

A New High Order Finite Difference Pair with Improved Properties

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Abstract

A tenth algebraic order P-stable symmetric three-stages two-step finite difference pair with vanished phase-lag and its derivatives up to order four is built, for the first time in the literature, in this paper. The methodology for the building of the new finite difference pair is based on the following steps:

- Satisfaction of the necessary and sufficient conditions for P-stability.
- Satisfaction of the condition of the vanishing of the phase-lag.
- Satisfaction of the conditions of the vanishing of the derivatives of the phase-lag up to order four.

The solution of the resulting system of equations, produced based on the above methodology, leads to the determination of the coefficients of the new proposed method.

As a result of the above procedure we obtain, for the first time in the literature, a three-stages P-stable tenth algebraic order symmetric two-step finite difference pair with vanished phase-lag and its first, second, third and fourth derivatives.

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We will also present a detailed theoretical and numerical analysis of the new obtained scheme, as follows:

- the building of the new proposed finite difference pair,
- the computation of its local truncation error (LTE),
- the denotation of the asymptotic form of the LTE, applying the new scheme to scalar problem of the radial Schrödinger equation,
- the stability analysis with the computation of the stability domain and the interval of periodicity,
- the denotation of an embedded pair for the LTE control procedure and the determination of variable step procedure for the change of the step length of the integration,
- the evaluation of the computational efficiency of the new built finite difference pair with application on:
 1. the resonance problem of the radial Schrödinger equation and on
 2. the coupled differential equations arising from the Schrödinger equation.

The above obtained results leads to the conclusion that the new obtained three-stages P-stable tenth algebraic order finite difference pair with vanished phase-lag and its derivatives up to order four is more efficient method than the existed ones.

1 Introduction

A new three stages P-stable symmetric two-step method with eliminated phase-lag and its derivatives up to order four is built, for the first time in the literature, in this paper. The building of the new finite difference method is based on the following steps:

- The conditions for the P-stability are satisfied.
- The conditions for the elimination of the phase-lag are satisfied.
- The conditions for the elimination of the derivatives of the phase-lag up to order four are satisfied.

The effectiveness of the new built finite difference pair is evaluated applying it to the following problems:

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

The efficient numerical solution of the above described problems is very important in Computational Chemistry (see [8] and references therein) since a critical part of the quantum chemical computations contains the Schrödinger equation (see [8] and references therein). We note also that in problems with more than one particle the approximate solution of the Schrödinger equation is necessary. The efficient approximate solution of the Schrödinger's equation (using numerical methods) gives us the following important information:

- numerical computations of molecular properties (vibrational energy levels and wave functions of systems) and
- numerical presentation of the electronic structure of the molecule (see for more details in [9–12]).

In this paper, and based on the new built finite difference pair, we also develop an embedded numerical pair which is based on an local truncation error control procedure and a variable-step algorithm.

The problems investigated in the present paper belong to the category of special problems which can be written as:

$$\varphi''(x) = f(x, \varphi), \quad \varphi(x_0) = \varphi_0 \quad \text{and} \quad \varphi'(x_0) = \varphi'_0. \quad (1)$$

and which they have periodical and/or oscillating solutions.

Below we give the main categories of numerical methods and their bibliography which was developed during the large research which has been done the last decades:

- Exponentially, trigonometrically and phase fitted Runge–Kutta and Runge–Kutta Nyström methods: [46], [49], [58], [61] – [66], [55], [77]. In this category of methods, Runge–Kutta and Runge–Kutta Nyström schemes are built. This category can be divided into two subcategories:
 - Numerical methods which have the property of exact integration of sets of functions of the form:

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

or sets of functions which are combination of the above functions.

- Numerical methods which have the property of elimination (or vanishing) of the phase-lag.

Remark 1. *The quantity ω in (2) determines the frequency of the problem.*

- Multistep exponentially, trigonometrically and phase fitted methods and multistep methods with minimal phase-lag: [1] – [7], [17] – [20], [24] – [27], [33], [37], [39], [43], [47] – [48], [52], [57], [59] – [60], [70] – [72], [78] – [81]. In this category of methods, multistep schemes are built. This category can be divided into two subcategories:
 - Multistep methods which have the property of exact integration of sets of functions of the form (2) or sets of functions which are combination of the functions mentioned in (2).
 - Multistep methods which have the property of elimination (or vanishing) of the phase-lag.
- Symplectic integrators: [41] – [42], [50], [53], [56], [66] – [69], [75]. In this category of numerical methods, algorithms for which the Hamiltonian energy of the system remains almost constant during the integration procedure, are built.
- Nonlinear methods: [51]. In this category of numerical methods, the schemes 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} , $j = 0, 1, 2, \dots$) is nonlinear) are built.
- General methods: [13] – [16], [21] – [23], [34] – [36], [40]. In the category of numerical methods, numerical pairs with constant coefficients are built.

2 General theory for the building of symmetric multistep finite difference pairs

In this section we describe the general theory for the building of the symmetric multistep methods. We focus our interest on these methods since the new proposed method belongs to this category.

Problems of the general form (1) can be numerically solved by discretization procedure. The integration domain $[a, b]$ is discretized using the $2m$ -step method (i.e. a finite difference method) presented below (3). In this type of discretization the quantity m determines the number of the discretization points.

In this section we will use the following symbols:

- h determines the stepsize of the integration which is the same with the step length of the discretization. It is defined as $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$ (i.e. the parameter i is moved between $1 - m$ and $m - 1$ with step 1) where
- x_n denotes the n -th point on the discretized area.
- φ_n denotes the approximated value of the function $\varphi(x)$ at the point x_n . We note here that the approximated value is computed using a numerical method and in our investigation we will use as numerical method, the $2m$ -step method (3) presented below

Let us consider the family of $2m$ -step methods:

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

The above family of finite difference pairs will be used for the numerical solution of the initial value problem (1) on the integration domain $[a, b]$. It is noted that α_i and β_i $i = -m(1)m$ are the coefficients of the $2m$ -step method.

Definition 1.

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

Definition 2.

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

Remark 2. The method $\Delta(m)$ is associated with the linear operator

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

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

Definition 3. [13] *The multistep method (3) is called of algebraic order τ , if the linear operator L (6) vanishes for any linear combination of the linearly independent functions $1, x, x^2, \dots, x^{\tau+1}$.*

Applying the symmetric $2m$ -step method $\Delta(m)$ to the scalar test problem

$$\varphi'' = -\phi^2 \varphi \quad (7)$$

we obtain the difference equation:

$$\begin{aligned} \Upsilon_m(v) \varphi_{n+m} + \dots + \Upsilon_1(v) \varphi_{n+1} + \Upsilon_0(v) \varphi_n \\ + \Upsilon_1(v) \varphi_{n-1} + \dots + \Upsilon_m(v) \varphi_{n-m} = 0 \end{aligned} \quad (8)$$

and its associated characteristic equation:

$$\begin{aligned} \Upsilon_m(v) \lambda^m + \dots + \Upsilon_1(v) \lambda + \Upsilon_0(v) \\ + \Upsilon_1(v) \lambda^{-1} + \dots + \Upsilon_m(v) \lambda^{-m} = 0. \end{aligned} \quad (9)$$

where

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

Definition 4. [14] *We call that a symmetric $2m$ -step method has an non zero interval of periodicity $(0, v_0^2)$, if its characteristic equation (9), for all $v \in (0, v_0^2)$, has the following roots :*

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

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

Definition 5. (see [14]) *We call a symmetric multistep method P -stable if its interval of periodicity is equal to $(0, \infty)$.*

Remark 3. We call a symmetric multistep method *P-stable* if the following necessary and sufficient conditions are hold:

$$|\lambda_1| = |\lambda_2| = 1 \quad (11)$$

$$|\lambda_j| \leq 1, j = 3(1)2m, \forall v. \quad (12)$$

Definition 6. We call a symmetric multistep method *singularly P-stable* if its interval of periodicity is equal to $(0, \infty) \setminus S$, where S is a finite set of points.

Definition 7. [15], [16] The symmetric multistep method with associated characteristic equation given by (9), has phase-lag which is defined as the leading term in the expansion of

$$t = v - \psi(v). \quad (13)$$

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

Definition 8. [17] We call a symmetric multistep method **phase-fitted** if its phase-lag is equal to zero.

Theorem 1. [15] For a symmetric $2m$ -step method with characteristic equation given by (9) a direct formula for the computation of the phase-lag order v and the phase-lag constant ϖ is given by

$$-\varpi v^{v+2} + O(v^{v+4}) = \frac{2 \Upsilon_m(v) \cos(mv) + \dots + 2 \Upsilon_j(v) \cos(jv) + \dots + \Upsilon_0(v)}{2m^2 \Upsilon_m(v) + \dots + 2j^2 \Upsilon_j(v) + \dots + 2 \Upsilon_1(v)} \quad (14)$$

Remark 4. For the symmetric two-step methods the phase-lag order v and the phase-lag constant ϖ are computed using the formula:

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

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

3 A new P-stable three-stages symmetric two-step finite difference pair with vanished phase-lag and its first, second, third and fourth derivatives

We consider the following family of methods

$$\hat{\varphi}_{n+1} = \varphi_{n+1} - h^2 \left(c_1 f_{n+1} - c_0 f_n + c_1 f_{n-1} \right)$$

$$\begin{aligned}\tilde{\varphi}_{n+1} &= \varphi_{n+1} - h^2 \left(c_3 \widehat{f}_{n+1} - c_2 f_n + c_3 f_{n-1} \right) \\ \varphi_{n+1} + a_1 \varphi_n + \varphi_{n-1} &= h^2 \left[b_1 \left(\tilde{f}_{n+1} + f_{n-1} \right) + b_0 f_n \right]\end{aligned}\quad (16)$$

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

Remark 5. *The new proposed finite difference pair is a nonlinear pair of three-stages. We note here that all the stages of the new scheme are based on approximations on the point x_{n+1} .*

We will study the following specific case:

$$b_0 = \frac{5}{6}, b_1 = \frac{1}{12}. \quad (17)$$

Remark 6. *We determine the above mentioned constant values of the coefficients of the family of finite difference pairs (16) requesting the maximum possible algebraic order.*

Application of the scheme (16) with the constant coefficients given by (17) to the scalar model problem (7), leads to the difference equation (8) with $m = 1$ and the corresponding characteristic equation (9) with $m = 1$ where:

$$\begin{aligned}\Upsilon_1(v) &= 1 + \frac{1}{12} v^2 \left(1 + v^2 c_3 + v^4 c_1 c_3 \right) \\ \Upsilon_0(v) &= a_1 + \frac{1}{12} v^2 \left(10 - v^2 c_2 - v^4 c_0 c_3 \right)\end{aligned}\quad (18)$$

The methodology of the building of the proposed finite difference pair is described in the flowchart of Figure 1 (for developing flowcharts in LaTeX one can see [89]):

3.1 Satisfaction of the P-stability properties

The procedure first introduced by Lambert and Watson [14] and Wang [82] is used in order to satisfy the P-stability properties for the new proposed method:

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

$$(e^{Iv})^2 \Upsilon_0(v) + e^{Iv} \Upsilon_1(v) + \Upsilon_0(v) = 0 \quad (19)$$

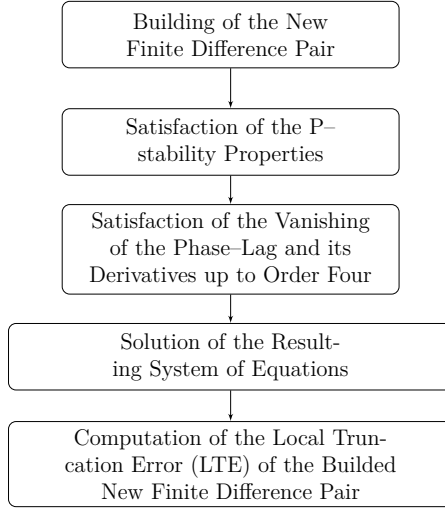


Figure 1. Flowchart for the methodology of the building of the new proposed P-stable three stages symmetric two-step scheme with vanished phase-lag and its derivatives up to order four

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

$$(e^{-Iv})^2 \Upsilon_0(v) + e^{-Iv} \Upsilon_1(v) + \Upsilon_0(v) = 0 \quad (20)$$

Remark 7. The above built conditions of P-stability are obtained based on the Definition 4 and taking into account that the new proposed new method has the characteristic equation given by (9) with $m = 1$, where Υ_j , $j = 0, 1$ are given by (18).

