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A High Order Multistage Scheme with Improved Properties

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Abstract

A high algebraic order P–stable symmetric multistage two–step scheme with eliminated phase–lag and its derivatives up to order five is obtained, for the first time in the literature, in this paper. In order to develop the new multistage scheme we follow the next steps:

- Gratification of the necessary and sufficient junctures for P–stability.
- Gratification of the juncture of the eliminating of the phase–lag.
- Gratification of the junctures of the eliminating of the derivatives of the phase–lag up to order five.

The above methodology, guides to the development of the coefficients of the new multistage scheme.

The achievement of the above developments is the construction, for the first time in the literature, of a multistage P–stable tenth algebraic order symmetric two–step scheme with eliminated phase–lag and its first, second, third, fourth and fifth derivatives.

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The new multistage scheme is analyzed numerically and theoretically, based on the following points:

- the construction of the new multistage scheme ,
- the calculation and the frmulation of its local truncation error (LTE),
- the determination of the asymptotic form of the LTE of the new multistage scheme,
- the stability and interval of periodicity analysis of the new multistage scheme,
- the determination of an embedded multistage scheme and the denotation of the variable step procedure for the changing of the step lengths,
- the testing of the computational effectiveness of the new multistage scheme with application on:
  - the resonance problem of the radial Schrödinger equation and on
  - the system of the coupled differential equations of the Schrödinger type.

The above analysis leads to the conclusion that the new multistage scheme is more efficient schem than the existed ones.

1 Introduction

A new multistage P–stable scheme with vanished phase–lag and its derivatives up to order five is obtained, for the first time in the literature, in this paper.

The construction of the new proposed scheme is based on the following stages:

- Satisfaction of the property of the P–stability.
- Satisfaction of the property for the vanishing of the phase–lag.
- Satisfaction of the properties for the vanishing of the derivatives of the phase–lag up to order five.

We will test the efficiency of the new proposed multistage scheme by applying it to:

- the radial time independent Schrödinger equation and
- Systems of coupled differential equations of the Schrödinger type.

The effective computational solution of the above mentioned problems is very important in Computational Chemistry (see [9] and references therein) since an important part of the quantum chemical computations contains the Schrödinger equation (see [9] and references therein). We mention here that in problems with more than one particle the computational solution of the Schrödinger equation is necessary. The effective computational solution of the Schrödinger's equation (via numerical schemes) gives us the following important information:

- numerical calculations of molecular properties (vibrational energy levels and wave functions of systems) and
- numerical presentment of the electronic structure of the molecule (see for more details in [10–13]).

Based on the new constructed multistage scheme, we will also construct an embedded computational scheme which is based on an local truncation error control technique and a variable–step method.

The problems studied in this paper belong to the following category of special problems:

$$\zeta''(x) = f(x, \zeta), \;\; \zeta(x_0) = \zeta_0 \;\; and \;\; \zeta'(x_0) = \zeta'_0. \tag{1}$$

which have periodical and/or oscillating solutions.

In the following we present the main classes of numerical schemes and their bibliography which is based on the large research which has been taken place the last decades:

- Exponentially, trigonometrically and phase fitted Runge–Kutta and Runge–Kutta Nyström schemes: [47], [50], [59], [62] – [67], [56] [78]. In this class of methods, Runge–Kutta and Runge–Kutta Nyström schemes are developed. This class can be divided into two subcategories:
  - Numerical schemes which have the property of accurate integration of sets of functions of the form:

$$\begin{aligned} x^i \, \cos(\omega\, x)\,,\; i = 0, 1, 2, \ldots \text{or} \;\; x^i \, \sin(\omega\, x)\,,\; i = 0, 1, 2, \ldots \\ \text{or} \;\; x^i \, \exp(\omega\, x)\,,\; i = 0, 1, 2, \ldots \end{aligned} \tag{2}$$

    or sets of functions which are combination of the above functions.
  - Numerical schemes which have the property of vanishing (or elimination) of the phase–lag.

Remark 1. *The frequency of the problem in (2) is denoted by the quantity* ω *.*

- Multistep exponentially, trigonometrically and phase fitted methods and multistep algorithms with minimal phase–lag: [1]– [7], [18]– [21], [25]– [28], [34], [38], [40], [44], [48]– [49], [53], [58], [60]– [61], [71]– [73], [79]– [82]. In this class of methods, multistep schemes are developed. This class can be divided into two subcategories:
  - Multistep schemes which have the property of accurate integration of sets of functions of the form (2) or sets of functions which are combination of the functions mentioned in (2).
  - Multistep schemes which have the property of vanishing (or elimination) of the phase–lag.
- Symplectic integrators: [42]– [43], [51], [54], [57], [67]– [70], [76]. In this class of numerical schemes, methods for which the Hamiltonian energy of the system remains almost constant during the integration procedure, are obtained.
- Nonlinear methods: [52]. In this category of numerical schemes, the algorithms have nonlinear form (i.e. the relation between several approximations of the function on several points of the integration domain (i.e. y_{n+j}, $j = 0, 1, 2, \ldots$) is nonlinear).
- General methods: [14]– [17], [22]– [24], [35]– [37], [41]. In the category of numerical schemes, numerical methods with constant coefficients are constructed.

2 Theory for the development of symmetric multistep schemes

The theory for the construction of the symmetric multistep schemes is described in this section.

The technique used for the numerical solution of the problems of the form (1) is the use of the discretization of the integration domain. In our case, the integration domain $[a, b]$ is discretized by using the $2\,m$-step scheme the formula of which is described below by the relation (3). For these type of algorithms their parameter m denotes the number of the discretization points.

The following symbols are used:

- h denotes the step length of the integration which is the same with the stepsize of the discretization. Is determined using the following relation: $h = |x_{i+1} - x_i|$,

$i = 1 - m(1)m - 1$ (i.e. the parameter i is moved between $1 - m$ and $m - 1$ with step 1) where

- x_n determines the n-th point on the discretized domain.
- ζ_n determines the approximation of the function $\zeta(x)$ at the point x_n. It is noted the in order to achieve the approximation ζ_n we use a numerical scheme and in our study we use the $2\,m$-step method (3) described below

We consider the family of $2\,m$-step schemes:

$$\Delta\,(m) : \sum_{i=-m}^{m} \alpha_i\,\zeta_{n+i} = h^2 \sum_{i=-m}^{m} \beta_i\,f(x_{n+i}, \zeta_{n+i}) \tag{3}$$

The above family of algorithms us used for the approximate solution of the initial value problem (1) on the integration domain $[a, b]$, where α_i and β_i $i = -m(1)m$ are the coefficients of the $2\,m$-step scheme.

Definition 1.

$$\Delta\,(m) \rightarrow \begin{cases} \beta_m \neq 0 & \textit{implicit;} \\ \beta_m = 0 & \textit{explicit.} \end{cases} \tag{4}$$

Definition 2.

$$\Delta\,(m) \;\; \textit{with}\; \alpha_{i-m} = \alpha_{m-i},\, \beta_{i-m} = \beta_{m-i},\, i = 0(1)m \rightarrow \textit{symmetric} \tag{5}$$

Remark 2. *The scheme $\Delta\,(m)$ is related with the following linear operator*

$$L(x) = \sum_{i=-m}^{m} \alpha_i\,\zeta(x + i\,h) - h^2 \sum_{i=-m}^{m} \beta_i\,\zeta''(x + ih) \tag{6}$$

where $\zeta \in \mathbb{C}^2$ (i.e. $\mathbb{C}^2 \equiv \mathbb{C}x\mathbb{C}$).

Definition 3. *[14] We call that the multistep scheme (3) has an algebraic order τ, if the linear operator L (6) is eliminated for any linear combination of the linearly independent functions* $1,\, x,\, x^2,\, \ldots,\, x^{\tau+1}$.

Application of the symmetric $2\,m$-step scheme $\Delta\,(m)$ to the test equation

$$\zeta'' = -\phi^2\,\zeta \tag{7}$$

leads to the difference equation:

$$\Upsilon_m(v)\,\zeta_{n+m} + ... + \Upsilon_1(v)\,\zeta_{n+1} + \Upsilon_0(v)\,\zeta_n$$
$$+\Upsilon_1(v)\,\zeta_{n-1} + ... + \Upsilon_m(v)\,\zeta_{n-m} = 0 \tag{8}$$

and its associated characteristic equation:

$$\Upsilon_m(v)\,\lambda^m + ... + \Upsilon_1(v)\,\lambda + \Upsilon_0(v)$$
$$+\Upsilon_1(v)\,\lambda^{-1} + ... + \Upsilon_m(v)\,\lambda^{-m} = 0. \tag{9}$$

where

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

Definition 4. [15] *A symmetric* $2\,m$*-step scheme is called that has an non zero interval of periodicity* $(0, v_0^2)$*, if its characteristic equation (9)has the following roots :*

$$\lambda_1 = e^{i\psi(v)},\ \lambda_2 = e^{-i\psi(v)},\ \text{and } |\lambda_\mathrm{i}| \leq 1,\ \mathrm{i} = 3(1)2\,\mathrm{m} \tag{10}$$

for all $v \in (0, v_0^2)$*, where* $\psi(v)$ *is a real function of* v*.*

Definition 5. *(see [15]) A symmetric multistep scheme is called* **P-stable** *it its interval of periodicity is equal to* $(0, \infty)$*.*

Remark 3. *A symmetric multistep scheme is called* **P-stable** *if the following necessary and sufficient conditions are hold:*

$$|\lambda_1| = |\lambda_2| = 1 \tag{11}$$
$$|\lambda_j| \leq 1, j = 3(1)2m,\ \forall v. \tag{12}$$

Definition 6. *A symmetric multistep scheme is called singularly P-stable if its interval of periodicity is equal to* $(0, \infty)\backslash S$*, where* S *is a finite set of points.*

Definition 7. [16], [17] *A symmetric multistep scheme with associated characteristic equation given by (9), has phase-lag which is defined by the leading term in the expansion of*

$$t = v - \psi(v). \tag{13}$$

If $t = O(v^{\gamma+1})$ *as* $v \to \infty$ *then the phase-lag order is called as equal to* γ.

Definition 8. *[18] A symmetric multistep scheme is called as* **phase-fitted** *if its phase-lag is equal to zero.*

Theorem 1. [16] *For a symmetric* $2\,m$*-step scheme, with characteristic equation given by (9), a direct formula for the computation of the phase-lag order* υ *and the phase-lag constant* ϖ *is given by*

$$-\varpi v^{\upsilon+2} + O(v^{\upsilon+4}) = \frac{2\,\Upsilon_m(v)\,\cos(m\,v) + \ldots + 2\,\Upsilon_j(v)\,\cos(j\,v) + \ldots + \Upsilon_0(v)}{2\,m^2\,\Upsilon_m(v) + \ldots + 2\,j^2\,\Upsilon_j(v) + \ldots + 2\,\Upsilon_1(v)} \tag{14}$$

Remark 4. *For the symmetric two–step methods the phase-lag order* υ *and the phase-lag constant* ϖ *can be directly computed using the formula:*

$$-\varpi v^{\upsilon+2} + O(v^{\upsilon+4}) = \frac{2\,\Upsilon_1(v)\,\cos(v) + \Upsilon_0(v)}{2\,\Upsilon_1(v)} \tag{15}$$

where $\Upsilon_j(v)\, j = 0, 1$ *are the stability polynomials.*

3 A new multistage P–stable symmetric scheme with eliminated phase–lag and its first, second, third, fourth and fifth derivatives

The following family of multistage schemes is considered:

$$\begin{aligned}
\widehat{\zeta}_{n+1} &= \zeta_{n+1} - h^2 \left(c_1\, f_{n+1} - c_0\, f_n + c_1\, f_{n-1} \right) \\
\tilde{\zeta}_{n+1} &= \zeta_{n+1} - h^2 \left(c_3\, \widehat{f}_{n+1} - c_2\, f_n + c_3\, f_{n-1} \right) \\
\zeta_{n+1} + a_1\, \zeta_n + \zeta_{n-1} &= h^2 \left[b_1 \left(\tilde{f}_{n+1} + f_{n-1} \right) + b_0\, f_n \right]
\end{aligned} \tag{16}$$

where $f_{n+i} = \zeta''\left(x_{n+i}, \zeta_{n+i}\right), i = -1(1)1,\ \widehat{f}_{n+1} = \zeta''\left(x_{n+1}, \widehat{q}_{n+1}\right),\ \tilde{f}_{n+1} = \zeta''\left(x_{n+1}, \tilde{\zeta}_{n+1}\right)$ and a_1, b_i, $i = 0,\ 1$ and c_j, $i = 0\,(1)\,3$ are parameters.

Remark 5. *The new multistage scheme is nonlinear. All the approximations are based on the point* x_{n+1}.

The following specific case is considered:

$$b_1 = \frac{1}{12}. \tag{17}$$

Remark 6. *The above set of parameters ensures that the new multistage scheme (16) will have the maximum possible algebraic order.*

If we apply the new proposed multistage pair (16) with the constant coefficient given by (17) to the scalar model (7), we obtain the difference equation (8) with $m = 1$ and the corresponding characteristic equation (9) with $m = 1$ with:

$$\begin{aligned} \Phi_1(v) &= 1 + \frac{1}{12} v^2 \left(1 + v^2 c_3 + v^4 c_1 c_3\right) \\ \Phi_0(v) &= a_1 + \frac{1}{12} v^2 \left(12 b_0 - v^2 c_2 - v^4 c_0 c_3\right) \end{aligned} \tag{18}$$

The stages for the construction of the new proposed multistage scheme are presented in the flowchart of Figure 1 (for developing flowcharts in LaTeX one can see [90]):

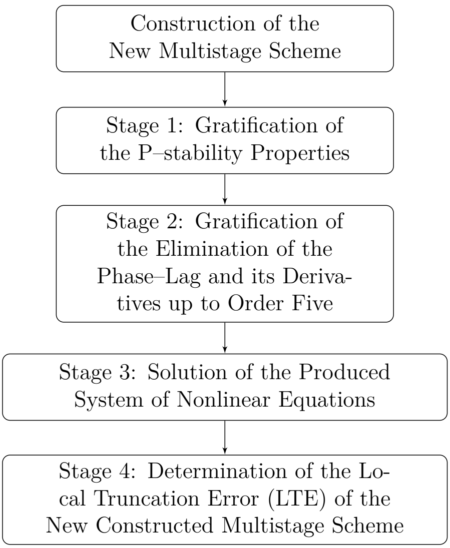

Figure 1. Flowchart for the stages requested for the development of the new proposed multistage scheme

3.1 Gratification of the property of the P–stability

We use the methodology first introduced by Lambert and Watson [15] and Wang [83] in order to determine the conditions of the P–stability for the new multistage scheme:

- Request of gratification of the characteristic equation given by (9) with $m = 1$ for $\lambda = e^{I\,v}$, where $I = \sqrt{-1}$, leads to the following equation:

$$\left(\mathrm{e}^{I\,v}\right)^2 \, \Phi_0\,(v) + \mathrm{e}^{I\,v}\,\Phi_1\,(v) + \Phi_0\,(v) = 0 \tag{19}$$

- Request of gratification of the characteristic equation given by (9) with $m = 1$ for $\lambda = e^{-I\,v}$, where $I = \sqrt{-1}$, leads to the following equation:

$$\left(\mathrm{e}^{-I\,v}\right)^2 \, \Phi_0\,(v) + \mathrm{e}^{-I\,v}\,\Phi_1\,(v) + \Phi_0\,(v) = 0 \tag{20}$$

Remark 7. *We obtain the above mentioned conditions for P–stability based on*

- *the Definition 4*
- *the characteristic equation given by (9) with $m = 1$, where Φ_j, $j = 0, 1$ given by (18).*

3.2 Gratification of the elimination of the phase–lag and its derivatives up to order five

The request of gratification of the elimination of the phase–lag and its derivatives up to order five for the new multistage scheme (16) with the coefficients given by (17), gives us the following system of equations:

$$\mathrm{Phase-Lag(PL)} = \frac{1}{2}\,\frac{\Upsilon_0\,(v)}{v^6 c_1 c_3 + v^4 c_3 + v^2 + 12} = 0 \tag{21}$$

$$\mathrm{First\,Derivative\,of\,the\,Phase-Lag} = \frac{\Upsilon_1\,(v)}{\left(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12\right)^2} = 0 \tag{22}$$

$$\mathrm{Second\,Derivative\,of\,the\,Phase-Lag} = \frac{\Upsilon_2\,(v)}{\left(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12\right)^3} = 0 \tag{23}$$

$$\mathrm{Third\,Derivative\,of\,the\,Phase-Lag} = \frac{\Upsilon_3\,(v)}{\left(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12\right)^4} = 0 \tag{24}$$

$$\mathrm{Fourth\,Derivative\,of\,the\,Phase-Lag} = \frac{\Upsilon_4\,(v)}{\left(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12\right)^5} = 0 \tag{25}$$

$$\text{Fifth Derivative of the Phase} - \text{Lag} = \frac{\Upsilon_5\left(v\right)}{\left(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12\right)^6} = 0 \tag{26}$$

where $\Upsilon_j\left(v\right), \, j = 0(1)5$ are given in the Appendix A.

