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# A New Algorithm for the Approximation of the Schrödinger Equation

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**Abstract:** In this paper a four stages twelfth algebraic order symmetric two-step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives is developed for the first time in the literature. For the new proposed method: (1) we will study the phase-lag analysis, (2) we will present the development of the new method, (3) the local truncation error (LTE) analysis will be studied. The analysis is based on a test problem which is the radial time independent Schrödinger equation, (4) the stability and the interval of periodicity analysis will be presented, (5) stepsize control technique will also be presented, (6) the examination of the accuracy and computational cost of the proposed algorithm which is based on the approximation of the Schrödinger equation.

**Keywords:** Phase-lag and its derivatives; two step methods; Schrödinger equation

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## 1 Introduction

A new algorithm for the solution of the special second order problems:

$$\varphi''(x) = \zeta(x, \varphi), \quad \varphi(x_0) = \varphi_0 \;\; and \;\; \varphi'(x_0) = \varphi_0' \tag{1}$$

is produced in this paper. Emphasis will be given on the problems (1) for which the solution behaves with periodical or/and oscillating form

The structure of the paper is:

– The basic theory for the construction of the new algorithm is given in Section 2.
– In Section 3 the new algorithm is constructed.
– The behavior of the error of the algorithm is shown in Section 4 using the Schrödinger equation as model problem.
– The stability analysis of the algorithm is shown in Section 5.
– In Section 6 the solution of a system of Schrödinger type equations is shown.
– Finally, in Section 7 we present remarks and conclusions .

## 2 Phase-lag and Stability Analysis of General Symmetric 2 *k*-Step Methods

We will present in this section the basic points of the phase-lag and the stability analysis of the general symmetric multistep algorithms. We consider the 2 $k$-Step algorithms:

$$\sum_{i=-k}^{k} \gamma_i \, \varphi_{n+i} = h^2 \sum_{i=-k}^{k} \delta_i \, \zeta(x_{n+i}, \varphi_{n+i}) \tag{2}$$

for approximation of (1) on the domain $[\alpha, \beta]$. The domain is determined by the user taking into account the properties of the application. The 2 $k$-step algorithm (2) is applied to the problem (1) by dividing the domain $[\alpha, \beta]$ into 2 $k$ areas of the same size i.e. $\{x_i\}_{i=-k}^{k} \in [\alpha, \beta]$. $h$ denotes the step length of the approximation procedure and is given by:

$$h = |x_{i+1} - x_i|, \; i = 1 - k(1)k - 1. \tag{3}$$

We have the following definitions:

**Definition 1.** *If for the algorithm (2) applies:*

$$\gamma_{-i} = \gamma_i, \; i = 0(1)k$$
$$\delta_{-i} = \delta_i, \; i = 0(1)k$$

*then we have a symmetric* 2 *k-step algorithm*

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**Remark 1.** *The operator:*

$$L(x) = \sum_{i=-k}^{k} \gamma_i \, \varphi(x + i\,h) - h^2 \sum_{i=-k}^{k} \delta_i \, \varphi''(x + ih) \tag{4}$$

*is related with the algorithm (2), where $y \in C^2$.*

**Definition 2.** [1] We call the algorithm (2) is of algebraic order $p$, if the operator $L$ determined by (4) eliminates for every possible combination of linear form of the functions $1,\, x,\, x^2,\, \ldots,\, x^{p+1}$.

In order to determine the stability polynomials for the specific algorithm (2) it is necessary to apply it to the problem

$$\varphi'' = -\phi^2 \, \varphi. \tag{5}$$

Then we achieve the following difference equation:

$$A_k(v)\,\varphi_{n+k} + \ldots + A_1(v)\,\varphi_{n+1} + A_0(v)\,\varphi_n + A_1(v)\,\varphi_{n-1} + \ldots + A_k(v)\,\varphi_{n-k} = 0 \tag{6}$$

For the above equation we have that:

- $v = \phi\, h$,
- $h$ is the stepsize and
- $A_j(v)\, j = 0(1)m$ are the stability polynomials for the specific algorithm and for the problem (5).

An equation which is related with (6) is:

$$A_k(v)\,\sigma^k + \ldots + A_1(v)\,\sigma + A_0(v) + A_1(v)\,\sigma^{-1} + \ldots + A_k(v)\,\sigma^{-k} = 0. \tag{7}$$

which is known as the characteristic equation of the algorithm for the problem (5).

**Definition 3.** [6] *If for the algorithm (2) we have the following roots $\sigma_i,\ i = 1(1)2\,k$ of its related equation (7) for all $v \in (0, v_0^2)$,:*

$$\sigma_1 = e^{i\theta(v)},\ \sigma_2 = e^{-i\theta(v)},\ and\ |\sigma_i| \le 1,\ i = 3(1)2\,k \tag{8}$$

*then we say that the algorithm (2) has an non empty interval of periodicity $(0, v_0^2)$. In the formula (8) $\theta(v)$ denotes a real function of $v$.*

**Definition 4.** *(see [6]) If the interval of periodicity of an algorithm (2) is computed as $(0, \infty)$, then we call this algorithm P-stable.*

**Definition 5.** *If the interval of periodicity of an algorithm (2) is computed as $(0, \infty)\backslash S$ [1], then we call the algorithm singularly P-stable.*

**1** where $S$ is a set of distinct points

**Definition 6.** [4], [5] *We call phase-lag of an algorithm (2) with the related characteristic equation (7) the dominant term of the expression*

$$\tau = v - \theta(v). \tag{9}$$

*The phase-lag is equal to $t$, if the relation $\tau = O(v^{t+1})$ as $v \to \infty$ is hold.*

**Definition 7.** *[2] If for an algorithm (2) the phase-lag is zero, then this algorithm is called* **phase-fitted***.*

**Theorem 1.** [4] *In order to compute the order of the phase-lag $t$ and the constant of the phase-lag $c$ for an algorithm (2) with the related equation (7), we use the direct formula:*

$$-\,c v^{t+2} + O(v^{t+4}) = \frac{2\,A_k(v)\,\cos(k\,v) + \ldots + 2\,A_j(v)\,\cos(j\,v) + \ldots + A_0(v)}{2\,k^2\,A_k(v) + \ldots + 2\,j^2\,A_j(v) + \ldots + 2\,A_1(v)} \tag{10}$$

## 3 The New Algorithm

We will examine the algorithm:

$$\begin{aligned}
\widehat{\varphi}_n &= \varphi_n - a_0\,h^2\left(\zeta_{n+1} - 2\,\zeta_n + \zeta_{n-1}\right) - 2a_1\,h^2\,\zeta_n \\
\widehat{\varphi}_{n+\frac{1}{2}} &= \frac{1}{2}\left(\varphi_n + \varphi_{n+1}\right) - h^2\left[a_2\,\widehat{\zeta}_n + \left(\frac{1}{8} - a_2\right)\zeta_{n+1}\right] \\
\widehat{\varphi}_{n-\frac{1}{2}} &= \frac{1}{2}\left(\varphi_n + \varphi_{n-1}\right) - h^2\left[a_2\,\widehat{\zeta}_n + \left(\frac{1}{8} - a_2\right)\zeta_{n-1}\right] \\
\varphi_{n+1} + a_3\,\varphi_n + \varphi_{n-1} &= h^2\Bigg[b_1\,(\zeta_{n+1} + \zeta_{n-1}) \\
&\quad + b_0\,\zeta_n + b_2\left(\widehat{\zeta}_{n+\frac{1}{2}} + \widehat{\zeta}_{n-\frac{1}{2}}\right)\Bigg]
\end{aligned} \tag{11}$$

where $\zeta_i = \varphi''(x_i, \varphi_i),\, i = -1\left(1\right)1$ and $a_\iota,\ \iota = 0(1)3$ $b_\lambda\,\lambda = 0(1)2$ are real numbers or functions of $v$, $\widehat{\zeta}_{n\pm\frac{1}{2}} = \varphi''\left(x_{n\pm\frac{1}{2}}, \widehat{\varphi}_{n\pm\frac{1}{2}}\right)$, $\widehat{\zeta}_n = \varphi''\left(x_n, \widehat{\varphi}_n\right)$ and

$$a_0 = -\frac{127}{2150064} \tag{12}$$

Application of the method (11) to the scalar test equation (5) leads to the difference equation given by (6) with:

$$\begin{aligned}
A_1(v) &= 1 + v^2\Bigg(b_1 + b_2\Bigg(\frac{1}{2} \\
&\quad + v^2\left(-\frac{127\,a_2 v^2}{2150064} + \frac{1}{8} - a_2\right) - \frac{127\,v^4 a_2}{2150064}\Bigg)\Bigg) \\
A_0(v) &= a_3 + v^2\Big(b_0 + b_2\Big(1
\end{aligned}$$

$$+ 2 v^2 a_2 \left(1 + \frac{127 v^2}{1075032} + 2 a_1 v^2\right)\bigg)\bigg) \quad (13)$$