3.2 Satisfaction of vanishing of the phase-lag of the pair and its derivatives up to order four

The requirement of satisfaction of the vanishing of the phase-lag and its derivatives up to order four for the new proposed scheme (16) with the coefficients given by (17) leads to the following system of equations:

$$\text{Phase - Lag(PL)} = \frac{1}{2} \frac{\Upsilon_2(v)}{v^6 c_1 c_3 + v^4 c_3 + v^2 + 12} = 0 \quad (21)$$

$$\text{First Derivative of the Phase - Lag} = \frac{\Upsilon_3(v)}{(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12)^2} = 0 \quad (22)$$

$$\text{Second Derivative of the Phase} - \text{Lag} = \frac{\Upsilon_4(v)}{(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12)^3} = 0 \quad (23)$$

$$\text{Third Derivative of the Phase} - \text{Lag} = \frac{\Upsilon_5(v)}{(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12)^4} = 0 \quad (24)$$

$$\text{Fourth Derivative of the Phase} - \text{Lag} = \frac{\Upsilon_6(v)}{(v^6 c_1 c_3 + v^4 c_3 + v^2 + 12)^5} = 0 \quad (25)$$

where $\Upsilon_j(v)$, $j = 2(1)6$ are given in the Appendix A.

3.3 Solution of the obtained system of equations

In order to obtain the determination of the coefficients of the new finite difference pair (16), the system of equations (19), (20), (21)–(25) is solved:

$$\begin{aligned} a_1 &= -\frac{1}{18} \frac{\Upsilon_7(v)}{Udenom_1(v)} \\ c_0 &= -\frac{1}{3} \frac{\Upsilon_8(v)}{Udenom_2(v)} \\ c_1 &= -\frac{1}{2} \frac{\Upsilon_9(v)}{Udenom_2(v)} \\ c_2 &= -2 \frac{\Upsilon_{10}(v)}{v^4 Udenom_1(v)} \\ c_3 &= -2 \frac{\Upsilon_{11}(v)}{v^4 Udenom_1(v)} \end{aligned} \quad (26)$$

where $\Upsilon_j(v)$, $j = 6(1)9$ and $Udenom_k(v)$, $j = 1, 2$ are given in the Appendix B.

Since there is the possibility to face cancellations or impossibility of determination of the coefficients (26), during computations (Example of a possible cancellation: Some of the denominators of the coefficients (26) lead to zero for some values of $|v|$), in the Appendix C, we give the truncated Taylor series expansions of the coefficients built in (26).

In Figure 1 we present the behavior of the coefficients.

Based on the methodology for the building of the new scheme, the last stage of the development consists the determination of its local truncation error (LTE), which is given by:

$$LTE_{NM3SPS4DV} = -\frac{1}{119750400} h^{12} \left(5 \varphi_n^{(12)} + 24 \phi^2 \varphi_n^{(10)} + 45 \phi^4 \varphi_n^{(8)} \right)$$

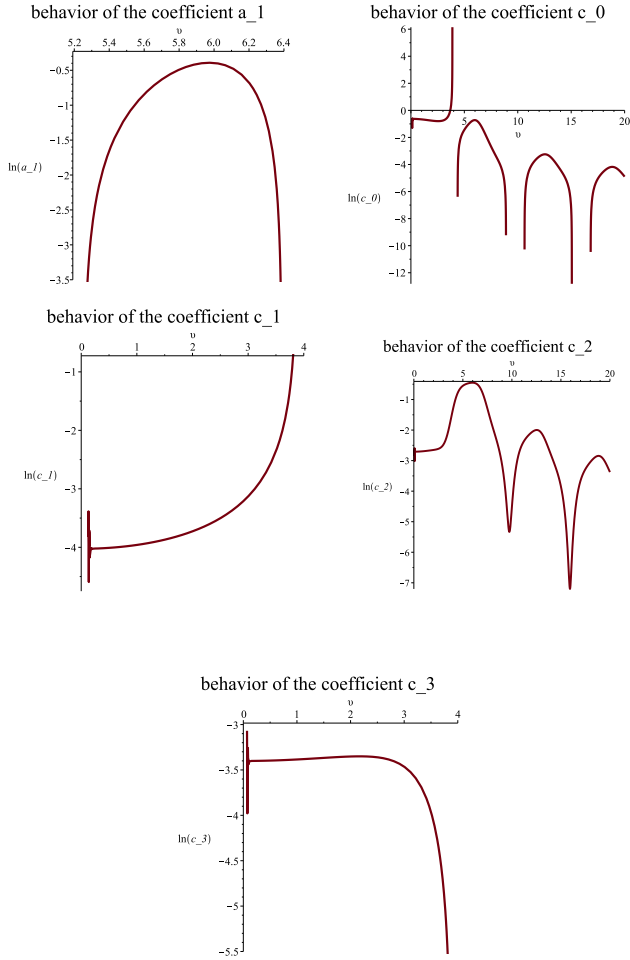


Figure 2. Plot of the behavior of the coefficients of the new proposed symmetric finite difference pair (16) given by (26) for several values of $v = \phi h$.

$$+40 \phi^6 \varphi_n^{(6)} + 15 \phi^8 \varphi_n^{(4)} - \phi^{12} \varphi_n^{(4)} \Big) + O(h^{14}). \quad (27)$$

We symbolized the new built method as *NM3SPS4DV*. The explanation of the abbreviation *NM3SPS4DV* is: New Method of Three-Stages P-Stable with Vanished Phase-Lag and its Derivatives up to Order Four.

Remark 8. *The computation of the formula of the local truncation error (27) is important for the determination of the algebraic order of the new proposed finite difference scheme. The formula of the LTE is also important for the computation of the asymptotic form of the local truncation error which is important for the local truncation error analysis and comparative error analysis.*

4 Local truncation error and stability analysis of the new proposed pair

4.1 Comparative error analysis

In the Section we will study the local truncation error of some finite difference pairs of similar form. The error analysis is based on the following scalar model problem:

$$\varphi''(x) = (V(x) - V_c + \Gamma) \varphi(x) \quad (28)$$

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. *The scalar model problem for the error analysis is the radial Schrödinger equation with potential $V(x)$.*

We will study the following methods:

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

$$LTE_{CL} = -\frac{1}{23950080} h^{12} \varphi_n^{(12)} + O(h^{14}). \quad (29)$$

4.1.2 P-stable linear six-step method of Wang [82]

$$LTE_{WANGPSL6S} = -\frac{81}{44800} h^{10} \left(\varphi_n^{(10)} + 10 \phi^{10} \varphi_n \right) + O(h^{12}). \quad (30)$$

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

$$LTE_{NM3SPS2DV} = -\frac{1}{47900160} h^{12} \left(2 \varphi_n^{(12)} - 9 \phi^4 \varphi_n^{(8)} - 8 \phi^6 \varphi_n^{(6)} - \phi^{12} \varphi_n \right) + O(h^{14}). \quad (31)$$

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

$$LTE_{NM3SPS3DV} = -\frac{1}{23950080} h^{12} \left(\varphi_n^{(12)} - 9 \phi^4 \varphi_n^{(8)} - 16 \phi^6 \varphi_n^{(6)} - 9 \phi^8 \varphi_n^{(4)} + \phi^{12} \varphi_n \right) + O(h^{14}). \quad (32)$$

4.1.5 P-stable scheme with vanished phase-lag and its first, second, third and fourth derivatives developed in section 3

The formula of the Local Truncation Error for this method is given by (27)

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

- Computation of the new expressions for the LTE formulae given by (29), (30), (31), (32) and (27) applying the model problem (28) (radial time independent Schrödinger equation). The new expressions are derived by substituting the derivatives of the function φ (which are produced based on the the test problem (28)) in the formulae given by (29), (30), (31), (32) and (27). We mention here the some expressions of the derivatives of the function φ are presented in the Appendix D.
- The above step leads to the new formulae of LTE for the methods under evaluation. The characteristic of these new formulae is the inclusion of the parameter Γ and the energy E .

The general form of the new formulae of LTE is given by:

$$LTE = h^p \sum_{j=0}^k \Phi_j \Gamma^j \quad (33)$$

with Φ_j are: 1) real numbers (frequency independent cases i.e. the classical case) or 2) formulae of v and Γ (frequency dependent cases), p is the algebraic order of

the specific finite difference pair and k is the maximum possible power of Γ in the formulae of LTE.

- Two cases for the parameter Γ will be studied:

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

Consequently:

$$\Gamma \approx 0 \Rightarrow \Gamma^i \approx 0, i = 1, 2, \dots \quad (34)$$

which leads to the form for the formula (33):

Remark 10.

$$LTE_{\Gamma=0} = h^k \Lambda_0 \quad (35)$$

We note here that the quantity Λ_0 is the same for all the finite difference pairs of the same family, i.e. $LTE_{CL} = LTE_{NM3SPS2DV} = LTE_{NM3SPS3DV} = LTE_{NM3SPS4DV} = h^{12} \Lambda_0$, where Λ_0 is given in the Appendix E.

Theorem 2. *The formula (34) leads us to the conclusion that for $\Gamma = V_c - E \approx 0$ the local truncation error of the classical method (constant coefficients - (29)), the local truncation error of the scheme with vanished phase-lag and its first and second derivatives developed in [6] (with LTE given by (31), 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 (32) and the local truncation error for the numerical pair with vanished phase-lag and its first, second, third and fourth derivatives developed in Section 3 (with LTE given by (27), are the same and equal to $h^{12} \Lambda_0$, where Λ_0 is given in the Appendix E.*

2. **The Potential and the Energy are far from each other.** Therefore,

$\Gamma \gg 0 \vee \Gamma \ll 0 \Rightarrow |\Gamma| \gg 0$. Consequently, the most accurate finite difference pair is the finite difference pair with formula of asymptotic form of LTE, given by (33), which contains the minimum power of Γ and the maximum value of p .

- The above analysis leads to the following asymptotic forms of the LTE formulae for the schemes which are under evaluation.

4.1.6 Classical method

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

$$LTE_{CL} = -\frac{1}{23950080} h^{12} \left(\varphi(x) \Gamma^6 + \dots \right) + O(h^{14}). \quad (36)$$

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

4.1.7 P-stable linear six-step method of Wang [82]

This is the method presented in Linear Six-step Method presented in [82] (see in [82] equations (23)-(27). We note also here that there is a missprint in the paper [82]. In formula (25) $2C_{3,0}y''_{k+2}$ must be replaced by the correct: $2C_{3,0}y''_{k+3}$.

$$LTE_{WANGPSL6S} = -\frac{81}{8960} h^{10} \left(\Xi(x) \varphi(x) \Gamma^4 + \dots \right) + O(h^{12}). \quad (37)$$

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

4.1.8 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].

$$\begin{aligned} LTE_{NM3SPS2DV} = & -\frac{1}{997920} h^{12} \left(\frac{d^4}{dx^4} \Xi(x) \varphi(x) \Gamma^4 \right. \\ & \left. + \dots \right) + O(h^{14}). \end{aligned} \quad (38)$$

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

4.1.9 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].

$$LTE_{NM3SPS3DV} = -\frac{1}{997920} h^{12} \left[\left[4 \Xi(x) \varphi(x) \frac{d^2}{dx^2} \Xi(x) + 7 \varphi(x) \frac{d^4}{dx^4} \Xi(x) \right. \right.$$

$$+2 \frac{d^3}{dx^3} \Xi(x) \frac{d}{dx} \varphi(x) + 3 \varphi(x) \left(\frac{d}{dx} \Xi(x) \right)^2 \Big] \Gamma^3 + \dots \Big] + O(h^{14}). \quad (39)$$

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

4.1.10 P-stable scheme with vanished phase-lag and its first, second, third and fourth derivatives developed in section 3

This is the P-stable method which we developed in Section 3.

$$LTE_{NM3SPS4DV} = -\frac{1}{1247400} h^{12} \left[\left[\varphi(x) \frac{d^4}{dx^4} \Xi(x) \right] \Gamma^3 + \dots \right] + O(h^{14}). \quad (40)$$

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

The above achievements lead 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 [82]: 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 Section 3: For this method the error increases as the third power of Γ , but the coefficient of the fourth power of Γ is much lower.*

Therefore, for the numerical solution of the time independent radial Schrödinger equation, which is the scalar model problem for the error analysis, the new P -stable tenth algebraic order method with vanished phase-lag and its derivatives up to order four is the most accurate one.

