v^8 + 765\,\cos(v)\,s^6v^3 - 11619\,\cos(v)\,s^2v^7 + 2700\,(\cos(v))^2\,s^6v \\
& - && 18900\,(\cos(v))^2\,s^4v^3 - 6480\,\sin(v)\,s^6v^2 + 15120\,\sin(v)\,s^2v^6 + 4320\,\cos(v)\sin(v)\,s^6 \\
& + && 8100\,\cos(v)\,s^6v + 28\,\cos(v)\,v^{13} - 24\,\sin(v)\,v^{12} + 1068\,\cos(v)\,v^{11} - 2016\,\sin(v)\,v^{10} \\
& - && 34020\,s^2v^5 + 14\,\cos(v)\,s^6v^7 - 42\,\cos(v)\,s^2v^{11} + 60\,\sin(v)\,s^6v^6 - 36\,\sin(v)\,s^2v^{10}
\end{aligned}
$$

$$
\begin{aligned}
&+ \; 8\,v^{13} + 15\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)s^{6}v^{6} - 9\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)s^{2}v^{10} \\
&+ \; 114\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)s^{6}v^{4} - 378\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)s^{2}v^{8} \\
&- \; 10080\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)s^{2}v^{6} - 945\,\left(\cos\left(v\right)\right)^{3}s^{6}v^{3} \\
&- \; 4401\,\left(\cos\left(v\right)\right)^{3}s^{2}v^{7} - 6048\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)v^{8} - 3780\,\left(\cos\left(v\right)\right)^{3}s^{6}v \\
&- \; 34020\,\left(\cos\left(v\right)\right)^{3}s^{2}v^{5} - 4320\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)s^{6} + 34020\,\left(\cos\left(v\right)\right)^{2}s^{2}v^{5} \\
&+ \; 34020\,\cos\left(v\right)s^{2}v^{5} - 3\,\left(\cos\left(v\right)\right)^{3}s^{2}v^{11} - 6\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)v^{12} \\
&- \; 57\,\left(\cos\left(v\right)\right)^{3}s^{6}v^{5} - 189\,\left(\cos\left(v\right)\right)^{3}s^{2}v^{9} - 6\,\cos\left(v\right)\sin\left(v\right)v^{12} \\
&- \; 504\,\left(\cos\left(v\right)\right)^{2}\sin\left(v\right)v^{10} + 882\,\left(\cos\left(v\right)\right)^{3}v^{9} + 2\,\left(\cos\left(v\right)\right)^{3}v^{13} \\
&- \; 2\,\left(\cos\left(v\right)\right)^{2}v^{13} + 102\,\left(\cos\left(v\right)\right)^{3}v^{11} + \left(\cos\left(v\right)\right)^{3}s^{6}v^{7}\,.
\end{aligned}
$$

Definition 5. *(see [9]) We call a multistep method P-stable if its interval of periodicity is equal to $(0,\infty)$.*

Definition 6. *We call a multistep method singularly almost P-stable if its interval of periodicity is equal to $(0,\infty) - S$ [2]. We use the term singularly almost P-stable method only in the cases when the frequency of the scalar test equation for the phase–lag analysis is equal with the frequency of the scalar test equation for the stability analysis, i.e., $\omega = \phi$.*

The $s - v$ plane for the method obtained in this paper is shown in Figure 2.

Remark 9. *Investigating the $s - v$ region we observe two areas:*

- *The shadowed area denotes where the method is stable,*
- *The white area denotes the region where the method is unstable.*

Remark 10. *The observation of* **the surroundings of the first diagonal of the $s - v$ plane** *is requested in the cases of problems for which the models require only one frequency per differential equation in the specific model. This is because in these cases the frequency of the scalar test equation used for the phase–lag analysis is equal with the frequency of the scalar test equation used for the stability analysis. One can find many problems in Sciences, Engineering and Technology for which their mathematical models are of the form described above. (for example the time independent Schrödinger equation and the coupled equations arising from the Schrödinger equation).*

[2] where S is a set of distinct points

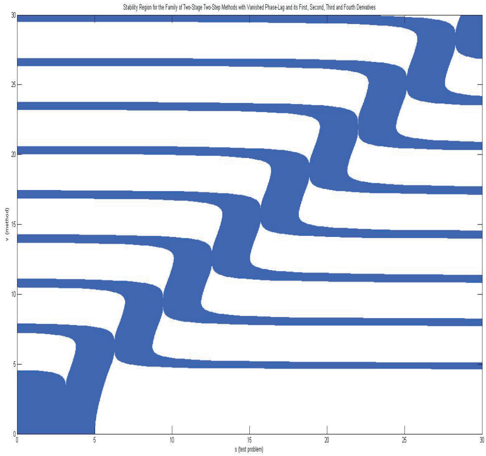

Figure 2: $s-v$ plane of the new obtained symmetric three stages two–step tenth algebraic order method with vanished phase–lag and its first, second, third and fourth derivatives.

Based on the above remark, we study the case where the frequency of the scalar test equation used for the stability analysis is equal with the frequency of the scalar test equation used for the phase–lag analysis , i.e., we investigate the case where $s = v$ (i.e., on the the $s - v$ plane see the surroundings of the first diagonal). Based on the above mentioned study we found that the interval of periodicity in the case $s = v$ is equal to: $(0, 21)$.

Based on the above we have the following theorem:

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

- *is of three stages*
- *is of tenth algebraic order,*
- *has the phase–lag and its first, second, third and fourth derivatives equal to zero*
- *has an interval of periodicity equals to:* $(0, 21)$, *when the frequency of the scalar test equation used for the phase–lag analysis is equal with the frequency of the scalar test equation used for the stability analysis*

6 Numerical results

In this section we will investigate the efficiency of the new obtained method by applying it on two problems :

1. the numerical solution of the radial time–independent Schrödinger equation and
2. the numerical solution of coupled differential equations of the Schrödinger type

6.1 Radial time–independent Schrödinger equation

The radial time independent Schrödinger equation can be written as :

$$q''(r) = [l(l+1)/r^2 + V(r) - k^2]\, q(r). \tag{35}$$

where

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

For the boundary value problems (like our problem (35)) it is necessary the boundary conditions to be defined. The initial value i.e. the condition on the initial point of integration gives the first boundary condition :

$$q(0) = 0$$

while the second boundary condition (at the end of the integration) is obtained , for large values of r, and is defined by physical considerations.

Since the new developed method has coefficients which are frequency dependent, it is necessary to define the parameter ϕ of the coefficients of the new obtained method ($v = \phi\, h$) in order to be possible to determine the coefficients. The parameter ϕ for the radial Schrödinger equation and for the case $l = 0$ is given by :

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

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

6.1.1 Woods–Saxon potential

For our numerical tests the well known Woods-Saxon potential is used. The Wood-Saxon potential can be written as :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{36}$$

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

The behavior of the Woods–Saxon potential is presented in Figure 3.

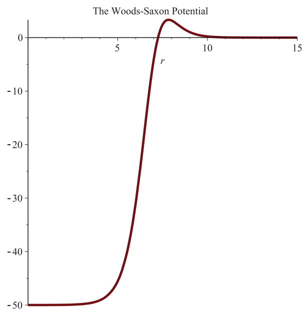

Figure 3: The Woods-Saxon potential.

Following the methodology proposed by Ixaru et al. ([13] [15]), we approximate the potential in some critical points. These approximations define the value of the parameter ϕ.