The request of elimination of the phase-lag and phase-lag's derivatives leads us to the following system of equations:

$$\text{Phase} - \text{Lag(PL)} = \frac{T_0}{T_{denom}} = 0 \quad (14)$$

$$\text{First Derivative of the Phase} - \text{Lag} = \frac{\partial PL}{\partial v} = 0 \quad (15)$$

$$\text{Second Derivative of the Phase} - \text{Lag} = \frac{\partial^2 PL}{\partial^2 v} = 0 \quad (16)$$

$$\text{Third Derivative of the Phase} - \text{Lag} = \frac{\partial^3 PL}{\partial^3 v} = 0 \quad (17)$$

$$\text{Fourth Derivative of the Phase} - \text{Lag} = \frac{\partial^4 PL}{\partial^4 v} = 0 \quad (18)$$

$$\text{Fifth Derivative of the Phase} - \text{Lag} = \frac{\partial^5 PL}{\partial^5 v} = 0 \quad (19)$$

where

$$\begin{aligned}
T_0 = {} & \left(-1075032 + 127 v^6 b_2 a_2 + 1075032 \left(a_2 - \frac{1}{8}\right)\right. \\
& \left. \cdot b_2 v^4 + (-1075032\, b_1 - 537516\, b_2) v^2\right) \cos(v) \\
& - 2150064 \left(a_1 + \frac{127}{2150064}\right) a_2 b_2 v^6 \\
& - 1075032\, b_2 v^4 a_2 + (-537516\, b_0 - 537516\, b_2) v^2 \\
& - 537516\, a_3 \\
T_{denom} = {} & -1075032 + 127 v^6 b_2 a_2 + 1075032 \\
& \left(a_2 - \frac{1}{8}\right) b_2 v^4 + (-1075032\, b_1 - 537516\, b_2) v^2
\end{aligned}$$

The solution of the above equations gives us the following parameters of the algorithm: $b_0$, $b_1$, $b_2$, $a_1$, $a_2$ and $a_3$:

$$\begin{aligned}
b_0 &= 12 \frac{T_1}{T_{denom1}}, \quad & b_1 &= -3 \frac{T_2}{T_{denom1}}, \\
b_2 &= 24 \frac{T_3}{T_{denom1}}, \quad & a_1 &= \frac{T_4}{T_{denom2}}, \\
a_2 &= 44793 \frac{T_5}{T_{denom3}}, \quad & a_3 &= -8 \frac{T_6}{T_{denom4}}
\end{aligned} \quad (20)$$

where $T_j$, $j = 1(1)6$, $T_{denom1}$, $T_{denom2}$, $T_{denom3}$ and $T_{denom4}$ are determined in Supplement Material A.

The avoidance of impossibility of definition of the parameters determined in (20) achieved via the the Taylor series expression given below:

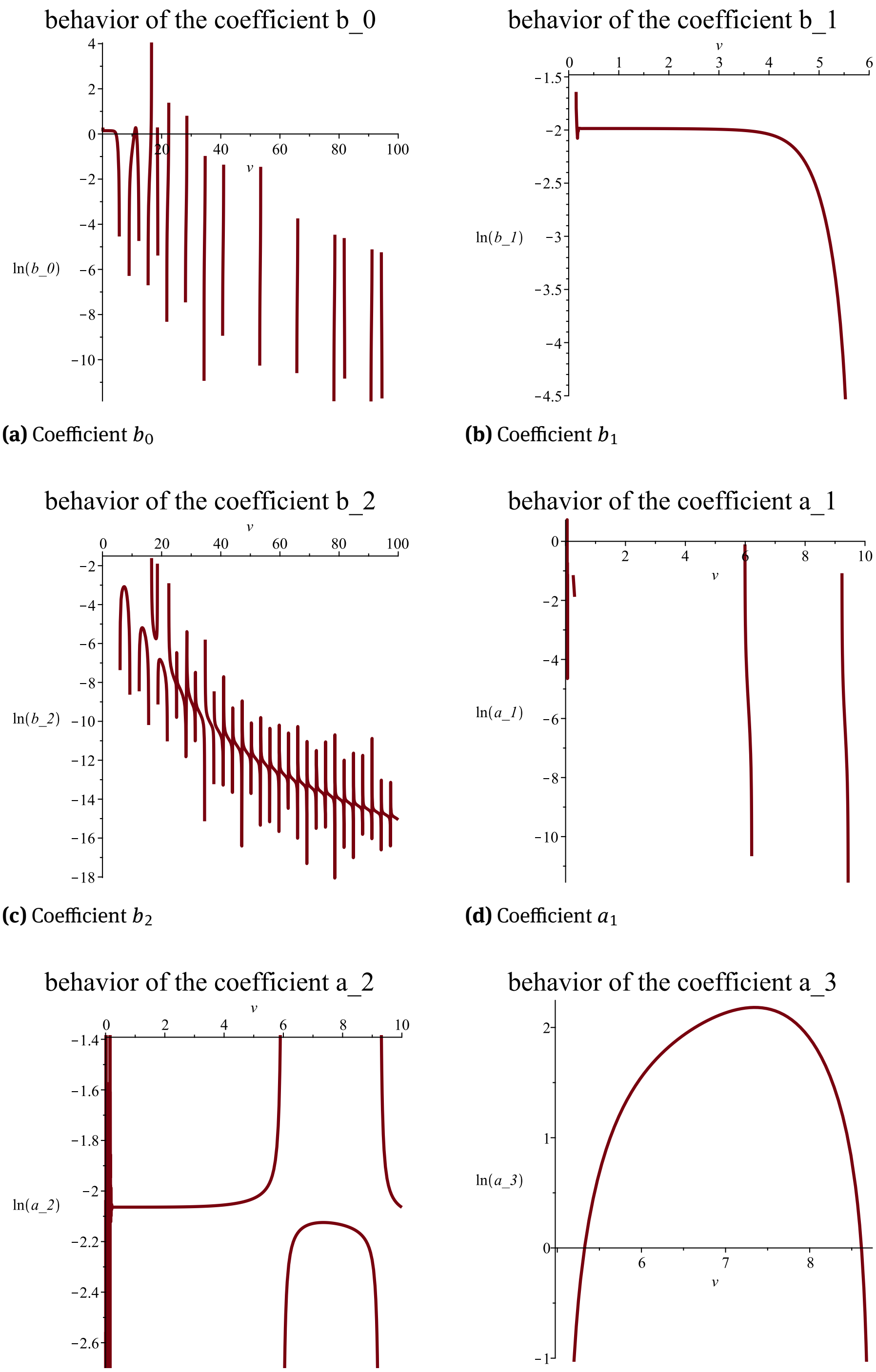
$$\begin{aligned}
b_0 = {} & \frac{4505}{3894} - \frac{4067611271 v^4}{55133728272480} \\
& + \frac{542817613251 v^6}{771026811981208640} \\
& + \frac{400038789030314774501 v^8}{29200231661822285547966912 00} \\
& - \frac{835633018590743592492184926 29 v^{10}}{571897803130169226731142088113 98784000} \\
& + \ldots
\end{aligned}$$

$$\begin{aligned}
b_1 = {} & \frac{1069}{7788} - \frac{4067611271 v^4}{330802369634880} \\
& + \frac{180939204417 v^6}{1542053623962417280} \\
& + \frac{400038789030314774501 v^8}{1752013899709337132878014720 0} \\
& - \frac{41224781806998621124747166231 v^{10}}{127088400695593161495809352914 21952000} \\
& + \ldots
\end{aligned}$$

$$\begin{aligned}
b_2 = {} & -\frac{140}{649} + \frac{4067611271 v^4}{82700592408720} \\
& - \frac{180939204417 v^6}{385513405990604320} \\
& - \frac{400038789030314774501 v^8}{4380034749273342832195036800} \\
& + \frac{11364658453051548734298574717 7 v^{10}}{285948901565084613365571044056 99392000} \\
& + \ldots
\end{aligned}$$

$$\begin{aligned}
a_1 = {} & -\frac{13}{1896} + \frac{14231797 v^4}{3350426302080} \\
& - \frac{5636191273 v^6}{23427297512910720} \\
& + \frac{2595679492029592027 v^8}{328427588575781431622645760} \\
& - \frac{589474110051330099313 v^{10}}{29218545755698476502637625456 00} \\
& + \ldots
\end{aligned}$$

$$\begin{aligned}
a_2 = {} & \frac{711}{5600} + \frac{3592051 v^4}{1554891520000} \\
& + \frac{1466269151 v^6}{17791068771840000} \\
& + \frac{284006254151551693 81 v^8}{1524191927736179436134400000 0} \\
& + \frac{569523423333851373951 1 v^{10}}{134997001620958863245341081600000} \\
& + \ldots
\end{aligned}$$




**(a)** Coefficient $b_0$ **(b)** Coefficient $b_1$

**(c)** Coefficient $b_2$ **(d)** Coefficient $a_1$

**(e)** Coefficient $a_2$ **(f)** Coefficient $a_3$

**Figure 1:** Plot of the parameters determined in (20).

$$a_3 = -2 + \frac{45469\, v^{14}}{282893554944000} + \dots \tag{21}$$

The plot of the parameters determined in (20) are shown in Figure 1.