3.3 Solution of the system of nonlinear equations determined by (19) - (26)

Solving the nonlinear system of equations (19), (20), (21)–(26), we obtain the coefficients of the new multistage scheme:

$$\begin{aligned} a_1 &= -\frac{1}{36}\frac{\Upsilon_6\left(v\right)}{\Upsilon_7\left(v\right)}, \quad c_0 = -\frac{1}{6}\frac{\Upsilon_8\left(v\right)}{\Upsilon_9\left(v\right)} \\ c_1 &= -\frac{1}{2}\frac{\Upsilon_{10}\left(v\right)}{\Upsilon_9\left(v\right)}, \quad c_2 = -\frac{\Upsilon_{11}\left(v\right)}{v^4\,\Upsilon_7\left(v\right)} \\ c_3 &= -2\,\frac{\Upsilon_{12}\left(v\right)}{v^4\,\Upsilon_7\left(v\right)}, \quad b_0 = -\frac{1}{12}\frac{\Upsilon_{13}\left(v\right)}{v\,\Upsilon_7\left(v\right)} \end{aligned} \tag{27}$$

where $\Upsilon_j\left(v\right), \, j = 6(1)13$ are given in the Appendix B.

The probability of cancellations or the probability of impossibility of computation of the coefficients (27), during the integration procedure (Example of cancellation: $|\Upsilon_j\left(v\right)| \Rightarrow 0$, $j = 7, \, 9$ for some values of $|v|$), leads us to give the truncated Taylor series expansions of the coefficients developed in (27) in the Appendix C.

The behavior of new obtained coefficients is presented in Figure 1.

Based on the Figure 1, the last stage of the construction of the new multistage scheme is the denotation of its local truncation error (LTE):

$$\begin{aligned} LTE_{NM3SPS5DV} = -\frac{1}{23950080}\,h^{12}\Big(&\zeta_n^{(12)} + 6\,\phi^2\,\zeta_n^{(10)} + 15\,\phi^4\,\zeta_n^{(8)} \\ &+20\,\phi^6\,\zeta_n^{(6)} + 15\,\phi^8\,\zeta_n^{(4)} + 6\,\phi^{10}\,\zeta_n^{(2)} + \phi^{12}\,\zeta_n\Big) + O\left(h^{14}\right). \end{aligned} \tag{28}$$

The new developed multistage scheme is defined as $NM3SPS5DV$. The explanation of the abbreviation $NM3SPS5DV$ is: New Method of Three–Stages P–Stable with Vanished Phase–Lag and its Derivatives up to Order Five.

Remark 8. *The LTE formula (28) is useful for*

- *the denotation of the algebraic order of the new multistage scheme*
- *for the development of the asymptotic form of the local error which is important for the evaluation of the efficiency of the new scheme.*

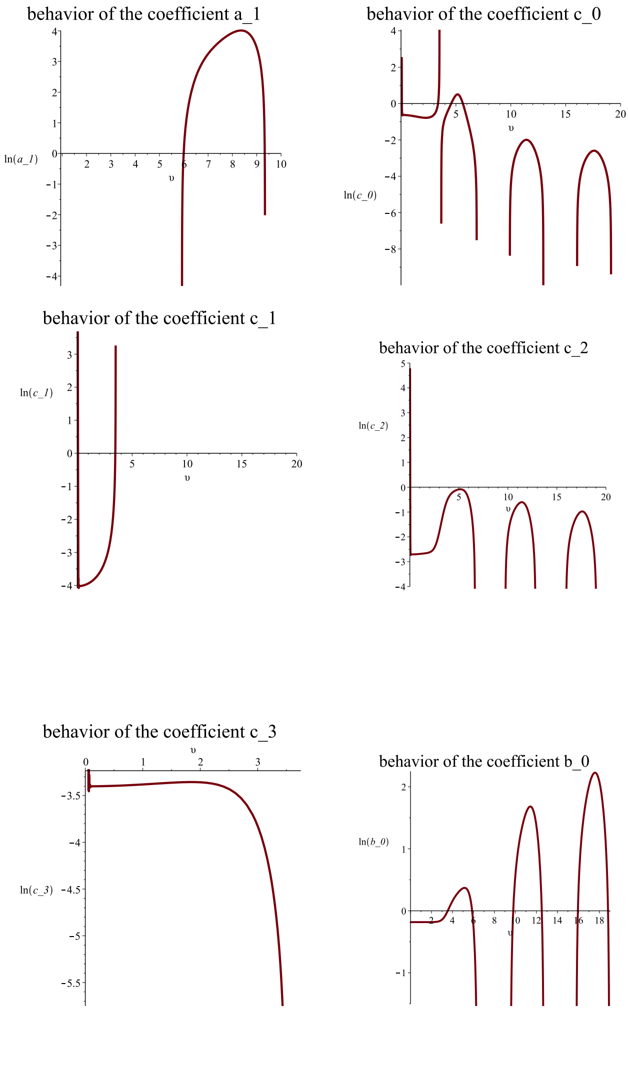

Figure 2. Presentation of the behavior of the coefficients of the new multistage scheme (16) given by (27) for several values of $v = \phi\, h$.

4 Local truncation error and stability analysis of the new multistage scheme

4.1 Comparative local truncation error analysis

In this chapter the local truncation error of some multistage schemes of similar form are evaluated. The model on which is based the above mentioned evaluation is given by:

$$\zeta''(x) \;=\; (V(x) - V_c + \Gamma)\;\zeta(x) \tag{29}$$

where

- $V(x)$ denotes the potential function,
- V_c denotes a constant approximation of the potential on the specific point x,
- $\Gamma = V_c - E$
- $\Xi(x) = V(x) - V_c$ and
- E denotes the energy.

Remark 9. *It is easy to see studying the equation (29) that the above mentioned model problem is the radial Schrödinger equation with potential $V(x)$.*

The following multistage schemes are evaluated:

4.1.1 Classical method (i.e., method (16) with constant coefficients)

$$LTE_{CL} = -\frac{1}{23950080}\,h^{12}\,\zeta_n^{(12)} + O\left(h^{14}\right). \tag{30}$$

4.1.2 P–stable linear six–step method of wang [83]

$$LTE_{WANGPSL6S} = -\frac{81}{44800}\,h^{10}\left(\zeta_n^{(10)} + 10\,\phi^{10}\,\zeta_n\right) + O\left(h^{12}\right). \tag{31}$$

4.1.3 P–stable method with vanished phase–lag and its first and second derivatives developed in [6]

$$LTE_{NM3SPS2DV} = -\frac{1}{47900160}\,h^{12}\Big(2\,\zeta_n^{(12)} - 9\,\phi^4\,\zeta_n^{(8)} - 8\,\phi^6\,\zeta_n^{(6)} - \phi^{12}\,\zeta_n\Big) + O\left(h^{14}\right). \tag{32}$$

4.1.4 P–stable scheme with vanished phase–lag and its first, second and third derivatives developed in [7]

$$LTE_{NM3SPS3DV} = -\frac{1}{23950080}\, h^{12} \Big(\zeta_n^{(12)} - 9\,\phi^4\,\zeta_n^{(8)} \\ -16\,\phi^6\,\zeta_n^{(6)} - 9\,\phi^8\,\zeta_n^{(4)} + \phi^{12}\,\zeta_n \Big) + O\left(h^{14}\right). \tag{33}$$

4.1.5 P–stable scheme with vanished phase–lag and its first, second, third and fourth derivatives developed in [8]

$$LTE_{NM3SPS4DV} = -\frac{1}{119750400}\, h^{12} \Big(5\,\zeta_n^{(12)} + 24\,\phi^2\,\zeta_n^{(10)} + 45\,\phi^4\,\zeta_n^{(8)} \\ +40\,\phi^6\,\zeta_n^{(6)} + 15\,\phi^8\,\zeta_n^{(4)} - \phi^{12}\,\zeta_n \Big) + O\left(h^{14}\right). \tag{34}$$

4.1.6 P–stable scheme with vanished phase–lag and its first, second, third, fourth and fifth derivatives developed in Section 3

The formula of the Local Truncation Error for this multistage scheme is given by (28)

The methodology for the comparative local truncation error analysis is the following:

- Step 1: Application of the LTE formulae given by (30), (31), (32), (33), (34) and (28) to the scalar problem (29).

- Step 2: Step 1 leads to the new formulae of LTE.

  Remark 10. *The derivation of the new expressions of LTE is based on the substitution of the derivatives of the function ζ (which are determined using the scalar problem (29)) in the formulae given by (30), (31), (32), (33), (34) and (28). We give some formulae of the derivatives of the function ζ in the Appendix D.*

- Step 3: Step 2 leads to the new formulae of LTE for the multistage schemes which are under evaluation.

  Remark 11. *Observing the new formulae of LTE it is easy to see that the characteristic of these formulae is the inclusion of the parameter Γ and the energy E.*

  The general form of the new formulae of LTE can be written as:

$$LTE = h^p \sum_{j=0}^{k} \Psi_j \, \Gamma^j \tag{35}$$

with Ψ_j:

1. real numbers (frequency independent cases i.e. the classical case) or
2. formulae of v and Γ (frequency dependent schemes),

p is the algebraic order of the multistage scheme and k is the maximum possible power of Γ in the formulae of LTE.

- Step 4: We investigate two set of values for the parameter Γ:

  1. **The Potential is Closed to the Energy.**

     Consequences:

$$\Gamma \approx 0 \Rightarrow \Gamma^i \approx 0, \; i = 1, 2, \ldots. \tag{36}$$

which leads to:

$$LTE_{\Gamma=0} = h^k \, \Lambda_0 \tag{37}$$

Remark 12. *The quantity Λ_0 is the same for all the multistage schemes of the same family, i.e. $LTE_{CL} = LTE_{NM3SPS2DV} = LTE_{NM3SPS3DV} = LTE_{NM3SPS4DV} = LTE_{NM3SPS5DV} = h^{12} \, \Lambda_0$. Λ_0 is given in the Appendix E.*

Theorem 2. *Based on the formula (36) we conclude that for $\Gamma = V_c - E \approx 0$ the local truncation error of the classical method (constant coefficients - (30)), the local truncation error of the scheme with vanished phase–lag and its first and second derivatives developed in [6] (with LTE given by (32), the local truncation error for the algorithm with vanished phase–lag and its first, second and third derivatives developed in [7] (with LTE given by (33), the local truncation error for the algorithm with vanished phase–lag and its first, second, third and fourth derivatives developed in [8] (with LTE given by (34)) and the local truncation error for the numerical pair with vanished phase–lag and its first, second, third, fourth and fifth derivatives developed in Section 3 (with*

LTE given by (28), are the same and equal to $h^{12}\,\Lambda_0$, where Λ_0 is given in the Appendix E.

2. **The Energy and the Potential are far from each other.** Therefore, $\Gamma >> 0 \vee \Gamma << 0 \Rightarrow |\Gamma| >> 0$.

   Consequences:

   The most accurate multistage scheme is the one with formula of its asymptotic form of LTE, given by (35), which contains the minimum power of Γ (i.e. minimum values for k) and the maximum value of p.

- Based on the above we obtain the following asymptotic forms of the LTE formulae for the multistage schemes which are under evaluation.

4.1.7 Classical method

The Classical Method is the method (16) with constant coefficients.

$$LTE_{CL} = -\frac{1}{23950080}\, h^{12} \left(\zeta\,(x)\; \Gamma^6 + \cdots \right) + O\left(h^{14}\right). \tag{38}$$

We present here the leading term in the asymptotic form of the Local Truncation Error. Consequently, the symbol $\cdots$ means that there are also terms for $\Gamma^j\; j = 0\,(1)\,5$.

4.1.8 4.1.7. P–stable linear six–step method of Wang [83]

This is the method presented in Linear Six–step Method presented in [83] (see in [83] equations (23)-(27). We note also here that there is a missprint in the paper [83]. In formula (25) $2\,C_{3,0}\,y''_{k+2}$ must be replaced by the correct: $2\,C_{3,0}\,y''_{k+3}$.

$$LTE_{WANGPSL6S} = -\frac{81}{8960}\, h^{10} \left(\Xi\,(x)\; \zeta\,(x)\; \Gamma^4 + \cdots \right) + O\left(h^{12}\right). \tag{39}$$

We present here the leading term in the asymptotic form of the Local Truncation Error. Consequently, the symbol $\cdots$ means that there are also terms for $\Gamma^j\; j = 0\,(1)\,3$.

4.1.9 P–stable method with vanished phase–lag and its first and second derivatives developed in [6].

This is the P–stable method which we developed in [6].

$$LTE_{NM3SPS2DV} = -\frac{1}{997920}\,h^{12}\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi\left(x\right)\zeta\left(x\right)\,\Gamma^4\right.$$
$$\left.+\cdots\right)+O\left(h^{14}\right). \tag{40}$$

We present here the leading term in the asymptotic form of the Local Truncation Error. Consequently, the symbol $\cdots$ means that there are also terms for $\Gamma^j\; j=0\,(1)\,3$.

4.1.10 P–stable scheme with vanished phase–lag and its first, second and third derivatives developed in [7]

This is the P–stable method which we developed in [7].

$$LTE_{NM3SPS3DV} = -\frac{1}{997920}\,h^{12}\left[\left[4\,\Xi\left(x\right)\,\zeta\left(x\right)\,\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi\left(x\right)+7\,\zeta\left(x\right)\,\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi\left(x\right)\right.\right.$$
$$\left.\left.+2\,\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi\left(x\right)\frac{\mathrm{d}}{\mathrm{d}x}\zeta\left(x\right)+3\,\zeta\left(x\right)\,\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)^2\right]\Gamma^3+\cdots\right]+O\left(h^{14}\right). \tag{41}$$

We present here the leading term in the asymptotic form of the Local Truncation Error. Consequently, the symbol $\cdots$ means that there are also terms for $\Gamma^j\; j=0\,(1)\,2$.

4.1.11 P–stable scheme with vanished phase–lag and its first, second, third and fourth derivatives developed in [8]

This is the P–stable method which we developed in [8].

$$LTE_{NM3SPS4DV} = -\frac{1}{1247400}\,h^{12}\left[\left[\zeta\left(x\right)\,\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi\left(x\right)\right]\Gamma^3\right.$$
$$\left.+\cdots\right]+O\left(h^{14}\right). \tag{42}$$

We present here the leading term in the asymptotic form of the Local Truncation Error. Consequently, the symbol $\cdots$ means that there are also terms for $\Gamma^j\; j=0\,(1)\,2$.

4.1.12 P–stable scheme with vanished phase–lag and its first, second, third, fourth and fifth derivatives developed in Section 3

$$LTE_{NM3SPS5DV} = -\frac{1}{1496880}\,h^{12}\left[\left[6\,\Xi\left(x\right)\,\zeta\left(x\right)\,\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi\left(x\right)\right.\right.$$

$$+15\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)\zeta\left(x\right)\,\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi\left(x\right)+2\,\frac{\mathrm{d}^{5}}{\mathrm{d}x^{5}}\Xi\left(x\right)\,\frac{\mathrm{d}}{\mathrm{d}x}\zeta\left(x\right)$$
$$+10\,\zeta\left(x\right)\,\left(\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi\left(x\right)\right)^{2}+5\,\zeta\left(x\right)\,\frac{\mathrm{d}^{6}}{\mathrm{d}x^{6}}\Xi\left(x\right)\Bigg]\,\Gamma^{2}+\cdots\Bigg]+O\left(h^{14}\right). \tag{43}$$

We present here the leading term in the asymptotic form of the Local Truncation Error. Consequently, the symbol $\cdots$ means that there are also terms for Γ^j $j = 0,\, 1$.

The above analysis leads to the following theorem:

Theorem 3.

- *Classical Method (i.e., the method (16) with constant coefficients): For this method the error increases as the sixth power of* Γ.

- *P–stable Linear Six–step Method of Wang [83]: For this method the error increases as the fourth power of* Γ.

- *P–Stable Tenth Algebraic Order Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in [6]: For this method the error increases as the fourth power of* Γ.

- *P–Stable Tenth Algebraic Order Method with Vanished Phase–Lag and Its First, Second and Third Derivatives Developed in [7]: For this method the error increases as the third power of* Γ.

- *P–Stable Tenth Algebraic Order Method with Vanished Phase–Lag and Its First, Second, Third and Fourth Derivatives Developed in [8]: For this method the error increases as the third power of* Γ.

- *P–Stable Tenth Algebraic Order Method with Vanished Phase–Lag and Its First, Second, Third, Fourth and Fifth Derivatives Developed in Section 3: For this method the error increases as the second power of* Γ.

Consequently, for the numerical solution of the time independent radial Schrödinger equation, which is the scalar model for the local truncation error analysis, the new multistage scheme with vanished phase–lag and its derivatives up to order five is the most accurate one.