4.2 Stability analysis

For the stability and interval of periodicity analysis the following scalar model problem is used:

$$\varphi'' = -\omega^2 \varphi. \quad (41)$$

where $\omega \neq \phi$, where ϕ is the frequency of the test problem (7) (phase-lag analysis) and ω is the frequency of the test problem (41) (stability analysis).

Application of the new built finite difference pair (16) to the scalar model problem (41) leads to the difference equation:

$$\Omega_1(s, v) (\varphi_{n+1} + \varphi_{n-1}) + \Omega_0(s, v) \varphi_n = 0 \quad (42)$$

and the corresponding characteristic equation:

$$\Omega_1(s, v) (\lambda^2 + 1) + \Omega_0(s, v) \lambda = 0 \quad (43)$$

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

$$\begin{aligned} \Omega_1(s, v) &= 1 + b_1 s^2 + c_3 b_1 s^4 + c_1 c_3 b_1 s^6 \\ \Omega_0(s, v) &= a_1 + b_0 s^2 - c_2 b_1 s^4 - c_0 c_3 b_1 s^6 \end{aligned} \quad (44)$$

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

Remark 11. Observing that some of the coefficients of (44) are dependent on v , we conclude that the formulae (44) have dependence on s and v , while the formulae (18) have dependence only on v .

if we substitute the coefficients b_j , $j = 0, 1$ from (17) and the coefficients a_1 , c_i $i = 0(1)3$ from (26) into the above stability polynomials, we obtain:

$$\Omega_1(s, v) = \frac{1}{12} \frac{\Upsilon_{12}(s, v)}{v^6 \Upsilon_{14}(s, v)}$$

$$\Omega_0(s, v) = -\frac{1}{18} \frac{\Upsilon_{13}(s, v)}{v^6 \Upsilon_{14}(s, v)} \quad (45)$$

where $\Upsilon_j(s, v)$, $j = 12(1)14$ are given in the Appendix F.

Remark 12. *We note here that the definitions of P -stability and singularly almost P -stability, which are given in Section 2, are corresponded with problems having frequency which satisfied the condition $\omega = \phi$.*

The finite difference pair (16) has a non zero interval of periodicity if the roots of its characteristic equation (43) satisfy the following condition:

$$|\lambda_{1,2}| \leq 1 \quad (46)$$

4.2.1 Methodology of the building of $s-v$ domain for the new finite difference pair

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

The methodology which is described in the flowchart of Figure 3 leads to the development of the $s-v$ domain plotted in Figure 4.

Remark 13. *Observing the $s-v$ domain plotted in Figure 4 we arrive to the following remarks:*

1. *The new proposed finite difference pair is stable within the shadowed area of the domain.*
2. *The new proposed finite difference pair is unstable within the white area of the domain.*

Remark 14. *The stability area on $s-v$ domain of the finite difference pair specifies the kind of problems for which the specific method is appropriate:*

1. **Categories of problems for which $\omega \neq \phi$.** *For these problems we have to study all the area of the $s-v$ domain excluding the area around the first diagonal of the domain.*
2. **Categories of problems for which $\omega = \phi$** *(see the Schrödinger equation and related problems). For these problems we have to study the area around the first diagonal of the figure of the $s-v$ domain.*

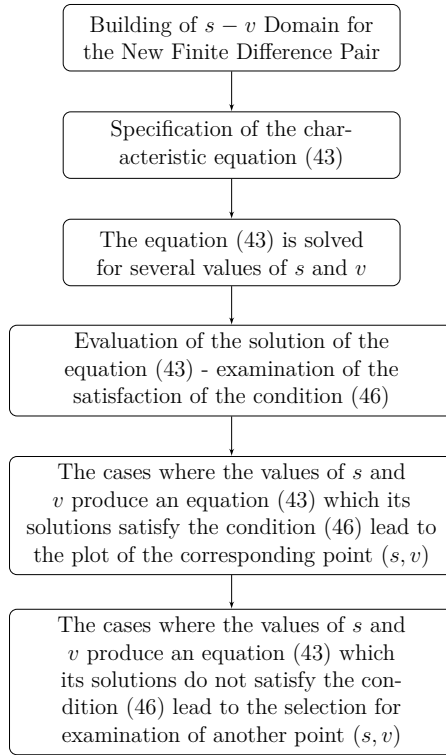


Figure 3. Flowchart for the methodology of the building of $s - v$ domain for the new finite difference pair

The methodology for the determination of the interval of periodicity of the new developed finite difference pair is as follows:

1. Substitution $s = v$ in the stability polynomials Ω_i , $i = 0, 1$ given by (45).
2. Investigation of the area around the first diagonal of the $s - v$ domain which is given in Figure 4.

Based on the above described methodology, the interval of periodicity of the new built method is found to be equal to $(0, \infty)$.

Remark 15. *The interval of periodicity is a property corresponding to categories of problems for which $s = v$.*

The above analysis leads to the following theorem:

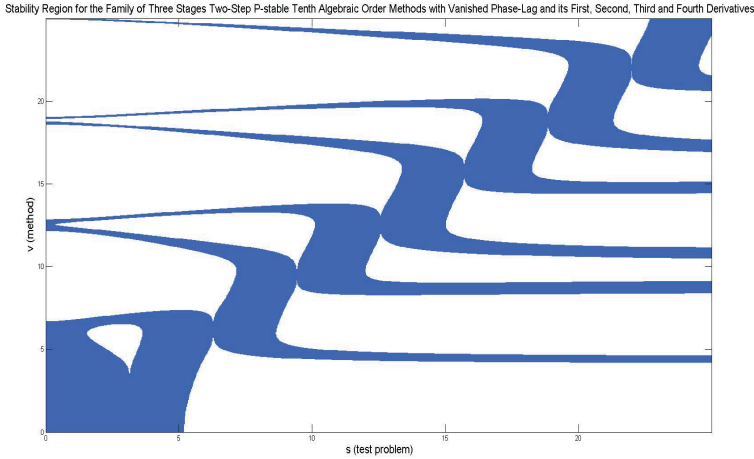


Figure 4. The plot of $s - v$ domain of the new developed P-stable two-stages pair with vanished phase-lag and its derivatives up to order three.

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

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

5 Numerical results

The evaluation of the efficiency of the new built finite difference pair is achieved via its application to the numerical solution of:

1. The radial time-independent Schrödinger equation and
2. The systems of coupled differential equations of the Schrödinger type.

5.1 Radial time-independent Schrödinger equation

The mathematical model of the radial time-independent Schrödinger equation is given by:

$$\varphi''(r) = [l(l+1)/r^2 + V(r) - k^2] \varphi(r), \quad (47)$$

where

1. The function $\Theta(r) = l(l+1)/r^2 + V(r)$ determines *the effective potential* which satisfies the following property : $\Theta(r) \rightarrow 0$ as $r \rightarrow \infty$.
2. $k^2 \in \mathbb{R}$ determines *the energy*.
3. $l \in \mathbb{Z}$ determines *the angular momentum*.
4. The function V determines *the potential*.

We note that the problem (47) is a boundary value one and therefore, the boundary conditions must be determined. These conditions are given by:

$$\varphi(0) = 0$$

and another boundary condition at the end point of integration domain which is denoted for large values of r from the physical considerations of the specific problem.

The new built finite difference pair is belonged to the frequency dependent methods (all or some of its coefficients are dependent from the $v = \phi h$), and consequently, the definition of the frequency ϕ is necessary, in order all or some coefficients of the new developed method to be computed and therefore to be possible the new finite difference pair to be applied on the numerical solution of the problem (47). In our numerical experiments and for (47) and $l = 0$ we have:

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

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

5.1.1 Woods–Saxon potential

Since the mathematical model of the problem (47) consists the potential $V(r)$, it is necessary its determination the mathematical form of the potential function before the numerical solution of the problem (47). In our numerical tests we will use the Wood–Saxon potential which is given by:

$$V(r) = \frac{\Psi_0}{1 + \xi} - \frac{\Psi_0 \xi}{a(1 + \xi)^2} \quad (48)$$

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

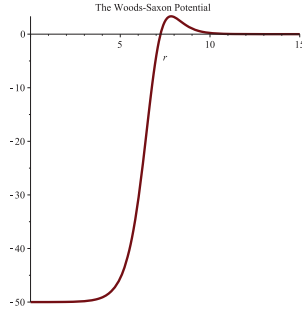


Figure 5. Behavior of the Woods–Saxon potential.

The plot of the Wood–Saxon potential for several values of r is presented in Figure 5.

The necessary values of the frequency ϕ are determined as follows (see for details [19] and [20]):

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

For the definition of the above values of the frequency ϕ , the methodology introduced by Ixaru et al. ([18] and [20]) is used. The specific methodology requests discrete approximations of the continuous function $V(r)$ by constant values on some critical points within the integration domain. Examples for the determination of the values of ϕ are given below:

1. On $r = 6.5 - h$, the value of ϕ is equal to: $\sqrt{-37.5 + E}$. Consequently, $v = \phi h = \sqrt{-37.5 + E} h$.
2. On $r = 6.5 - 3h$, the value of ϕ is equal to: $\sqrt{-50 + E}$. Consequently, $v = \phi h = \sqrt{-50 + E} h$.

It is noted that the potential $V(r)$ is defined by the user. Many potentials are of great interest in several scientific disciplines of Chemistry. Very few of them have known their eigenenergies. The selection of the Woods–Saxon potential was done based on the fact that for this potential the eigenenergies are known.

5.1.2 The resonance problem of the radial Schrödinger equation

We will solve numerically the problem (47):

- with $l = 0$ and
- using the Woods-Saxon potential (48)

By theory, the interval of integration for the problem described above is equal to $(0, \infty)$. Therefore and in order the above mentioned problem to be solved numerically, an approximation of the infinite interval of integration $(0, \infty)$ by a finite one is necessary. For our numerical tests we approximate the infinite interval of integration by $r \in [0, 15]$. For our numerical experiments we also apply the finite difference methods to be examined on a wide range of energies: $E \in [1, 1000]$.

The radial Schrödinger equation (47) can be written as:

$$\varphi''(r) + \left(k^2 - \frac{l(l+1)}{r^2} \right) \varphi(r) = 0 \quad (49)$$

when $r \rightarrow \infty$, because in these cases, for positive energies the potential $V(r)$ vanished faster than the term $\frac{l(l+1)}{r^2}$. We note also that in (49) the linearly independent solutions of the above model are given by $kr j_l(kr)$ and $kr n_l(kr)$, with $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively (see [83]).

Therefore, the asymptotic form of the solution of equation (47) (when $r \rightarrow \infty$) is given by:

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

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

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

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 $S(r) = kr j_l(kr)$ and $C(r) = -kr n_l(kr)$. The above mentioned problem is an initial-value one and consequently, the values of φ_j , $j = 0, 1$ must be

computed in order a two-step scheme to be applied. The value φ_0 is defined by the initial condition of the problem. The value φ_1 is computed using the high order Runge-Kutta-Nyström methods (see [21] and [22]). The computation of the values φ_i , $i = 0, 1$ leads to the computation of the phase shift δ_l at the point r_2 of the asymptotic region. It is noted that φ_j is the approximation of the function φ at the point x_j .