In (22) we determine the LTE of the algorithm (symbolized as $4 - St - 2S - 12 - 5D$):

$$LTE_{4-St-2S-12-5D} = -\frac{45469}{1697361329664000}\, h^{14}$$

$$\left( \varphi_n^{(14)} - 21\,\phi^4\,\varphi_n^{(10)} - 70\,\phi^6\,\varphi_n^{(8)} - 105\,\phi^8\,\varphi_n^{(6)} \right.$$
$$\left. - 84\,\phi^{10}\,\varphi_n^{(4)} - 35\,\phi^{12}\,\varphi_n^{(2)} - 6\,\phi^{14}\,\varphi_n \right) + O\left(h^{16}\right) \quad (22)$$

# 4 Comparative Error Analysis

For the error analysis the following problem is used:

$$\varphi''(x) = \left(V(x) - V_c + \Gamma\right)\,\varphi(x) \quad (23)$$

(1) $V(x)$ is a function which is called potential, (2) $V_c$ is real number denoting an approximate value of the function $V(x)$ at $x$, (3) $\Gamma = V_c - E$, (4) The energy is denoted as $E$.

**Remark 2.** *The above mentioned test equation is the time independent radial Schrödinger equation.*

Our study will be focused on the local truncation errors of the following methods of the same family:

## 4.1 Classical Algorithm (i.e. the algorithm (11) with constant coefficients)

$$LTE_{CL} = -\frac{45469}{1697361329664000}\,h^{14}\,\varphi_n^{(14)} + O\left(h^{16}\right) \quad (24)$$

## 4.2 Algorithm Produced in [23]

$$LTE_{4-St-2S-12-1D} = -\frac{45469}{1697361329664000}\,h^{14}$$
$$\left( \varphi_n^{(14)} + 6\,\phi^{10}\,\varphi_n^{(4)} + 5\,\phi^{12}\,\varphi_n^{(2)} \right) + O\left(h^{16}\right) \quad (25)$$

## 4.3 Algorithm Obtained in [25]

$$LTE_{4-St-2S-12-2D} = -\frac{45469}{1697361329664000}\,h^{14}$$
$$\left( \varphi_n^{(14)} - 15\,\phi^8\,\varphi_n^{(6)} \right.$$
$$\left. - 24\,\phi^{10}\,\varphi_n^{(4)} - 10\,\phi^{12}\,\varphi_n^{(2)} \right) + O\left(h^{16}\right) \quad (26)$$

## 4.4 Algorithm Produced in Section 3

$$LTE_{4-St-2S-12-5D} = -\frac{45469}{1697361329664000}\,h^{14}$$
$$\left( \varphi_n^{(14)} - 21\,\phi^4\,\varphi_n^{(10)} - 70\,\phi^6\,\varphi_n^{(8)} - 105\,\phi^8\,\varphi_n^{(6)} \right.$$
$$\left. - 84\,\phi^{10}\,\varphi_n^{(4)} - 35\,\phi^{12}\,\varphi_n^{(2)} - 6\,\phi^{14}\,\varphi_n \right) + O\left(h^{16}\right) \quad (27)$$

Our analysis is based on the following algorithm :

- The local truncation error (LTE) formulae are expressed via the test equation (23).
- More specifically, we substitute the derivatives of the function $\varphi$ which are included in the LTE formulae, with results based on the problem (23). Some of the results are shown in Appendix A .
- The previous step leads to new formulae for the LTE which have the form:

$$LTE = \sum_{i=0}^{m} P_i\,\Gamma^i \quad (28)$$

  where $P_i,\ i = 0, 1, \ldots$ are quantities which can have two forms:

  - real numbers in cases that the algorithm use coefficients which are real numbers or
  - functions of $v$ in the other cases.
- Two cases for the parameter $\Gamma$ are examined:
  - First Case: $V_c - E = \Gamma \approx 0$: The Potential and the Energy are closed each other. This leads to a form of the LTE given by (28) which is approximately equal to $LTE = P_0$ (since $\Gamma^j = 0$, $j = 1, 2, \ldots$). Consequently, all the formulae of the LTE of the algorithms under comparison are approximately the same i.e. $LTE \approx P_0$ for all the algorithms under comparison. This achievement leads to the conclusion that for these values of $\Gamma$, the algorithms under comparison are of comparable accuracy.
  - Second Case: $\Gamma >> 0$ or $\Gamma << 0$. Consequently, $|\Gamma|$ is a very big number. The Potential is much greater or much smaller than the Energy. Consequently, for the algorithms under comparison, the most accurate one is the algorithm with asymptotic form of the expression of its LTE given by (28) with the minimum value of $m$.

The above achievements lead to the following asymptotic forms of the LTE formuale:

### 4.5 Classical Algorithm

$$LTE_{CL} = -\frac{45469}{1697361329664000}\, h^{14} \left( \varphi(x)\, \Gamma^7 + \cdots \right) + O\left(h^{16}\right) \tag{29}$$

### 4.6 Algorithm Produced in [23]

$$\begin{aligned} LTE_{4-St-2S-12-1D} &= -\frac{45469}{339472265932800}\, h^{14} \\ &\left[ \left( 3\,\xi(x)^2\, \varphi(x) + 31\,\xi''(x)\, \varphi(x) \right.\right. \\ &\left.\left. + 6\,\xi'(x)^2\, \varphi'(x) \right) \Gamma^5 + \cdots \right] + O\left(h^{16}\right) \end{aligned} \tag{30}$$

### 4.7 Algorithm Produced in [25]

$$LTE_{4-St-2S-12-2D} = -\frac{45469}{21217016620800}\, h^{14} \left[ \left( \xi''(x)\, \varphi(x) \right) \Gamma^5 + \cdots \right] + O\left(h^{16}\right) \tag{31}$$

### 4.8 Algorithm Produced in Section 3

$$\begin{aligned} LTE_{4-St-2S-12-5D} &= -\frac{1}{106085083104000}\, h^{14} \\ &\left[ \left( -1773291\,\xi^{(6)}(x)\, \varphi(x) - 636566\,\xi^{(5)}(x)\, \varphi'(x) \right.\right. \\ &- 1909698\,\xi^{(4)}(x)\, \varphi(x)\, \xi(x) \\ &- 4774245\,\xi^{(3)}(x)\, \varphi(x)\, \xi'(x) \\ &\left.\left. - 3182830\,\xi^{(2)}(x)^2\, \varphi(x) \right) \Gamma^3 + \cdots \right] + O\left(h^{16}\right) \end{aligned} \tag{32}$$

We have the following theorem:

**Theorem 2.** *For the four symmetric two-step algorithms investigated in this section we have the following conclusions:*

- *The algebraic order of all algorithms under comparison is twelve.*
- *For the Classical algorithm, the error is dependent from the seventh power of $\Gamma$.*
- *For the algorithm developed in [23], the error is dependent from the fifth power of $\Gamma$.*
- *For the algorithm developed in [25], the error is dependent from the fifth power of $\Gamma$.*
- *For the algorithm produced in Section 3, the error is dependent from the third power of $\Gamma$.*

*The above conclusions lead to the following: For the approximation of the problem (23) the new produced in Section 3 algorithm is the most effective one in the cases of very big values of $|\Gamma|$.*

## 5 Stability Analysis

Our study is based on the following chart:

- The scalar test equation for the stability analysis is given by:

$$\varphi'' = -\omega^2\, \varphi. \tag{33}$$

**Remark 3.** *It is easy for one to see that $\omega \neq \phi$.*

- The difference equation mentioned below is produced by applying the algorithm to the problem (33):

$$A_1(s,v)\,(\varphi_{n+1} + \varphi_{n-1}) + A_0(s,v)\,\varphi_n = 0 \tag{34}$$

where

$$A_1(s,v) = \frac{T_7}{T_{denom5}},\quad A_0(s,v) = \frac{T_8}{T_{denom6}} \tag{35}$$

where $s = \omega\, h$ and $v = \phi\, h$ and $T_j$, $j = 7, 8$, $T_{denom5}$ and $T_{denom6}$ are given in Supplement Material B.
The $s - v$ domain for the new algorithm is presented in Figure 2.
Observing the $s - v$ domain we have the following remarks:

**Remark 4.**
- *The algorithm is stable within the shadowed area of the $s - v$ domain.*
- *The algorithm is unstable within the white area of the $s - v$ domain.*