4.2 Stability analysis

We will use for our analysis the following test equation:

$$\zeta'' = -\omega^2 \, \zeta. \tag{44}$$

Remark 13. *Observing (7) and (44) we conclude that $\omega \neq \phi$, where ϕ is the frequency of the test problem (7) (phase–lag analysis) and ω is the frequency of the test problem (44) (stability analysis).*

If we apply the new multistage scheme (16) to the test equation (44) we obtain the difference equation:

$$\Omega_1 \left(s, v\right) \, \left(\zeta_{n+1} + \zeta_{n-1}\right) + \Omega_0 \left(s, v\right) \, \zeta_n = 0 \tag{45}$$

and the corresponding characteristic equation:

$$\Omega_1 \left(s, v\right) \, \left(\lambda^2 + 1\right) + \Omega_0 \left(s, v\right) \, \lambda \, = \, 0 \tag{46}$$

where the stability polynomials $\Omega_j \left(s, v\right), \, j = 0, 1$ are given by:

$$\begin{aligned} \Omega_1 \left(s, v\right) &= 1 + b_1 \, s^2 + c_3 \, b_1 \, s^4 + c_1 \, c_3 \, b_1 \, s^6 \\ \Omega_0 \left(s, v\right) &= a_1 + b_0 \, s^2 - c_2 \, b_1 \, s^4 - c_0 \, c_3 \, b_1 \, s^6 \end{aligned} \tag{47}$$

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

Remark 14. *Observation of the expression (47), we conclude that the formulae (47) are dependent on s and v, while the formulae (18) are dependent only on v.*

Substitution of the coefficients b_1 given by (17) and the coefficients a_1, $c_i \, i = 0(1)3, b_0$ given by (27) into the stability polynomials (47), leads to the following formulae for the stability polynomials $\Omega_j \left(s, v\right), \, j = 0, 1$:

$$\begin{aligned} \Omega_1 \left(s, v\right) &= \frac{1}{12} \, \frac{\Upsilon_{14} \left(s, v\right)}{v^6 \, \Upsilon_{15} \left(s, v\right)} \\ \Omega_0 \left(s, v\right) &= -\frac{1}{18} \, \frac{\Upsilon_{16} \left(s, v\right)}{v^6 \, \Upsilon_{15} \left(s, v\right)} \end{aligned} \tag{48}$$

where $\Upsilon_j \left(s, v\right), \, j = 14(1)16$ are given in the Appendix F.

Remark 15. *It is noted that the conditions and definitions of P–stability and singularly almost P–stability, which are given in Section 2, are referred to problems which have frequency with satisfaction of the condition $\omega = \phi$.*

The multistage scheme (16) satisfies the condition of a non zero interval of periodicity if for the roots of its characteristic equation (46) the following condition is hold:

$$|\lambda_{1,2}| \leq 1 \tag{49}$$

4.2.1 Procedure for the development of the $s - v$ domain for the new multistage scheme

The development of the $s - v$ domain for the new scheme is based on the flowchart of Figure 3.

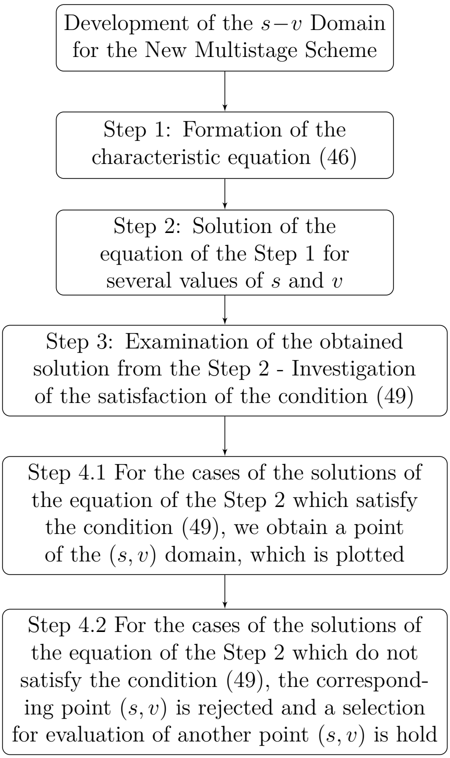

Figure 3. Flowchart for the development of the $s-v$ domain for the new multistage scheme

The procedure presented in the flowchart of Figure 3 leads to the construction of the $s-v$ domain which is builded in Figure 4.

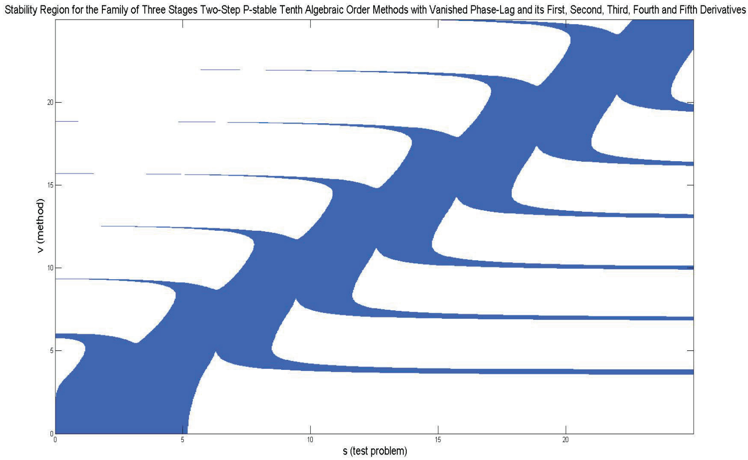

Figure 4. The plot of $s-v$ domain of the new obtained multistage P–stable scheme with vanished phase–lag and its derivatives up to order five.

Remark 16. *The examination of the produced in Figure 4 $s-v$ domain leads us to the following remarks:*

1. *The new obtained multistage P–stable scheme is stable within the shadowed area of the domain.*

2. *The new obtained multistage P–stable scheme is unstable within the white area of the domain.*

Remark 17. *Each of the above mentioned areas for the $s-v$ domain new obtained multistage P–stable scheme corresponds to the possibility of the efficient solution of problem which are categorized as follows:*

1. **Problems for which** $\omega \neq \phi$. *For these kind of problems, the most efficient methods are those with $s-v$ domain within the shadowed area of the Figure 4* **excluding** *the area around the first diagonal.*

2. **Problems for which** $\omega = \phi$ *(see the Schrödinger equation and related problems). For these kind of problems the most efficient methods are those with* $s - v$ *domain equal with the area around the first diagonal of the Figure 4.*

The procedure for the denotation of the interval of periodicity of the new obtained multistage P–stable scheme is as follows:

1. We substitute $s = v$ in the stability polynomials Ω_i, $i = 0, 1$ given by (48).
2. We evaluate the area around the first diagonal of the $s - v$ domain defined in Figure 4.

The above presented procedure leads us to the conclusion that the interval of periodicity of the new obtained multistage P–stable scheme is equal to $(0, \infty)$.

The above achievements lead to the following theorem:

Theorem 4. *The multistage scheme developed in Section 3:*

- *is of three stages*
- *is of tenth algebraic order,*
- *has vanished the phase–lag and its derivatives up to order five and*
- *is P–stable i.e. has an interval of periodicity equals to:* $(0, \infty)$.

5 Numerical results

We will evaluate the effectiveness of the new developed multistage scheme applying it to the numerical solution of:

1. The radial time–independent Schrödinger equation and
2. The systems of coupled differential equations arising from the Schrödinger equation.

5.1 Radial time–independent Schrödinger equation

The radial time–independent Schrödinger equation is given by:

$$\zeta''(r) = \left[l(l+1)/r^2 + V(r) - k^2 \right] \zeta(r), \tag{50}$$

where

1. The function $\Theta(r) = l(l+1)/r^2 + V(r)$ denotes *the effective potential* satisfying the following relation: $\Theta(r) \to 0$ as $r \to \infty$.

2. $k^2 \in \mathbb{R}$ denotes *the energy.*

3. $l \in \mathbb{Z}$ denotes *the angular momentum.*

4. The function V denotes *the potential.*

Since the the problem (50) is a boundary value one, the boundary conditions are given by:

$$\zeta(0) = 0$$

and another the integration's end point condition which is denoted for large values of r from the physical characteristics and properties of the specific problem.

The new obtained multistage scheme has some of its coefficients are dependent from the quantity $v = \phi\, h$, where ϕ is the frequency of the specific problem. Therefore in order the coefficients of the new multistage scheme to be possible to be computed during the integration procedure, it is necessary the denotation of their frequency ϕ. In our numerical tests and for (50) and $l = 0$ we have:

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

where $V\,(r)$ denotes the potential and $E = k^2$ denotes the energy.

5.1.1 Woods–Saxon potential

Observing the model of (50) it is easy to see that it consists the potential $V\,(r)$. Consequently, in order to be possible to computer the values of the potential $V\,(r)$, it is necessary to denote the the function of the potential $V\,(r)$. In our numerical experiments we will use the Wood–Saxon potential which is given by:

$$V\,(r) = \frac{\Psi_0}{1+\xi} - \frac{\Psi_0\,\xi}{a\,(1+\xi)^2} \tag{51}$$

with $\xi = \exp\left[\frac{r-X_0}{a}\right],\ \Psi_0 = -50,\ a = 0.6$, and $X_0 = 7.0$.

In Figure 5 we present the form of the Wood–Saxon potential for several values of r.

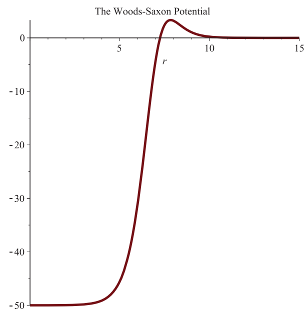

Figure 5. Form of the Woods–Saxon potential for several values of r.

In the following we give the values of the frequency ϕ (see for details [20] and [21]):

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

For the denotation of the above values of the frequency ϕ, the technique introduced by Ixaru et al. ([19] and [21]) is used. This technique approximates the continuous function $V(r)$ by discrete constant values on some specific points within the integration domain. Below we give some examples of this technique:

1. On $r = 6.5 - h$, the value of ϕ is approximated by the value: $\sqrt{-37.5+E}$. Consequently, $v = \phi\, h = \sqrt{-37.5+E}\, h$.

2. On $r = 6.5 - 3\,h$, the value of ϕ is approximated by the value: $\sqrt{-50+E}$. Consequently, $v = \phi\, h = \sqrt{-50+E}\, h$.

The potential $V(r)$ is a user defined function. There are a lot of potentials which are of great interest in several disciplines of Chemistry. For the most of them, their their eigenenergies are unknown. We selected the Woods–Saxon potential since for this potential the eigenenergies are known.

5.1.2 The resonance problem of the radial Schrödinger equation

In this section we will present the numerical solution of the problem (50):

- with $l = 0$ and
- using the Woods-Saxon potential (51)

Theoretically the interval of integration for the problem presented above is equal to $(0, \infty)$. In order the above problem to be solved numerically, it is necessary the infinite interval of integration $(0, \infty)$ to be approximated by a finite one. We approximate the above infinite interval by $r \in [0, 15]$ for the needs of our numerical experiments. We note also that the numerical schemes which will be evaluated will be applied on a wide range of energies: $E \in [1, 1000]$.

Since for positive energies the potential $V(r)$ vanished faster than the term $\frac{l(l+1)}{r^2}$, the equation (50) can be written as:

$$\zeta''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) \zeta(r) = 0 \tag{52}$$

when $r \to \infty$. It is noted that in (52) the solutions of the above model are given by $k\,r\,j_l(k\,r)$ and $k\,r\,n_l(k\,r)$, which are linearly independent, with $j_l(k\,r)$ and $n_l(k\,r)$ to be the spherical Bessel and Neumann functions respectively (see [84]).

Consequently, the asymptotic form of the solution of equation (50) (i.e. in the case where $r \to \infty$) is given by:

$$\begin{aligned} \zeta(r) &\approx A\,krj_l(kr) - B\,krn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned}$$

where δ_l is the phase shift and A, B, $AC \in \mathbb{R}$. The computation of the phase shift is given by the following direct formula:

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

where r_1 and r_2 are distinct points in the asymptotic region (we chosen $r_1 = 15$ and $r_2 = r_1 - h$) with $S(r) = k\,r\,j_l(k\,r)$ and $C(r) = -k\,r\,n_l(k\,r)$. The problem described above is an initial–value one. Consequently, it is necessary to compute the values of $\zeta_j,\ j = 0, 1$ before starting the application of a two–step finite difference pair. The value ζ_0 is determined by the initial condition of the problem. The value ζ_1 is computed using the high order Runge–Kutta–Nyström methods (see [22] and [23]). Using the computation of the values ζ_i, $i = 0, 1$, we compute the phase shift δ_l at the point r_2 of the asymptotic region. We note that ζ_j is the approximation of the function ζ at the point x_j.

We solve numerically the above described problem for positive energies. Consequently, two are the possible results of the solution:

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

For our numerical experiments the second problem is solved, which is known as **the resonance problem**.

The boundary conditions are:

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

The following schemes are used for the computation of the the positive eigenenergies of the resonance problem presented above:

- **Method QT8**: the eighth order multi–step method developed by Quinlan and Tremaine [24];
- **Method QT10**: the tenth order multi–step method developed by Quinlan and Tremaine [24];
- **Method QT12**: the twelfth order multi–step method developed by Quinlan and Tremaine [24];
- **Method MCR4**: the fourth algebraic order method of Chawla and Rao with minimal phase–lag [25];
- **Method RA**: the exponentially–fitted method of Raptis and Allison [26];
- **Method MCR6**: the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase–lag [27];
- **Method NMPF1**: the Phase-Fitted Method (Case 1) developed in [14];
- **Method NMPF2**: the Phase-Fitted Method (Case 2) developed in [14];
- **Method NMC2**: the Method developed in [28] (Case 2);

- **Method NMC1**: the method developed in [28] (Case 1);
- **Method NM2SH2DV**: the Two-Step Hybrid Method developed in [1];
- **Method WPS2S**: the Two–Step P–stable Method developed in [83];
- **Method WPS4S**: the Four–Step P–stable Method developed in [83];
- **Method WPS6S**: the Six–Step P–stable Method developed in [83];
- **Method NM3SPS2DV**: the Three Stages Tenth Algebraic Order P–stable Symmetric Two–Step method with vanished phase-lag and its first and second derivatives developed in [6];
- **Method NM3SPS3DV**: the Three Stages Tenth Algebraic Order P–stable Symmetric Two–Step method with vanished phase-lag and its first, second and third derivatives developed in [7].
- **Method NM3SPS4DV**: the Three Stages Tenth Algebraic Order P–stable Symmetric Two–Step method with vanished phase-lag and its first, second, third and fourth derivatives developed in [7].
- **Method NM3SPS5DV**: the Three Stages Tenth Algebraic Order P–stable Symmetric Two–Step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives developed in Section 3.

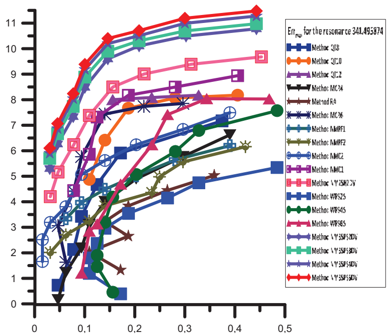

Figure 6. Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

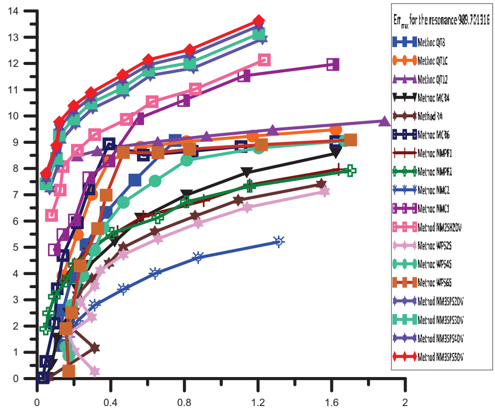

Figure 7. Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

The maximum absolute errors Err_{max}, which are determined by:

$Err_{max} = max|\log_{10}(Err)|$ where

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

are presented in Figures 6 and 7.

The determination of the absolute error Err is achieved using two values of the specific eigenenergy:

1. The computed eigenenergies. The computed eigenenergies are denoted as $E_{calculated}$ and are computed using each of the 18 numerical methods mentioned above.

2. The accurate eigenenergies (or as also called **reference values** for the eigenenergies). The accurate eigenenergies are denoted as $E_{accurate}$ and are computed using the well known two-step method of Chawla and Rao [27].

In Figures 6 and 7 we present the following:

- the maximum absolute errors Err_{max} for the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$, respectively, and for the 18 numerical methods mentioned above for several values of CPU time (in seconds).
- the needed CPU time (in seconds) (as mentioned above).

The symbols E_2 and E_3 for the eigenenergies in our numerical tests are used since it is known that the Woods–Saxon potential has also the eigenenergies E_0 and E_1. We chose the eigenenergies E_2 and E_3 because for these eigenenergies the solution has stiffer behavior and consequently the newly developed scheme can show efficiently its effectiveness.

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

The results presented in Figures 6 and 7 lead to the following conclusions:

- **Method QT10** is more efficient than **Method MCR4** and **Method QT8**.
- **Method QT10** is more efficient than **Method MCR6** for large CPU time and less efficient than **Method MCR6** for small CPU time.
- **Method QT12** is more efficient than **Method QT10**
- **Method NMPF1** is more efficient than **Method RA**, **Method NMPF2** and **Method WPS2S**
- **Method WPS4S** is more efficient than **Method MCR4**, **Method NMPF1** and **Method NMC2**.
- **Method WPS6S** is more efficient than **Method WPS4S**.
- **Method NMC1**, is more efficient than all the other methods mentioned above.
- **Method NM2SH2DV**, is more efficient than all the other methods mentioned above.
- **Method NM3SPS2DV**, is more efficient than all the other methods mentioned above.
- **Method NM3SPS3DV**, is more efficient than all the other methods mentioned above.

- **Method NM3SPS4DV**, is more efficient than all the other methods mentioned above.

- **Method NM3SPS5DV**, is the most efficient one.

5.2 Error estimation

In our numerical tests we will use also the numerical solution of systems of coupled differential equations of the Schrödinger type.

The above problem will be solved using the so called variable–step schemes.