The above mentioned problem is solved for positive energies and therefore, 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:

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

The following methods are evaluated for the computation of the the positive eigenenergies of the resonance problem described above:

- **Method QT8**: the eighth order multi-step method developed by Quinlan and Tremaine [23];
- **Method QT10**: the tenth order multi-step method developed by Quinlan and Tremaine [23];
- **Method QT12**: the twelfth order multi-step method developed by Quinlan and Tremaine [23];
- **Method MCR4**: the fourth algebraic order method of Chawla and Rao with minimal phase-lag [24];
- **Method RA**: the exponentially-fitted method of Raptis and Allison [25];
- **Method MCR6**: the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [26];
- **Method NMPF1**: the Phase-Fitted Method (Case 1) developed in [13];

- **Method NMPF2:** the Phase-Fitted Method (Case 2) developed in [13];
- **Method NMC2:** the Method developed in [27] (Case 2);
- **Method NMC1:** the method developed in [27] (Case 1);
- **Method NM2SH2DV:** the Two-Step Hybrid Method developed in [1];
- **Method WPS2S:** the Two-Step P-stable Method developed in [82];
- **Method WPS4S:** the Four-Step P-stable Method developed in [82];
- **Method WPS6S:** the Six-Step P-stable Method developed in [82];
- **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 Section 3.

In Figures 6 and 7 we present the maximum absolute error Err_{max} , which is defined by: $Err_{max} = \max |\log_{10}(Err)|$ where

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

In order to compute the absolute error Err two values of the specific eigenenergy are used:

1. The computed eigenenergies. The computed eigenenergies are determined as $E_{calculated}$ and are computed using each of the 17 numerical methods mentioned above.
2. The accurate eigenenergies (the reference values for the eigenenergies). The accurate eigenenergies are determined as $E_{accurate}$ and are computed using the well known two-step method of Chawla and Rao [26]. .

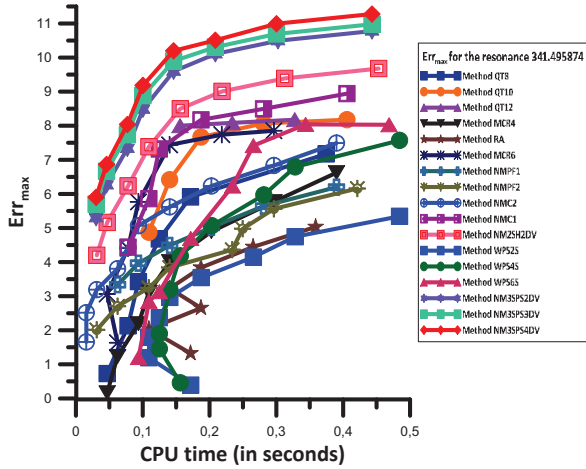


Figure 6. Accuracy (Digits) for several values of *CPU* Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

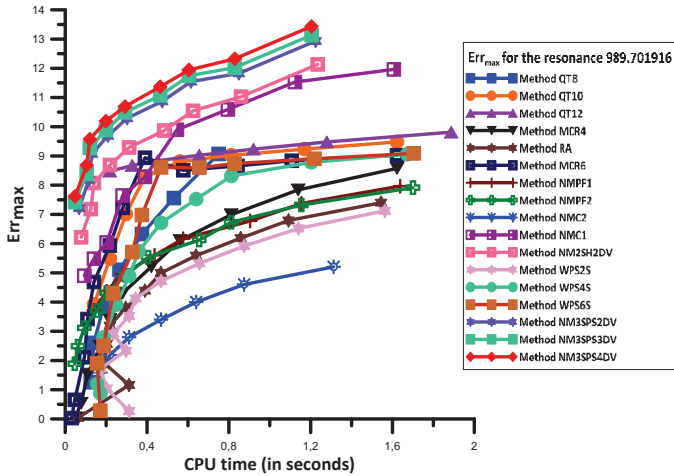


Figure 7. Accuracy (Digits) for several values of *CPU* Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

In Figures 6 and 7 we present the maximum absolute errors Err_{max} for the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$, respectively, and for the 17 numerical methods mentioned above for several values of CPU time (in seconds). The symbolizations E_2 and E_3 for the computed eigenenergies in our numerical experiments are given since it is known that the Woods–Saxon potential has also the eigenenergies E_0 and E_1 . The choice of the eigenenergies E_2 and E_3 was done because for these eigenenergies the solution has stiffer behavior and therefore the new built method can show effectively its efficiency.

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

Our numerical experiments 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 the most efficient one.

5.2 Error estimation

The second problem which we will solve in our numerical experiments, is the numerical solution of the coupled differential equations arising from the Schrödinger equation.

We will solve the above problem using a so called variable-step pair.

Definition 9. We denote a numerical pair as variable-step numerical pair if the stepsize of integration is changed during the integration process.

Definition 10. We call Local truncation error estimation procedure(LTEEPR), the process which is used in order a variable-step pair to change the stepsize during the integration.

We note that during the last decades much research has been done on the building of numerical schemes of constant or variable stepsize for the numerical solution of problems of the form of the Schrödinger equation (see for example [13]– [82]).

As we mentioned previously, we solve numerically the systems of coupled differential equations arising from the Schrödinger equation using the variable-step pairs determined above. We also mentioned above that the variable-step pairs are based on the LTEEPR procedure determined above. The categories of the LTEEPR procedures are shown in Figure 8.

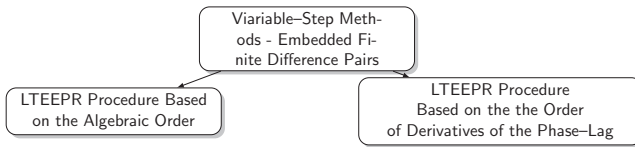


Figure 8. Categories of LTEEPR Procedures used for Building Embedded Finite Difference Pairs for Problems with Oscillatory and/or Periodical solutions

The following formula for the estimation of the local truncation error (LTE) in the lower order solution φ_{n+1}^L is used:

$$LTE = | \varphi_{n+1}^H - \varphi_{n+1}^L | \quad (50)$$

where φ_{n+1}^L and φ_{n+1}^H are

- **LTEEPR Procedure based on the algebraic order of the pairs.** For this procedure, φ_{n+1}^L determines the finite difference pair with the lower algebraic order solution and φ_{n+1}^H determines the finite difference pair with the higher algebraic order solution.

- **LTEE Procedure 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 finite difference pairs which participate in this procedure are p and s respectively, where $p < s$. For this procedure φ_{n+1}^L determines the finite difference pair with eliminated higher order derivative of the phase-lag equal to p and φ_{n+1}^H determines the finite difference pair with eliminated higher order derivative of the phase-lag equal to s .

For our numerical experiments we use the first LTEEPR procedure for the estimation of the local truncation error. Consequently, we use:

As φ_{n+1}^L we use the eighth algebraic order method developed in [81] and as φ_{n+1}^H we use the tenth algebraic order method developed in Section 3.

In Figure 9 we present the variable-step procedure via the Local Truncation Error Control Procedure *LTEEPR*. This is the procedure which we use in our numerical experiments. We note that:

- h_n is denoted the stepsize which is used for the n^{th} step of the integration and
- acc is denoted the accuracy of the local truncation error *LTE* which is determined by the user.

Remark 16. *In our numerical tests the known as **local extrapolation** technique is used. Based on this technique for the approximation of the solution at each point of the integration domain we use the higher order solution φ_{n+1}^H although the local error estimation is based on the lower order solution φ_{n+1}^L .*

5.3 Coupled differential equations arising from the Schrödinger equation

Systems of coupled differential equations of the Schrödinger type are appeared in mathematical models of problems in many scientific disciplines like:

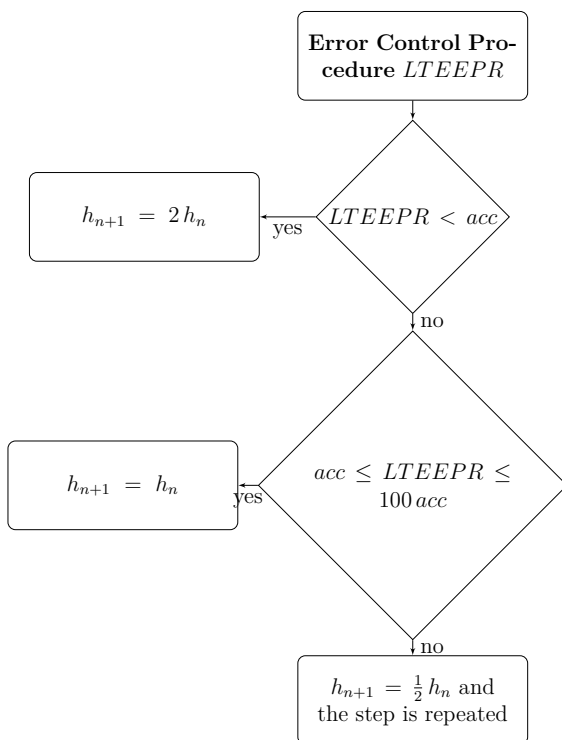


Figure 9. Flowchart for the Local Truncation Error Control Procedure *LTEEPR*. The parameter *acc* is defined by the user

- quantum chemistry,
- material science,
- theoretical physics,
- quantum physics,
- atomic physics,
- physical chemistry
- chemical physics,
- quantum chemistry,
- electronics,

- etc.

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

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

for $1 \leq i \leq N$ and $m \neq i$. This problem is a boundary value problem.

The boundary conditions are given by (see for details [28]):

$$\begin{aligned} \varphi_{ij} &= 0 \text{ at } x = 0 \\ \varphi_{ij} &\sim k_i x j_{l_i}(k_i x) \delta_{ij} + \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x) \end{aligned} \quad (51)$$

Remark 17. *The finite difference pair built in this paper and the resulting embedded pair can be applied effectively to both open and close channels problem.*

The analysis fully described in [28] leads to the new formulae of the asymptotic condition (51):

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

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

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

We will investigate the rotational excitation of a diatomic molecule by neutral particle impact. We can meet this problem in many scientific disciplines 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. The form of the above presented problem contains the close-coupling Schrödinger equations (see [8], [9–12], [84] – [88]). We use the determinations:

- quantum numbers (j, l) which denote the entrance channel (see for details in [28]),
- quantum numbers (j', l') which denote the exit channels and

- $J = j + l = j' + l'$ which denote the total angular momentum.

and we obtain:

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

where

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

and E determines the kinetic energy of the incident particle in the center-of-mass system, I determines the moment of inertia of the rotator, μ determines 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 experiments, we use the following potential V (see [28]):

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

and consequently, the coupling matrix contains elements of the form:

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

where f_2 coefficients are determined from formulae presented by Bernstein et al. [29] 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 [30]). We note also that $V_0(x)$ and $V_2(x)$ are potential functions defined by the user. The above analysis leads to the following new expressions of the boundary conditions:

$$\varphi_{j'l'}^{Jjl}(x) = 0 \text{ at } x = 0 \quad (52)$$

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

where S matrix. For K matrix of (51) we use the following formula:

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

The methodology fully described in [28] is used for the numerical solution of the above presented problem. The methodology contains the numerical method built in this paper for the integration from the initial value point to the matching points.

For our numerical tests the following parameters for the **S** matrix are used:

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

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

In our numerical tests we chose (see for full details in [28]) $J = 6$ and for the excitation of the rotator the value $j = 0$ state to levels up to $j' = 2, 4$ and 6 . The above values leads to systems of **four, nine and sixteen coupled differential equations arising from the Schrödinger equation**, respectively. Following the theory fully described in [30] and [28], the potential is considered infinite for x less than x_0 . Consequently, the boundary condition (52) can be written now as

$$\varphi_{j'v}^{Jjl}(x_0) = 0.$$

For the approximate solution of the above presented problem, we use the following methods:

- the Iterative Numerov method of Allison [28] which is indicated as **Method I²**,
- the variable-step method of Raptis and Cash [31] 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 [22] which is indicated as **Method III**,
- the embedded Runge-Kutta method ERK4(2) developed in Simos [32] 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**.