**Remark 5.** *In the cases of problems where where their mathematical models have only one frequency*

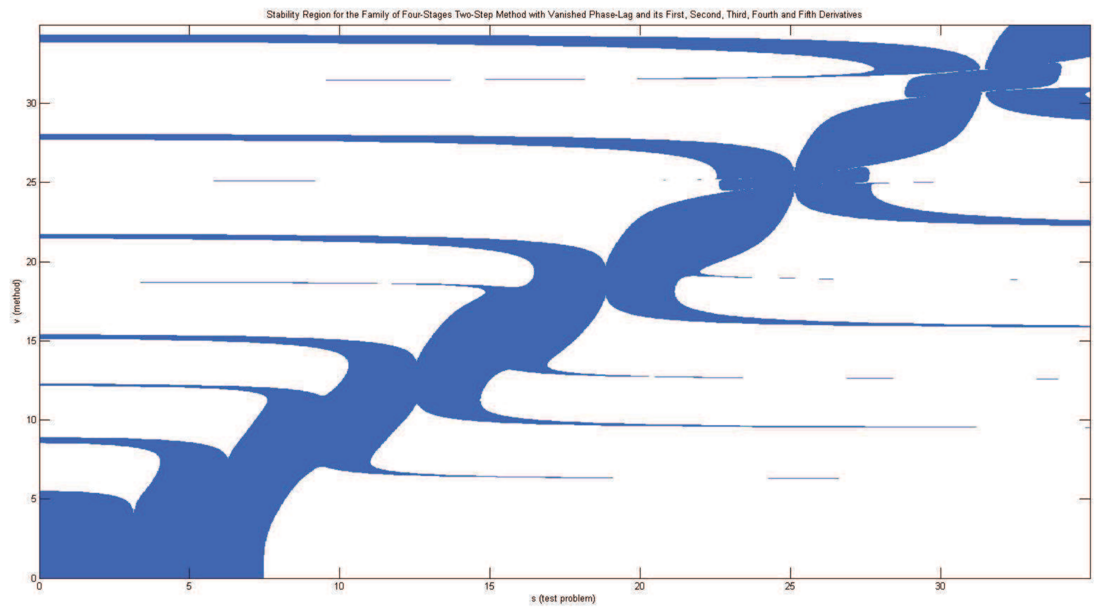



**Figure 2:** $s-v$ domain of the new algorithm

*per differential equation, we have to observe on $s-v$ domain the area where $\omega = \phi$ or $s = v$.*

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**Remark 6.** *In the cases where $s = v$, the interval of periodicity for the new algorithm is equal to:* $(0, \infty)$, *i.e. it is P-stable.*

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We have the following theorem:

**Theorem 3.** *The new algorithm obtained in Section 3:*

- *is of twelfth algebraic order,*
- *has eliminated the phase-lag and its derivatives up to order four,*
- *has a $s-v$ region presented in Figure 2*
- *is P-stable i.e. its interval of periodicity is equal to:* $(0, \infty)$ *(in the cases where $s = v$).*

# 6 Numerical Results

In this section we will present the application of the new developed method to the numerical solution of the coupled differential equations arising from the Schrödinger equation.

## 6.1 Error Estimation

The numerical example contains a variable-step algorithm and therefore an error estimation procedure .

We mention here that in the literature the last decades there are several variable step procedures for the approximation of the solution for systems of Schrödinger type equations [1–14].

Basic methodologies for the local truncation error estimation (see for example [15–27]) are based on:

- the order $q$ in $h^q$ in the LTE expressions of the algorithms,
- the maximum order $p$ in the expressions $x^p \, exp\,(\pm w\, x)$ or in the expressions $x^p \cos(\pm w\, x)$ and/or $x^p \sin(\pm w\, x)$ which are the algorithm integrates exactly,
- order of the phase-lag of the algorithms (i.e. zero order of the phase-lag is for eliminated phase-lag algorithms, first order of the phase-lag is for the algorithms with eliminated the phase-lag the derivative of the first order, $n$-th order of the phase-lag order is for the algorithms with eliminated phase-lag and its derivatives up to order $n$.

We will use the first of the above mentioned methodologies. Our embedded pair is based

- on the order $q$ in $h^q$ in the LTE expressions of the algorithms

- on the fact that in order to obtain highly accurate numerical solutions, the maximum algebraic order $q$ of an algorithm must be used .

**Definition 8.** *The local truncation error in $y^L_{n+1}$ is estimated by*

$$LTE = \mid y^H_{n+1} - y^L_{n+1} \mid \tag{36}$$

*where $y^L_{n+1}$ is the low order approximation and we use for this approximation the algorithm obtained in [24] and $y^H_{n+1}$ is the high order approximation and we use for this approximation the algorithm produced in Section 3.*

For our numerical example we reduced the changes of the step sizes on its duplication . More specifically :

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

where $h_n$ the size of the step used for the $n^{th}$ step of integration and $acc$ is the accuracy defined by the user.

**Remark 7.** *For our numerical tests we used the local extrapolation technique, i.e. while we use the lower algebraic order solution $y^L_{n+1}$ for an estimation of the local truncation error less than $acc$, we accept at each point of integration the higher algebraic order solution $y^H_{n+1}$ as approximation of the solution.*

## 6.2 Coupled differential equations

The coupled differential equations of the Schrödinger type can be found in several scientific areas. The general form of the close-coupling differential equations arising from the Schrödinger equation is of the form:

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii}\right]\varphi_{ij} = \sum_{m=1}^{N} V_{im}\varphi_{mj} \tag{37}$$

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

There are two cases for the above system of differential equations: (1) the open channels case and (2) the close channels case. We will study the first case with conditions on boundaries [16] (we note here that the new algorithm can be applied to close channels case also):

$$\varphi_{ij} = 0 \quad \text{at} \quad x = 0 \tag{38}$$

$$\varphi_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x) \tag{39}$$

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

For the details on the model of the problem one can see [16]. Based on the analysis presented in [16], the following matrix $K'$ and diagonal matrices $M$, $N$ are defined as:

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

and the boundary condition (39) now is given by:

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

The close-coupling differential equations arising from the Schrödinger equation of the our numerical test describe, under environment of neutral particle impact, the phenomenon of the rotational excitation of a diatomic molecule. We use the same notations, as in [16]:

- for the entrance channel we use the quantum numbers $(j, l)$,
- for the exit channels we use the quantum numbers $(j', l')$ and
- for the total angular momentum we use the notation $J = j + l = j' + l'$.

Based on the above notations we have the following form of the problem:

$$\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2}\right]\varphi^{Jjl}_{j'l'}(x) = \frac{2\mu}{\hbar^2}\sum_{j''}\sum_{l''} < j'l'; J \mid V \mid j''l''; J > \varphi^{Jjl}_{j''l''}(x) \tag{40}$$

where

$$k_{j'j}^2 = \frac{2\mu}{\hbar^2}[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}] \tag{41}$$

$E$ is the energy of the corresponding system, $I$ is the moment of inertia of the rotator, and $\mu$ is the mass of the corresponding system.

The function $V$ is given by ([16]):

$$V(x, \hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}), \tag{42}$$

The coupling matrix element can be written as

$$< j'l'; J \mid V \mid j''l''; J >= \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x) \tag{43}$$

where the $f_2$ coefficients can are given via the formulae mentioned in Bernstein et al. [18] and $\hat{\mathbf{k}}_{j'j}$ is a vector parallel to the vector $\mathbf{k}_{j'j}$ and $P_i$, $i = 0, 2$ are Legendre polynomials (see for details [19]). Now we have the following form for the boundary conditions :

$$\varphi^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \tag{44}$$

$$\varphi^{Jjl}_{j'l'}(x) \sim \delta_{jj'}\delta_{ll'} \exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp[i(k_{j'j}x - 1/2l'\pi)] \tag{45}$$

where:

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1} \tag{46}$$

A program was developed for the numerical solution of this problem. With this program we calculated cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles ([16], [17]). We included also a subroutine for the numerical integration from the initial value to the matching points and we applied the variable step method described in the previous subsection.

We made the computations using the following parameters:

$$\frac{2\mu}{\hbar^2} = 1000.0, \ \frac{\mu}{I} = 2.351, \ E = 1.1,$$
$$V_0(x) = \frac{1}{x^{12}} - 2\frac{1}{x^6}, \ V_2(x) = 0.2283V_0(x).$$

As we mentioned previously we followed the procedure described in [16]. We taken the values $J = 6$ and from $j = 0$ to $j' = 2, 4$ and 6 and therefore, we have sets of **four, nine and sixteen coupled differential equations**, respectively. We used the methodology obtained by Bernstein [19] and Allison [16] and consequently, for $x$ less than some $x_0$, the potential tends to infinite. For this case we have for $x_0$:

$$y^{Jjl}_{j'l'}(x_0) = 0 \tag{47}$$

We solved the above described problems using the algorithms:

- the Iterative Numerov algorithm of Allison [16] which is symbolized as **Algorithm I**,
- the variable-step algorithm of Raptis and Cash [15] which is symbolized as **Algorithm II**,
- the embedded Runge-Kutta Dormand and Prince algorithm 5(4) [13] which is symbolized as **Algorithm III**,
- the embedded Runge-Kutta algorithm ERK4(2) introduced in Simos [20] which is symbolized as **Algorithm IV**,
- the introduced embedded symmetric two-step algorithm introduced in [22] which is symbolized as **Algorithm V**
- the introduced embedded symmetric two-step algorithm introduced in [23] which is symbolized as **Algorithm VI**
- the introduced embedded symmetric two-step algorithm introduced in [23] which is symbolized as **Algorithm VII**