Definition 9. *We determine a numerical scheme as a variable–step method if the step length of used by the numerical scheme is changed during the integration procedure.*

Definition 10. *A technique is called as Local truncation error estimation technique (LTEETQ), if it uses a variable–step scheme in order to change the step length during the integration.*

During the last decades much research has been done on the development of numerical methods of constant or variable step length for the approximate solution of problems of the form of the Schrödinger equation (see for example [14]– [83]).

The categories of the LTEETQ procedures are shown in Figure 8.

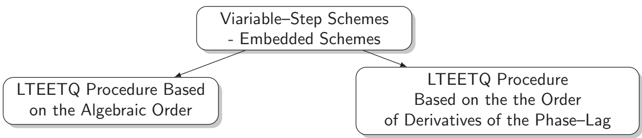

Figure 8. Categories of LTEETQ Procedures used for the Development of Embedded Schemes for the Problems with Oscillatory and/or Periodical Solutions

For the change of the step length we use the following relation for the estimation of the local truncation error (LTE) in the lower order solution ζ_{n+1}^{L}:

$$LTE = \mid \zeta_{n+1}^{H} - \zeta_{n+1}^{L} \mid \tag{53}$$

where ζ_{n+1}^{L} and ζ_{n+1}^{H} are

- **LTEETQ Technique which is based on the algebraic order of the numerical schemes**. For this procedure, ζ_{n+1}^{L} denotes the numerical scheme with the lower algebraic order solution and ζ_{n+1}^{H} denotes the numerical scheme pair with the higher algebraic order solution.
- **LTEETQ Technique which is based on the order of the derivatives of the phase–lag**. Let us consider that the higher order of the derivatives of the phase–lag which are eliminated for the numerical schemes which participate in this technique are p and s respectively, where $p < s$. For this procedure ζ_{n+1}^{L} denotes the numerical scheme with eliminated higher order derivative of the phase–lag equal to p and ζ_{n+1}^{H} denotes the numerical scheme with eliminated higher order derivative of the phase–lag equal to s .

For our numerical tests we use the first LTEETQ technique for the estimation of the local truncation error. Consequently, we use:

As ζ_{n+1}^{L} we use the eighth algebraic order method developed in [82] and as ζ_{n+1}^{H} we use the tenth algebraic order method developed in Section 3.

In Figure 9 we present the variable–step process used in our numerical tests. This process uses the Local Truncation Error Control Technique $LTEETQ$. We note that:

- h_n is determined as the stepsize which is used during the n^{th} step of the integration procedure and
- acc is determined as the accuracy of the local truncation error LTE which is defined by the user.

Remark 18. *For our numerical tests we use the well known methodology called as* **local extrapolation**. *Using this methodology, the approximation of the solution at each point of the integration domain is done via the higher order solution ζ_{n+1}^{H} although the local truncation error estimation is based on the lower order solution ζ_{n+1}^{L}.*

5.3 The system of coupled differential equations of the Schrödinger type

We can find systems of coupled differential equations arising from the Schrödinger equation in many scientific areas like: quantum chemistry, material science, theoretical physics, quantum physics, atomic physics, physical chemistry, chemical physics, quantum chemistry, electronics, etc.

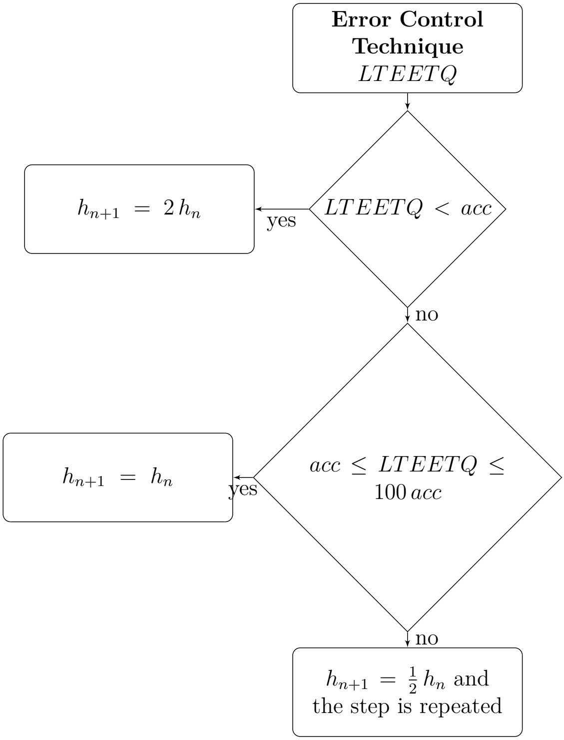

Figure 9. Flowchart for the Local Truncation Error Control Technique $LTEETQ$. The parameter acc is defined by the user

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

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

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

Since the above problem is a boundary value one, the boundary conditions, which must be determined, are given by (see for details [29]):

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

$$\zeta_{ij} \sim k_i\,x j_{l_i}\,(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}\,k_i\,x\,n_{li}\,(k_i x) \tag{54}$$

Remark 19. *The multistage schem obtained in this paper and the produced embedded finite difference method, which is based on the multistage scheme, can be applied efficiently to both open and close channels problem.*

Following the analysis fully presented in [29] we produce the new formulae of the asymptotic condition (54):

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

where the matrix $\mathbf{K}'$ and diagonal matrices $\mathbf{M}$, $\mathbf{N}$ are give by :

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

The rotational excitation of a diatomic molecule by neutral particle impact is studied in our paper. In many scientific areas like quantum chemistry, theoretical chemistry, theoretical physics, quantum physics, material science, atomic physics, molecular physics, in technical applications in the analysis of gas dynamics and stratification of chemically reacting flows, dispersed flows, including with nano-sized particles etc, we can find the above mentioned problem. The model of the above problem contains the close–coupling Schrödinger equations (see [9], [10–13], [85] - [89]). Using the denotations:

- quantum numbers (j, l) which determine the entrance channel (see for details in [29]),
- quantum numbers (j', l') which determine the exit channels and
- $J = j + l = j' + l'$ which determine the total angular momentum.

we obtain:

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

where

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

and E denotes the kinetic energy of the incident particle in the center-of-mass system, I denotes the moment of inertia of the rotator, μ denotes the reduced mass of the system, Jjl is angular momentum of the quantum numbers (j, l) and j'' and l'' are quantum numbers.

For our numerical tests, we use the following potential V (see [29]):

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

and therefore, the coupling matrix has elements of the form:

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

where f_2 coefficients are denoted from formulae described by Bernstein et al. [30] 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 [31]). We note also that $V_0(x)$ and $V_2(x)$ denote potential functions defined by the user. Based on the above achievements, we obtain the following new formulae of the boundary conditions:

$$\zeta^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \tag{55}$$

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

where S matrix. For K matrix of (54) we use the following formula:

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

The procedure fully presented in [29] is used in order to approximate the solution of the above mentioned problem. The procedure contains the multistage scheme developed in this paper in order to obtain the integration from the initial point to the matching points.

For our numerical experiments the following parameters for the $\mathbf{S}$ matrix are used:

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

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

For our experiments we use (see in [29]) $J = 6$ and for the excitation of the rotator the value $j = 0$ state to levels up to $j' = 2, 4$ and 6. These values produce systems of **four, nine and sixteen coupled differential equations of the Schrödinger type**, respectively. We follow the theory fully presented in [31] and [29] and consequently the potential is considered infinite for x less than x_0. Therefore, the boundary condition (55) can be written now as

$$\zeta^{Jjl}_{j'l'}(x_0) = 0.$$

For the numerical solution of the above described problem, the following schemes are used:

- the Iterative Numerov method of Allison [29] which is indicated as **Method I**[2],
- the variable–step method of Raptis and Cash [32] which is indicated as **Method II**,
- the embedded Runge–Kutta Dormand and Prince method 5(4) (5(4) means: Runge–Kutta method of variable step which uses the fourth algebraic order part in order to control the error of the the fifth algebraic order part) which is developed in [23] which is indicated as **Method III**,
- the embedded Runge–Kutta method ERK4(2) developed in Simos [33] which is indicated as **Method IV**,
- the embedded two–step method developed in [1] which is indicated as **Method V**,
- the embedded two–step method developed in [2] which is indicated as **Method VI**.
- the embedded two–step method developed in [3] which is indicated as **Method VII**.
- the new developed embedded two–step method with error control based on the algebraic order of the method developed in [6] which is indicated as **Method VIII**.
- the new developed embedded two–step method with error control based on the algebraic order of the method developed in [7] which is indicated as **Method IX**.
- the new developed embedded two–step method with error control based on the algebraic order of the method developed in [8] which is indicated as **Method X**.
- the new developed embedded two–step method with error control based on the algebraic order of the method developed in this paper which is indicated as **Method X**.

In Table 2 we present:

- the real time of computation requested by the schemes I-XI introduced above in order to calculate the square of the modulus of the **S** matrix for the sets of 4, 9 and 16 of systems of coupled differential equations respectively,

[2]We note here that Iterative Numerov method developed by Allison [29] is one of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation

- the maximum error in the computation of the square of the modulus of the **S** matrix.

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

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 VIII. acc=10^{-6}. Note that hmax is the maximum stepsize. N indicates the number of equations of the set of coupled differential equations

Method	N	hmax	RTC	MErr
Method I	4	0.014	3.25	1.2×10^{-3}
	9	0.014	23.51	5.7×10^{-2}
	16	0.014	99.15	6.8×10^{-1}
Method II	4	0.056	1.55	8.9×10^{-4}
	9	0.056	8.43	7.4×10^{-3}
	16	0.056	43.32	8.6×10^{-2}
Method III	4	0.007	45.15	9.0×10^{0}
	9			
	16			
Method IV	4	0.112	0.39	1.1×10^{-5}
	9	0.112	3.48	2.8×10^{-4}
	16	0.112	19.31	1.3×10^{-3}
Method V	4	0.448	0.20	1.1×10^{-6}
	9	0.448	2.07	5.7×10^{-6}
	16	0.448	11.18	8.7×10^{-6}
Method VI	4	0.448	0.15	3.2×10^{-7}
	9	0.448	1.40	4.3×10^{-7}
	16	0.448	10.13	5.6×10^{-7}
Method VII	4	0.448	0.10	2.5×10^{-7}
	9	0.448	1.10	3.9×10^{-7}
	16	0.448	9.43	4.2×10^{-7}
Method VIII	4	0.896	0.04	3.8×10^{-8}
	9	0.896	0.55	5.6×10^{-8}
	16	0.896	8.45	6.5×10^{-8}
Method IX	4	0.896	0.03	3.2×10^{-8}
	9	0.896	0.50	4.1×10^{-8}
	16	0.896	8.35	5.0×10^{-8}
Method X	4	0.896	0.02	2.7×10^{-8}
	9	0.896	0.44	3.3×10^{-8}
	16	0.896	8.01	4.2×10^{-8}
Method XI	4	0.896	0.01	1.9×10^{-8}
	9	0.896	0.39	2.7×10^{-8}
	16	0.896	7.12	3.6×10^{-8}

6 Conclusions

A new P–stable multistage scheme with vanished phase–lag and its derivatives up to order five was developed in this paper.

The development was based on the following stages:

1. Satisfaction of the P–stability properties introduced by Lambert and Watson [15] and Wang [83].
2. Satisfaction of the property of the vanishing of the phase–lag.
3. Satisfaction of the properties of the vanishing of the derivatives of the phase–lag up to order five.

The above technique for the construction of P–stable numerical schemes was first introduced by Medvedev and Simos [6].

We analyzed the new proposed multistage scheme as follows:

- Computation of the local truncation error (LTE).
- Computation of the asymptotic form of the LTE
- Comparison of the asymptotic form of the LTE of new multistage method with the asymptotic forms of the LTE of similar methods.
- Study of the stability and the interval of periodicity properties of the new multistage scheme.
- Study of the computational efficiency of the new multistage scheme.

Based on the above analysis we arrived to the conclusion that the theoretical, computational and numerical results developed in this paper, proved the efficiency of the new multistage scheme compared with other well known and recently obtained methods of the literature for the numerical solution of the Schrödinger equation.

Appendix A: Formulae for the $\Upsilon_i\,(v)$, $i = 0(1)5$

$$
\begin{aligned}
\Upsilon_0\,(v) &= 2\,\cos\,(v)\,v^6c_1c_3 - v^6c_0c_3 \\
&+ 2\,\cos\,(v)\,v^4c_3 - v^4c_2 \\
&+ 2\,\cos\,(v)\,v^2 + 12\,v^2b_0 \\
&+ 24\,\cos\,(v) + 12\,a_1 \\
\Upsilon_1\,(v) &= -\sin\,(v)\,v^{12}{c_1}^2{c_3}^2 \\
&- 2\,\sin\,(v)\,v^{10}c_1{c_3}^2 - v^9c_0{c_3}^2 \\
&+ v^9c_1c_2c_3 - 2\,\sin\,(v)\,v^8c_1c_3 \\
&- \sin\,(v)\,v^8{c_3}^2 - 24\,v^7b_0c_1c_3 \\
&- 24\,\sin\,(v)\,v^6c_1c_3 - 2\,v^7c_0c_3 \\
&- 2\,\sin\,(v)\,v^6c_3 - 36\,v^5a_1c_1c_3 \\
&- 12\,v^5b_0c_3 - 36\,v^5c_0c_3 \\
&- 24\,\sin\,(v)\,v^4c_3 - v^5c_2 \\
&- \sin\,(v)\,v^4 - 24\,v^3a_1c_3 \\
&- 24\,v^3c_2 - 24\,\sin\,(v)\,v^2 \\
&- 12\,va_1 + 144\,vb_0 - 144\,\sin\,(v) \\
\Upsilon_2\,(v) &= -2160\,v^4c_0c_3 - 204\,v^6c_0c_3 \\
&- 432\,\cos\,(v)\,v^4c_3 - 1728\,v^4b_0c_3 \\
&+ 120\,v^6c_2c_3 - 12\,v^6b_0c_3 \\
&+ 108\,v^4a_1c_3 - 864\,v^2a_1c_3 \\
&- 3\,\cos\,(v)\,v^8c_3 - 36\,\cos\,(v)\,v^8{c_3}^2 \\
&- \cos\,(v)\,v^{12}{c_3}^3 - 3\,\cos\,(v)\,v^{10}{c_3}^2 \\
&- v^{12}c_0{c_3}^3 - 72\,\cos\,(v)\,v^6c_3 \\
&- 3\,v^{10}c_0{c_3}^2 + 36\,v^8b_0{c_3}^2 \\
&- 6\,v^8c_0c_3 + 3\,v^8c_2c_3 \\
&+ 120\,v^6a_1{c_3}^2 - 3\,\cos\,(v)\,v^{10}c_1c_3 \\
&- 72\,\cos\,(v)\,v^8c_1c_3 - 72\,\cos\,(v)\,v^{10}c_1{c_3}^2 \\
&- 6\,\cos\,(v)\,v^{12}c_1{c_3}^2
\end{aligned}
$$

$$
\begin{aligned}
& - && 36\,\cos(v)\,v^{12}{c_1}^2{c_3}^2 - 3\,\cos(v)\,v^{14}c_1{c_3}^3 \\
& - && 3\,\cos(v)\,v^{14}{c_1}^2{c_3}^2 - 2160\,v^4a_1c_1c_3 \\
& - && 3\,\cos(v)\,v^{16}{c_1}^2{c_3}^3 - \cos(v)\,v^{18}{c_1}^3{c_3}^3 \\
& - && 1728\,\cos(v) - 3600\,v^6b_0c_1c_3 \\
& + && 96\,v^6a_1c_1c_3 + 324\,v^8c_1c_2c_3 \\
& - && 72\,v^8b_0c_1c_3 + 12\,v^{10}c_1c_2c_3 \\
& + && 324\,v^8a_1c_1{c_3}^2 + v^{12}c_1c_2{c_3}^2 \\
& + && 252\,v^{10}c_0c_1{c_3}^2 + 108\,v^{10}b_0c_1{c_3}^2 \\
& + && 252\,v^{10}a_1{c_1}^2{c_3}^2 + 10\,v^{12}c_0c_1{c_3}^2 \\
& - && 3\,v^{14}{c_1}^2c_2{c_3}^2 - 144\,a_1 \\
& + && 120\,v^{12}b_0{c_1}^2{c_3}^2 + 3\,v^{14}c_0c_1{c_3}^3 \\
& + && 1728\,b_0 - 864\,v^2c_2 - 36\,v^4c_2 \\
& - && 432\,v^2b_0 - \cos(v)\,v^6 - 432\,\cos(v)\,v^2 \\
& - && v^6c_2 + 36\,v^2a_1 \\
& - && 432\,\cos(v)\,v^6c_1c_3 - 36\,\cos(v)\,v^4 \\
\Upsilon_3(v) & = && -103680\,v^3a_1c_1c_3 + 58752\,v^9b_0c_1{c_3}^2 \\
& - && 1440\,v^9a_1c_1{c_3}^2 + 60480\,v^9a_1{c_1}^2{c_3}^2 \\
& + && 60\,v^{11}c_1c_2c_3 - 2592\,v^{11}c_1c_2{c_3}^2 \\
& + && 60480\,v^9c_0c_1{c_3}^2 - 144\,v^9b_0c_1c_3 \\
& + && 864\,\sin(v)\,v^4 + 4896\,v^{11}c_0c_1{c_3}^2 \\
& + && 6912\,\sin(v)\,v^6c_1c_3 + 2592\,v^9c_1c_2c_3 \\
& + && 864\,\sin(v)\,v^{12}{c_1}^2{c_3}^2 + 1728\,\sin(v)\,v^{10}c_1{c_3}^2 \\
& + && 1728\,\sin(v)\,v^8c_1c_3 + 13824\,v^5a_1c_1c_3 \\
& + && 62208\,v^7a_1c_1{c_3}^2 + 6912\,\sin(v)\,v^2 \\
& - && 10368\,v^5c_0c_3 + 6912\,\sin(v)\,v^4c_3 \\
& + && 1728\,\sin(v)\,v^6c_3 - 103680\,v^3b_0c_3 \\
& - && 103680\,v^3c_0c_3 + 864\,v^9c_0{c_3}^2 \\
& - && 576\,v^7c_0c_3 + 6912\,v^5b_0c_3 \\
& + && 10368\,v^3a_1c_3 + 864\,\sin(v)\,v^8{c_3}^2
\end{aligned}
$$