We choose ϕ as follows (see for details [14] and [15]) :

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

For example, on the point of the integration region $r = 6.5 - h$, the value of ϕ is equal to: $\sqrt{-37.5+E}$. Therefore, $w = \phi\, h = \sqrt{-37.5+E}\, h$. On the point of the integration region $r = 6.5 - 3\,h$, the value of ϕ is equal to: $\sqrt{-50+E}$, etc.

6.1.2 Radial Schrödinger equation – the resonance problem

The numerical solution of the one–dimensional time independent Schrödinger equation (35) with the Woods-Saxon potential (36) consists of our first numerical test .

The above described problem has an infinite interval of integration i.e., its interval of integration is equal to $r \in \Big(0, \infty\Big)$. Therefore, in order to be solved numerically, it is necessary to be approximated with a finite one. Consequently, the integration interval $r \in [0, 15]$ is used for our numerical test . For our test the domain of energies : $E \in [1, 1000]$ is also used .

Since in our problem for the case of positive energies, $E = k^2$, the potential decays faster than the term $\frac{l(l+1)}{r^2}$ for radius r greater than some value R , the radial Schrödinger equation effectively reduces to:

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{37}$$

In the above mentioned model (37) the reduced differential equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Consequently, the solution of equation (35) (when $r \to \infty$), has the asymptotic form

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

where δ_l is the phase shift. We note here that the phase shift can be calculated from the formula

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

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. As we mentioned above in our numerical test, the problem is treated as an initial–value problem, and therefore we need q_j , $j = 0, 1$ before starting a two-step method. The value q_0 is obtained from the initial condition . The value q_1 is obtained by using high order Runge–Kutta–Nyström methods (see [16] and [17]). With these starting (initial) values, we evaluate at r_2 of the asymptotic region the phase shift δ_l.

In the case of positive energies the problem described above is called resonance problem . This problem is expressed by two forms :

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

We actually solve the latter problem, known as **the resonance problem**.

The boundary conditions for this problem are:

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

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

- the eighth order multi–step method developed by Quinlan and Tremaine [18], which is indicated as **Method QT8**;
- the tenth order multi–step method developed by Quinlan and Tremaine [18], which is indicated as **Method QT10**;
- the twelfth order multi–step method developed by Quinlan and Tremaine [18], which is indicated as **Method QT12**;
- the fourth algebraic order method of Chawla and Rao with minimal phase–lag [19], which is indicated as **Method MCR4**;
- the exponentially–fitted method of Raptis and Allison [20], which is indicated as **Method MRA** ;
- the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase–lag [21], which is indicated as **Method MCR6**;
- the Phase-Fitted Method (Case 1) developed in [8], which is indicated as **Method NMPF1**;
- the Phase-Fitted Method (Case 2) developed in [8], which is indicated as **Method NMPF2**;
- the Method developed in [22] (Case 2), which is indicated as **Method NMC2**;
- the method developed in [22] (Case 1), which is indicated as **Method NMC1**;

- the Two-Step Hybrid Method developed in [1], which is indicated as **Method NM2SH2DV**;
- the new obtained Two–Step Runge–Kutta type method developed in [2], which is indicated as **Method NM2SH3DV**;
- the new obtained Three Stages Two–Step method developed in Section 3, which is indicated as **Method NM2SH4DV**

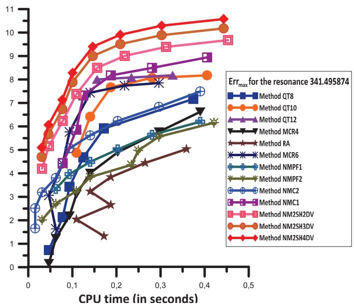

Figure 4: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

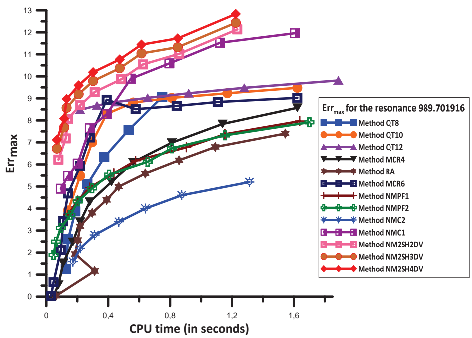

Figure 5: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

Using the well known two-step method of Chawla and Rao [21] with small step size for the integration, we compute the reference values . The procedure which we follow consists of the numerical computation of the eigenenergies and after that the comparison of the numerically computed eigenenergies with the reference values. In Figures 4 and 5, we present the maximum absolute error $Err_{max} = |\log_{10}(Err)|$ where

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

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of CPU time (in seconds). We note that the CPU time (in seconds) counts the computational cost for each method.

6.1.3 Remarks on the numerical results for the radial Schrödinger equation

Based on the numerical results given above, we have the following:

1. The tenth algebraic order multistep method developed by Quinlan and Tremaine [18], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase–lag [19], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [18], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase–lag [21], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.

2. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [18], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [18], which is indicated as **Method QT10**

3. The Phase-Fitted Method (Case 1) developed in [8], which is indicated as **Method NMPF1** is more efficient than the exponentially-fitted method of Raptis and Allison [20] and the Phase-Fitted Method (Case 2) developed in [8], which is indicated as **Method NMPF2**

4. The Method developed in [22] (Case 2), which is indicated as **Method NMC2** is more efficient than the exponentially-fitted method of Raptis and Allison [20], which

is indicated as **Method MRA** and the Phase-Fitted Method (Case 2) developed in [8], which is indicated as **Method NMPF2** and the Phase-Fitted Method (Case 1) developed in [8], which is indicated as **Method NMPF1**

5. The Method developed in [22] (Case 1), which is indicated as **Method NMC1**, is more efficient than all the other methods mentioned above.

6. The Two-Step Hybrid Method developed in [1] , which is indicated as **Method NM2SH2DV**, is more efficient than all the other methods mentioned above.

7. The Two-Step Runge–Kutta type Method developed in in [2], which is indicated as **Method NM2SH3DV**, is more efficient than all the above mentioned methods.

8. Finally, the new Three–Stages Tenth Algebraic Order Method developed in Section 3, which is indicated as **Method NM2SH4DV**, is the most efficient one.

6.2 Error estimation

The variable–step schemes are based on the estimation of the local truncation error (LTE) . In the literature one can find several methodologies and several algorithms of variable–step form for the numerical integration of systems of differential equations which have been developed the last decades (see for example [8]– [65]).

The variable step algorithm which we develop in this paper is based on:

- an embedded pair of multistep methods with a local error estimation technique and

- the fact that with the maximum possible algebraic order of a method we obtain better approximate solution for the problems with oscillatory or periodical solution.

We use as lower order solution y_{n+1}^{L}, for the purpose of local error estimation, the method developed in [65] - which is of eight algebraic order and has vanished the phase-lag and its first, second, third and fourth derivatives. As higher order solution y_{n+1}^{H} we use the method obtained in the present paper - which is of tenth algebraic order has vanished the phase-lag and its first, second, third and fourth derivatives. Now, the local truncation error in y_{n+1}^{L} is estimated by

$$LTE = \left| y_{n+1}^{H} - y_{n+1}^{L} \right| .$$

The estimated step size for the $(n+1)^{st}$ step, for a required local error of acc, for a step size used for the n^{th} step equal to h_n and for which would give a local error equal to acc, is given by

$$h_{n+1} = h_n \left(\frac{acc}{LTE}\right)^{\frac{1}{p}}$$

where p is the algebraic order of the method.