**Table 1: System of Differential Equations of the Schrödinger type.** Computational cost (in seconds) (CC) and maximum value of the absolute error (MErr) of the computation of $|S|^2$ for the Algorithm I - Algorithm X. $acc$=$10^{-6}$. hmax: maximum step length

| Algorithm | N | hmax | CC | MErr |
|---|---|---|---|---|
| Algorithm I | 4 | 0.014 | 3.25 | $1.2\times10^{-3}$ |
| | 9 | 0.014 | 23.51 | $5.7\times10^{-2}$ |
| | 16 | 0.014 | 99.15 | $6.8\times10^{-1}$ |
| Algorithm II | 4 | 0.056 | 1.55 | $8.9\times10^{-4}$ |
| | 9 | 0.056 | 8.43 | $7.4\times10^{-3}$ |
| | 16 | 0.056 | 43.32 | $8.6\times10^{-2}$ |
| Algorithm III | 4 | 0.007 | 45.15 | $9.0\times10^{0}$ |
| | 9 | | | |
| | 16 | | | |
| Algorithm IV | 4 | 0.112 | 0.39 | $1.1\times10^{-5}$ |
| | 9 | 0.112 | 3.48 | $2.8\times10^{-4}$ |
| | 16 | 0.112 | 19.31 | $1.3\times10^{-3}$ |
| Algorithm V | 4 | 0.448 | 0.14 | $3.4\times10^{-7}$ |
| | 9 | 0.448 | 1.37 | $5.8\times10^{-7}$ |
| | 16 | 0.448 | 9.58 | $8.2\times10^{-7}$ |
| Algorithm VI | 4 | 0.448 | 0.09 | $2.9\times10^{-7}$ |
| | 9 | 0.448 | 1.10 | $4.5\times10^{-7}$ |
| | 16 | 0.448 | 8.57 | $7.4\times10^{-7}$ |
| Algorithm VII | 4 | 0.448 | 0.06 | $1.3\times10^{-7}$ |
| | 9 | 0.448 | 1.04 | $1.7\times10^{-7}$ |
| | 16 | 0.448 | 7.58 | $2.9\times10^{-7}$ |
| Algorithm VIII | 4 | 0.448 | 0.04 | $8.8\times10^{-8}$ |
| | 9 | 0.448 | 1.02 | $9.2\times10^{-8}$ |
| | 16 | 0.448 | 7.48 | $8.9\times10^{-8}$ |
| Algorithm IX | 4 | 0.448 | 0.04 | $9.7\times10^{-8}$ |
| | 9 | 0.448 | 1.01 | $1.2\times10^{-7}$ |
| | 16 | 0.448 | 7.15 | $2.3\times10^{-7}$ |
| Algorithm X | 4 | 0.896 | 0.01 | $6.3\times10^{-8}$ |
| | 9 | 0.896 | 0.47 | $5.9\times10^{-8}$ |
| | 16 | 0.896 | 6.05 | $6.9\times10^{-8}$ |

– the introduced embedded symmetric two-step algorithm introduced in [25] which is symbolized as **Algorithm VIII**
– the introduced embedded symmetric two-step algorithm introduced in [26] which is symbolized as **Algorithm IX**
– the introduced embedded symmetric two-step algorithm introduced in this paper which is symbolized as **Algorithm X**

Table 1 shows the computational cost (in seconds) requested by the algorithms I-X mentioned above for the computation of $| S |^2$ for the system of N differential equations. The same Table shows also the maximum error of the computation of $| S |^2$. $N \in \{4, 9, 16\}$ symbolizes the number of equations of the system of the Schrödinger type differential equations.

## 7 Conclusions

A new algorithm with eliminated phase-lag and its derivatives up to order five is produced, for the first time in the literature, in the present paper. More specifically for the new algorithm we presented:

1. its construction,
2. the analysis of its error,
3. the analysis of its stability,
4. the analysis of its effectiveness by applying it to the numerical solution of systems of Schrödinger type equations.

The theoretical and numerical achievements lead to the conclusion that the new algorithm is more effective than other known ones or recently constructed for the approximation of systems of equations of the Schrödinger type.

We used for our computations a IBM PC-AT compatible 80486 using arithmetic with 16 significant digits accuracy (IEEE standard).

## Appendix A: Expressions of the Derivatives of $\varphi_n$

Here we present expressions of the derivatives of $\varphi_n$ using the test equation (23):

$$\varphi_n^{(2)} = \left(V(x) - V_c + \Gamma\right)\, \varphi(x)$$

$$\varphi_n^{(3)} = \left(\frac{d}{dx}\xi(x)\right)\varphi(x) + (\xi(x)+\Gamma)\,\frac{d}{dx}\varphi(x)$$

$$\varphi_n^{(4)} = \left(\frac{d^2}{dx^2}\xi(x)\right)\varphi(x) + 2\left(\frac{d}{dx}\xi(x)\right)\frac{d}{dx}\varphi(x) + (\xi(x)+\Gamma)^2\,\varphi(x)$$

$$\varphi_n^{(5)} = \left(\frac{d^3}{dx^3}\xi(x)\right)\varphi(x) + 3\left(\frac{d^2}{dx^2}\xi(x)\right)\frac{d}{dx}\varphi(x) + 4\,(\xi(x)+\Gamma)\,\varphi(x)\,\frac{d}{dx}\xi(x) + (\xi(x)+\Gamma)^2\,\frac{d}{dx}\varphi(x)$$

$$\varphi_n^{(6)} = \left(\frac{d^4}{dx^4}\xi(x)\right)\varphi(x) + 4\left(\frac{d^3}{dx^3}\xi(x)\right)\frac{d}{dx}\varphi(x) + 7\,(\xi(x)+\Gamma)\,\varphi(x)\,\frac{d^2}{dx^2}\xi(x) + 4\left(\frac{d}{dx}\xi(x)\right)^2\varphi(x) + 6\,(\xi(x)+\Gamma)\left(\frac{d}{dx}\varphi(x)\right)\frac{d}{dx}\xi(x) + (\xi(x)+\Gamma)^3\,\varphi(x)$$

$$\varphi_n^{(7)} = \left(\frac{d^5}{dx^5}\xi(x)\right)\varphi(x) + 5\left(\frac{d^4}{dx^4}\xi(x)\right)\frac{d}{dx}\varphi(x) + 11\,(\xi(x)+\Gamma)\,\varphi(x)\,\frac{d^3}{dx^3}\xi(x) + 15\left(\frac{d}{dx}\xi(x)\right)\varphi(x)\,\frac{d^2}{dx^2}\xi(x) + 13\,(\xi(x)+\Gamma)\left(\frac{d}{dx}\varphi(x)\right)\frac{d^2}{dx^2}\xi(x) + 10\left(\frac{d}{dx}\xi(x)\right)^2\frac{d}{dx}\varphi(x) + 9\,(\xi(x)+\Gamma)^2\,\varphi(x)\,\frac{d}{dx}\xi(x) + (\xi(x)+\Gamma)^3\,\frac{d}{dx}\varphi(x)$$

$$\varphi_n^{(8)} = \left(\frac{d^6}{dx^6}\xi(x)\right)\varphi(x) + 6\left(\frac{d^5}{dx^5}\xi(x)\right)\frac{d}{dx}\varphi(x) + 16\,(\xi(x)+\Gamma)\,\varphi(x)\,\frac{d^4}{dx^4}\xi(x) + 26\left(\frac{d}{dx}\xi(x)\right)\varphi(x)\,\frac{d^3}{dx^3}\xi(x) + 24\,(\xi(x)+\Gamma)\left(\frac{d}{dx}\varphi(x)\right)\frac{d^3}{dx^3}\xi(x) + 15\left(\frac{d^2}{dx^2}\xi(x)\right)^2\varphi(x)\,48\left(\frac{d}{dx}\xi(x)\right)\left(\frac{d}{dx}\varphi(x)\right)\frac{d^2}{dx^2}\xi(x) + 22\,(\xi(x)+\Gamma)^2\,\varphi(x)\,\frac{d^2}{dx^2}\xi(x) + 28\,(\xi(x)+\Gamma)\,\varphi(x)\left(\frac{d}{dx}\xi(x)\right)^2 + 12\,(\xi(x)+\Gamma)^2\left(\frac{d}{dx}\varphi(x)\right)\frac{d}{dx}\xi(x) + (\xi(x)+\Gamma)^4\,\varphi(x)\ldots$$

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# SUPPLEMENT MATERIAL A

$$
\begin{aligned}
T_1 &= 193505760 - 86002560\,v^2 - 193505760\,\cos(v) \\
&+ 17200512\,v^4 - 5786844\,v^6 + 7112\,v^{10} + 50800\,v^8 \\
&- 28448\,\cos(v)\sin(v)\,v^9 + 26670\,(\cos(v))^3\sin(v)\,v^5 \\
&- 11430\,(\cos(v))^3\sin(v)\,v^7 - 4645772\,(\cos(v))^2\sin(v)\,v^7 \\
&+ 11413668\,\cos(v)\sin(v)\,v^5 + 43001280\,\cos(v)\sin(v)\,v^3 \\
&- 45720\,\cos(v)\sin(v)\,v^7 - 1016\,(\cos(v))^3\sin(v)\,v^9 \\
&- 265670370\,(\cos(v))^2\sin(v)\,v^3 \\
&+ 96752880\,(\cos(v))^2\sin(v)\,v \\
&- 387011520\,\cos(v)\sin(v)\,v + 179426\,(\cos(v))^2\sin(v)\,v^9 \\
&- 48798386\,(\cos(v))^2\sin(v)\,v^5 + 193505760\,(\cos(v))^3 \\
&- 193505760\,(\cos(v))^2 + 290258640\,v\sin(v) \\
&- 5023928\,v^9\sin(v) - 14704804\,v^7\sin(v) \\
&- 104763652\,v^5\sin(v) + 319421970\,v^3\sin(v) \\
&+ 127\,(\cos(v))^4 v^{10} + 3810\,(\cos(v))^4 v^8 \\
&+ 2150064\,(\cos(v))^3 v^8 + 25800768\,(\cos(v))^3 v^6 \\
&+ 25600743\,(\cos(v))^2 v^4 + 279508320\,(\cos(v))^2 v^2 \\
&- 397761840\,\cos(v)\,v^2 + 66675\,(\cos(v))^4 v^6 \\
&+ 200025\,(\cos(v))^4 v^4 + 156954672\,(\cos(v))^3 v^4 \\
&+ 204256080\,(\cos(v))^3 v^2 + 8636\,(\cos(v))^2 v^{10} \\
&+ 91440\,(\cos(v))^2 v^8 - 20067264\,\cos(v)\,v^8 \\
&- 1220016\,(\cos(v))^2 v^6 - 109958268\,\cos(v)\,v^6 \\
&- 103203072\,\cos(v)\,v^4
\end{aligned}
$$