$$
\begin{aligned}
- &\quad 576\, v^7 a_1 c_1 c_3 + 1728\, v^3 c_2 - 20736\, v b_0 \\
+ &\quad 864\, v^{11} b_0 c_1 {c_3}^2 + 60480\, v^{11} b_0 {c_1}^2 {c_3}^2 \\
- &\quad 144\, v^{11} a_1 {c_1}^2 {c_3}^2 - 48\, v^{13} c_1 c_2 {c_3}^2 \\
+ &\quad 120\, v^{13} c_0 c_1 {c_3}^2 - 3744\, v^{13} {c_1}^2 c_2 {c_3}^2 \\
- &\quad 576\, v^{13} b_0 c_1 {c_3}^3 + 1440\, v^{13} b_0 {c_1}^2 {c_3}^2 \\
- &\quad 3744\, v^{13} a_1 {c_1}^2 {c_3}^3 - 2736\, v^{11} a_1 c_1 {c_3}^3 \\
- &\quad 120\, v^{15} {c_1}^2 c_2 {c_3}^2 + 48\, v^{15} c_0 c_1 {c_3}^3 \\
- &\quad 864\, v^{15} b_0 {c_1}^2 {c_3}^3 - 2016\, v^{15} a_1 {c_1}^3 {c_3}^3 \\
- &\quad 12\, v^{17} {c_1}^2 c_2 {c_3}^3 + 12\, v^{17} c_0 c_1 {c_3}^4 \\
- &\quad 60\, v^{17} c_0 {c_1}^2 {c_3}^3 - 2016\, v^{15} c_0 {c_1}^2 {c_3}^3 \\
- &\quad 720\, v^{17} b_0 {c_1}^3 {c_3}^3 + 12\, v^{19} {c_1}^3 c_2 {c_3}^3 \\
- &\quad 12\, v^{19} c_0 {c_1}^2 {c_3}^4 + 144\, \sin(v)\, v^{10} c_1 c_3 \\
+ &\quad 288\, \sin(v)\, v^{12} c_1 {c_3}^2 + 12\, \sin(v)\, v^{14} c_1 {c_3}^2 \\
+ &\quad 144\, \sin(v)\, v^{14} c_1 {c_3}^3 + 4\, \sin(v)\, v^{12} c_1 c_3 \\
+ &\quad 144\, \sin(v)\, v^{14} {c_1}^2 {c_3}^2 + 12\, \sin(v)\, v^{16} c_1 {c_3}^3 \\
+ &\quad 144\, \sin(v)\, v^{16} {c_1}^2 {c_3}^3 + 4\, \sin(v)\, v^{18} c_1 {c_3}^4 \\
+ &\quad 12\, \sin(v)\, v^{18} {c_1}^2 {c_3}^3 + 6\, \sin(v)\, v^{16} {c_1}^2 {c_3}^2 \\
+ &\quad 48\, \sin(v)\, v^{18} {c_1}^3 {c_3}^3 + 6\, \sin(v)\, v^{20} {c_1}^2 {c_3}^4 \\
+ &\quad 4\, \sin(v)\, v^{22} {c_1}^3 {c_3}^4 + \sin(v)\, v^{24} {c_1}^4 {c_3}^4 \\
+ &\quad 44928\, v^7 c_1 c_2 c_3 + 4\, \sin(v)\, v^{20} {c_1}^3 {c_3}^3 \\
- &\quad 290304\, v^5 b_0 c_1 c_3 - 20736\, v a_1 c_3 \\
+ &\quad 4\, \sin(v)\, v^{10} c_3 + 144\, \sin(v)\, v^{10} {c_3}^2 \\
+ &\quad 17280\, v^5 c_2 c_3 + 48\, \sin(v)\, v^{12} {c_3}^3 \\
+ &\quad \sin(v)\, v^{16} {c_3}^4 + 6\, \sin(v)\, v^{12} {c_3}^2 \\
+ &\quad 4\, \sin(v)\, v^{14} {c_3}^3 - 20736\, v c_2 \\
+ &\quad 1728\, v a_1 - 144\, v^3 a_1 + 1728\, v^3 b_0 \\
+ &\quad \sin(v)\, v^8 + 48\, \sin(v)\, v^6 \\
+ &\quad 17280\, v^5 a_1 {c_3}^2 + 144\, \sin(v)\, v^8 c_3 \\
- &\quad 576\, v^5 a_1 c_3 + 17280\, v^7 c_0 {c_3}^2
\end{aligned}
$$

$$
\begin{aligned}
& + \quad 576\,v^7c_2c_3 + 12\,v^9c_2c_3 \\
& - \quad 864\,v^7a_1{c_3}^2 - 12\,v^9c_0c_3 \\
& + \quad 17280\,v^7b_0{c_3}^2 - 144\,v^{11}c_0{c_3}^3 \\
& - \quad 144\,v^{11}b_0{c_3}^3 + 144\,v^9b_0{c_3}^2 \\
& + \quad 12\,v^{11}c_0{c_3}^2 - 720\,v^9a_1{c_3}^3 \\
& - \quad 12\,v^{11}c_2{c_3}^2 - 720\,v^9c_2{c_3}^2 \\
& + \quad 20736\,\sin(v) \\
\Upsilon_4(v) & = \quad -60\,v^{14}c_0{c_3}^3 + 60\,v^{14}c_2{c_3}^3 \\
& + \quad 5040\,v^{12}a_1{c_3}^4 - 1440\,v^{12}b_0{c_3}^3 \\
& + \quad 5040\,v^{12}c_2{c_3}^3 + 120\,v^{12}c_0{c_3}^2 \\
& - \quad 120\,v^{12}c_2{c_3}^2 + \cos(v)\,v^{10} \\
& + \quad 20\,\cos(v)\,v^{16}c_1{c_3}^2 - 174528\,v^{10}c_0{c_3}^3 \\
& - \quad 7488\,v^{10}c_2{c_3}^2 + 720\,\cos(v)\,v^{16}c_1{c_3}^3 \\
& + \quad 7056\,v^{10}a_1{c_3}^3 - 174528\,v^{10}b_0{c_3}^3 \\
& - \quad 12\,v^{10}c_0c_3 + 12\,v^{10}c_2c_3 \\
& - \quad 267840\,v^8a_1{c_3}^3 + 144\,v^{10}b_0{c_3}^2 \\
& + \quad 7200\,v^8a_1{c_3}^2 + 240\,\cos(v)\,v^{12}c_1c_3 \\
& + \quad 540\,v^{18}{c_1}^2c_2{c_3}^3 + 60\,v^{18}c_0c_1{c_3}^4 \\
& + \quad 30\,\cos(v)\,v^{18}c_1{c_3}^3 + 360\,\cos(v)\,v^{16}{c_1}^2{c_3}^2 \\
& + \quad 10\,\cos(v)\,v^{18}{c_1}^2{c_3}^2 + 240\,\cos(v)\,v^{18}c_1{c_3}^4 \\
& + \quad 20\,\cos(v)\,v^{20}c_1{c_3}^4 + 30\,\cos(v)\,v^{20}{c_1}^2{c_3}^3 \\
& + \quad 720\,\cos(v)\,v^{14}c_1{c_3}^2 + 720\,\cos(v)\,v^{18}{c_1}^2{c_3}^3 \\
& + \quad 1440\,\cos(v)\,v^{12}{c_3}^3 - 248832\,c_2 + 20736\,a_1 \\
& - \quad 248832\,b_0 - 259200\,v^6a_1{c_3}^2 \\
& + \quad 248832\,\cos(v) + 360\,\cos(v)\,v^{20}{c_1}^2{c_3}^4 \\
& + \quad 5\,\cos(v)\,v^{22}c_1{c_3}^5 + 30\,\cos(v)\,v^{22}{c_1}^2{c_3}^4 \\
& + \quad 10\,\cos(v)\,v^{22}{c_1}^3{c_3}^3 + 240\,\cos(v)\,v^{20}{c_1}^3{c_3}^3 \\
& + \quad 240\,\cos(v)\,v^{22}{c_1}^3{c_3}^4 + 10\,\cos(v)\,v^{24}{c_1}^2{c_3}^5 \\
& + \quad 103680\,\cos(v)\,v^6c_1c_3 + 5\,\cos(v)\,v^{14}c_1c_3
\end{aligned}
$$

$$- \quad 6480\, v^{12} c_0 {c_3}^3 + 518400\, v^2 a_1 c_3$$
$$+ \quad 4320\, \cos(v)\, v^{10} {c_3}^2 + 17280\, \cos(v)\, v^8 {c_3}^2$$
$$+ \quad 4320\, \cos(v)\, v^8 c_3 + 1244160\, v^4 b_0 c_3$$
$$+ \quad 7632\, v^{10} c_0 {c_3}^2 + 720\, v^8 c_2 c_3$$
$$- \quad 103680\, v^4 c_0 c_3 - 17280\, v^6 c_0 c_3$$
$$- \quad 267840\, v^8 c_2 {c_3}^2 - 3732480\, v^2 b_0 c_3$$
$$- \quad 3732480\, v^2 c_0 c_3 + 103680\, \cos(v)\, v^4 c_3$$
$$+ \quad 2799360\, v^6 b_0 {c_3}^2 + 2799360\, v^6 c_0 {c_3}^2$$
$$- \quad 112320\, v^4 a_1 c_3 + 190080\, v^8 c_0 {c_3}^2$$
$$+ \quad 3600\, v^6 a_1 c_3 + 1347840\, v^4 a_1 {c_3}^2$$
$$+ \quad 5\, \cos(v)\, v^{18} {c_3}^4 + 60\, \cos(v)\, v^{16} {c_3}^4$$
$$+ \quad 10\, \cos(v)\, v^{16} {c_3}^3 + 10\, \cos(v)\, v^{14} {c_3}^2$$
$$+ \quad 240\, \cos(v)\, v^{14} {c_3}^3 + 5\, \cos(v)\, v^{12} c_3$$
$$+ \quad 360\, \cos(v)\, v^{12} {c_3}^2 + 720\, v^{14} b_0 {c_3}^4$$
$$+ \quad 240\, \cos(v)\, v^{10} c_3 + 720\, v^{14} c_0 {c_3}^4$$
$$+ \quad 34560\, \cos(v)\, v^6 c_3 + 207360\, v^2 c_2$$
$$- \quad 8640\, v^4 c_2 + 207360\, v^2 b_0 + 1440\, \cos(v)\, v^6$$
$$+ \quad 103680\, \cos(v)\, v^2 + 17280\, \cos(v)\, v^4$$
$$+ \quad 720\, v^4 a_1 + 1347840\, v^4 c_2 c_3 - 720\, v^8 c_0 c_3$$
$$- \quad 25920\, v^6 c_2 c_3 + \cos(v)\, v^{20} {c_3}^5$$
$$- \quad 43200\, v^6 b_0 c_3 - 77760\, v^8 b_0 {c_3}^2$$
$$+ \quad 4320\, \cos(v)\, v^{10} c_1 c_3 + 34560\, \cos(v)\, v^{10} c_1 {c_3}^2$$
$$+ \quad 8640\, \cos(v)\, v^{12} c_1 {c_3}^2 + 34560\, \cos(v)\, v^8 c_1 c_3$$
$$+ \quad 17280\, \cos(v)\, v^{12} {c_1}^2 {c_3}^2 + 4320\, \cos(v)\, v^{14} c_1 {c_3}^3$$
$$+ \quad 4320\, \cos(v)\, v^{14} {c_1}^2 {c_3}^2 + 4320\, \cos(v)\, v^{16} {c_1}^2 {c_3}^3$$
$$+ \quad 1440\, \cos(v)\, v^{18} {c_1}^3 {c_3}^3 + 1347840\, v^4 a_1 c_1 c_3$$
$$+ \quad 1347840\, v^6 b_0 c_1 c_3 - 129600\, v^6 a_1 c_1 c_3$$
$$- \quad 51840\, v^8 b_0 c_1 c_3 - 587520\, v^8 a_1 c_1 {c_3}^2$$
$$+ \quad 10512\, v^{10} c_1 c_2 c_3 + 198720\, v^8 c_1 c_2 c_3$$

$$
\begin{aligned}
&+ \quad 903744\,v^{10}c_0c_1{c_3}^2 + 41472\,v^{10}b_0c_1{c_3}^2 \\
&- \quad 221184\,v^{10}a_1{c_1}^2{c_3}^2 - 43200\,v^{12}c_1c_2{c_3}^2 \\
&+ \quad 43200\,v^{12}c_0c_1{c_3}^2 + 406080\,v^{12}b_0{c_1}^2{c_3}^2 \\
&- \quad 79200\,v^{14}{c_1}^2c_2{c_3}^2 - 28800\,v^{14}c_0c_1{c_3}^3 \\
&- \quad 17280\,v^2a_1 - 3732480\,v^2a_1c_1c_3 \\
&- \quad 1860\,v^{18}c_0{c_1}^2{c_3}^3 + 43920\,v^{18}{c_1}^3c_2{c_3}^3 \\
&- \quad 720\,v^{18}c_0{c_1}^2{c_3}^4 + 60\,\cos(v)\,v^8 \\
&- \quad 248832\,a_1c_3 - 8640\,v^4b_0 \\
&+ \quad 7200\,v^{18}b_0{c_1}^2{c_3}^4 - 22320\,v^{18}b_0{c_1}^3{c_3}^3 \\
&+ \quad 43200\,v^{18}a_1{c_1}^3{c_3}^4 - 12\,v^{20}{c_1}^2c_2{c_3}^4 \\
&+ \quad 1212\,v^{20}{c_1}^3c_2{c_3}^3 + 12\,v^{20}c_0c_1{c_3}^5 \\
&- \quad 624\,v^{20}c_0{c_1}^2{c_3}^4 - 17418240\,v^4b_0c_1c_3 \\
&+ \quad 18144\,v^{20}c_0{c_1}^3{c_3}^4 + 7056\,v^{20}b_0{c_1}^3{c_3}^4 \\
&+ \quad 18144\,v^{20}a_1{c_1}^4{c_3}^4 + 120\,v^{22}{c_1}^3c_2{c_3}^4 \\
&- \quad 120\,v^{22}c_0{c_1}^2{c_3}^5 + 420\,v^{22}c_0{c_1}^3{c_3}^4 \\
&- \quad 60\,v^{24}{c_1}^4c_2{c_3}^4 + 60\,v^{24}c_0{c_1}^3{c_3}^5 \\
&+ \quad 20\,\cos(v)\,v^{24}{c_1}^3{c_3}^4 + 5040\,v^{22}b_0{c_1}^4{c_3}^4 \\
&+ \quad 60\,\cos(v)\,v^{24}{c_1}^4{c_3}^4 + 10\,\cos(v)\,v^{26}{c_1}^3{c_3}^5 \\
&+ \quad 5\,\cos(v)\,v^{28}{c_1}^4{c_3}^5 + \cos(v)\,v^{30}{c_1}^5{c_3}^5 \\
&+ \quad 4250880\,v^6c_1c_2c_3 + 5\,\cos(v)\,v^{26}{c_1}^4{c_3}^4 \\
&+ \quad 7050240\,v^6a_1c_1{c_3}^2 + 3600\,v^8a_1c_1c_3 \\
&+ \quad 11715840\,v^8b_0c_1{c_3}^2 + 8709120\,v^8a_1{c_1}^2{c_3}^2 \\
&- \quad 144\,v^{10}b_0c_1c_3 - 1074816\,v^{10}c_1c_2{c_3}^2 \\
&+ \quad 14688\,v^{10}a_1c_1{c_3}^2 + 13499136\,v^{10}b_0{c_1}^2{c_3}^2 \\
&- \quad 1249344\,v^{10}a_1c_1{c_3}^3 + 180\,v^{12}c_1c_2c_3 \\
&+ \quad 3600\,v^{12}b_0c_1{c_3}^2 - 1347840\,v^{12}{c_1}^2c_2{c_3}^2 \\
&- \quad 717120\,v^{12}c_0c_1{c_3}^3 - 794880\,v^{12}b_0c_1{c_3}^3 \\
&+ \quad 16560\,v^{12}a_1c_1{c_3}^3 + 9360\,v^{12}a_1{c_1}^2{c_3}^2 \\
&- \quad 2064960\,v^{12}a_1{c_1}^2{c_3}^3 - 720\,v^{14}c_1c_2{c_3}^2
\end{aligned}
$$