²We note here that Iterative Numerov method developed by Allison [28] is one of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation

- 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 this paper which is indicated as **Method X**.

The real time of computation required by the numerical methods I-X presented above in order to calculate the square of the modulus of the **S** matrix for the sets of 4, 9 and 16 coupled differential equations respectively, is presented in Table 2. The maximum error in the computation of the square of the modulus of the **S** matrix is also presented in the same table.

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}

6 Conclusions

In the present paper a new P-stable symmetric two-step finite difference pair with eliminated phase-lag and its derivatives up to order four was built. The three stages of the building of the new proposed scheme are as follows:

1. In the first stage the P-stability conditions introduced by Lambert and Watson [14] and Wang [82] are satisfied.
2. In the second stage, the condition for the elimination of the phase-lag is satisfied.
3. In the third stage, the conditions for the elimination of the derivatives of the phase-lag up to order four are satisfied.

The above methodology for the building of P-stable symmetric finite difference pairs was first introduced in the paper of Medvedev and Simos [6].

The analysis of the new built scheme consisted from the following parts:

- The determination of the local truncation error (LTE) was done.
- The asymptotic form of the LTE was computed and the asymptotic form of the LTE of new built scheme was compared with the asymptotic forms of the LTE of similar methods.
- The stability and the interval of periodicity properties of the new built finite difference method was investigated.
- The computational effectiveness of the new built pair was also investigated.

Based on the above studies we conclude that the theoretical, computational and numerical results presented in this paper, proved the effectiveness of the new built method compared with other well known and recently obtained methods of the literature for the numerical solution of the radial Schrödinger equation and of the systems of coupled differential equations arising from the Schrödinger equation.

Appendix A: Formulae for the $\Upsilon_i(v)$, $i = 2(1)6$

$$\begin{aligned}
\Upsilon_2(v) &= 2 \cos(v) v^6 c_1 c_3 - v^6 c_0 c_3 + 2 \cos(v) v^4 c_3 - v^4 c_2 \\
&+ 2 \cos(v) v^2 + 10 v^2 + 24 \cos(v) + 12 a_1 \\
\Upsilon_3(v) &= -\sin(v) v^{12} c_1^2 c_3^2 - 2 \sin(v) v^{10} c_1 c_3^2 - v^9 c_0 c_3^2 \\
&+ v^9 c_1 c_2 c_3 - 2 \sin(v) v^8 c_1 c_3 - \sin(v) v^8 c_3^2 - 24 \sin(v) v^6 c_1 c_3 \\
&- 2 v^7 c_0 c_3 - 20 v^7 c_1 c_3 - 2 \sin(v) v^6 c_3 - 36 v^5 a_1 c_1 c_3 \\
&- 36 v^5 c_0 c_3 - 24 \sin(v) v^4 c_3 - v^5 c_2 - 10 v^5 c_3 - \sin(v) v^4 - 24 v^3 a_1 c_3 \\
&- 24 v^3 c_2 - 24 \sin(v) v^2 - 12 v a_1 - 144 \sin(v) + 120 v \\
\Upsilon_4(v) &= 1440 - 204 v^6 c_0 c_3 + 120 v^6 c_2 c_3 - 432 \cos(v) v^4 c_3 \\
&+ 108 v^4 a_1 c_3 - 864 v^2 a_1 c_3 - \cos(v) v^{12} c_3^3 - 3 \cos(v) v^{10} c_3^2 \\
&- 3 \cos(v) v^8 c_3 - 36 \cos(v) v^8 c_3^2 - 72 \cos(v) v^6 c_3 - 3 v^{10} c_0 c_3^2 \\
&- 3 v^{14} c_1^2 c_2 c_3^2 + 10 v^{12} c_0 c_1 c_3^2 + v^{12} c_1 c_2 c_3^2 \\
&+ 252 v^{10} a_1 c_1^2 c_3^2 + 252 v^{10} c_0 c_1 c_3^2 + 12 v^{10} c_1 c_2 c_3 \\
&+ 324 v^8 a_1 c_1 c_3^2 + 3 v^8 c_2 c_3 - 6 v^8 c_0 c_3 - v^{12} c_0 c_3^3 \\
&+ 120 v^6 a_1 c_3^2 - 432 \cos(v) v^2 - 10 v^6 c_3 - 3 \cos(v) v^{14} c_1 c_3^3 \\
&- 1440 v^4 c_3 - 864 v^2 c_2 - 36 v^4 c_2 - \cos(v) v^6 - 72 \cos(v) v^8 c_1 c_3 \\
&- 3 \cos(v) v^{10} c_1 c_3 - 72 \cos(v) v^{10} c_1 c_3^2 - 6 \cos(v) v^{12} c_1 c_3^2 \\
&- \cos(v) v^{18} c_1^3 c_3^3 - 2160 v^4 a_1 c_1 c_3 + 96 v^6 a_1 c_1 c_3 \\
&+ 324 v^8 c_1 c_2 c_3 + 3 v^{14} c_0 c_1 c_3^3 - 3 \cos(v) v^{14} c_1^2 c_3^2 \\
&- 432 \cos(v) v^6 c_1 c_3 - 3 \cos(v) v^{16} c_1^2 c_3^3 + 36 v^2 a_1 \\
&- 36 \cos(v) v^4 - v^6 c_2 - 2160 v^4 c_0 c_3 - 3000 v^6 c_1 c_3 - 36 \cos(v) v^{12} c_1^2 c_3^2 \\
&+ 30 v^8 c_3^2 - 1728 \cos(v) - 144 a_1 - 360 v^2 - 60 v^8 c_1 c_3 + 100 v^{12} c_1^2 c_3^2 \\
&+ 90 v^{10} c_1 c_3^2 \\
\Upsilon_5(v) &= -17280 v + 6912 \sin(v) v^6 c_1 c_3 + 2592 v^9 c_1 c_2 c_3 \\
&+ 13824 v^5 a_1 c_1 c_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^8 c_1 c_3 + 1728 \sin(v) v^6 c_3 + 6912 \sin(v) v^2 + 1728 v^3 c_2 \\
&+ 5760 v^5 c_3 - 86400 v^3 c_3 + 864 \sin(v) v^8 c_3^2 + 10368 v^3 a_1 c_3
\end{aligned}$$

$$\begin{aligned}
& - 576 v^7 c_0 c_3 + 864 v^9 c_0 c_3^2 - 241920 v^5 c_1 c_3 - 20736 v a_1 c_3 \\
& - 103680 v^3 c_0 c_3 - 103680 v^3 a_1 c_1 c_3 - 2016 v^{15} a_1 c_1^3 c_3^3 \\
& - 12 v^{17} c_1^2 c_2 c_3^3 + 12 v^{17} c_0 c_1 c_3^4 - 60 v^{17} c_0 c_1^2 c_3^3 \\
& + 12 v^{19} c_1^3 c_2 c_3^3 - 12 v^{19} c_0 c_1^2 c_3^4 + 1728 v a_1 \\
& - 20736 v c_2 - 144 v^3 a_1 + 14400 v^7 c_3^2 + 120 v^9 c_3^2 - 120 v^{11} c_3^3 \\
& + 144 \sin(v) v^{10} c_1 c_3 + 4 \sin(v) v^{12} c_1 c_3 + 288 \sin(v) v^{12} c_1 c_3^2 \\
& + 12 \sin(v) v^{14} c_1 c_3^2 + 144 \sin(v) v^{14} c_1 c_3^3 + 144 \sin(v) v^{14} c_1^2 c_3^2 \\
& + 12 \sin(v) v^{16} c_1 c_3^3 + 6 \sin(v) v^{16} c_1^2 c_3^2 + 144 \sin(v) v^{16} c_1^2 c_3^3 \\
& + 4 \sin(v) v^{18} c_1 c_3^4 + 12 \sin(v) v^{18} c_1^2 c_3^3 + 48 \sin(v) v^{18} c_1^3 c_3^3 \\
& + 6 \sin(v) v^{20} c_1^2 c_3^4 + 4 \sin(v) v^{20} c_1^3 c_3^3 + 4 \sin(v) v^{22} c_1^3 c_3^4 \\
& + \sin(v) v^{24} c_1^4 c_3^4 + 44928 v^7 c_1 c_2 c_3 - 576 v^7 a_1 c_1 c_3 \\
& + 62208 v^7 a_1 c_1 c_3^2 + 60480 v^9 c_0 c_1 c_3^2 - 1440 v^9 a_1 c_1 c_3^2 \\
& + 48 \sin(v) v^{12} c_3^3 + 60480 v^9 a_1 c_1^2 c_3^2 + 60 v^{11} c_1 c_2 c_3 \\
& - 2592 v^{11} c_1 c_2 c_3^2 + 4896 v^{11} c_0 c_1 c_3^2 - 2736 v^{11} a_1 c_1 c_3^3 \\
& - 144 v^{11} a_1 c_1^2 c_3^2 - 48 v^{13} c_1 c_2 c_3^2 \\
& + 120 v^{13} c_0 c_1 c_3^2 - 3744 v^{13} c_1^2 c_2 c_3^2 \\
& - 3744 v^{13} a_1 c_1^2 c_3^3 - 120 v^{15} c_1^2 c_2 c_3^2 \\
& + 48 v^{15} c_0 c_1 c_3^3 - 2016 v^{15} c_0 c_1^2 c_3^3 + \sin(v) v^8 \\
& + 864 \sin(v) v^4 + 48 \sin(v) v^6 + 4 \sin(v) v^{14} c_3^3 + \sin(v) v^{16} c_3^4 - 576 v^5 a_1 c_3 \\
& + 17280 v^5 c_2 c_3 + 17280 v^5 a_1 c_3^2 + 576 v^7 c_2 c_3 \\
& - 864 v^7 a_1 c_3^2 + 17280 v^7 c_0 c_3^2 - 120 v^9 c_1 c_3 + 12 v^9 c_2 c_3 \\
& - 720 v^9 c_2 c_3^2 - 12 v^9 c_0 c_3 - 720 v^9 a_1 c_3^3 + 48960 v^9 c_1 c_3^2 \\
& - 12 v^{11} c_2 c_3^2 + 720 v^{11} c_1 c_3^2 - 144 v^{11} c_0 c_3^3 \\
& + 12 v^{11} c_0 c_3^2 + 50400 v^{11} c_1^2 c_3^2 - 720 v^{15} c_1^2 c_3^3 \\
& + 144 \sin(v) v^{10} c_3^2 + 4 \sin(v) v^{10} c_3 + 6912 \sin(v) v^4 c_3 - 10368 v^5 c_0 c_3 \\
& + 6 \sin(v) v^{12} c_3^2 - 600 v^{17} c_1^3 c_3^3 - 480 v^{13} c_1 c_3^3 \\
& + 144 \sin(v) v^8 c_3 + 1200 v^{13} c_1^2 c_3^2 + 1440 v^3 + 20736 \sin(v) \\
\Upsilon_6(v) &= -207360 + 240 \cos(v) v^{18} c_1 c_3^4 + 10 \cos(v) v^{18} c_1^2 c_3^2
\end{aligned}$$