$$
\begin{aligned}
T_2 &= -387011520 + 494514720\,v^2 + 387011520\,\cos(v) \\
&+ 223606656\,v^4 - 160538112\,v^6 + 5733504\,v^8 \\
&- 1475921\,(\cos(v))^2\sin(v)\,v^7 \\
&- 151937856\,\cos(v)\sin(v)\,v^5 \\
&- 731021760\,\cos(v)\sin(v)\,v^3 \\
&- 194305860\,(\cos(v))^2\sin(v)\,v^3 \\
&- 193505760\,(\cos(v))^2\sin(v)\,v \\
&+ 774023040\,\cos(v)\sin(v)\,v - 4826\,(\cos(v))^2\sin(v)\,v^9 \\
&- 26018573\,(\cos(v))^2\sin(v)\,v^5 \\
&- 127\,(\cos(v))^2\sin(v)\,v^{11} \\
&- 387011520\,(\cos(v))^3 + 387011520\,(\cos(v))^2 \\
&- 580517280\,v\sin(v) + 35814\,v^9\sin(v) \\
&+ 40079918\,v^7\sin(v) \\
&+ 220210949\,v^5\sin(v) - 558216540\,v^3\sin(v) \\
&+ 33020\,(\cos(v))^3 v^8 - 8413566\,(\cos(v))^3 v^6 \\
&+ 12900384\,(\cos(v))^2 v^4 - 881526240\,(\cos(v))^2 v^2 \\
&+ 1118033280\,\cos(v)\,v^2 - 120003534\,(\cos(v))^3 v^4 \\
&- 731021760\,(\cos(v))^3 v^2 + 1433376\,(\cos(v))^2 v^8 \\
&+ 148590\,\cos(v)\,v^8 + 45868032\,(\cos(v))^2 v^6 \\
&+ 80429076\,\cos(v)\,v^6 + 335009934\,\cos(v)\,v^4 \\
&+ 762\,(\cos(v))^3 v^{10} - 7112\,\cos(v)\,v^{10} \\
&+ 3556\,v^{11}\sin(v)
\end{aligned}
$$

$$
\begin{aligned}
T_3 &= 96752880 - 43001280\,v^2 - 96752880\,\cos(v) \\
&+ 8600256\,v^4 - 2866752\,v^6 + 145129320\,v\sin(v) \\
&- 3556\,v^9\sin(v) - 10039982\,v^7\sin(v) \\
&- 55069406\,v^5\sin(v) + 139554135\,v^3\sin(v) \\
&+ 2150064\,(\cos(v))^3 v^6 + 12900384\,(\cos(v))^2 v^4 \\
&+ 139754160\,(\cos(v))^2 v^2 - 279508320\,\cos(v)\,v^2 \\
&+ 30100896\,(\cos(v))^3 v^4 \\
&+ 182755440\,(\cos(v))^3 v^2 \\
&- 716688\,(\cos(v))^2 v^6 - 20040594\,\cos(v)\,v^6 \\
&+ 21500640\,\cos(v)\sin(v)\,v^3 \\
&- 193505760\,\cos(v)\sin(v)\,v \\
&+ 364694\,(\cos(v))^2\sin(v)\,v^7 \\
&+ 48376440\,(\cos(v))^2\sin(v)\,v \\
&+ 5733504\,\cos(v)\sin(v)\,v^5 \\
&+ 48576465\,(\cos(v))^2\sin(v)\,v^3 \\
&+ 127\,(\cos(v))^2\sin(v)\,v^9 \\
&+ 6507977\,(\cos(v))^2\sin(v)\,v^5 \\
&+ 96752880\,(\cos(v))^3 - 96752880\,(\cos(v))^2 \\
&- 83852496\,\cos(v)\,v^4
\end{aligned}
$$

$$
\begin{aligned}
T_4 &= 2032\,\sin(v)(\cos(v))^3 v^6 \\
&+ 56896\,\cos(v)\sin(v)\,v^6 \\
&- 360630\,(\cos(v))^2\sin(v)\,v^6 \\
&- 48393585\,(\cos(v))^2\sin(v)\,v^2 \\
&- 127\,(\cos(v))^2\sin(v)\,v^8 \\
&+ 30480\,\cos(v)\sin(v)\,v^4 \\
&+ 7620\,\sin(v)(\cos(v))^3 v^4 \\
&- 68580\,\sin(v)(\cos(v))^3 v^2 \\
&- 6467337\,(\cos(v))^2\sin(v)\,v^4 \\
&+ 137160\,v^2\sin(v)\cos(v) \\
&- 48376440\,(\cos(v))^2\sin(v) \\
&- 96804315\,v^2\sin(v) \\
&+ 3556\,\sin(v)\,v^8 + 10053190\,\sin(v)\,v^6 \\
&+ 6400662\,\sin(v)\,v^4 + 96851940\,v^3\cos(v) \\
&+ 34290\,\cos(v)\,v + 243840\,(\cos(v))^2 v^3 \\
&- 34290\,(\cos(v))^2 v + 34290\,(\cos(v))^4 v \\
&- 4572\,(\cos(v))^4 v^5 - 49530\,(\cos(v))^4 v^3
\end{aligned}
$$

$$- 34290\,(\cos(v))^3\,v + 254\,(\cos(v))^4\,v^7 - 10668\,(\cos(v))^3\,v^5 - 64770\,(\cos(v))^3\,v^3 - 762\,(\cos(v))^3\,v^7 + 7112\,\cos(v)\,v^7 + 17272\,(\cos(v))^2\,v^7 - 18288\,(\cos(v))^2\,v^5 + 29718\,\cos(v)\,v^5 + 14224\,v^7 + 60960\,v^5 - 228600\,v^3 + 48376440\,\sin(v)$$

$$T_5 = (\cos(v))^2\sin(v)\,v^7 + 6\,(\cos(v))^3\,v^6 + 18\,(\cos(v))^2\sin(v)\,v^5 - 28\,v^7\sin(v) + 84\,(\cos(v))^3\,v^4 - 56\,\cos(v)\,v^6 + 135\,(\cos(v))^2\sin(v)\,v^3 - 154\,v^5\sin(v) + 510\,(\cos(v))^3\,v^2 - 234\,\cos(v)\,v^4 + 135\,(\cos(v))^2\sin(v)\,v + 390\,v^3\sin(v) + 270\,(\cos(v))^3 - 780\,\cos(v)\,v^2 + 405\,v\sin(v) - 270\,\cos(v)$$

$$T_6 = 72564660\,\cos(v) + 22860\,v^4 - 60960\,v^6 + 60470550\,v\sin(v) + 2508408\,v^7\sin(v) - 47838924\,v^5\sin(v) + 72564660\,v^3\sin(v) - 1612548\,(\cos(v))^3\,v^6 + 76200\,(\cos(v))^2\,v^4 - 120015\,(\cos(v))^2\,v^2 - 48376440\,\cos(v)\,v^2 + 33325992\,(\cos(v))^3\,v^4 + 120941100\,(\cos(v))^3\,v^2 + 71628\,(\cos(v))^2\,v^6 + 15050448\,\cos(v)\,v^6 - 8636\,(\cos(v))^2\,v^8 - 127\,(\cos(v))^4\,v^8 + 8382\,(\cos(v))^4\,v^6 + 55245\,(\cos(v))^4\,v^4 + 120015\,(\cos(v))^4\,v^2 - 7112\,v^8 - 68580\,\cos(v)\sin(v)\,v^3 - 89586\,(\cos(v))^2\sin(v)\,v^7 - 205599870\,(\cos(v))^2\sin(v)\,v + 15240\,\cos(v)\sin(v)\,v^5 - 12094110\,(\cos(v))^2\sin(v)\,v^3 + 11287836\,(\cos(v))^2\sin(v)\,v^5 - 72564660\,(\cos(v))^3 - 105890652\,\cos(v)\,v^4 + 34290\,(\cos(v))^3\sin(v)\,v^3 + 56896\,\cos(v)\sin(v)\,v^7 + 2032\,(\cos(v))^3\sin(v)\,v^7 + 3810\,(\cos(v))^3\sin(v)\,v^5$$