$$
\begin{aligned}
& + \quad 780\, v^{14} c_0 c_1 {c_3}^2 + 23760\, v^{14} c_1 c_2 {c_3}^3 \\
& - \quad 9360\, v^{14} b_0 c_1 {c_3}^3 + 8709120\, v^{8} c_0 c_1 {c_3}^2 \\
& + \quad 9360\, v^{14} b_0 {c_1}^2 {c_3}^2 - 1270080\, v^{14} c_0 {c_1}^2 {c_3}^3 \\
& - \quad 1339200\, v^{14} b_0 {c_1}^2 {c_3}^3 + 24480\, v^{14} a_1 c_1 {c_3}^4 \\
& + \quad 3600\, v^{14} a_1 {c_1}^2 {c_3}^3 - 1270080\, v^{14} a_1 {c_1}^3 {c_3}^3 \\
& + \quad 300\, v^{16} c_1 c_2 {c_3}^3 - 1620\, v^{16} {c_1}^2 c_2 {c_3}^2 \\
& - \quad 180\, v^{16} c_0 c_1 {c_3}^3 + 42480\, v^{16} {c_1}^2 c_2 {c_3}^3 \\
& + \quad 4320\, v^{16} c_0 c_1 {c_3}^4 - 90000\, v^{16} c_0 {c_1}^2 {c_3}^3 \\
& + \quad 3600\, v^{16} b_0 c_1 {c_3}^4 - 21600\, v^{16} b_0 {c_1}^2 {c_3}^3 \\
& - \quad 933120\, v^{16} b_0 {c_1}^3 {c_3}^3 + 46800\, v^{16} a_1 {c_1}^2 {c_3}^4 \\
& - \quad 12240\, v^{16} a_1 {c_1}^3 {c_3}^3 \\
\Upsilon_5(v) & = \quad -8640\, \sin(v)\, v^{10} c_3 - 360\, \sin(v)\, v^{14} c_1 c_3 \\
& + \quad 328320\, v^{23} b_0 {c_1}^4 {c_3}^4 - 4560\, v^{15} c_1 c_2 {c_3}^2 \\
& + \quad 336960\, v^{19} a_1 {c_1}^3 {c_3}^4 + 34800\, v^{21} {c_1}^3 c_2 {c_3}^3 \\
& - \quad 404974080\, v^{13} c_0 {c_1}^2 {c_3}^3 - 617725440\, v^{13} b_0 {c_1}^2 {c_3}^3 \\
& + \quad 22498560\, v^{13} a_1 c_1 {c_3}^4 - 1866240\, v^{13} b_0 c_1 {c_3}^3 \\
& - \quad 103680\, \sin(v)\, v^{10} c_1 c_3 - 4320\, v^{13} b_0 {c_3}^3 \\
& + \quad 3360\, v^{15} c_0 c_1 {c_3}^2 - 69120\, v^{15} b_0 c_1 {c_3}^3 \\
& + \quad 648000\, v^{15} c_1 c_2 {c_3}^3 - 404974080\, v^{13} a_1 {c_1}^3 {c_3}^3 \\
& + \quad 665280\, v^{19} c_0 {c_1}^2 {c_3}^4 - 60480\, v^{13} a_1 {c_3}^4 \\
& - \quad 15\, \sin(v)\, v^{28} {c_1}^2 {c_3}^6 - 60\, \sin(v)\, v^{28} {c_1}^3 {c_3}^5 \\
& + \quad 777600\, v^{9} c_0 {c_3}^2 - 622080\, v^{5} c_0 c_3 \\
& - \quad 47278080\, v^{7} a_1 {c_3}^3 - 1492992\, \sin(v)\, v^{4} c_3 - 15\, \sin(v)\, v^{28} {c_1}^4 {c_3}^4 \\
& + \quad 1200\, v^{15} c_2 {c_3}^3 + 103680\, v^{17} b_0 c_1 {c_3}^4 + 4458240\, v^{11} a_1 {c_1}^2 {c_3}^2 \\
& - \quad 2985984\, \sin(v) + 1866240\, v^{13} b_0 {c_3}^4 \\
& - \quad 4320\, v^{17} c_0 {c_3}^5 + 360\, v^{17} c_0 {c_3}^4 \\
& + \quad 15655680\, v^{11} a_1 c_1 {c_3}^3 + 14394240\, v^{21} b_0 {c_1}^4 {c_3}^4 \\
& + \quad 725760\, v^{11} b_0 {c_3}^3 + 95040\, v^{13} c_2 {c_3}^3 \\
& + \quad 1909440\, v^{19} {c_1}^3 c_2 {c_3}^3 - 72\, \sin(v)\, v^{20} {c_3}^5
\end{aligned}
$$

$$- \quad 40320\, v^{15} a_1 {c_3}^5 - 103680\, \sin(v)\, v^{10} {c_3}^2$$
$$- \quad 9953280\, v^3 a_1 c_3 + 54120960\, v^{17} a_1 {c_1}^3 {c_3}^4$$
$$- \quad 1440\, \sin(v)\, v^{16} c_1 {c_3}^2 - 6\, \sin(v)\, v^{16} c_1 c_3$$
$$- \quad 30\, \sin(v)\, v^{18} c_1 {c_3}^2 + 3939840\, v^{11} c_2 {c_3}^3$$
$$- \quad 34560\, \sin(v)\, v^6 - 2160\, \sin(v)\, v^{18} c_1 {c_3}^3$$
$$- \quad 120683520\, v^7 a_1 c_1 {c_3}^2 + 94556160\, v^3 a_1 c_1 c_3$$
$$+ \quad 14400\, v^{15} b_0 {c_3}^4 - 99360\, v^{13} c_0 {c_3}^3$$
$$+ \quad 7464960\, v c_2 - 25920\, \sin(v)\, v^{14} c_1 {c_3}^2$$
$$- \quad 20\, \sin(v)\, v^{30} {c_1}^3 {c_3}^6 - 360\, \sin(v)\, v^{22} c_1 {c_3}^5$$
$$+ \quad 233280\, v^{13} c_0 c_1 {c_3}^2 + 94556160\, v^3 b_0 c_3$$
$$- \quad 2073600\, v^3 c_2 + 209018880\, v^5 b_0 c_1 c_3$$
$$- \quad 720\, \sin(v)\, v^{14} {c_3}^2 - 13582080\, v^{15} b_0 {c_1}^2 {c_3}^3$$
$$- \quad 328320\, v^{13} c_1 c_2 {c_3}^2 - 47278080\, v^7 c_2 {c_3}^2$$
$$- \quad 622080\, v a_1 - 354240\, v^{15} a_1 {c_1}^2 {c_3}^3$$
$$+ \quad 268738560\, v^5 c_0 {c_3}^2 + 1624320\, v^{17} {c_1}^2 c_2 {c_3}^3$$
$$- \quad 4320\, v^{17} b_0 {c_3}^5 + 26853120\, v^{19} b_0 {c_1}^3 {c_3}^4$$
$$- \quad 360\, v^{29} c_0 {c_1}^4 {c_3}^6 - 60\, \sin(v)\, v^{20} c_1 {c_3}^3$$
$$- \quad 720\, \sin(v)\, v^{18} {c_1}^2 {c_3}^2 + 69672960\, v^3 a_1 {c_3}^2$$
$$- \quad 1440\, \sin(v)\, v^{20} c_1 {c_3}^4 - 15\, \sin(v)\, v^{20} {c_1}^2 {c_3}^2$$
$$- \quad 60\, \sin(v)\, v^{22} c_1 {c_3}^4 - 2160\, \sin(v)\, v^{20} {c_1}^2 {c_3}^3$$
$$- \quad 18040320\, v^5 a_1 c_1 c_3 - 60\, \sin(v)\, v^{22} {c_1}^2 {c_3}^3$$
$$- \quad 311040\, \sin(v)\, v^{12} {c_1}^2 {c_3}^2 - 622080\, \sin(v)\, v^{10} c_1 {c_3}^2$$
$$- \quad 622080\, \sin(v)\, v^8 c_1 c_3 - 1492992\, \sin(v)\, v^6 c_1 c_3$$
$$- \quad 16174080\, v^7 b_0 c_1 c_3 + 14929920\, v a_1 c_3$$
$$- \quad 311040\, \sin(v)\, v^8 {c_3}^2 + 1088640\, v^9 c_1 c_2 c_3$$
$$- \quad 622080\, \sin(v)\, v^6 c_3 - 1719360\, v^{17} c_0 {c_1}^2 {c_3}^3$$
$$- \quad 60134400\, v^9 b_0 {c_3}^3 - 836075520\, v^3 b_0 c_1 c_3$$
$$- \quad 1200\, v^{27} {c_1}^4 c_2 {c_3}^5 - 578880\, v^{19} a_1 {c_1}^2 {c_3}^5$$
$$- \quad 103680\, \sin(v)\, v^{14} {c_1}^2 {c_3}^2 - 449141760\, v^{15} b_0 {c_1}^3 {c_3}^3$$

$$- \quad 8640\,\sin(v)\,v^{12}c_1c_3 - 838080\,v^{15}{c_1}^2c_2{c_3}^2$$
$$- \quad 360\,\sin(v)\,v^{18}{c_3}^4 - 30\,\sin(v)\,v^{30}{c_1}^4{c_3}^5$$
$$+ \quad 2177280\,v^{11}b_0c_1{c_3}^2 - 720\,\sin(v)\,v^{16}{c_3}^3$$
$$- \quad 12960\,\sin(v)\,v^{12}{c_3}^2 - 72\,\sin(v)\,v^{30}{c_1}^5{c_3}^5$$
$$- \quad 360\,\sin(v)\,v^{28}{c_1}^4{c_3}^5 - 3214080\,v^{11}c_0{c_3}^3$$
$$- \quad 14307840\,v^5b_0c_3 - 250560\,v^{17}b_0{c_1}^2{c_3}^3$$
$$- \quad 64800\,v^{21}b_0{c_1}^2{c_3}^5 + 26127360\,v^{11}b_0{c_1}^2{c_3}^2$$
$$- \quad 79004160\,v^9a_1{c_1}^2{c_3}^2 + 7672320\,v^9a_1c_1{c_3}^2$$
$$+ \quad 417600\,v^{21}b_0{c_1}^3{c_3}^4 - 3006720\,v^{15}a_1{c_1}^3{c_3}^3$$
$$- \quad 518400\,v^{23}a_1{c_1}^4{c_3}^5 + 352800\,v^{21}a_1{c_1}^4{c_3}^4$$
$$- \quad 25920\,v^7a_1c_3 + 3525120\,v^{13}b_0{c_1}^2{c_3}^2$$
$$- \quad 15\,\sin(v)\,v^{20}{c_3}^4 - 40320\,v^{15}c_2{c_3}^4$$
$$- \quad 1200\,v^{15}c_0{c_3}^3 - 1492992\,\sin(v)\,v^2$$
$$+ \quad 1347840\,v^7a_1c_1c_3 - 544320\,v^{23}{c_1}^4c_2{c_3}^4$$
$$+ \quad 268738560\,v^5b_0{c_3}^2 - 20\,\sin(v)\,v^{18}{c_3}^3$$
$$+ \quad 24675840\,v^{19}a_1{c_1}^4{c_3}^4 - 103680\,\sin(v)\,v^8c_3$$
$$- \quad 311040\,\sin(v)\,v^4 - 69672960\,v^9b_0c_1{c_3}^2$$
$$+ \quad 6635520\,v^{11}c_0c_1{c_3}^2 - 360\,v^{17}c_2{c_3}^4$$
$$+ \quad 360\,v^{25}{c_1}^3c_2{c_3}^5 + 1552320\,v^{21}c_0{c_1}^3{c_3}^4$$
$$- \quad 103680\,\sin(v)\,v^{14}c_1{c_3}^3 + 777600\,v^9b_0{c_3}^2$$
$$- \quad 20373120\,v^{13}{c_1}^2c_2{c_3}^2 + 313528320\,v^5c_1c_2c_3$$
$$- \quad 60134400\,v^9c_0{c_3}^3 + 11612160\,v^{13}a_1{c_1}^2{c_3}^3$$
$$- \quad 181440\,v^{25}a_1{c_1}^5{c_3}^5 - 3732480\,v^7c_1c_2c_3$$
$$+ \quad 311040\,v^9b_0c_1c_3 - 175680\,v^{15}a_1c_1{c_3}^4$$
$$- \quad 6\,\sin(v)\,v^{34}{c_1}^5{c_3}^6 - 15\,\sin(v)\,v^{32}{c_1}^4{c_3}^6$$
$$- \quad 38568960\,v^7b_0{c_3}^2 + 8709120\,v^7c_0{c_3}^2$$
$$- \quad 36080640\,v^5a_1{c_3}^2 - 5400\,v^{21}{c_1}^2c_2{c_3}^4$$
$$- \quad 40435200\,v^{15}c_0{c_1}^2{c_3}^3 - 90720\,v^{21}c_0{c_1}^2{c_3}^5$$
$$+ \quad 7920\,v^{25}c_0{c_1}^3{c_3}^5 - 360\,v^{25}c_0{c_1}^2{c_3}^6$$

$$- \quad 12960\, v^{25} {c_1}^4 c_2 {c_3}^4 - 6\, \sin{(v)}\, v^{32} {c_1}^5 {c_3}^5$$
$$- \quad 650880\, v^{21} {c_1}^3 c_2 {c_3}^4 + 1866240\, v^{13} c_0 {c_3}^4$$
$$+ \quad 25920\, v^{11} c_1 c_2 c_3 - 648000\, v^{15} c_0 c_1 {c_3}^3$$
$$- \quad 7983360\, v^{11} c_1 c_2 {c_3}^2 + 69672960\, v^3 c_2 c_3$$
$$- \quad 17729280\, v^{17} b_0 {c_1}^3 {c_3}^3 + 3525120\, v^7 a_1 {c_3}^2$$
$$- \quad 741600\, v^{21} a_1 {c_1}^3 {c_3}^5 + 54720\, v^{15} c_0 {c_3}^4$$
$$- \quad 207360\, \sin{(v)}\, v^{12} c_1 {c_3}^2 + 24883200\, v^3 c_0 c_3$$
$$+ \quad 328320\, v^{17} c_0 c_1 {c_3}^4 + 5011200\, v^9 a_1 {c_3}^3$$
$$- \quad 25920\, v^{11} c_2 {c_3}^2 - 12960\, \sin{(v)}\, v^{16} {c_1}^2 {c_3}^2$$
$$- \quad 4320\, v^5 a_1 - 25920\, \sin{(v)}\, v^{16} c_1 {c_3}^3$$
$$- \quad \sin{(v)}\, v^{12} - 72\, \sin{(v)}\, v^{10} - 2160\, \sin{(v)}\, v^8$$
$$- \quad 15\, \sin{(v)}\, v^{16} {c_3}^2 - 103680\, \sin{(v)}\, v^{16} {c_1}^2 {c_3}^3$$
$$- \quad 8640\, \sin{(v)}\, v^{18} c_1 {c_3}^4 - 25920\, \sin{(v)}\, v^{18} {c_1}^2 {c_3}^3$$
$$+ \quad 25920\, v^{11} c_0 {c_3}^2 - 34560\, \sin{(v)}\, v^{18} {c_1}^3 {c_3}^3$$
$$- \quad 2160\, v^{19} c_1 c_2 {c_3}^4 - 8640\, \sin{(v)}\, v^{20} {c_1}^3 {c_3}^3$$
$$- \quad 8640\, \sin{(v)}\, v^{22} {c_1}^3 {c_3}^4 - 2160\, \sin{(v)}\, v^{24} {c_1}^4 {c_3}^4$$
$$- \quad 6\, \sin{(v)}\, v^{26} c_1 {c_3}^6 - 60\, \sin{(v)}\, v^{26} {c_1}^2 {c_3}^5$$
$$- \quad 60\, \sin{(v)}\, v^{26} {c_1}^3 {c_3}^4 - 12960\, \sin{(v)}\, v^{20} {c_1}^2 {c_3}^4$$
$$- \quad 720\, \sin{(v)}\, v^{26} {c_1}^3 {c_3}^5 - 360\, \sin{(v)}\, v^{26} {c_1}^4 {c_3}^4$$
$$+ \quad 20632320\, v^{13} c_1 c_2 {c_3}^3 - 19491840\, v^{13} c_0 c_1 {c_3}^3$$
$$- \quad 6\, \sin{(v)}\, v^{22} {c_3}^5 - \sin{(v)}\, v^{24} {c_3}^6$$
$$+ \quad 22320\, v^{19} {c_1}^2 c_2 {c_3}^3 + 8640\, v^{13} b_0 c_1 {c_3}^2$$
$$+ \quad 2160\, v^{19} c_0 c_1 {c_3}^4 - 90\, \sin{(v)}\, v^{24} {c_1}^2 {c_3}^4$$
$$- \quad 720\, \sin{(v)}\, v^{24} {c_1}^2 {c_3}^5 - 1440\, \sin{(v)}\, v^{24} {c_1}^3 {c_3}^4$$
$$- \quad 8640\, \sin{(v)}\, v^{14} {c_3}^3 - 2160\, \sin{(v)}\, v^{16} {c_3}^4$$
$$- \quad 552960\, v^{19} {c_1}^2 c_2 {c_3}^4 - 20\, \sin{(v)}\, v^{24} {c_1}^3 {c_3}^3$$
$$- \quad 86400\, v^{11} a_1 {c_3}^3 + 3939840\, v^{11} a_1 {c_3}^4$$
$$+ \quad 360\, v^{13} c_0 {c_3}^2 - 272160\, v^{13} a_1 c_1 {c_3}^3$$
$$- \quad 60480\, v^{13} a_1 {c_1}^2 {c_3}^2 - 360\, v^{13} c_2 {c_3}^2$$