$$\begin{aligned} & + 30 \cos(v) v^{18} c_1 c_3^3 + 360 \cos(v) v^{16} c_1^2 c_3^2 + 720 \cos(v) v^{16} c_1 c_3^3 \\ & + 20 \cos(v) v^{16} c_1 c_3^2 + 720 \cos(v) v^{14} c_1 c_3^2 + 5 \cos(v) v^{14} c_1 c_3 \\ & + 240 \cos(v) v^{12} c_1 c_3 - 12 v^{20} c_1^2 c_2 c_3^4 + 43200 v^{18} a_1 c_1^3 c_3^4 \\ & + 5880 v^{20} c_1^3 c_3^4 + 30 \cos(v) v^{20} c_1^2 c_3^3 + 20 \cos(v) v^{20} c_1 c_3^4 \\ & + 720 \cos(v) v^{18} c_1^2 c_3^3 + 5 \cos(v) v^{22} c_1 c_3^5 + 240 \cos(v) v^{20} c_1^3 c_3^3 \\ & + 360 \cos(v) v^{20} c_1^2 c_3^4 + 10 \cos(v) v^{22} c_1^3 c_3^3 + 30 \cos(v) v^{22} c_1^2 c_3^4 \\ & - 1270080 v^{14} a_1 c_1^3 c_3^3 + 103680 \cos(v) v^6 c_1 c_3 \\ & + 780 v^{14} c_0 c_1 c_3^2 + 23760 v^{14} c_1 c_2 c_3^3 + 24480 v^{14} a_1 c_1 c_3^4 \\ & - 1270080 v^{14} c_0 c_1^2 c_3^3 - 248832 a_1 c_3 + 198720 v^8 c_1 c_2 c_3 \\ & - 120 v^{10} c_1 c_3 + 60 \cos(v) v^8 + 1212 v^{20} c_1^3 c_2 c_3^3 \\ & + 7800 v^{14} c_1^2 c_3^2 + 540 v^{18} c_1^2 c_2 c_3^3 - 1860 v^{18} c_0 c_1^2 c_3^3 \\ & + 60 v^{18} c_0 c_1 c_3^4 + 43920 v^{18} c_1^3 c_2 c_3^3 \\ & - 720 v^{18} c_0 c_1^2 c_3^4 + 3000 v^{12} c_1 c_3^2 - 12240 v^{16} a_1 c_1^3 c_3^3 \\ & + 600 v^{14} c_3^4 - 3110400 v^2 c_3 + 1036800 v^4 c_3 + 207360 v^2 c_2 \\ & - 8640 v^4 c_2 + 1440 \cos(v) v^6 - 25920 v^6 c_2 c_3 - 7800 v^{14} c_1 c_3^3 \\ & + 103680 \cos(v) v^2 - 36000 v^6 c_3 + 5040 v^{12} a_1 c_3^4 + 3000 v^{16} c_1 c_3^4 \\ & + 2332800 c_3^2 v^6 + 4200 v^{22} c_1^4 c_3^4 + 46800 v^{16} a_1 c_1^2 c_3^4 \\ & - 90000 v^{16} c_0 c_1^2 c_3^3 + 17280 \cos(v) v^4 + 11249280 v^{10} c_1^2 c_3^2 \\ & - 662400 v^{12} c_1 c_3^3 + 720 v^{14} c_0 c_3^4 + 60 v^{14} c_2 c_3^3 \\ & - 60 v^{14} c_0 c_3^3 + 12 v^{10} c_2 c_3 + 1347840 v^4 c_2 c_3 \\ & + 4320 \cos(v) v^8 c_3 + 17280 \cos(v) v^8 c_3^2 - 18600 v^{18} c_1^3 c_3^3 \\ & + 4320 \cos(v) v^{10} c_3^2 + \cos(v) v^{10} - 1116000 v^{14} c_1^2 c_3^3 - 2064960 v^{12} a_1 c_1^2 c_3^3 \\ & - 720 v^{14} c_1 c_2 c_3^2 - 18000 v^{16} c_1^2 c_3^3 + 120 v^{10} c_3^2 \\ & - 1200 v^{12} c_3^3 + 9763200 v^8 c_1 c_3^2 - 7488 v^{10} c_2 c_3^2 \\ & - 64800 v^8 c_3^2 - 12 v^{10} c_0 c_3 + 3600 v^{14} a_1 c_1^2 c_3^3 \\ & - 129600 v^6 a_1 c_1 c_3 + 1347840 v^4 a_1 c_1 c_3 \\ & + 1440 \cos(v) v^{18} c_1^3 c_3^3 + 4320 \cos(v) v^{16} c_1^2 c_3^3 \\ & + 4320 \cos(v) v^{14} c_1^2 c_3^2 - 145440 v^{10} c_3^3 + 240 \cos(v) v^{22} c_1^3 c_3^4 \end{aligned}$$

$$\begin{aligned}
& - 17280 v^2 a_1 + 60 \cos(v) v^{24} c_1^4 c_3^4 + 10 \cos(v) v^{24} c_1^2 c_3^5 \\
& + 7200 v^8 a_1 c_3^2 + 20 \cos(v) v^{24} c_1^3 c_3^4 + 10 \cos(v) v^{26} c_1^3 c_3^5 \\
& + 5 \cos(v) v^{26} c_1^4 c_3^4 + 5 \cos(v) v^{28} c_1^4 c_3^5 + \cos(v) v^{30} c_1^5 c_3^5 \\
& + 300 v^{16} c_1 c_2 c_3^3 - 1620 v^{16} c_1^2 c_2 c_3^2 \\
& - 180 v^{16} c_0 c_1 c_3^3 + 42480 v^{16} c_1^2 c_2 c_3^3 \\
& + 4250880 v^6 c_1 c_2 c_3 + 7050240 v^6 a_1 c_1 c_3^2 \\
& + 3600 v^8 a_1 c_1 c_3 + 8709120 v^8 c_0 c_1 c_3^2 + 8709120 v^8 a_1 c_1^2 c_3^2 \\
& - 777600 v^{16} c_1^3 c_3^3 + 6000 c_1^2 c_3^4 v^{18} + 12 v^{20} c_0 c_1 c_3^5 \\
& - 624 v^{20} c_0 c_1^2 c_3^4 + 18144 v^{20} c_0 c_1^3 c_3^4 \\
& + 18144 v^{20} a_1 c_1^4 c_3^4 + 120 v^{22} c_1^3 c_2 c_3^4 \\
& - 120 v^{22} c_0 c_1^2 c_3^5 + 420 v^{22} c_0 c_1^3 c_3^4 + 4320 v^{16} c_0 c_1 c_3^4 \\
& - 1074816 v^{10} c_1 c_2 c_3^2 - 43200 v^8 c_1 c_3 + 34560 v^{10} c_1 c_3^2 \\
& + 338400 v^{12} c_1^2 c_3^2 + 34560 \cos(v) v^8 c_1 c_3 + 4320 \cos(v) v^{10} c_1 c_3 \\
& + 20736 a_1 + 248832 \cos(v) - 7200 v^4 - 248832 c_2 + 172800 v^2 \\
& + 240 \cos(v) v^{10} c_3 + 5 \cos(v) v^{12} c_3 + 10 \cos(v) v^{14} c_3^2 + 4320 \cos(v) v^{14} c_1 c_3^3 \\
& + 17280 \cos(v) v^{12} c_1^2 c_3^2 + 8640 \cos(v) v^{12} c_1 c_3^2 \\
& - 3732480 v^2 a_1 c_1 c_3 + 34560 \cos(v) v^{10} c_1 c_3^2 \\
& + 240 \cos(v) v^{14} c_3^3 + 360 \cos(v) v^{12} c_3^2 + 10 \cos(v) v^{16} c_3^3 - 60 v^{24} c_1^4 c_2 c_3^4 \\
& + 60 v^{24} c_0 c_1^3 c_3^5 + 60 \cos(v) v^{16} c_3^4 + 5 \cos(v) v^{18} c_3^4 \\
& + \cos(v) v^{20} c_3^5 - 28800 v^{14} c_0 c_1 c_3^3 - 79200 v^{14} c_1^2 c_2 c_3^2 \\
& + 1347840 v^4 a_1 c_3^2 + 3600 v^6 a_1 c_3 + 43200 v^{12} c_0 c_1 c_3^2 \\
& - 43200 v^{12} c_1 c_2 c_3^2 + 2799360 v^6 c_0 c_3^2 + 720 v^4 a_1 \\
& - 221184 v^{10} a_1 c_1^2 c_3^2 - 267840 v^8 c_2 c_3^2 + 1440 \cos(v) v^{12} c_3^3 \\
& + 518400 v^2 a_1 c_3 - 112320 v^4 a_1 c_3 - 174528 v^{10} c_0 c_3^3 \\
& - 259200 v^6 a_1 c_3^2 + 720 v^8 c_2 c_3 - 720 v^8 c_0 c_3 + 7632 v^{10} c_0 c_3^2 \\
& - 6480 v^{12} c_0 c_3^3 + 14688 v^{10} a_1 c_1 c_3^2 - 1249344 v^{10} a_1 c_1 c_3^3 \\
& + 180 v^{12} c_1 c_2 c_3 - 1347840 v^{12} c_1^2 c_2 c_3^2 \\
& - 717120 v^{12} c_0 c_1 c_3^3 + 16560 v^{12} a_1 c_1 c_3^3
\end{aligned}$$

$$\begin{aligned}
& + 9360 v^{12} a_1 c_1^2 c_3^2 + 34560 \cos(v) v^6 c_3 + 190080 v^8 c_0 c_3^2 \\
& - 267840 v^8 a_1 c_3^3 + 103680 \cos(v) v^4 c_3 - 17280 v^6 c_0 c_3 \\
& - 14515200 v^4 c_1 c_3 - 103680 v^4 c_0 c_3 + 1123200 v^6 c_1 c_3 \\
& - 3732480 v^2 c_0 c_3 + 7056 v^{10} a_1 c_3^3 - 120 v^{12} c_2 c_3^2 \\
& + 120 v^{12} c_0 c_3^2 + 5040 v^{12} c_2 c_3^3 + 903744 v^{10} c_0 c_1 c_3^2 \\
& + 10512 v^{10} c_1 c_2 c_3 - 587520 v^8 a_1 c_1 c_3^2.
\end{aligned}$$

Appendix B: Formulae for the $\Upsilon_j(v)$, $j = 7(1)11$ and $Udenom_k(v)$, $k = 1, 2$

$$\begin{aligned}
\Upsilon_7(v) &= (\cos(v))^3 v^6 - 9 (\cos(v))^2 \sin(v) v^5 + 5 (\cos(v))^2 v^6 \\
&+ 15 (\cos(v))^3 v^4 + 45 \cos(v) \sin(v) v^5 \\
&+ 14 \cos(v) v^6 - 486 (\cos(v))^2 \sin(v) v^3 \\
&- 105 (\cos(v))^2 v^4 - 36 \sin(v) v^5 - 20 v^6 \\
&- 1665 (\cos(v))^3 v^2 + 90 \cos(v) \sin(v) v^3 \\
&+ 462 \cos(v) v^4 - 1080 (\cos(v))^2 \sin(v) v \\
&- 225 (\cos(v))^2 v^2 - 1836 \sin(v) v^3 \\
&- 210 v^4 - 3780 (\cos(v))^3 - 3195 \cos(v) v^2 \\
&+ 2160 \sin(v) v + 225 v^2 + 3780 \cos(v) \\
\Upsilon_8(v) &= 2 (\cos(v))^3 v^6 + 18 (\cos(v))^2 \sin(v) v^5 - 5 (\cos(v))^2 v^6 \\
&+ 30 (\cos(v))^3 v^4 - 105 \cos(v) \sin(v) v^5 \\
&+ 28 \cos(v) v^6 + 480 (\cos(v))^2 \sin(v) v^3 \\
&+ 825 (\cos(v))^2 v^4 + 72 \sin(v) v^5 + 20 v^6 \\
&+ 450 (\cos(v))^3 v^2 + 2850 \cos(v) \sin(v) v^3 \\
&+ 1260 \cos(v) v^4 + 8280 (\cos(v))^2 \sin(v) v \\
&- 4275 (\cos(v))^2 v^2 + 2160 \sin(v) v^3 \\
&+ 450 v^4 - 5400 (\cos(v))^3 - 1800 \cos(v) \sin(v) v \\
&+ 3150 \cos(v) v^2 - 17280 \sin(v) v \\
&+ 6075 v^2 + 5400 \cos(v)
\end{aligned}$$