The lower order solution y_{n+1}^L is the basis of our local truncation error estimate . However , in our numerical tests we apply the widely used procedure of performing local extrapolation, for a requirement of an error estimate less than acc. Thus, although the lower order solution y_{n+1}^L is used for the control of the estimation of the local error , it is the higher order solution y_{n+1}^H which is accepted at each point.

6.3 Coupled differential equations

In many problems within quantum chemistry, material science, theoretical physics, atomic physics, physical chemistry and chemical physics, etc. one can find models which consist of coupled differential equations of the Schrödinger type.

We write the close-coupling differential equations of the Schrödinger type with the form:

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

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

In this paper we will investigate the case in which all channels are open. Consequently, the following boundary conditions are hold (see for details [23]):

$$q_{ij} = 0 \;\; at \;\; x = 0$$

$$q_{ij} \sim k_i\, x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}\, k_i\, x\, n_{li}(k_i x) \tag{38}$$

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

Remark 11. *The new developed method can also be used in case of problems involving closed channels.*

Defining a matrix K' and diagonal matrices M, N by (see for detailed analysis in [23]):

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

$$N_{ij} \;\; = \;\; k_i x n_{l_i}(k_i x)\delta_{ij}$$

we find that the asymptotic condition (38) can be written as:

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

The rotational excitation of a diatomic molecule by neutral particle impact is an important real problem in quantum chemistry, theoretical physics, material science, atomic physics and molecular physics with its model to be expressed with close–coupling differential equations of the Schrödinger type. The entrance channel is denoted (see for details in [23]) by the quantum numbers (j, l), the exit channels by (j', l'), and the total angular momentum by $J = j + l = j' + l'$. Based on the above notations we find that

$$\left[\frac{d^2}{dx^2} + k^2_{j'j} - \frac{l'(l'+1)}{x^2}\right] q^{Jjl}_{j'l'}(x) = \frac{2\mu}{\hbar^2}\sum_{j''}\sum_{l''} < j'l'; J \mid V \mid j''l''; J > q^{Jjl}_{j''l''}(x)$$

where

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

E is the kinetic energy of the incident particle in the center-of-mass system, I is the moment of inertia of the rotator, and μ is the reduced mass of the system.

The potential V is given by (see for details [23]):

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

and consequently, the coupling matrix element may then be written as

$$< j'l'; J \mid V \mid j''l''; J >= \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x)$$

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [24] 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 [25]). The boundary conditions are given by

$$q^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \tag{39}$$

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

where the relation of scattering S matrix with K matrix of (38) is given by

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

The algorithm which is used for the computation of the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles consists of the numerical method for step-by-step integration from the initial value to matching points . The method used in our numerical tests is based on an analogous algorithm which has been developed for the numerical tests of [23].

For our numerical experiments we choose the **S** matrix which is calculated using the following parameters

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

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

As is described in [23], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of **four, nine and sixteen coupled differential equations**, respectively. Following the procedure obtained by Bernstein [25] and Allison [23] the potential is considered infinite for values of x less than some x_0. The wave functions then zero in this region and effectively the boundary condition (39) may be written as

$$q_{j'l'}^{Jjl}(x_0) = 0 \,.$$

For the numerical solution of the above described problem we have used the following methods:

- the Iterative Numerov method of Allison [23] which is indicated as **Method I**[3],
- the variable-step method of Raptis and Cash [26] which is indicated as **Method II**,
- the embedded Runge–Kutta Dormand and Prince method 5(4) [17] which is indicated as **Method III**,
- the embedded Runge–Kutta method ERK4(2) developed in Simos [27] which is indicated as **Method IV**,
- the embedded two-step method developed in [1] which is indicated as **Method V**,

[3] We note here that Iterative Numerov method developed by Allison [23] is one of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation

- the embedded two-step method developed in [2] which is indicated as **Method VI** .
- the new developed embedded two-step method which is indicated as **Method VII** .

The real time of computation required by the methods mentioned above in order to calculate the square of the modulus of the **S** matrix for sets of 4, 9 and 16 coupled differential equations is presented in Table 1 . The maximum error in the calculation of the square of the modulus of the **S** matrix is also presented . In Table 1 N indicates the number of equations of the set of coupled differential equations.

Table 1: **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.

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}

7 Conclusions

A family of tenth algebraic order two-step methods is investigated in this paper. More specifically, we investigated:

- the development of the method using the methodology of vanishing of the phase–lag and its first, second, third and fourth derivatives,
- the comparative local truncation error analysis,
- the stability (interval of periodicity) analysis and
- the computational efficiency of the new produced method on the numerical solution of the radial Schrödinger equation and of the coupled Schrödinger equations (which are of high importance for chemistry).

From the theoretical analysis and numerical results given above, it is easy to see the efficiency of the new obtained method for the numerical solution of the radial Schrödinger equation and of the coupled Schrödinger equations.

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

Appendix A: Formulae for the Derivatives of T_j, $j = 0(1)3$

$$\begin{aligned}
T_0 &= 2\left(1 + v^2\left(1/12 + b_0\,a_2\,v^2\left(-2\,a_0\,v^2 + 1\right)\right)\right)\cos(v) + a_3 \\
&+ v^2\,b_0\left(1 + a_2\,v^2\left(4\,a_0\,v^2 - 4\,a_1\,v^2 - 2\right)\right) \\
T_1 &= -576\,\sin(v)\,v^{12}\,{a_0}^2\,{a_2}^2\,{b_0}^2 + 576\,\sin(v)\,v^{10}\,a_0\,{a_2}^2\,{b_0}^2 \\
&- 576\,v^9\,a_1\,{a_2}^2\,{b_0}^2 - 144\,\sin(v)\,v^8\,{a_2}^2\,{b_0}^2 + 48\,\sin(v)\,v^8\,a_0\,a_2\,b_0 \\
&+ 576\,v^7 a_0\,a_2\,{b_0}^2 + 576\,\sin(v)\,v^6\,a_0\,a_2\,b_0 + 96\,v^7\,a_0\,a_2\,b_0 \\
&- 96\,v^7\,a_1\,a_2\,b_0 - 24\,\sin(v)\,v^6\,a_2\,b_0 + 864\,v^5 a_0\,a_2\,a_3\,b_0 \\
&+ 1728\,v^5\,a_0\,a_2\,b_0 - 1728\,v^5\,a_1\,a_2\,b_0 - 144\,v^5\,a_2\,{b_0}^2 \\
&- 288\,\sin(v)\,v^4\,b_0\,a_2 - 24\,v^5 a_2\,b_0 - 288\,v^3\,a_2\,a_3\,b_0 \\
&- \sin(v)\,v^4 - 576\,b_0\,a_2\,v^3 - 24\,\sin(v)\,v^2 - 12\,v\,a_3 + 144\,v\,b_0 - 144\,\sin(v)
\end{aligned}$$