$$
\begin{aligned}
&+ \ 311040\, v^7 b_0 c_3 - 25920\, v^{19} c_0 c_1 {c_3}^5 \\
&+ \ 50492160\, v^{15} a_1 {c_1}^2 {c_3}^4 - 60480\, v^{25} b_0 {c_1}^4 {c_3}^5 \\
&+ \ 940584960\, v^7 c_0 c_1 {c_3}^2 + 1507921920\, v^7 b_0 c_1 {c_3}^2 \\
&+ \ 940584960\, v^7 a_1 {c_1}^2 {c_3}^2 - 25920\, v^9 a_1 c_1 c_3 \\
&- \ 223534080\, v^9 c_1 c_2 {c_3}^2 + 2072770560\, v^9 b_0 {c_1}^2 {c_3}^2 \\
&- \ 283668480\, v^9 a_1 c_1 {c_3}^3 - 129600\, v^{11} a_1 c_1 {c_3}^2 \\
&- \ 296110080\, v^{11} {c_1}^2 c_2 {c_3}^2 - 274959360\, v^{11} c_0 c_1 {c_3}^3 \\
&- \ 322237440\, v^{11} b_0 c_1 {c_3}^3 + 293760\, v^{19} b_0 {c_1}^2 {c_3}^4 \\
&- \ 328320\, v^{19} b_0 {c_1}^3 {c_3}^3 + 360\, v^{13} c_1 c_2 c_3 \\
&- \ 181440\, v^{25} c_0 {c_1}^4 {c_3}^5 - 27360\, v^{19} c_0 {c_1}^2 {c_3}^3 \\
&- \ 89579520\, v c_0 c_3 + 40320\, v^{15} b_0 {c_1}^2 {c_3}^2 \\
&+ \ 40435200\, v^{15} {c_1}^2 c_2 {c_3}^3 - 25920\, v^{19} b_0 c_1 {c_3}^5 \\
&+ \ 10056960\, v^{15} c_0 c_1 {c_3}^4 + 172800\, v^3 a_1 \\
&- \ 360\, \sin{(v)}\, v^{12} c_3 + 24675840\, v^{19} c_0 {c_1}^3 {c_3}^4 \\
&+ \ 93726720\, v^9 c_0 c_1 {c_3}^2 - 34560\, \sin{(v)}\, v^{12} {c_3}^3 \\
&+ \ 10540800\, v^{15} b_0 c_1 {c_3}^4 - 13685760\, v^5 c_2 c_3 \\
&- \ 2073600\, v^3 b_0 + 33747840\, v^{17} {c_1}^3 c_2 {c_3}^3 \\
&+ \ 20373120\, v^{17} c_0 {c_1}^2 {c_3}^4 + 1244160\, v^5 a_1 c_3 \\
&+ \ 23898240\, v^{17} b_0 {c_1}^2 {c_3}^4 - 237600\, v^{17} a_1 c_1 {c_3}^5 \\
&+ \ 1200\, v^{27} c_0 {c_1}^3 {c_3}^6 + 8280\, v^{17} c_1 c_2 {c_3}^3 \\
&- \ 89579520\, v b_0 c_3 - 38880\, v^{17} a_1 {c_1}^2 {c_3}^4 \\
&+ \ 51840\, v^5 c_2 - 6\, \sin{(v)}\, v^{14} c_3 \\
&+ \ 311040\, v^7 c_2 c_3 - 3360\, v^{27} c_0 {c_1}^4 {c_3}^5 \\
&- \ 12960\, v^{17} {c_1}^2 c_2 {c_3}^2 - 7920\, v^{17} c_0 c_1 {c_3}^3 \\
&- \ 233280\, v^{17} c_1 c_2 {c_3}^4 - 40320\, v^{27} b_0 {c_1}^5 {c_3}^5 \\
&- \ 64800\, v^9 a_1 {c_3}^2 - 571069440\, v^{11} a_1 {c_1}^2 {c_3}^3 \\
&+ \ 25920\, v^{23} c_0 {c_1}^3 {c_3}^5 - 86400\, v^{23} b_0 {c_1}^3 {c_3}^5 \\
&- \ 5040\, v^{23} {c_1}^3 c_2 {c_3}^4 + 7464960\, v b_0 \\
&+ \ 51840\, v^5 b_0 - 2160\, v^{23} c_0 {c_1}^2 {c_3}^5
\end{aligned}
$$

$$
\begin{aligned}
&- \sin(v)\, v^{36} {c_1}^6 {c_3}^6 - 89579520\, v a_1 c_1 c_3 \\
&+ 582266880\, v^5 a_1 c_1 {c_3}^2 - 241920\, v^{17} a_1 {c_1}^3 {c_3}^3 \\
&+ 27360\, v^{23} c_0 {c_1}^3 {c_3}^4 + 360\, v^{29} {c_1}^5 c_2 {c_3}^5 \\
&- 2160 \sin(v)\, v^{22} {c_1}^2 {c_3}^4 - 720 \sin(v)\, v^{22} {c_1}^3 {c_3}^3 \\
&- 30 \sin(v)\, v^{24} c_1 {c_3}^5.
\end{aligned}
$$

Appendix B: Formulae for the $\Upsilon_j(v)$, $j = 6(1)13$

$$
\begin{aligned}
\Upsilon_6(v) &= (\cos(v))^2 \sin(v)\, v^9 + 54\, (\cos(v))^2 \sin(v)\, v^7 \\
&+ 216\, (\cos(v))^3 v^6 + 783\, (\cos(v))^2 \sin(v)\, v^5 \\
&- 1026 \sin(v)\, v^7 + 6480\, (\cos(v))^3 v^4 \\
&- 2286 \cos(v)\, v^6 + 4995\, (\cos(v))^2 \sin(v)\, v^3 \\
&+ 14310 \sin(v)\, v^5 + 87480\, (\cos(v))^3 v^2 \\
&- 46440 \cos(v)\, v^4 + 4860\, (\cos(v))^2 \sin(v)\, v \\
&+ 117585 \sin(v)\, v^3 + 113400\, (\cos(v))^3 \\
&+ 110160 \cos(v)\, v^2 - 89100 \sin(v)\, v \\
&- 113400 \cos(v) - 28 \sin(v)\, v^9 \\
\Upsilon_7(v) &= (\cos(v))^2 v^6 + 24 \cos(v) \sin(v)\, v^5 \\
&+ 4\, v^6 - 210\, (\cos(v))^2 v^4 - 750 \cos(v) \sin(v)\, v^3 \\
&+ 420\, v^4 + 765\, (\cos(v))^2 v^2 \\
&- 1170 \cos(v) \sin(v)\, v + 1980\, v^2 \\
&+ 1575\, (\cos(v))^2 - 1575 \\
\Upsilon_8(v) &= -(\cos(v))^2 \sin(v)\, v^9 + 18\, (\cos(v))^3 v^8 \\
&+ 28 \sin(v)\, v^9 + 60\, (\cos(v))^3 v^6 - 168 \cos(v)\, v^8 \\
&+ 945\, (\cos(v))^2 \sin(v)\, v^5 + 90\, (\cos(v))^2 \sin(v)\, v^7 \\
&+ 1290 \sin(v)\, v^7 + 2970\, (\cos(v))^3 v^4 \\
&- 6630 \cos(v)\, v^6 + 10125\, (\cos(v))^2 \sin(v)\, v^3 \\
&- 2430 \sin(v)\, v^5 + 20250\, (\cos(v))^3 v^2 \\
&+ 57780 \cos(v)\, v^4 + 72900\, (\cos(v))^2 \sin(v)\, v
\end{aligned}
$$

$$
\begin{aligned}
& + \quad 54675\ \sin(v)\, v^3 - 32400\ (\cos(v))^3 \\
& + \quad 12150\ \cos(v)\, v^2 - 137700\ \sin(v)\, v + 32400\ \cos(v) \\
\Upsilon_9(v) \quad & = \quad v^2 \Big((\cos(v))^2\, v^8 + 16\ \cos(v) \sin(v)\, v^7 \\
& - \quad 48\ (\cos(v))^2\, v^6 + 4\, v^8 + 174\ \cos(v) \sin(v)\, v^5 \\
& + \quad 105\ (\cos(v))^2\, v^4 + 168\, v^6 \\
& + \quad 1890\ \cos(v) \sin(v)\, v^3 + 8505\ (\cos(v))^2\, v^2 \\
& - \quad 5460\, v^4 - 3780\ \cos(v) \sin(v)\, v \\
& + \quad 28350\ (\cos(v))^2 + 23625\, v^2 - 28350 \Big) \\
\Upsilon_{10}(v) \quad & = \quad (\cos(v))^2\, v^8 + 8\ \cos(v) \sin(v)\, v^7 \\
& + \quad 4\, v^8 + 90\ \cos(v) \sin(v)\, v^5 + 765\ (\cos(v))^2\, v^4 \\
& + \quad 188\, v^6 - 1890\ \cos(v) \sin(v)\, v^3 \\
& + \quad 1215\ (\cos(v))^2\, v^2 - 3060\, v^4 \\
& - \quad 10800\ \cos(v) \sin(v)\, v - 5400\ (\cos(v))^2 + 4185\, v^2 \\
& + \quad 5400 + 22\ (\cos(v))^2\, v^6 \\
\Upsilon_{11}(v) \quad & = \quad -(\cos(v))^2 \sin(v)\, v^9 + 12\ (\cos(v))^3\, v^8 \\
& + \quad 28\ \sin(v)\, v^9 + 432\ (\cos(v))^3\, v^6 - 112\ \cos(v)\, v^8 \\
& + \quad 81\ (\cos(v))^2 \sin(v)\, v^5 - 6\ (\cos(v))^2 \sin(v)\, v^7 \\
& + \quad 1522\ \sin(v)\, v^7 + 7980\ (\cos(v))^3\, v^4 \\
& - \quad 4362\ \cos(v)\, v^6 - 2835\ (\cos(v))^2 \sin(v)\, v^3 \\
& + \quad 8490\ \sin(v)\, v^5 + 49140\ (\cos(v))^3\, v^2 \\
& + \quad 38640\ \cos(v)\, v^4 + 3780\ (\cos(v))^2 \sin(v)\, v \\
& - \quad 23625\ \sin(v)\, v^3 + 113400\ (\cos(v))^3 \\
& + \quad 79380\ \cos(v)\, v^2 - 18900\ \sin(v)\, v - 113400\ \cos(v) \\
\Upsilon_{12}(v) \quad & = \quad (\cos(v))^2\, v^8 + 16\ \cos(v) \sin(v)\, v^7 \\
& - \quad 48\ (\cos(v))^2\, v^6 + 4\, v^8 \\
& + \quad 174\ \cos(v) \sin(v)\, v^5 + 105\ (\cos(v))^2\, v^4 \\
& + \quad 168\, v^6 + 1890\ \cos(v) \sin(v)\, v^3 + 8505\ (\cos(v))^2\, v^2 \\
& - \quad 5460\, v^4 - 3780\ \cos(v) \sin(v)\, v \\
& + \quad 28350\ (\cos(v))^2 + 23625\, v^2 - 28350
\end{aligned}
$$

$$
\begin{aligned}
\Upsilon_{13}\left(v\right) &= -\sin\left(v\right) v^{8} \left(\cos\left(v\right)\right)^{2} + 6\, \left(\cos\left(v\right)\right)^{3} v^{7} \\
&+ 28\, \sin\left(v\right) v^{8} + 180\, \left(\cos\left(v\right)\right)^{3} v^{5} \\
&- 56\, v^{7} \cos\left(v\right) - 1935\, \left(\cos\left(v\right)\right)^{2} \sin\left(v\right) v^{4} \\
&+ 1434\, \sin\left(v\right) v^{6} + 2430\, \left(\cos\left(v\right)\right)^{3} v^{3} \\
&- 750\, v^{5} \cos\left(v\right) - 39555\, \left(\cos\left(v\right)\right)^{2} \sin\left(v\right) v^{2} \\
&+ 4530\, \sin\left(v\right) v^{4} + 3150\, \left(\cos\left(v\right)\right)^{3} v \\
&+ 64620\, \cos\left(v\right) v^{3} - 56700\, \left(\cos\left(v\right)\right)^{2} \sin\left(v\right) \\
&- 81045\, \sin\left(v\right) v^{2} - 3150\, \cos\left(v\right) v \\
&+ 56700\, \sin\left(v\right) - 54\, \sin\left(v\right) v^{6} \left(\cos\left(v\right)\right)^{2} .
\end{aligned}
$$

Appendix C: Truncated Taylor Series Expansion Formulae for the coefficients of the new proposed multistage scheme given by (27)

$$
\begin{aligned}
a_{1} &= -2 - \frac{v^{12}}{23950080} - \frac{4457\, v^{14}}{1307674368000} - \frac{2767\, v^{16}}{10984464691200} \\
&- \frac{106679737\, v^{18}}{862719856846848000} + \cdots \\
c_{0} &= \frac{15}{28} - \frac{575\, v^{2}}{19404} + \frac{4887391\, v^{4}}{1864646784} + \frac{15077\, v^{6}}{134604189720} \\
&+ \frac{84186356129\, v^{8}}{26061476937560064} + \frac{154226125707413\, v^{10}}{8578786670921334067200} \\
&+ \frac{3080113830519428490 31\, v^{12}}{2225845126607912600008458 2400} \\
&+ \frac{281090859355362774 1\, v^{14}}{26020760336357682722770944 00} \\
&+ \frac{9287240278093570364153717761\, v^{16}}{1073288523936179345169649710142586880 00} \\
&+ \frac{1302156515867258642643820022837\, v^{18}}{1859472367719430715506418122822031769 60000} + \cdots \\
c_{1} &= \frac{1}{56} + \frac{5\, v^{2}}{3528} + \frac{206263\, v^{4}}{1695133440} + \frac{2022851\, v^{6}}{195787912320}
\end{aligned}
$$

$$
\begin{aligned}
& + \frac{61297160059\,v^{8}}{7107675528425472 0} + \frac{3468098943931\,v^{10}}{487431060847803072 00} \\
& + \frac{2359972324490615 3507\,v^{12}}{404699113928711381819719 6800} \\
& + \frac{2560426008760631776 7231\,v^{14}}{537541598075810892902042664 96000} \\
& + \frac{1263359942925797796682921363\,v^{16}}{3252389466473270742938332454977536 0000} \\
& + \frac{5350970486623998983625292 3301\,v^{18}}{169042942519948246864219829347457433 60000} + \cdots \\
c_2 &= \frac{1}{15} + \frac{v^{2}}{693} - \frac{11267\,v^{4}}{151351200} - \frac{10391\,v^{6}}{635675040} \\
& + \frac{972045013\,v^{8}}{166419725472000} + \frac{46267062131\,v^{10}}{7968176455599360 0} \\
& + \frac{1230391596534229\,v^{12}}{26103746068543503360000} \\
& + \frac{83598456817075157\,v^{14}}{3081982285826036296704 0000} \\
& + \frac{187537763777 2463417\,v^{16}}{2329978608084483440308 2240000} \\
& - \frac{318786439217896549 7\,v^{18}}{611619384622176903080908 800000} + \cdots \\
c_3 &= \frac{1}{30} + \frac{v^{2}}{1386} - \frac{11267\,v^{4}}{302702400} - \frac{10391\,v^{6}}{1271350080} \\
& - \frac{278704487\,v^{8}}{332839450944000} - \frac{49075415171\,v^{10}}{796817645559936000} \\
& - \frac{165555536796521\,v^{12}}{52207492137087006720000} \\
& - \frac{387466496860559\,v^{14}}{684884952405785843712 0000} \\
& + \frac{510183980580548867\,v^{16}}{46599572161689668806164480000}
\end{aligned}
$$

$$+ \quad \frac{50607729096627067\,v^{18}}{2895239690519180606300160000} + \cdots$$

$$b_0 = \frac{5}{6} + \frac{v^{10}}{3991680} + \frac{11353\,v^{12}}{523069747200}$$

$$+ \quad \frac{178109\,v^{14}}{109844646912000} + \frac{141929317\,v^{16}}{1725439713693696000}$$

$$+ \quad \frac{18408898661\,v^{18}}{1376900891527569408000} + \cdots$$

Appendix D: Expressions for the Derivatives of ζ_n

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

$$\zeta^{(2)} = (V(x) - V_c + \Gamma)\ \zeta(x) = (\Xi(x) + \Gamma)\ \zeta(x)$$

$$\zeta^{(3)} = \left(\frac{d}{dx}\Xi(x)\right)\zeta(x) + (\Xi(x) + \Gamma)\frac{d}{dx}\zeta(x)$$

$$\zeta^{(4)} = \left(\frac{d^2}{dx^2}\Xi(x)\right)\zeta(x) + 2\left(\frac{d}{dx}\Xi(x)\right)\frac{d}{dx}\zeta(x) + (\Xi(x) + \Gamma)^2\zeta(x)$$

$$\zeta^{(5)} = \left(\frac{d^3}{dx^3}\Xi(x)\right)\zeta(x) + 3\left(\frac{d^2}{dx^2}\Xi(x)\right)\frac{d}{dx}\zeta(x)$$

$$+ \quad 4(\Xi(x) + \Gamma)\zeta(x)\frac{d}{dx}\Xi(x) + (\Xi(x) + \Gamma)^2\frac{d}{dx}\zeta(x)$$

$$\zeta^{(6)} = \left(\frac{d^4}{dx^4}\Xi(x)\right)\zeta(x) + 4\left(\frac{d^3}{dx^3}\Xi(x)\right)\frac{d}{dx}\zeta(x)$$