$$\begin{aligned}\Upsilon_9(v) &= (\cos(v))^2 v^6 + \cos(v) \sin(v) v^5 \\ &+ 43 (\cos(v))^2 v^4 - 4 v^6 \\ &- 110 \cos(v) \sin(v) v^3 - 40 \cos(v) v^4 + 555 (\cos(v))^2 v^2 \\ &- 400 \sin(v) v^3 - 138 v^4 \\ &- 3000 \cos(v) \sin(v) v + 600 \cos(v) v^2 \\ &- 1800 (\cos(v))^2 - 600 \sin(v) v + 645 v^2 + 1800 \\ \Upsilon_{10}(v) &= (\cos(v))^3 v^6 + 3 (\cos(v))^2 \sin(v) v^5 - 5 (\cos(v))^2 v^6 \\ &+ 63 (\cos(v))^3 v^4 - 85 \cos(v) \sin(v) v^5 \\ &+ 14 \cos(v) v^6 + 126 (\cos(v))^2 \sin(v) v^3 \\ &+ 465 (\cos(v))^2 v^4 + 12 \sin(v) v^5 + 20 v^6 \\ &+ 1467 (\cos(v))^3 v^2 + 510 \cos(v) \sin(v) v^3 \\ &+ 670 \cos(v) v^4 + 3360 (\cos(v))^2 \sin(v) v \\ &+ 1905 (\cos(v))^2 v^2 + 108 \sin(v) v^3 \\ &+ 530 v^4 + 11340 (\cos(v))^3 + 4200 \cos(v) \sin(v) v \\ &+ 3873 \cos(v) v^2 - 5040 \sin(v) v \\ &+ 1575 v^2 - 11340 \cos(v) \\ \Upsilon_{11}(v) &= (\cos(v))^2 v^6 + 7 \cos(v) \sin(v) v^5 \\ &+ 29 (\cos(v))^2 v^4 - 4 v^6 \\ &+ 102 \cos(v) \sin(v) v^3 - 20 \cos(v) v^4 \\ &+ 891 (\cos(v))^2 v^2 - 360 \sin(v) v^3 - 90 v^4 \\ &- 840 \cos(v) \sin(v) v + 1740 \cos(v) v^2 \\ &+ 5670 (\cos(v))^2 + 2100 \sin(v) v + 1779 v^2 - 5670 \\ Udenom_1(v) &= (\cos(v))^2 v^4 + 13 \cos(v) \sin(v) v^3 \\ &- 4 v^4 - 45 (\cos(v))^2 v^2 \\ &+ 30 \cos(v) \sin(v) v - 90 v^2 - 105 (\cos(v))^2 + 105 \\ Udenom_2(v) &= v^2 \left((\cos(v))^2 v^6 + 7 \cos(v) \sin(v) v^5 \right. \\ &+ 29 (\cos(v))^2 v^4 - 4 v^6 + 102 \cos(v) \sin(v) v^3 \\ &\left. - 20 \cos(v) v^4 + 891 (\cos(v))^2 v^2 \right)\end{aligned}$$

$$\begin{aligned}
 & - 360 \sin(v) v^3 - 90 v^4 - 840 \cos(v) \sin(v) v + 1740 \cos(v) v^2 \\
 & + 5670 (\cos(v))^2 + 2100 \sin(v) v + 1779 v^2 - 5670 \Big).
 \end{aligned}$$

Appendix C: Truncated Taylor Series Expansion Formulae for the coefficients of the new obtained method given by (26)

$$\begin{aligned}
 a_1 &= -2 + \frac{v^{12}}{119750400} + \frac{37 v^{14}}{74724249600} + \frac{3823 v^{16}}{131813576294400} \\
 &+ \frac{8082727 v^{18}}{6470398926351360000} + \dots \\
 c_0 &= \frac{15}{28} - \frac{115 v^2}{4851} + \frac{4183181 v^4}{2796970176} + \frac{43290661 v^6}{8614668142080} \\
 &+ \frac{26855116571749 v^8}{15832347239567738880} + \frac{13069268523635959 v^{10}}{138976344068925611888640} \\
 &+ \frac{36995398988232494879 v^{12}}{5891942982197415705904742400} \\
 &+ \frac{4794898835302746891443 v^{14}}{11568830045544625738543961702400} \\
 &+ \frac{44791008915154857836703317699 v^{16}}{1630056945728072380476405497279053824000} \\
 &+ \frac{36614245294685173091989320114727 v^{18}}{20082301571369851727469315726477943111680000} + \dots \\
 c_1 &= \frac{1}{56} + \frac{v^2}{882} + \frac{39001 v^4}{508540032} + \frac{8111861 v^6}{1566303298560} \\
 &+ \frac{4995247059577 v^8}{14393042945061580800} + \frac{14616813578053517 v^{10}}{631710654858752781312000} \\
 &+ \frac{36868361335551830789 v^{12}}{23962447535252647607746560000} \\
 &+ \frac{154491264866748824244067 v^{14}}{1511835744588218136286994995200000} \\
 &+ \frac{62828772349636551906828658211 v^{16}}{9261687191636774889070485779994624000000}
 \end{aligned}$$

$$\begin{aligned}
& + \frac{205504627149665352212652766877947 v^{18}}{456415944803860266533393539238135070720000000} + \dots \\
c_2 = & \frac{1}{15} + \frac{4 v^2}{3465} - \frac{1801 v^4}{45405360} - \frac{52079 v^6}{7628100480} \\
& + \frac{8651507759 v^8}{8986665175488000} + \frac{199398453803 v^{10}}{2758214926938240000} \\
& + \frac{5608485889441381 v^{12}}{1174668573084457651200000} + \frac{1572019742188578791 v^{14}}{6569488556629182632448000000} \\
& + \frac{1378327386753952656761 v^{16}}{157273556045702632220805120000000} \\
& + \frac{7994388728944332905833 v^{18}}{66054893539195105532738150400000000} + \dots \\
c_3 = & \frac{1}{30} + \frac{2 v^2}{3465} - \frac{1801 v^4}{90810720} - \frac{52079 v^6}{15256200960} \\
& - \frac{4856586841 v^8}{17973330350976000} - \frac{1143449026051 v^{10}}{71713588100394240000} \\
& - \frac{1715515200063719 v^{12}}{2349337146168915302400000} - \frac{294832409423618959 v^{14}}{13138977113258365264896000000} \\
& + \frac{932778876735780883 v^{16}}{18502771299494427320094720000000} \\
& + \frac{9778995804489942605833 v^{18}}{132109787078390211065476300800000000} + \dots
\end{aligned}$$

Appendix D: Expressions for the Derivatives of φ_n

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

$$\begin{aligned}
\varphi^{(2)} &= (V(x) - V_c + \Gamma) \varphi(x) \\
\varphi^{(3)} &= \left(\frac{d}{dx} \Xi(x) \right) \varphi(x) + (\Xi(x) + \Gamma) \frac{d}{dx} \varphi(x) \\
\varphi^{(4)} &= \left(\frac{d^2}{dx^2} \Xi(x) \right) \varphi(x) + 2 \left(\frac{d}{dx} \Xi(x) \right) \frac{d}{dx} \varphi(x) + (\Xi(x) + \Gamma)^2 \varphi(x)
\end{aligned}$$

$$\begin{aligned}\varphi^{(5)} &= \left(\frac{d^3}{dx^3} \Xi(x) \right) \varphi(x) + 3 \left(\frac{d^2}{dx^2} \Xi(x) \right) \frac{d}{dx} \varphi(x) \\ &+ 4 (\Xi(x) + \Gamma) \varphi(x) \frac{d}{dx} \Xi(x) + (\Xi(x) + \Gamma)^2 \frac{d}{dx} \varphi(x) \\ \varphi^{(6)} &= \left(\frac{d^4}{dx^4} \Xi(x) \right) \varphi(x) + 4 \left(\frac{d^3}{dx^3} \Xi(x) \right) \frac{d}{dx} \varphi(x) \\ &+ 7 (\Xi(x) + \Gamma) \varphi(x) \frac{d^2}{dx^2} \Xi(x) + 4 \left(\frac{d}{dx} \Xi(x) \right)^2 \varphi(x) \\ &+ 6 (\Xi(x) + \Gamma) \left(\frac{d}{dx} \varphi(x) \right) \frac{d}{dx} \Xi(x) + (\Xi(x) + \Gamma)^3 \varphi(x) \\ \varphi^{(7)} &= \left(\frac{d^5}{dx^5} \Xi(x) \right) \varphi(x) + 5 \left(\frac{d^4}{dx^4} \Xi(x) \right) \frac{d}{dx} \varphi(x) \\ &+ 11 (\Xi(x) + \Gamma) \varphi(x) \frac{d^3}{dx^3} \Xi(x) + 15 \left(\frac{d}{dx} \Xi(x) \right) \varphi(x) \\ &+ \frac{d^2}{dx^2} \Xi(x) + 13 (\Xi(x) + \Gamma) \left(\frac{d}{dx} \varphi(x) \right) \frac{d^2}{dx^2} \Xi(x) \\ &+ 10 \left(\frac{d}{dx} \Xi(x) \right)^2 \frac{d}{dx} \varphi(x) + 9 (\Xi(x) + \Gamma)^2 \varphi(x) \\ &+ \frac{d}{dx} \Xi(x) + (\Xi(x) + \Gamma)^3 \frac{d}{dx} \varphi(x) \\ \varphi^{(8)} &= \left(\frac{d^6}{dx^6} \Xi(x) \right) \varphi(x) + 6 \left(\frac{d^5}{dx^5} \Xi(x) \right) \frac{d}{dx} \varphi(x) \\ &+ 16 (\Xi(x) + \Gamma) \varphi(x) \frac{d^4}{dx^4} \Xi(x) + 26 \left(\frac{d}{dx} \Xi(x) \right) \varphi(x) \\ &+ \frac{d^3}{dx^3} \Xi(x) + 24 (\Xi(x) + \Gamma) \left(\frac{d}{dx} \varphi(x) \right) \frac{d^3}{dx^3} \Xi(x) \\ &+ 15 \left(\frac{d^2}{dx^2} \Xi(x) \right)^2 \varphi(x) + 48 \left(\frac{d}{dx} \Xi(x) \right) \\ &+ \left(\frac{d}{dx} \varphi(x) \right) \frac{d^2}{dx^2} \Xi(x) + 22 (\Xi(x) + \Gamma)^2 \varphi(x)\end{aligned}$$

$$\begin{aligned}
& + \frac{d^2}{dx^2} \Xi(x) + 28 (\Xi(x) + \Gamma) \varphi(x) \left(\frac{d}{dx} \Xi(x) \right)^2 \\
& + 12 (\Xi(x) + \Gamma)^2 \left(\frac{d}{dx} \varphi(x) \right) \frac{d}{dx} \Xi(x) + (\Xi(x) + \Gamma)^4 \varphi(x) \\
& \dots
\end{aligned}$$