$$\begin{aligned}
T_2 &= \cos(v)\,v^6 + 36\,\cos(v)\,v^4 + 432\,\cos(v)\,v^2 + 1728\,\cos(v) - 36\,v^2\,a_3 + 20736\,b_0\,a_2\,v^2 \\
&- 10368\,\cos(v)\,v^6\,a_0\,a_2\,b_0 - 1728\,\cos(v)\,v^8\,a_0\,a_2\,b_0 - 72\,\cos(v)\,v^{10}\,a_0\,a_2\,b_0 \\
&- 20736\,\cos(v)\,v^{10}\,a_0\,{a_2}^2\,{b_0}^2 - 1728\,\cos(v)\,v^{12}\,a_0\,{a_2}^2\,{b_0}^2 \\
&+ 20736\,\cos(v)\,v^{12}\,{a_0}^2\,{a_2}^2\,{b_0}^2 + 1728\,\cos(v)\,v^{14}\,{a_0}^2\,{a_2}^2\,{b_0}^2 \\
&- 10368\,\cos(v)\,v^{14}\,a_0\,{a_2}^3\,{b_0}^3 + 20736\,\cos(v)\,v^{16}\,{a_0}^2\,{a_2}^3\,{b_0}^3 \\
&- 13824\,\cos(v)\,v^{18}\,{a_0}^3\,{a_2}^3\,{b_0}^3 - 51840\,v^4\,a_0\,a_2\,a_3\,b_0 \\
&+ 2304\,v^6\,a_0\,a_2\,a_3\,b_0 + 93312\,v^8\,a_0\,{a_2}^2\,a_3\,{b_0}^2 \\
&+ 290304\,v^{10}\,a_0\,a_1\,{a_2}^2\,{b_0}^2 - 145152\,v^{10}\,{a_0}^2\,{a_2}^2\,a_3\,{b_0}^2 \\
&+ 11520\,v^{12}\,a_0\,a_1\,{a_2}^2\,{b_0}^2 + 41472\,v^{14}\,a_0\,a_1\,{a_2}^3\,{b_0}^3 \\
&+ 432\,v^2\,b_0 + 1728\,v^{10}\,a_1\,{a_2}^2\,{b_0}^2 + 31104\,v^{10}\,a_0\,{a_2}^2\,{b_0}^3 \\
&- 290304\,v^{10}\,{a_0}^2\,{a_2}^2\,{b_0}^2 + 6912\,v^{12}\,a_1\,{a_2}^3\,{b_0}^3 \\
&+ 103680\,v^4\,a_1\,a_2\,b_0 - 69120\,v^{12}\,{a_0}^2\,{a_2}^2\,{b_0}^3 \\
&+ 5184\,\cos(v)\,v^4\,b_0\,a_2 + 864\,\cos(v)\,v^6\,a_2\,b_0 + 36\,\cos(v)\,v^8\,a_2\,b_0 \\
&+ 5184\,\cos(v)\,v^8\,{a_2}^2\,{b_0}^2 + 1728\,\cos(v)\,v^{12}\,{a_2}^3\,{b_0}^3 + 432\,\cos(v)\,v^{10}\,{a_2}^2\,{b_0}^2 \\
&+ 10368\,v^2\,a_2\,a_3\,b_0 - 1296\,v^4\,a_2\,a_3\,b_0 + 288\,v^8\,a_1\,a_2\,b_0 \\
&- 17280\,v^6\,{a_2}^2\,a_3\,{b_0}^2 - 1728\,v^8\,a_0\,a_2\,{b_0}^2 + 186624\,v^8\,a_0\,{a_2}^2\,{b_0}^2 \\
&- 86400\,v^6\,a_0\,a_2\,{b_0}^2 + 9792\,v^6\,a_1\,a_2\,b_0 - 11520\,v^{12}\,{a_0}^2\,{a_2}^2\,{b_0}^2 \\
&+ 5184\,v^{10}\,a_0\,{a_2}^2\,{b_0}^2 - 288\,v^8\,a_0\,a_2\,b_0 - 103680\,v^4\,a_0\,a_2\,b_0 \\
&- 9792\,v^6\,a_0\,a_2\,b_0 + 20736\,v^4\,a_2\,{b_0}^2 - 864\,v^8\,{a_2}^2\,{b_0}^2 \\
&+ 24\,v^6\,a_2\,b_0 + 144\,v^6\,a_2\,{b_0}^2 - 34560\,v^6\,{a_2}^2\,{b_0}^2 - 5184\,v^8\,{a_2}^2\,{b_0}^3 \\
&+ 864\,v^4\,a_2\,b_0 + 144\,a_3 - 1728\,b_0 \\
T_3 &= 864\,\sin(v)\,v^4 + 6912\,\sin(v)\,v^2 + 48\,\sin(v)\,v^6 + \sin(v)\,v^8 \\
&+ 20736\,\sin(v) - 41472\,\sin(v)\,v^8\,a_0\,a_2\,b_0 \\
&- 165888\,\sin(v)\,v^6\,a_0\,a_2\,b_0 + 497664\,\sin(v)\,v^{12}\,{a_0}^2\,{a_2}^2\,{b_0}^2 \\
&- 497664\,\sin(v)\,v^{10}\,a_0\,{a_2}^2\,{b_0}^2 - 331776\,v^5\,a_0\,a_2\,a_3\,b_0 \\
&+ 497664\,\sin(v)\,v^{20}\,{a_0}^2\,{a_2}^4\,{b_0}^4 - 663552\,\sin(v)\,v^{22}\,{a_0}^3\,{a_2}^4\,{b_0}^4 \\
&+ 331776\,\sin(v)\,v^{24}\,{a_0}^4\,{a_2}^4\,{b_0}^4 + 576\,v^9\,a_0\,a_2\,b_0 \\
&+ 3456\,v^9\,a_0\,a_2\,{b_0}^2 + 331776\,v^{13}\,a_0\,{a_2}^3\,{b_0}^3 + 829440\,v^{13}\,{a_0}^2\,{a_2}^2\,{b_0}^3
\end{aligned}$$