$$+ \quad 7(\Xi(x) + \Gamma)\zeta(x)\frac{d^2}{dx^2}\Xi(x) + 4\left(\frac{d}{dx}\Xi(x)\right)^2\zeta(x)$$

$$+ \quad 6(\Xi(x) + \Gamma)\left(\frac{d}{dx}\zeta(x)\right)\frac{d}{dx}\Xi(x) + (\Xi(x) + \Gamma)^3\zeta(x)$$

$$\zeta^{(7)} = \left(\frac{d^5}{dx^5}\Xi(x)\right)\zeta(x) + 5\left(\frac{d^4}{dx^4}\Xi(x)\right)\frac{d}{dx}\zeta(x)$$

$$+ \quad 11(\Xi(x) + \Gamma)\zeta(x)\frac{d^3}{dx^3}\Xi(x) + 15\left(\frac{d}{dx}\Xi(x)\right)\zeta(x)$$

$$
\begin{aligned}
& + \quad \frac{d^2}{dx^2}\Xi(x) + 13\,(\Xi(x)+\Gamma)\left(\frac{d}{dx}\zeta(x)\right)\frac{d^2}{dx^2}\Xi(x) \\
& + \quad 10\left(\frac{d}{dx}\Xi(x)\right)^2\frac{d}{dx}\zeta(x) + 9\,(\Xi(x)+\Gamma)^2\zeta(x) \\
& + \quad \frac{d}{dx}\Xi(x) + (\Xi(x)+\Gamma)^3\frac{d}{dx}\zeta(x) \\
\zeta^{(8)} \quad = & \quad \left(\frac{d^6}{dx^6}\Xi(x)\right)\zeta(x) + 6\left(\frac{d^5}{dx^5}\Xi(x)\right)\frac{d}{dx}\zeta(x) \\
& + \quad 16\,(\Xi(x)+\Gamma)\,\zeta(x)\frac{d^4}{dx^4}\Xi(x) + 26\left(\frac{d}{dx}\Xi(x)\right)\zeta(x) \\
& + \quad \frac{d^3}{dx^3}\Xi(x) + 24\,(\Xi(x)+\Gamma)\left(\frac{d}{dx}\zeta(x)\right)\frac{d^3}{dx^3}\Xi(x) \\
& + \quad 15\left(\frac{d^2}{dx^2}\Xi(x)\right)^2\zeta(x) + 48\left(\frac{d}{dx}\Xi(x)\right) \\
& + \quad \left(\frac{d}{dx}\zeta(x)\right)\frac{d^2}{dx^2}\Xi(x) + 22\,(\Xi(x)+\Gamma)^2\zeta(x) \\
& + \quad \frac{d^2}{dx^2}\Xi(x) + 28\,(\Xi(x)+\Gamma)\,\zeta(x)\left(\frac{d}{dx}\Xi(x)\right)^2 \\
& + \quad 12\,(\Xi(x)+\Gamma)^2\left(\frac{d}{dx}\zeta(x)\right)\frac{d}{dx}\Xi(x) + (\Xi(x)+\Gamma)^4\zeta(x) \\
& \ldots
\end{aligned}
$$

We compute the j-th derivative of the function ζ at the point x_n, i.e. $\zeta_n^{(j)}$, substituting in the above formulae x with x_n.

Appendix E: Formula for the quantity $\mathbf{\Lambda_0}$

$$
\begin{aligned}
\Lambda_0 \quad = & \quad -\frac{239\,(\Xi(x))^2\zeta(x)\frac{\mathrm{d}^6}{\mathrm{d}x^6}g(x)}{23950080} - \frac{19\,(\Xi(x))^4\zeta(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}g(x)}{4790016} \\
- & \quad \frac{1201\,(\Xi(x))^2\zeta(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2}{23950080} - \frac{109\,\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\zeta(x)\right)\frac{\mathrm{d}^3}{\mathrm{d}x^3}g(x)}{1197504}
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{(\Xi(x))^6 \zeta(x)}{23950080} - \frac{31 \left(\frac{d}{dx}\Xi(x)\right)\left(\frac{d}{dx}\zeta(x)\right)\left(\frac{d^2}{dx^2}\Xi(x)\right)^2}{266112} \\
&- \frac{\left(\frac{d}{dx}\Xi(x)\right)^4 \zeta(x)}{85536} - \frac{g(x)\left(\frac{d}{dx}\zeta(x)\right)\frac{d^7}{dx^7}g(x)}{187110} - \frac{13 (\Xi(x))^3 \zeta(x)\left(\frac{d}{dx}\Xi(x)\right)^2}{1197504} \\
&- \frac{5\, g(x)\left(\frac{d}{dx}\zeta(x)\right)\left(\frac{d}{dx}\Xi(x)\right)^3}{199584} - \frac{(\Xi(x))^4\left(\frac{d}{dx}\zeta(x)\right)\frac{d}{dx}g(x)}{798336} \\
&- \frac{\left(\frac{d^3}{dx^3}\Xi(x)\right)\left(\frac{d}{dx}\zeta(x)\right)\frac{d^4}{dx^4}g(x)}{16632} - \frac{5 (\Xi(x))^3\left(\frac{d}{dx}\zeta(x)\right)\frac{d^3}{dx^3}g(x)}{598752} \\
&- \frac{\left(\frac{d^{10}}{dx^{10}}\Xi(x)\right)\zeta(x)}{23950080} - \frac{\left(\frac{d^9}{dx^9}\Xi(x)\right)\frac{d}{dx}\zeta(x)}{2395008} - \frac{17\left(\frac{d^2}{dx^2}\Xi(x)\right)\zeta(x)\frac{d^6}{dx^6}g(x)}{1596672} \\
&- \frac{23\, g(x)\left(\frac{d}{dx}\zeta(x)\right)\left(\frac{d^4}{dx^4}\Xi(x)\right)\frac{d}{dx}g(x)}{299376} - \frac{43\, g(x)\zeta(x)\left(\frac{d^3}{dx^3}\Xi(x)\right)^2}{748440} \\
&- \frac{37 (\Xi(x))^3\zeta(x)\frac{d^4}{dx^4}g(x)}{2993760} - \frac{\left(\frac{d}{dx}\Xi(x)\right)^2\zeta(x)\frac{d^4}{dx^4}g(x)}{19008} \\
&- \frac{353\left(\frac{d}{dx}\Xi(x)\right)\zeta(x)\left(\frac{d^3}{dx^3}\Xi(x)\right)\frac{d^2}{dx^2}g(x)}{2395008} - \frac{743\, g(x)\zeta(x)\left(\frac{d}{dx}\Xi(x)\right)^2\frac{d^2}{dx^2}g(x)}{5987520} \\
&- \frac{13\, g(x)\zeta(x)\left(\frac{d^4}{dx^4}\Xi(x)\right)\frac{d^2}{dx^2}g(x)}{136080} - \frac{157 (\Xi(x))^2\left(\frac{d}{dx}\zeta(x)\right)\frac{d^5}{dx^5}g(x)}{11975040} \\
&- \frac{23\, g(x)\zeta(x)\frac{d^8}{dx^8}g(x)}{11975040} - \frac{5\left(\frac{d^2}{dx^2}\Xi(x)\right)^3\zeta(x)}{177408} - \frac{\left(\frac{d^4}{dx^4}\Xi(x)\right)^2\zeta(x)}{114048} \\
&- \frac{31\left(\frac{d^3}{dx^3}\Xi(x)\right)\zeta(x)\frac{d^5}{dx^5}g(x)}{1995840} - \frac{73\, g(x)\left(\frac{d}{dx}\zeta(x)\right)\left(\frac{d^3}{dx^3}\Xi(x)\right)\frac{d^2}{dx^2}g(x)}{598752} \\
&- \frac{323\, g(x)\zeta(x)\left(\frac{d^5}{dx^5}\Xi(x)\right)\frac{d}{dx}g(x)}{5987520} - \frac{7\left(\frac{d}{dx}\Xi(x)\right)\left(\frac{d}{dx}\zeta(x)\right)\frac{d^6}{dx^6}g(x)}{342144} \\
&- \frac{5 (\Xi(x))^2\left(\frac{d}{dx}\zeta(x)\right)\left(\frac{d}{dx}\Xi(x)\right)\frac{d^2}{dx^2}g(x)}{99792} - \frac{313 (\Xi(x))^2\zeta(x)\left(\frac{d}{dx}\Xi(x)\right)\frac{d^3}{dx^3}g(x)}{3991680} \\
&- \frac{13\left(\frac{d}{dx}\Xi(x)\right)\zeta(x)\frac{d^7}{dx^7}g(x)}{2395008} - \frac{19\left(\frac{d^2}{dx^2}\Xi(x)\right)\left(\frac{d}{dx}\zeta(x)\right)\frac{d^5}{dx^5}g(x)}{443520}
\end{aligned}
$$

at every point $x = x_n$.

Appendix F: Formulae for the $\Upsilon_j(v)$, $j = 14(1)16$

$$
\begin{aligned}
\Upsilon_{14}(s,v) &= 8 \sin(v)\cos(v)\, s^6 v^7 - 32 \sin(v)\cos(v)\, s^4 v^9 \\
&+ 90 \sin(v)\cos(v)\, s^6 v^5 - 348 \sin(v)\cos(v)\, s^4 v^7 \\
&- 750 \sin(v)\cos(v)\, s^2 v^9 - 1890 \sin(v)\cos(v)\, s^6 v^3 \\
&- 3780 \sin(v)\cos(v)\, s^4 v^5 - 1170 \sin(v)\cos(v)\, s^2 v^7
\end{aligned}
$$

$$
\begin{aligned}
&- && 10800\,\sin(v)\cos(v)\,s^6v+7560\,\sin(v)\cos(v)\,s^4v^3\\
&+ && 765\,(\cos(v))^2\,s^2v^8-56700\,(\cos(v))^2\,s^4v^2\\
&- && 2\,(\cos(v))^2\,s^4v^{10}+24\,\sin(v)\cos(v)\,s^2v^{11}\\
&+ && (\cos(v))^2\,s^2v^{12}-17010\,(\cos(v))^2\,s^4v^4\\
&- && 210\,(\cos(v))^2\,s^4v^6+5040\,v^{10}\\
&- && 9000\,\sin(v)\cos(v)\,v^9+1215\,(\cos(v))^2\,s^6v^2\\
&+ && (\cos(v))^2\,s^6v^8+22\,(\cos(v))^2\,s^6v^6\\
&+ && 288\,\sin(v)\cos(v)\,v^{11}+1575\,(\cos(v))^2\,s^2v^6\\
&- && 210\,(\cos(v))^2\,s^2v^{10}+96\,(\cos(v))^2\,s^4v^8\\
&+ && 23760\,v^8+1980\,s^2v^8+765\,(\cos(v))^2\,s^6v^4\\
&- && 1575\,s^2v^6-336\,s^4v^8+420\,s^2v^{10}\\
&+ && 10920\,s^4v^6-47250\,s^4v^4+56700\,s^4v^2\\
&+ && 4\,s^6v^8-8\,s^4v^{10}+4\,s^2v^{12}+188\,s^6v^6\\
&- && 3060\,s^6v^4+4185\,s^6v^2+12\,(\cos(v))^2\,v^{12}\\
&- && 2520\,(\cos(v))^2\,v^{10}-5400\,(\cos(v))^2\,s^6\\
&+ && 18900\,(\cos(v))^2\,v^6-14040\,\sin(v)\cos(v)\,v^7\\
&- && 18900\,v^6+48\,v^{12}+5400\,s^6+9180\,(\cos(v))^2\,v^8\\
\Upsilon_{15}(s,v) &= && v^6\Big((\cos(v))^2\,v^6+24\,\sin(v)\cos(v)\,v^5\\
&+ && 4\,v^6-210\,(\cos(v))^2\,v^4-750\,\sin(v)\,v^3\cos(v)\\
&+ && 420\,v^4+765\,(\cos(v))^2\,v^2\\
&- && 1170\,\sin(v)\cos(v)\,v+1980\,v^2\\
&+ && 1575\,(\cos(v))^2-1575\Big)\\
\Upsilon_{16}(s,v) &= && 2970\,(\cos(v))^3\,s^6v^4+9450\,(\cos(v))^3\,s^2v^6\\
&+ && 783\,\sin(v)\,(\cos(v))^2\,v^{11}+84\,\sin(v)\,s^2v^{13}\\
&+ && 13086\,\cos(v)\,s^4v^8-36\,(\cos(v))^3\,s^4v^{10}\\
&- && 168\,\cos(v)\,s^2v^{12}-115920\,\cos(v)\,s^4v^6\\
&+ && 193860\,\cos(v)\,s^2v^8+54675\,\sin(v)\,s^6v^3\\
&+ && 70875\,\sin(v)\,s^4v^5-243135\,\sin(v)\,s^2v^7\\
&- && 340200\,(\cos(v))^3\,s^4v^2+12150\,\cos(v)\,s^6v^2
\end{aligned}
$$

$$
\begin{aligned}
&- \; 238140 \, \cos(v) \, s^4 v^4 - 9450 \, \cos(v) \, s^2 v^6 \\
&- \; 137700 \, \sin(v) \, s^6 v + 18 \, (\cos(v))^3 \, s^6 v^8 \\
&+ \; 28 \, \sin(v) \, s^6 v^9 + 4860 \, \sin(v) \, (\cos(v))^2 \, v^7 \\
&+ \; 20250 \, (\cos(v))^3 \, s^6 v^2 - 23940 \, (\cos(v))^3 \, s^4 v^6 \\
&+ \; 60 \, (\cos(v))^3 \, s^6 v^6 + 4302 \, \sin(v) \, s^2 v^{11} \\
&- \; 2430 \, \sin(v) \, s^6 v^5 - 84 \, \sin(v) \, s^4 v^{11} \\
&- \; 6630 \, \cos(v) \, s^6 v^6 + 18 \, (\cos(v))^3 \, s^2 v^{12} \\
&- \; 1296 \, (\cos(v))^3 \, s^4 v^8 - 25470 \, \sin(v) \, s^4 v^7 \\
&+ \; 336 \, \cos(v) \, s^4 v^{10} + 117585 \, \sin(v) \, v^9 \\
&+ \; 113400 \, (\cos(v))^3 \, v^6 - 89100 \, \sin(v) \, v^7 \\
&- \; 113400 \, \cos(v) \, v^6 + 87480 \, (\cos(v))^3 \, v^8 \\
&+ \; 110160 \, \cos(v) \, v^8 - 28 \, \sin(v) \, v^{15} \\
&+ \; 216 \, (\cos(v))^3 \, v^{12} - 1026 \, \sin(v) \, v^{13} \\
&+ \; 6480 \, (\cos(v))^3 \, v^{10} + 4995 \, \sin(v) \, (\cos(v))^2 \, v^9 \\
&- \; 2286 \, \cos(v) \, v^{12} + 14310 \, \sin(v) \, v^{11} \\
&- \; 46440 \, \cos(v) \, v^{10} - 32400 \, (\cos(v))^3 \, s^6 \\
&+ \; 32400 \, \cos(v) \, s^6 + 56700 \, \sin(v) \, s^4 v^3 \\
&+ \; 170100 \, \sin(v) \, s^2 v^5 + 340200 \, \cos(v) \, s^4 v^2 \\
&- \; \sin(v) \, (\cos(v))^2 \, s^6 v^9 + 3 \, \sin(v) \, (\cos(v))^2 \, s^4 v^{11} \\
&+ \; 7290 \, (\cos(v))^3 \, s^2 v^8 + 13590 \, \sin(v) \, s^2 v^9 \\
&+ \; 54 \, \sin(v) \, (\cos(v))^2 \, v^{13} - 3 \, \sin(v) \, (\cos(v))^2 \, s^2 v^{13} \\
&+ \; 57780 \, \cos(v) \, s^6 v^4 + \sin(v) \, (\cos(v))^2 \, v^{15} \\
&+ \; 540 \, (\cos(v))^3 \, s^2 v^{10} - 2250 \, \cos(v) \, s^2 v^{10} \\
&- \; 4566 \, \sin(v) \, s^4 v^9 - 168 \, \cos(v) \, s^6 v^8 \\
&- \; 147420 \, (\cos(v))^3 \, s^4 v^4 + 1290 \, \sin(v) \, s^6 v^7 \\
&+ \; 90 \, \sin(v) \, (\cos(v))^2 \, s^6 v^7 \\
&+ \; 18 \, \sin(v) \, (\cos(v))^2 \, s^4 v^9 - 162 \, \sin(v) \, (\cos(v))^2 \, s^2 v^{11} \\
&+ \; 945 \, \sin(v) \, (\cos(v))^2 \, s^6 v^5 - 243 \, \sin(v) \, (\cos(v))^2 \, s^4 v^7 \\
&+ \; 10125 \, \sin(v) \, (\cos(v))^2 \, s^6 v^3 + 8505 \, \sin(v) \, (\cos(v))^2 \, s^4 v^5
\end{aligned}
$$

$$
\begin{aligned}
&- \quad 118665 \sin(v) (\cos(v))^2 s^2 v^7 - 5805 \sin(v) (\cos(v))^2 s^2 v^9 \\
&+ \quad 72900 \sin(v) (\cos(v))^2 s^6 v - 11340 \sin(v) (\cos(v))^2 s^4 v^3 \\
&- \quad 170100 \sin(v) (\cos(v))^2 s^2 v^5 .
\end{aligned}
$$

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