$$T_{denom1} = v^4\Big(-290258640 - 387011520\,v^2 + 197805888\,v^4 + 8600256\,v^6 + 3810\,(\cos(v))^2\sin(v)\,v^7 + 17200512\,\cos(v)\sin(v)\,v^5 + 193505760\,\cos(v)\sin(v)\,v^3 + 257175\,(\cos(v))^2\sin(v)\,v^3 + 580517280\,\cos(v)\sin(v)\,v - 127\,(\cos(v))^2\sin(v)\,v^9 + 165735\,(\cos(v))^2\sin(v)\,v^5 + 290258640\,(\cos(v))^2 + 3556\,v^9\sin(v) + 65278\,v^7\sin(v) + 300990\,v^5\sin(v) - 120015\,v^3\sin(v) + 1524\,(\cos(v))^3\,v^8 + 27432\,(\cos(v))^3\,v^6 - 4300128\,(\cos(v))^2\,v^4 + 96752880\,(\cos(v))^2\,v^2 + 480060\,\cos(v)\,v^2 - 175260\,(\cos(v))^3\,v^4 - 480060\,(\cos(v))^3\,v^2 - 14224\,\cos(v)\,v^8 + 2150064\,(\cos(v))^2\,v^6 - 297942\,\cos(v)\,v^6 - 441960\,\cos(v)\,v^4\Big)$$

$$T_{denom2} = 2150064\,v\Big((\cos(v))^2\sin(v)\,v^7 + 6\,(\cos(v))^3\,v^6 + 18\,(\cos(v))^2\sin(v)\,v^5 - 28\,v^7\sin(v) + 84\,(\cos(v))^3\,v^4 - 56\,\cos(v)\,v^6 + 135\,(\cos(v))^2\sin(v)\,v^3 - 154\,v^5\sin(v) + 510\,(\cos(v))^3\,v^2 - 234\,\cos(v)\,v^4 + 135\,(\cos(v))^2\sin(v)\,v + 390\,v^3\sin(v) + 270\,(\cos(v))^3 - 780\,\cos(v)\,v^2 + 405\,v\sin(v) - 270\,\cos(v)\Big)$$

$$T_{denom3} = 96752880 - 43001280\,v^2 - 96752880\,\cos(v) + 8600256\,v^4 - 2866752\,v^6 + 145129320\,v\sin(v) - 3556\,v^9\sin(v) - 10039982\,v^7\sin(v) - 55069406\,v^5\sin(v) + 139554135\,v^3\sin(v) + 2150064\,(\cos(v))^3\,v^6 + 12900384\,(\cos(v))^2\,v^4 + 139754160\,(\cos(v))^2\,v^2 - 279508320\,\cos(v)\,v^2 + 30100896\,(\cos(v))^3\,v^4 + 182755440\,(\cos(v))^3\,v^2 - 716688\,(\cos(v))^2\,v^6 - 20040594\,\cos(v)\,v^6 + 21500640\,\cos(v)\sin(v)\,v^3 - 193505760\,\cos(v)\sin(v)\,v + 364694\,(\cos(v))^2\sin(v)\,v^7 + 48376440\,(\cos(v))^2\sin(v)\,v + 5733504\,\cos(v)\sin(v)\,v^5 + 48576465\,(\cos(v))^2\sin(v)\,v^3 + 127\,(\cos(v))^2\sin(v)\,v^9 + 6507977\,(\cos(v))^2\sin(v)\,v^5 + 96752880\,(\cos(v))^3 - 96752880\,(\cos(v))^2 - 83852496\,\cos(v)\,v^4$$

$$T_{denom4} = 290258640 + 387011520\,v^2 - 197805888\,v^4$$

$$- 8600256\, v^6 - 3556\, v^9 \sin(v)$$
$$- 65278\, v^7 \sin(v) - 300990\, v^5 \sin(v)$$
$$+ 120015\, v^3 \sin(v) - 27432\, (\cos(v))^3\, v^6$$
$$+ 4300128\, (\cos(v))^2\, v^4$$
$$- 96752880\, (\cos(v))^2\, v^2$$
$$- 480060\, \cos(v)\, v^2 + 175260\, (\cos(v))^3\, v^4$$
$$+ 480060\, (\cos(v))^3\, v^2$$
$$- 2150064\, (\cos(v))^2\, v^6$$
$$+ 297942\, \cos(v)\, v^6 - 1524\, (\cos(v))^3\, v^8$$
$$+ 14224\, \cos(v)\, v^8 - 193505760\, \cos(v) \sin(v)\, v^3$$
$$- 580517280\, \cos(v) \sin(v)\, v$$
$$- 3810\, (\cos(v))^2 \sin(v)\, v^7$$
$$- 17200512\, \cos(v) \sin(v)\, v^5$$
$$- 257175\, (\cos(v))^2 \sin(v)\, v^3$$
$$+ 127\, (\cos(v))^2 \sin(v)\, v^9$$
$$- 165735\, (\cos(v))^2 \sin(v)\, v^5$$
$$- 290258640\, (\cos(v))^2 + 441960\, \cos(v)\, v^4$$

## SUPPLEMENT MATERIAL B

$$T_7 = 580517280\, v^4 + 1354540320\, v^6$$
$$- 1011555\, \sin(v)\, s^2 v^7$$
$$+ 201930\, \cos(v)\, s^6 v^2 + 2293620\, \cos(v)\, v^8$$
$$- 480060\, \cos(v)\, v^6 - 1369695\, v^9 \sin(v)$$
$$+ 222885\, v^7 \sin(v) + 40005\, s^2 v^5 \sin(3\, v)$$
$$+ 600075\, s^4 v^3 \sin(3\, v) - 1935057600\, s^2 v^2 \cos(2\, v)$$
$$- 1161034560\, v^5 \sin(2\, v) + 175260\, v^8 \cos(3\, v)$$
$$+ 8600256\, s^2 v^8 \cos(2\, v) + 52324\, \cos(v)\, v^{12}$$
$$- 580517280\, v^4 \cos(2\, v) - 257175\, v^7 \sin(3\, v)$$
$$- 51435\, s^2 v^7 \sin(3\, v) + 99060\, s^2 v^8 \cos(3\, v)$$
$$- 10668\, s^6 v^4 \cos(3\, v) - 12954\, s^2 v^9 \sin(3\, v)$$
$$- 3810\, v^{11} \sin(3\, v) - 1524\, v^{12} \cos(3\, v)$$
$$- 38701152\, v^{10} - 782623296\, v^8 + 320040\, \cos(v)\, s^4 v^6$$
$$+ 2080260\, \cos(v)\, s^2 v^8 - 387011520\, v^7 \sin(2\, v)$$
$$- 38701152\, s^4 v^6 + 180605376\, s^4 v^4$$
$$+ 322509600\, s^4 v^2 - 1161034560\, s^4 v \sin(2\, v)$$
$$+ 2286\, s^2 v^{10} \cos(3\, v) - 127\, s^6 v^7 \sin(3\, v)$$
$$- 4300128\, s^4 v^6 \cos(2\, v) + 77402304\, s^4 v^4 \cos(2\, v)$$
$$+ 4880610\, \cos(v)\, s^2 v^6 + 1560195\, \sin(v)\, s^4 v^5$$
$$- 17145\, s^6 v \sin(3\, v) + 26162\, \cos(v)\, s^6 v^6$$
$$+ 14097\, \sin(v)\, s^6 v^7 - 1800225\, \sin(v)\, s^4 v^3$$
$$- 381\, s^2 v^{11} \sin(3\, v) + 34290\, \cos(v)\, s^6$$
$$+ 34401024\, s^4 v^5 \sin(2\, v) + 77402304\, s^2 v^8$$
$$- 14097\, \sin(v)\, v^{13} - 42291\, \sin(v)\, s^4 v^9$$
$$+ 42291\, \sin(v)\, s^2 v^{11} - 64770\, s^6 v^2 \cos(3\, v)$$
$$- 193505760\, v^6 \cos(2\, v) + 480060\, v^6 \cos(3\, v)$$
$$+ 19050\, s^4 v^7 \sin(3\, v) - 264922\, v^{11} \sin(v)$$
$$+ 1109472\, \cos(v)\, v^{10} - 17145\, s^6 v^3 \sin(3\, v)$$
$$+ 127\, v^{13} \sin(3\, v) - 4300128\, v^{10} \cos(2\, v)$$
$$+ 75946\, \sin(v)\, s^6 v^5 + 246126\, \sin(v)\, s^2 v^9$$
$$- 774023040\, s^2 v^5 \sin(2\, v) + 129003840\, s^4 v^3 \sin(2\, v)$$
$$+ 381\, s^4 v^9 \sin(3\, v) - 3870115200\, s^2 v^3 \sin(2\, v)$$
$$- 165735\, v^9 \sin(3\, v) - 78486\, \cos(v)\, s^2 v^{10}$$
$$- 1806053760\, s^2 v^6 + 3483103680\, s^2 v^4$$
$$+ 1935057600\, s^2 v^2$$
$$- 57150\, \sin(v)\, s^4 v^7 + 86868\, \cos(v)\, s^6 v^4$$
$$+ 580517280\, s^4 + 8600256\, v^8 \cos(2\, v)$$
$$- 215265\, \sin(v)\, s^6 v^3 - 34290\, s^6 \cos(3\, v)$$
$$- 762\, s^6 v^6 \cos(3\, v) + 387011520\, s^2 v^4 \cos(2\, v)$$
$$- 580517280\, s^4 \cos(2\, v) - 760095\, \sin(v)\, s^2 v^5$$
$$- 2286\, s^6 v^5 \sin(3\, v) + 258007680\, s^2 v^6 \cos(2\, v)$$
$$+ 560070\, s^2 v^6 \cos(3\, v) - 34401024\, v^9 \sin(2\, v)$$
$$+ 173355\, s^4 v^5 \sin(3\, v) - 222885\, \sin(v)\, s^6 v$$
$$+ 1200150\, s^2 v^4 \cos(3\, v) + 838524960\, s^4 v^2 \cos(2\, v)$$
$$- 27432\, v^{10} \cos(3\, v) - 1200150\, \cos(v)\, s^2 v^4$$
$$T_8 = -1161034560\, s^2 v^5 \cos(3\, v) + 254\, s^6 v^7 \cos(4\, v)$$
$$- 220980\, v^9 \cos(4\, v) + 290258640\, \sin(v)\, s^6$$
$$- 4572\, s^6 v^5 \cos(4\, v) - 2613660\, v^9 + 480060\, v^7$$
$$+ 79552368\, \sin(v)\, s^6 v^6 + 183642\, s^6 v^7$$
$$- 550926\, s^2 v^{11} + 400812\, s^6 v^5 - 400050\, s^2 v^7 \cos(4\, v)$$
$$- 480060\, v^7 \cos(4\, v) - 258007680\, s^2 v^7 \cos(3\, v)$$
$$+ 3773362320\, \sin(v)\, s^4 v^2 - 2103120\, v^9 \cos(2\, v)$$
$$+ 64501920\, s^2 v^8 \sin(3\, v) + 777240\, s^6 v^3 \cos(2\, v)$$
$$- 442913184\, \cos(v)\, v^{11} + 508\, v^{13} \cos(4\, v)$$
$$+ 140208\, v^{13} \cos(2\, v) - 79552368\, \sin(v)\, v^{12}$$
$$+ 180605376\, s^4 v^5 \cos(3\, v) + 34290\, s^6 v \cos(4\, v)$$
$$- 91440\, s^6 v^5 \cos(2\, v) - 4701540\, s^2 v^9$$
$$- 1002030\, s^6 v^3 - 3760470\, s^2 v^7$$
$$+ 2588677056\, \cos(v)\, v^9$$
$$+ 741772080\, s^2 v^6 \sin(3\, v) - 96752880\, s^6 \sin(3\, v)$$