$$- \; 51757056\, v^{13}\, {a_0}^2\, {a_2}^3\, {b_0}^3 + 1990656\, v^{13}\, a_0\, {a_2}^3\, {b_0}^4$$
$$- \; 995328\, v^{15}\, {a_0}^2\, {a_2}^3\, {b_0}^3 - 5971968\, v^{15}\, {a_0}^2\, {a_2}^3\, {b_0}^4$$
$$+ \; 1658880\, v^{17}\, {a_0}^3\, {a_2}^3\, {b_0}^3 + 55738368\, v^{15}\, {a_0}^3\, {a_2}^3\, {b_0}^3$$
$$+ \; 5640192\, v^{11}\, {a_0}^2\, {a_2}^2\, {b_0}^2 - 995328\, v^{11}\, a_1\, {a_2}^3\, {b_0}^3$$
$$+ \; 18911232\, v^{11}\, a_0\, {a_2}^3\, {b_0}^3 + 34836480\, v^{11}\, {a_0}^2\, {a_2}^2\, {b_0}^3$$
$$+ \; 138240\, v^{13}\, {a_0}^2\, {a_2}^2\, {b_0}^2 - 248832\, v a_2\, a_3\, b_0$$
$$- \; 55296\, \sin{(v)}\, v^{20}\, {a_0}^3\, {a_2}^3\, {b_0}^3 + 9953280\, v^{17}\, {a_0}^3\, {a_2}^3\, {b_0}^4$$
$$+ \; 13824\, v^7\, a_0\, a_2\, a_3\, b_0 - 248832\, v^{11}\, a_0\, {a_2}^2\, {b_0}^3$$
$$- \; 41472\, v^{11}\, a_0\, {a_2}^2\, {b_0}^2 + 6912\, v^{11}\, a_1\, {a_2}^2\, {b_0}^2$$
$$+ \; 1728\, v a_3 - 20736\, v\, b_0 + 82944\, \sin{(v)}\, v^{14}\, {a_0}^2\, {a_2}^2\, {b_0}^2 - 497664\, \sin{(v)}\, v^{14}\, a_0\, {a_2}^3\, {b_0}^3$$
$$+ \; 3456\, \sin{(v)}\, v^{16}\, {a_0}^2\, {a_2}^2\, {b_0}^2 + 1728\, \sin{(v)}\, v^8\, a_2\, b_0$$
$$+ \; 48\, \sin{(v)}\, v^{10}\, a_2\, b_0 + 20736\, \sin{(v)}\, v^{10}\, {a_2}^2\, {b_0}^2 + 864\, \sin{(v)}\, v^{12}\, {a_2}^2\, {b_0}^2$$
$$- \; 82944\, v^{11}\, {a_0}^2\, {a_2}^2\, a_3\, {b_0}^2 - 4976640\, v^3\, a_1\, a_2\, b_0$$
$$+ \; 9455616\, v^{11}\, a_0\, {a_2}^3\, a_3\, {b_0}^3 - 138240\, v^{13}\, a_0\, a_1\, {a_2}^2\, {b_0}^2$$
$$- \; 25878528\, v^{13}\, {a_0}^2\, {a_2}^3\, a_3\, {b_0}^3 - 663552\, v^{15}\, a_0\, a_1\, {a_2}^3\, {b_0}^3$$
$$- \; 55738368\, v^{15}\, {a_0}^2\, a_1\, {a_2}^3\, {b_0}^3 + 27869184\, v^{15}\, {a_0}^3\, {a_2}^3\, a_3\, {b_0}^3$$
$$- \; 576\, v^9\, a_1\, a_2\, b_0 - 35831808\, v^7\, a_0\, {a_2}^2\, {b_0}^2 + 9953280\, v^7\, a_1\, {a_2}^2\, {b_0}^2$$
$$- \; 124416\, v^7\, {a_2}^2\, a_3\, {b_0}^2 - 5640192\, v^{11}\, a_0\, a_1\, {a_2}^2\, {b_0}^2$$
$$+ \; 34836480\, v^9\, {a_0}^2\, {a_2}^2\, a_3\, {b_0}^2 + 2488320\, v^5\, {a_2}^2\, a_3\, {b_0}^2$$
$$+ \; 6967296\, v^5\, a_0\, a_2\, {b_0}^2 - 6912\, v^5\, a_2\, a_3\, b_0 + 20736\, \sin{(v)}\, v^{16}\, {a_2}^4\, {b_0}^4$$
$$- \; 69672960\, v^9\, a_0\, a_1\, {a_2}^2\, {b_0}^2 + 414720\, v^9\, a_0\, {a_2}^2\, a_3\, {b_0}^2$$
$$- \; 41472\, \sin{(v)}\, v^{16}\, a_0\, {a_2}^3\, {b_0}^3 - 1990656\, v^9\, a_0\, {a_2}^2\, {b_0}^2$$
$$- \; 16920576\, v^9\, a_0\, {a_2}^2\, {b_0}^3 + 69672960\, v^9\, {a_0}^2\, {a_2}^2\, {b_0}^2$$
$$- \; 1244160\, v^9\, {a_2}^3\, a_3\, {b_0}^3 - 17915904\, v^7\, a_0\, {a_2}^2\, a_3\, {b_0}^2$$
$$+ \; 6912\, \sin{(v)}\, v^{14}\, {a_2}^3\, {b_0}^3 + 82944\, \sin{(v)}\, v^{12}\, {a_2}^3\, {b_0}^3$$
$$+ \; 995328\, \sin{(v)}\, v^{16}\, {a_0}^2\, {a_2}^3\, {b_0}^3 + 82944\, \sin{(v)}\, v^{18}\, {a_0}^2\, {a_2}^3\, {b_0}^3$$
$$- \; 165888\, \sin{(v)}\, v^{18}\, a_0\, {a_2}^4\, {b_0}^4 - 663552\, \sin{(v)}\, v^{18}\, {a_0}^3\, {a_2}^3\, {b_0}^3$$
$$+ \; 2488320\, v^3\, a_0\, a_2\, a_3\, b_0 - 1658880\, v^{17}\, {a_0}^2\, a_1\, {a_2}^3\, {b_0}^3$$

$$
\begin{aligned}
& - \ 1990656\,v^{17}\,a_0\,a_1\,{a_2}^4\,{b_0}^4 + 1728\,v^3\,b_0 - 144\,v^3\,a_3 \\
& - \ 3981312\,v^{19}\,{a_0}^2\,a_1\,{a_2}^4\,{b_0}^4 - 3456\,\sin(v)\,v^{10}\,a_0\,a_2\,b_0 \\
& - \ 96\,\sin(v)\,v^{12}\,a_0\,a_2\,b_0 - 82944\,\sin(v)\,v^{12}\,a_0\,{a_2}^2\,{b_0}^2 \\
& - \ 3456\,\sin(v)\,v^{14}\,a_0\,{a_2}^2\,{b_0}^2 + 124416\,\sin(v)\,v^8\,{a_2}^2\,{b_0}^2 \\
& + \ 20736\,\sin(v)\,v^6\,a_2\,b_0 + 82944\,\sin(v)\,v^4\,b_0\,a_2 + 497664\,v^9\,a_1\,{a_2}^2\,{b_0}^2 \\
& + \ 27648\,v^7\,a_0\,a_2\,b_0 - 27648\,v^7\,a_1\,a_2\,b_0 + 124416\,v^3\,a_2\,a_3\,b_0 \\
& + \ 4976640\,b_0\,a_2\,v^3\,a_0 + 497664\,v^5\,a_0\,a_2\,b_0 - 497664\,v^5\,a_1\,a_2\,b_0 \\
& + \ 3456\,v^9\,{a_2}^2\,{b_0}^2 + 2488320\,v^7\,{a_2}^2\,{b_0}^3 + 4976640\,v^5\,{a_2}^2\,{b_0}^2 \\
& + \ 20736\,v^9\,{a_2}^2\,{b_0}^3 - 41472\,v^{11}\,{a_2}^3\,{b_0}^3 - 248832\,v^{11}\,{a_2}^3\,{b_0}^4 \\
& - \ 1244160\,v^3\,a_2\,{b_0}^2 - 2488320\,v^9\,{a_2}^3\,{b_0}^3 + 82944\,v^5\,a_2\,{b_0}^2 \\
& + \ 165888\,v^7\,{a_2}^2\,{b_0}^2 - 497664\,b_0\,a_2 v + 41472\,b_0\,a_2\,v^3 \\
T_4 & = \ -1440\,\cos(v)\,v^6 - 17280\,\cos(v)\,v^4 - 103680\,\cos(v)\,v^2 - 248832\,\cos(v) \\
& + \ 34560\,v^8\,a_1\,a_2\,b_0 + 44789760\,v^{12}\,a_1\,{a_2}^3\,{b_0}^3 + 17280\,v^2\,a_3 + 37324800\,v^6\,{a_2}^2\,a_3\,{b_0}^2 \\
& - \ 414720\,\cos(v)\,v^6\,a_2\,b_0 + 1170505728\,v^{20}\,{a_0}^3\,{a_2}^4\,{b_0}^5 \\
& - \ 12039487488\,v^{20}\,{a_0}^4\,{a_2}^4\,{b_0}^4 - 1244160\,\cos(v)\,v^4\,b_0\,a_2 \\
& - \ 1672151040\,v^{22}\,{a_0}^4\,{a_2}^4\,{b_0}^5 - 278691840\,v^{22}\,{a_0}^4\,{a_2}^4\,{b_0}^4 \\
& - \ 6220800\,v^2\,a_2\,a_3\,b_0 - 4396032\,v^{10}\,a_1\,{a_2}^2\,{b_0}^2 \\
& - \ 622080\,\cos(v)\,v^{10}\,{a_2}^2\,{b_0}^2 - 2488320\,\cos(v)\,v^{12}\,{a_2}^3\,{b_0}^3 \\
& - \ 51840\,\cos(v)\,v^8\,a_2\,b_0 - 829440\,v^6\,a_0\,a_2\,b_0 - 207360\,\cos(v)\,v^{16}\,{a_0}^2\,{a_2}^2\,{b_0}^2 \\
& + \ 5971968\,b_0\,a_2 + 5760\,\cos(v)\,v^{16}\,a_0\,{a_2}^2\,{b_0}^2 - 8635465728\,v^{10}\,a_0\,{a_2}^3\,{b_0}^3 \\
& - \ 2488320\,\cos(v)\,v^8\,{a_2}^2\,{b_0}^2 - 4317732864\,v^{10}\,a_0\,{a_2}^3\,a_3\,{b_0}^3 \\
& - \ 597196800\,v^{18}\,{a_0}^2\,{a_2}^4\,{b_0}^5 + 11943936\,v^{10}\,a_0\,{a_2}^2\,{b_0}^3 \\
& + \ 14332723200\,v^{18}\,{a_0}^3\,{a_2}^4\,{b_0}^4 + 195084288\,v^{20}\,{a_0}^3\,{a_2}^4\,{b_0}^4 \\
& - \ 418037760\,v^4\,a_0\,a_2\,{b_0}^2 + 223948800\,v^8\,a_0\,{a_2}^2\,{b_0}^2 \\
& - \ 1244160\,v^8\,a_0\,a_2\,{b_0}^2 + 120\,\cos(v)\,v^{14}\,a_0\,a_2\,b_0 + 207360\,\cos(v)\,v^{14}\,a_0\,{a_2}^2\,{b_0}^2 \\
& - \ 233902080\,v^{12}\,{a_0}^2\,{a_2}^2\,{b_0}^3 + 4976640\,v^4\,a_1\,a_2\,b_0 \\
& + \ 1347840\,v^4\,a_2\,a_3\,b_0 - 60\,\cos(v)\,v^8 + 2985984\,a_2\,a_3\,b_0 \\
& - \ 403107840\,v^6\,{a_2}^2\,{b_0}^3 + 25878528\,v^{10}\,{a_2}^3\,{b_0}^3 - 20736\,v^{10}\,{a_2}^2\,{b_0}^3
\end{aligned}
$$