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

Appendix E: Formula for the quantity Λ_0

$$\begin{aligned}
\Lambda_0 = & - \frac{\left(\frac{d^9}{dx^9} \Xi(x) \right) \frac{d}{dx} \varphi(x)}{2395008} - \frac{353 \left(\frac{d}{dx} \Xi(x) \right) \varphi(x) \left(\frac{d^3}{dx^3} \Xi(x) \right) \frac{d^2}{dx^2} \Xi(x)}{2395008} \\
& - \frac{743 \Xi(x) \varphi(x) \left(\frac{d}{dx} \Xi(x) \right)^2 \frac{d^2}{dx^2} \Xi(x)}{5987520} - \frac{5 (\Xi(x))^2 \left(\frac{d}{dx} \varphi(x) \right) \left(\frac{d}{dx} \Xi(x) \right) \frac{d^2}{dx^2} \Xi(x)}{99792} \\
& - \frac{313 (\Xi(x))^2 \varphi(x) \left(\frac{d}{dx} \Xi(x) \right) \frac{d^3}{dx^3} \Xi(x)}{3991680} - \frac{23 \Xi(x) \left(\frac{d}{dx} \varphi(x) \right) \left(\frac{d^4}{dx^4} \Xi(x) \right) \frac{d}{dx} \Xi(x)}{299376} \\
& - \frac{73 \Xi(x) \left(\frac{d}{dx} \varphi(x) \right) \left(\frac{d^3}{dx^3} \Xi(x) \right) \frac{d^2}{dx^2} \Xi(x)}{598752} - \frac{323 \Xi(x) \varphi(x) \left(\frac{d^5}{dx^5} \Xi(x) \right) \frac{d}{dx} \Xi(x)}{5987520} \\
& - \frac{13 \Xi(x) \varphi(x) \left(\frac{d^4}{dx^4} \Xi(x) \right) \frac{d^2}{dx^2} \Xi(x)}{136080} - \frac{31 \left(\frac{d}{dx} \Xi(x) \right) \left(\frac{d}{dx} \varphi(x) \right) \left(\frac{d^2}{dx^2} \Xi(x) \right)^2}{266112} \\
& - \frac{19 \left(\frac{d^2}{dx^2} \Xi(x) \right) \left(\frac{d}{dx} \varphi(x) \right) \frac{d^5}{dx^5} \Xi(x)}{443520} - \frac{7 \left(\frac{d}{dx} \Xi(x) \right) \left(\frac{d}{dx} \varphi(x) \right) \frac{d^6}{dx^6} \Xi(x)}{342144} \\
& - \frac{5 \left(\frac{d^2}{dx^2} \Xi(x) \right)^3 \varphi(x)}{177408} - \frac{\left(\frac{d^4}{dx^4} \Xi(x) \right)^2 \varphi(x)}{114048} - \frac{13 \left(\frac{d}{dx} \Xi(x) \right) \varphi(x) \frac{d^7}{dx^7} \Xi(x)}{2395008} \\
& - \frac{19 (\Xi(x))^4 \varphi(x) \frac{d^2}{dx^2} \Xi(x)}{4790016} - \frac{13 (\Xi(x))^3 \varphi(x) \left(\frac{d}{dx} \Xi(x) \right)^2}{1197504} \\
& - \frac{(\Xi(x))^6 \varphi(x)}{23950080} - \frac{\left(\frac{d^{10}}{dx^{10}} \Xi(x) \right) \varphi(x)}{23950080} - \frac{17 \left(\frac{d^2}{dx^2} \Xi(x) \right) \varphi(x) \frac{d^6}{dx^6} \Xi(x)}{1596672} \\
& - \frac{\left(\frac{d^3}{dx^3} \Xi(x) \right) \left(\frac{d}{dx} \varphi(x) \right) \frac{d^4}{dx^4} \Xi(x)}{16632} - \frac{\left(\frac{d}{dx} \Xi(x) \right)^2 \varphi(x) \frac{d^4}{dx^4} \Xi(x)}{19008} \\
& - \frac{5 \Xi(x) \left(\frac{d}{dx} \varphi(x) \right) \left(\frac{d}{dx} \Xi(x) \right)^3}{199584} - \frac{43 \Xi(x) \varphi(x) \left(\frac{d^3}{dx^3} \Xi(x) \right)^2}{748440} \\
& - \frac{\left(\frac{d}{dx} \Xi(x) \right)^4 \varphi(x)}{85536} - \frac{(\Xi(x))^4 \left(\frac{d}{dx} \varphi(x) \right) \frac{d}{dx} \Xi(x)}{798336}
\end{aligned}$$

$$\begin{aligned}
& - \frac{109 \left(\frac{d}{dx} \Xi(x) \right)^2 \left(\frac{d}{dx} \varphi(x) \right) \frac{d^3}{dx^3} \Xi(x)}{1197504} - \frac{5 \left(\Xi(x) \right)^3 \left(\frac{d}{dx} \varphi(x) \right) \frac{d^3}{dx^3} \Xi(x)}{598752} \\
& - \frac{1201 \left(\Xi(x) \right)^2 \varphi(x) \left(\frac{d^2}{dx^2} \Xi(x) \right)^2}{23950080} - \frac{37 \left(\Xi(x) \right)^3 \varphi(x) \frac{d^4}{dx^4} \Xi(x)}{2993760} \\
& - \frac{23 \Xi(x) \varphi(x) \frac{d^8}{dx^8} \Xi(x)}{11975040} - \frac{\Xi(x) \left(\frac{d}{dx} \varphi(x) \right) \frac{d^7}{dx^7} \Xi(x)}{187110} \\
& - \frac{31 \left(\frac{d^3}{dx^3} \Xi(x) \right) \varphi(x) \frac{d^5}{dx^5} \Xi(x)}{1995840} - \frac{157 \left(\Xi(x) \right)^2 \left(\frac{d}{dx} \varphi(x) \right) \frac{d^5}{dx^5} \Xi(x)}{11975040} \\
& - \frac{239 \left(\Xi(x) \right)^2 \varphi(x) \frac{d^6}{dx^6} \Xi(x)}{23950080}
\end{aligned}$$

at every point $x = x_n$.

Appendix F: Formulae for the $\Upsilon_j(v)$, $j = 12(1)14$

$$\begin{aligned}
\Upsilon_{12}(s, v) = & -1260 (\cos(v))^2 v^6 + 105 s^2 v^6 \\
& + 180 s^4 v^6 - 90 s^2 v^8 - 3558 s^4 v^4 \\
& + 11340 s^4 v^2 - 4 s^6 v^6 + 8 s^4 v^8 - 4 s^2 v^{10} \\
& - 138 s^6 v^4 + 645 s^6 v^2 + 12 (\cos(v))^2 v^{10} \\
& - 540 (\cos(v))^2 v^8 - 1800 (\cos(v))^2 s^6 \\
& - 1080 v^8 - 3480 \cos(v) s^4 v^4 \\
& - 40 \cos(v) s^6 v^4 + 43 (\cos(v))^2 s^6 v^4 \\
& - 45 (\cos(v))^2 s^2 v^8 + \cos(v) \sin(v) s^6 v^5 \\
& - 14 \cos(v) \sin(v) s^4 v^7 + 13 \cos(v) \sin(v) s^2 v^9 \\
& - 110 \cos(v) \sin(v) s^6 v^3 - 204 \cos(v) \sin(v) s^4 v^5 \\
& + 30 \cos(v) \sin(v) s^2 v^7 - 3000 \cos(v) \sin(v) s^6 v \\
& + 1680 \cos(v) \sin(v) s^4 v^3 - 58 (\cos(v))^2 s^4 v^6 \\
& - 400 \sin(v) s^6 v^3 + 720 \sin(v) s^4 v^5 - 4200 \sin(v) s^4 v^3 \\
& + 360 \cos(v) \sin(v) v^7 - 600 \sin(v) s^6 v \\
& - 2 (\cos(v))^2 s^4 v^8 - 105 (\cos(v))^2 s^2 v^6 \\
& + 40 \cos(v) s^4 v^6 + (\cos(v))^2 s^6 v^6 \\
& - 1782 (\cos(v))^2 s^4 v^4 + 555 (\cos(v))^2 s^6 v^2 \\
& - 11340 (\cos(v))^2 s^4 v^2 + 156 \cos(v) \sin(v) v^9
\end{aligned}$$

$$\begin{aligned} & + 600 \cos(v) s^6 v^2 + (\cos(v))^2 s^2 v^{10} \\ & + 1260 v^6 - 48 v^{10} + 1800 s^6 \\ \Upsilon_{13}(s, v) = & (\cos(v))^3 v^{12} - 20 v^{12} - 3 (\cos(v))^3 s^4 v^8 - 1575 s^2 v^6 \\ & - 1590 s^4 v^6 + 1350 s^2 v^8 - 4725 s^4 v^4 + 20 s^6 v^6 \\ & - 60 s^4 v^8 + 60 s^2 v^{10} + 450 s^6 v^4 \\ & + 6075 s^6 v^2 - 105 (\cos(v))^2 v^{10} \\ & - 225 (\cos(v))^2 v^8 + 5400 \cos(v) s^6 \\ & - 36 \sin(v) s^4 v^7 + 72 \sin(v) s^6 v^5 + 225 v^8 \\ & - 11619 \cos(v) s^4 v^4 + 1260 \cos(v) s^6 v^4 \\ & + 825 (\cos(v))^2 s^6 v^4 + 675 (\cos(v))^2 s^2 v^8 - 105 \cos(v) \sin(v) s^6 v^5 \\ & + 255 \cos(v) \sin(v) s^4 v^7 - 195 \cos(v) \sin(v) s^2 v^9 \\ & + 2850 \cos(v) \sin(v) s^6 v^3 - 1530 \cos(v) \sin(v) s^4 v^5 \\ & - 450 \cos(v) \sin(v) s^2 v^7 - 1800 \cos(v) \sin(v) s^6 v \\ & - 12600 \cos(v) \sin(v) s^4 v^3 - 1395 (\cos(v))^2 s^4 v^6 \\ & + 2160 \sin(v) s^6 v^3 - 324 \sin(v) s^4 v^5 + 15120 \sin(v) s^4 v^3 \\ & - 17280 \sin(v) s^6 v + 15 (\cos(v))^2 s^4 v^8 \\ & + 1575 (\cos(v))^2 s^2 v^6 - 2010 \cos(v) s^4 v^6 \\ & - 5 (\cos(v))^2 s^6 v^6 - 5715 (\cos(v))^2 s^4 v^4 \\ & - 4275 (\cos(v))^2 s^6 v^2 + 90 \cos(v) \sin(v) v^9 \\ & + 3150 \cos(v) s^6 v^2 - 15 (\cos(v))^2 s^2 v^{10} \\ & + 14 \cos(v) v^{12} - 36 \sin(v) v^{11} + 462 \cos(v) v^{10} \\ & - 1836 \sin(v) v^9 - 3195 \cos(v) v^8 + 2160 \sin(v) v^7 \\ & - 5400 (\cos(v))^3 s^6 + 15 (\cos(v))^3 v^{10} \\ & - 1665 (\cos(v))^3 v^8 + 5 v^{12} (\cos(v))^2 \\ & - 42 \cos(v) s^4 v^8 + 28 \cos(v) s^6 v^6 \\ & - 9 (\cos(v))^2 \sin(v) v^{11} + 8280 (\cos(v))^2 \sin(v) s^6 v \\ & - 10080 (\cos(v))^2 \sin(v) s^4 v^3 - 210 v^{10} \\ & - 3780 (\cos(v))^3 v^6 + 3780 \cos(v) v^6 \end{aligned}$$

$$\begin{aligned}
 & + 18 (\cos(v))^2 \sin(v) s^6 v^5 - 9 (\cos(v))^2 \sin(v) s^4 v^7 \\
 & + 480 (\cos(v))^2 \sin(v) s^6 v^3 - 378 (\cos(v))^2 \sin(v) s^4 v^5 \\
 & + 45 \cos(v) \sin(v) v^{11} - 486 (\cos(v))^2 \sin(v) v^9 \\
 & - 1080 (\cos(v))^2 \sin(v) v^7 - 34020 (\cos(v))^3 s^4 v^2 \\
 & + 34020 \cos(v) s^4 v^2 + 30 (\cos(v))^3 s^6 v^4 \\
 & - 189 (\cos(v))^3 s^4 v^6 + 450 (\cos(v))^3 s^6 v^2 \\
 & - 4401 (\cos(v))^3 s^4 v^4 + 2 (\cos(v))^3 s^6 v^6 \\
 \Upsilon_{14}(s, v) = & (\cos(v))^2 v^4 + 13 \cos(v) \sin(v) v^3 \\
 & - 4 v^4 - 45 (\cos(v))^2 v^2 + 30 \cos(v) \sin(v) v \\
 & - 90 v^2 - 105 (\cos(v))^2 + 105.
 \end{aligned}$$

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