$$+ 367284 v^{13} + 704088 v^{11} - 49530 s^6 v^3 \cos(4v)$$
$$- 15240 v^{10} \sin(4v) - 926592 v^{12} \sin(2v)$$
$$- 12900384 s^6 v^4 \sin(3v) + 411480 s^6 v^2 \sin(2v)$$
$$- 580517280 \cos(v) s^4 v + 1440542880 \sin(v) v^{10}$$
$$+ 290258640 s^4 v^4 \sin(3v) - 290258640 \sin(v) v^6$$
$$- 1354540320 \cos(v) v^7 + 231648 s^6 v^6 \sin(2v)$$
$$- 8128 v^{12} \sin(4v) + 2418822000 \sin(v) s^2 v^4$$
$$- 6720840 s^2 v^7 \cos(2v) - 762 s^2 v^{11} \cos(4v)$$
$$- 580517280 \cos(v) v^5 - 2225316240 \sin(v) v^8$$
$$- 210312 s^2 v^{11} \cos(2v) + 3644358480 \sin(v) s^4 v^4$$
$$- 137160 v^8 \sin(4v) - 967528800 v^7 \cos(3v)$$
$$- 1200150 s^2 v^5 \cos(4v) + 1096532640 s^4 v^3 \cos(3v)$$
$$+ 38701152 s^4 v^6 \sin(3v) + 70104 s^6 v^7 \cos(2v)$$
$$+ 12900384 s^4 v^7 \cos(3v) - 22860 s^2 v^9 \cos(4v)$$
$$- 33528 v^{11} \cos(4v) - 1280160 v^{11} \cos(2v)$$
$$+ 137160 s^6 v^4 \sin(2v) + 1234440 s^2 v^8 \sin(2v)$$
$$+ 68580 s^2 v^8 \sin(4v) - 96752880 s^6 v^2 \sin(3v)$$
$$+ 7620 s^6 v^4 \sin(4v) + 2150064 s^4 v^8 \sin(3v)$$
$$- 2150064 s^2 v^{10} \sin(3v) + 1935057600 s^2 v^3 \cos(3v)$$
$$+ 38701152 \sin(v) s^6 v^4 - 1935057600 \cos(v) s^2 v^3$$
$$- 238657104 \sin(v) s^4 v^8 + 960120 s^2 v^6 \sin(2v)$$
$$+ 822960 v^8 \sin(2v) + 716688 v^{12} \sin(3v)$$
$$- 90302688 v^{10} \sin(3v) - 1285738272 \sin(v) s^4 v^6$$
$$- 25800768 s^2 v^9 \cos(3v) - 160020 s^2 v^6 \sin(4v)$$
$$- 68580 s^6 v^2 \sin(4v) - 34290 s^6 v + 1200150 s^2 v^5$$
$$- 716688 s^6 v^6 \sin(3v) - 266607936 v^9 \cos(3v)$$
$$+ 12900384 v^{11} \cos(3v) - 442913184 \cos(v) s^4 v^7$$
$$+ 6096 s^2 v^{10} \sin(4v) + 885826368 \cos(v) s^2 v^9$$
$$- 3418601760 \cos(v) s^4 v^3 + 774023040 \cos(v) s^6 v^3$$
$$- 1470643776 \cos(v) s^4 v^5 + 2580076800 \cos(v) s^2 v^7$$
$$+ 2032 s^6 v^6 \sin(4v) + 4353879600 s^2 v^4 \sin(3v)$$
$$+ 238657104 \sin(v) s^2 v^{10} - 6579195840 \cos(v) s^2 v^5$$
$$+ 580517280 s^4 v \cos(3v) + 483764400 \sin(v) s^2 v^6$$
$$+ 580517280 v^5 \cos(3v) - 2286000 s^2 v^9 \cos(2v)$$
$$- 193505760 \sin(v) s^2 v^8 + 290258640 s^4 v^2 \sin(3v)$$
$$+ 694944 s^2 v^{10} \sin(2v) - 274320 v^{10} \sin(2v)$$
$$+ 96752880 v^8 \sin(3v) + 1644798960 v^6 \sin(3v)$$
$$- 870775920 \sin(v) s^6 v^2$$

$$T_{denom5} = 580517280 v^4 + 1354540320 v^6$$
$$+ 2293620 \cos(v) v^8$$
$$- 480060 \cos(v) v^6 - 1369695 v^9 \sin(v)$$
$$+ 222885 v^7 \sin(v) - 1161034560 v^5 \sin(2v)$$
$$+ 175260 v^8 \cos(3v) + 52324 \cos(v) v^{12}$$
$$- 580517280 v^4 \cos(2v) - 257175 v^7 \sin(3v)$$
$$- 3810 v^{11} \sin(3v) - 1524 v^{12} \cos(3v)$$
$$- 38701152 v^{10} - 782623296 v^8 - 387011520 v^7 \sin(2v)$$
$$- 14097 \sin(v) v^{13} - 193505760 v^6 \cos(2v)$$
$$+ 480060 v^6 \cos(3v) - 264922 v^{11} \sin(v)$$
$$+ 1109472 \cos(v) v^{10} + 127 v^{13} \sin(3v)$$
$$- 4300128 v^{10} \cos(2v) - 165735 v^9 \sin(3v)$$
$$+ 8600256 v^8 \cos(2v) - 34401024 v^9 \sin(2v)$$
$$- 27432 v^{10} \cos(3v)$$

$$T_{denom6} = -782623296 v^9 + 1354540320 v^7$$
$$+ 580517280 v^5 + 8600256 v^9 \cos(2v) + 52324 \cos(v) v^{13}$$
$$- 1524 \cos(3v) v^{13} - 580517280 v^5 \cos(2v)$$
$$+ 1109472 \cos(v) v^{11} - 264922 \sin(v) v^{12}$$
$$+ 2293620 \cos(v) v^9 - 38701152 v^{11} - 1369695 \sin(v) v^{10}$$
$$- 480060 \cos(v) v^7 - 1161034560 v^6 \sin(2v)$$
$$- 14097 \sin(v) v^{14} + 127 \sin(3v) v^{14}$$
$$+ 222885 \sin(v) v^8 + 480060 v^7 \cos(3v)$$
$$- 4300128 v^{11} \cos(2v) - 387011520 v^8 \sin(2v)$$
$$- 3810 v^{12} \sin(3v) - 165735 v^{10} \sin(3v)$$
$$+ 175260 v^9 \cos(3v) - 27432 v^{11} \cos(3v)$$
$$- 34401024 v^{10} \sin(2v) - 193505760 v^7 \cos(2v)$$
$$- 257175 v^8 \sin(3v)$$