$$+ \quad 301584384\, v^{10}\, {a_2}^3\, {b_0}^4 - 5391360\, v^{12}\, {a_0}^2\, {a_2}^2\, a_3\, {b_0}^2$$
$$+ \quad 2488320\, v^{12}\, {a_2}^3\, {b_0}^4 - 209018880\, v^{12}\, {a_2}^4\, {b_0}^4 - 2488320\, v^{14}\, {a_2}^4\, {b_0}^4$$
$$- \quad 14929920\, v^{14}\, {a_2}^4\, {b_0}^5 + 7464960\, v^6\, {a_2}^2\, {b_0}^2 + 518400\, v^6\, a_2\, {b_0}^2$$
$$- \quad \cos(v)\, v^{10} + 11197440\, v^8\, {a_2}^2\, {b_0}^3 + 4230144\, v^{10}\, a_0\, {a_2}^2\, a_3\, {b_0}^2$$
$$+ \quad 19906560\, \cos(v)\, v^{26}\, {a_0}^3\, {a_2}^5\, {b_0}^5 - 207360\, v^8\, {a_2}^2\, {b_0}^2$$
$$- \quad 14929920\, v^4\, a_2\, {b_0}^2 - 4976640\, b_0\, a_2\, v^2 - 1658880\, \cos(v)\, v^{26}\, {a_0}^4\, {a_2}^4\, {b_0}^4$$
$$+ \quad 138240\, \cos(v)\, v^{22}\, {a_0}^3\, {a_2}^3\, {b_0}^3 + 7962624\, \cos(v)\, v^{30}\, {a_0}^5\, {a_2}^5\, {b_0}^5$$
$$- \quad 29859840\, \cos(v)\, v^{20}\, {a_0}^2\, {a_2}^4\, {b_0}^4 - 5016453120\, v^8\, {a_0}^2\, {a_2}^2\, a_3\, {b_0}^2$$
$$- \quad 19906560\, \cos(v)\, v^{28}\, {a_0}^4\, {a_2}^5\, {b_0}^5 - 1041113088\, v^{10}\, {a_0}^2\, {a_2}^2\, {b_0}^2$$
$$+ \quad 179159040\, v^2\, a_1\, a_2\, b_0 + 8640\, v^4\, b_0 - 207360\, v^2\, b_0 - 2488320\, \cos(v)\, v^{22}\, {a_0}^2\, {a_2}^4\, {b_0}^4$$
$$+ \quad 2488320\, \cos(v)\, v^{22}\, a_0\, {a_2}^5\, {b_0}^5 + 39813120\, \cos(v)\, v^{22}\, {a_0}^3\, {a_2}^4\, {b_0}^4$$
$$+ \quad 3317760\, \cos(v)\, v^{24}\, {a_0}^3\, {a_2}^4\, {b_0}^4 - 9953280\, \cos(v)\, v^{24}\, {a_0}^2\, {a_2}^5\, {b_0}^5$$
$$- \quad 19906560\, \cos(v)\, v^{24}\, {a_0}^4\, {a_2}^4\, {b_0}^4 - 169205760\, v^8\, a_0\, {a_2}^2\, a_3\, {b_0}^2$$
$$+ \quad 1041113088\, v^{10}\, a_0\, a_1\, {a_2}^2\, {b_0}^2 + 127401984\, v^{10}\, {a_0}^2\, {a_2}^2\, a_3\, {b_0}^2$$
$$+ \quad 49766400\, v^{12}\, a_0\, a_1\, {a_2}^2\, {b_0}^2 - 398131200\, v^{14}\, a_0\, a_1\, {a_2}^3\, {b_0}^3$$
$$- \quad 34560\, v^8\, a_0\, a_2\, b_0 + 32348160\, v^6\, a_0\, a_2\, {b_0}^2 - 179159040\, b_0\, a_2\, v^2\, a_0$$
$$+ \quad 829440\, v^6\, a_1\, a_2\, b_0 - 49766400\, v^{12}\, {a_0}^2\, {a_2}^2\, {b_0}^2$$
$$+ \quad 10450944\, v^{10}\, a_0\, {a_2}^2\, {b_0}^2 - 4976640\, v^4\, a_0\, a_2\, b_0$$
$$- \quad 720\, v^4\, a_3 - 194088960\, v^4\, {a_2}^2\, a_3\, {b_0}^2 - 43200\, v^6\, a_2\, a_3\, b_0$$
$$- \quad 1612431360\, v^6\, a_1\, {a_2}^2\, {b_0}^2 - 1036800\, v^8\, {a_2}^2\, a_3\, {b_0}^2$$
$$- \quad 109486080\, v^8\, a_1\, {a_2}^2\, {b_0}^2 + 576\, v^{10}\, a_1\, a_2\, b_0$$
$$+ \quad 3374161920\, v^8\, a_0\, {a_2}^2\, {b_0}^3 - 3456\, v^{10}\, a_0\, a_2\, {b_0}^2$$
$$+ \quad 462827520\, v^8\, {a_2}^3\, a_3\, {b_0}^3 - 12192768\, v^{10}\, {a_2}^3\, a_3\, {b_0}^3$$
$$+ \quad 1206337536\, v^{10}\, a_1\, {a_2}^3\, {b_0}^3 - 7775502336\, v^{10}\, {a_0}^2\, {a_2}^2\, {b_0}^3$$
$$+ \quad 248832\, b_0 - 20736\, a_3 - 3881779200\, v^{16}\, {a_0}^2\, {a_2}^4\, a_3\, {b_0}^4$$
$$+ \quad 716636160\, v^{16}\, a_0\, a_1\, {a_2}^4\, {b_0}^4 - 169205760\, v^{16}\, {a_0}^3\, {a_2}^3\, a_3\, {b_0}^3$$
$$+ \quad 5760\, \cos(v)\, v^{12}\, a_0\, a_2\, b_0 + 57231360\, v^{12}\, a_0\, {a_2}^3\, a_3\, {b_0}^3$$
$$- \quad 9913466880\, v^{12}\, a_0\, a_1\, {a_2}^3\, {b_0}^3 + 898560\, v^{14}\, a_0\, a_1\, {a_2}^2\, {b_0}^2$$

$$+ \quad 14273003520\, v^{12}\, a_0{}^2\, a_2{}^3\, a_3\, b_0{}^3 + 2030469120\, v^6\, a_0\, a_2{}^2\, a_3\, b_0{}^2$$
$$+ \quad 86400\, v^8\, a_0\, a_2\, a_3\, b_0 + 10032906240\, v^8\, a_0\, a_1\, a_2{}^2\, b_0{}^2$$
$$- \quad 89579520\, v^2\, a_0\, a_2\, a_3\, b_0 - 24883200\, v^{14}\, a_0{}^2\, a_2{}^3\, a_3\, b_0{}^3$$
$$+ \quad 35115171840\, v^{14}\, a_0{}^2\, a_1\, a_2{}^3\, b_0{}^3 + 1015234560\, v^{14}\, a_0\, a_2{}^4\, a_3\, b_0{}^4$$
$$+ \quad 207360\, v^4\, a_2\, b_0 - 17557585920\, v^{14}\, a_0{}^3\, a_2{}^3\, a_3\, b_0{}^3$$
$$- \quad 207360\, \cos(v)\, v^{20}\, a_0{}^2\, a_2{}^3\, b_0{}^3 + 829440\, \cos(v)\, v^{20}\, a_0\, a_2{}^4\, b_0{}^4$$
$$+ \quad 3317760\, \cos(v)\, v^{20}\, a_0{}^3\, a_2{}^3\, b_0{}^3 - 2880\, \cos(v)\, v^{10}\, a_2\, b_0$$
$$- \quad 60\, \cos(v)\, v^{12}\, a_2\, b_0 - 51840\, \cos(v)\, v^{12}\, a_2{}^2\, b_0{}^2 - 1440\, \cos(v)\, v^{14}\, a_2{}^2\, b_0{}^2$$
$$- \quad 414720\, \cos(v)\, v^{14}\, a_2{}^3\, b_0{}^3 - 17280\, \cos(v)\, v^{16}\, a_2{}^3\, b_0{}^3$$
$$- \quad 1244160\, \cos(v)\, v^{16}\, a_2{}^4\, b_0{}^4 - 103680\, \cos(v)\, v^{18}\, a_2{}^4\, b_0{}^4$$
$$- \quad 248832\, \cos(v)\, v^{20}\, a_2{}^5\, b_0{}^5 + 44789760\, v^2\, a_2\, b_0{}^2 + 414720\, v^{12}\, a_2{}^3\, b_0{}^3$$
$$+ \quad 2488320\, \cos(v)\, v^6\, a_0\, a_2\, b_0 + 829440\, \cos(v)\, v^8\, a_0\, a_2\, b_0$$
$$+ \quad 103680\, \cos(v)\, v^{10}\, a_0\, a_2\, b_0 + 9953280\, \cos(v)\, v^{10}\, a_0\, a_2{}^2\, b_0{}^2$$
$$+ \quad 2488320\, \cos(v)\, v^{12}\, a_0\, a_2{}^2\, b_0{}^2 - 9953280\, \cos(v)\, v^{12}\, a_0{}^2\, a_2{}^2\, b_0{}^2$$
$$- \quad 2488320\, \cos(v)\, v^{14}\, a_0{}^2\, a_2{}^2\, b_0{}^2 + 14929920\, \cos(v)\, v^{14}\, a_0\, a_2{}^3\, b_0{}^3$$
$$- \quad 29859840\, \cos(v)\, v^{16}\, a_0{}^2\, a_2{}^3\, b_0{}^3 + 19906560\, \cos(v)\, v^{18}\, a_0{}^3\, a_2{}^3\, b_0{}^3$$
$$+ \quad 32348160\, v^4\, a_0\, a_2\, a_3\, b_0 - 388177920\, v^4\, a_2{}^2\, b_0{}^2$$
$$- \quad 3456\, v^{10}\, a_2{}^2\, b_0{}^2 - 3110400\, v^6\, a_0\, a_2\, a_3\, b_0 + 2488320\, \cos(v)\, v^{16}\, a_0\, a_2{}^3\, b_0{}^3$$
$$+ \quad 9953280\, \cos(v)\, v^{18}\, a_0\, a_2{}^4\, b_0{}^4 - 4976640\, \cos(v)\, v^{18}\, a_0{}^2\, a_2{}^3\, b_0{}^3$$
$$+ \quad 103680\, \cos(v)\, v^{18}\, a_0\, a_2{}^3\, b_0{}^3 + 24883200\, v^{16}\, a_0{}^2\, a_2{}^3\, b_0{}^3$$
$$- \quad 5391360\, v^{14}\, a_0\, a_2{}^3\, b_0{}^3 - 898560\, v^{14}\, a_0{}^2\, a_2{}^2\, b_0{}^2$$
$$+ \quad 172800\, v^{12}\, a_0\, a_2{}^2\, b_0{}^2 - 576\, v^{10}\, a_0\, a_2\, b_0 - 2488320\, v^{16}\, a_0\, a_1\, a_2{}^3\, b_0{}^3$$
$$+ \quad 2488320000\, v^{16}\, a_0{}^2\, a_1\, a_2{}^3\, b_0{}^3 + 149299200\, v^{16}\, a_0{}^2\, a_2{}^3\, b_0{}^4$$
$$+ \quad 24883200\, v^{16}\, a_0\, a_2{}^4\, b_0{}^4 + 9256550400\, v^{14}\, a_0{}^2\, a_2{}^3\, b_0{}^4$$
$$+ \quad 2030469120\, v^{14}\, a_0\, a_2{}^4\, b_0{}^4 - 59719680\, v^{14}\, a_1\, a_2{}^4\, b_0{}^4$$
$$+ \quad 1492992000\, v^{14}\, a_0{}^2\, a_2{}^3\, b_0{}^3 - 5760\, \cos(v)\, v^{18}\, a_0{}^2\, a_2{}^2\, b_0{}^2$$
$$+ \quad 477757440\, v^{24}\, a_0{}^3\, a_1\, a_2{}^5\, b_0{}^5 + 477757440\, v^{22}\, a_0{}^2\, a_1\, a_2{}^5\, b_0{}^5$$
$$+ \quad 278691840\, v^{22}\, a_0{}^3\, a_1\, a_2{}^4\, b_0{}^4 - 6019743744\, v^{20}\, a_0{}^4\, a_2{}^4\, a_3\, b_0{}^4$$

$$
\begin{aligned}
&+ \; 12039487488\, v^{20}\, {a_0}^3\, a_1\, {a_2}^4\, {b_0}^4 + 23887872\, v^{20}\, a_0\, a_1\, {a_2}^5\, {b_0}^5 \\
&+ \; 207028224\, v^{20}\, {a_0}^2\, a_1\, {a_2}^4\, {b_0}^4 + 7166361600\, v^{18}\, {a_0}^3\, {a_2}^4\, a_3\, {b_0}^4 \\
&+ \; 238878720\, v^{18}\, {a_0}^2\, a_1\, {a_2}^4\, {b_0}^4 + 9953280\, v^{18}\, a_0\, a_1\, {a_2}^4\, {b_0}^4 \\
&+ \; 51425280\, v^{18}\, {a_0}^2\, a_1\, {a_2}^3\, {b_0}^3 - 2488320000\, v^{16}\, {a_0}^3\, {a_2}^3\, {b_0}^3 \\
&+ \; 149299200\, v^{16}\, a_0\, {a_2}^4\, {b_0}^5 - 7763558400\, v^{16}\, {a_0}^2\, {a_2}^4\, {b_0}^4 \\
&- \; 12899450880\, v^{16}\, {a_0}^3\, {a_2}^3\, {b_0}^4 - 99532800\, v^{18}\, {a_0}^2\, {a_2}^4\, {b_0}^4 \\
&- \; 308551680\, v^{18}\, {a_0}^3\, {a_2}^3\, {b_0}^4 + 925655040\, v^{8}\, {a_2}^3\, {b_0}^3 \\
&+ \; 28546007040\, v^{12}\, {a_0}^2\, {a_2}^3\, {b_0}^3 - 35115171840\, v^{14}\, {a_0}^3\, {a_2}^3\, {b_0}^3 \\
&+ \; 4060938240\, v^{6}\, a_0\, {a_2}^2\, {b_0}^2 - 10032906240\, v^{8}\, {a_0}^2\, {a_2}^2\, {b_0}^2 \\
&- \; 51425280\, v^{18}\, {a_0}^3\, {a_2}^3\, {b_0}^3 + 414720\, v^{14}\, a_1\, {a_2}^3\, {b_0}^3 \\
&- \; 5391360\, v^{14}\, {a_0}^2\, {a_2}^2\, {b_0}^3 - 32348160\, v^{14}\, a_0\, {a_2}^3\, {b_0}^4 \\
&- \; 69120\, v^{12}\, a_1\, {a_2}^2\, {b_0}^2 + 1036800\, v^{12}\, a_0\, {a_2}^2\, {b_0}^3 \\
&- \; 343388160\, v^{12}\, a_0\, {a_2}^3\, {b_0}^3 - 2747105280\, v^{12}\, a_0\, {a_2}^3\, {b_0}^4 \\
&- \; 104509440\, v^{12}\, {a_2}^4\, a_3\, {b_0}^4\, .
\end{aligned}
$$

Appendix B: Formulae for the Derivatives of p_n

Formulae of the derivatives which presented in the formulae of the Local Truncation Errors:

$$
\begin{aligned}
q_n^{(2)} &= (V(x) - V_c + G)\; q(x) \\
q_n^{(3)} &= \left(\frac{d}{dx} g\,(x)\right) q\,(x) + (g\,(x) + G)\, \frac{d}{dx} q\,(x) \\
q_n^{(4)} &= \left(\frac{d^2}{dx^2} g\,(x)\right) q\,(x) + 2\, \left(\frac{d}{dx} g\,(x)\right) \frac{d}{dx} q\,(x) + (g\,(x) + G)^2\, q\,(x) \\
q_n^{(5)} &= \left(\frac{d^3}{dx^3} g\,(x)\right) q\,(x) + 3\, \left(\frac{d^2}{dx^2} g\,(x)\right) \frac{d}{dx} q\,(x) \\
&+ \; 4\,(g\,(x) + G)\, q\,(x)\, \frac{d}{dx} g\,(x) + (g\,(x) + G)^2\, \frac{d}{dx} q\,(x) \\
q_n^{(6)} &= \left(\frac{d^4}{dx^4} g\,(x)\right) q\,(x) + 4\, \left(\frac{d^3}{dx^3} g\,(x)\right) \frac{d}{dx} q\,(x)
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad 7\left(g\left(x\right)+G\right)q\left(x\right)\frac{d^2}{dx^2}g\left(x\right)+4\left(\frac{d}{dx}g\left(x\right)\right)^2 q\left(x\right) \\
&+ \quad 6\left(g\left(x\right)+G\right)\left(\frac{d}{dx}q\left(x\right)\right)\frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^3 q\left(x\right) \\
q_n^{(7)} &= \quad \left(\frac{d^5}{dx^5}g\left(x\right)\right)q\left(x\right)+5\left(\frac{d^4}{dx^4}g\left(x\right)\right)\frac{d}{dx}q\left(x\right) \\
&+ \quad 11\left(g\left(x\right)+G\right)q\left(x\right)\frac{d^3}{dx^3}g\left(x\right)+15\left(\frac{d}{dx}g\left(x\right)\right)q\left(x\right) \\
&+ \quad \frac{d^2}{dx^2}g\left(x\right)+13\left(g\left(x\right)+G\right)\left(\frac{d}{dx}q\left(x\right)\right)\frac{d^2}{dx^2}g\left(x\right) \\
&+ \quad 10\left(\frac{d}{dx}g\left(x\right)\right)^2\frac{d}{dx}q\left(x\right)+9\left(g\left(x\right)+G\right)^2 q\left(x\right) \\
&+ \quad \frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^3\frac{d}{dx}q\left(x\right) \\
q_n^{(8)} &= \quad \left(\frac{d^6}{dx^6}g\left(x\right)\right)q\left(x\right)+6\left(\frac{d^5}{dx^5}g\left(x\right)\right)\frac{d}{dx}q\left(x\right) \\
&+ \quad 16\left(g\left(x\right)+G\right)q\left(x\right)\frac{d^4}{dx^4}g\left(x\right)+26\left(\frac{d}{dx}g\left(x\right)\right)q\left(x\right) \\
&+ \quad \frac{d^3}{dx^3}g\left(x\right)+24\left(g\left(x\right)+G\right)\left(\frac{d}{dx}q\left(x\right)\right)\frac{d^3}{dx^3}g\left(x\right) \\
&+ \quad 15\left(\frac{d^2}{dx^2}g\left(x\right)\right)^2 q\left(x\right)+48\left(\frac{d}{dx}g\left(x\right)\right) \\
&+ \quad \left(\frac{d}{dx}q\left(x\right)\right)\frac{d^2}{dx^2}g\left(x\right)+22\left(g\left(x\right)+G\right)^2 q\left(x\right) \\
&+ \quad \frac{d^2}{dx^2}g\left(x\right)+28\left(g\left(x\right)+G\right)q\left(x\right)\left(\frac{d}{dx}g\left(x\right)\right)^2 \\
&+ \quad 12\left(g\left(x\right)+G\right)^2\left(\frac{d}{dx}q\left(x\right)\right)\frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^4 q\left(x\right) \\
&\ldots
\end{aligned}
$$

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