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An Optimized Multistage Complete in Phase P–Stable Algorithm

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Abstract

A fourteen algebraic order P–stable symmetric four–stages two–step scheme with expunged phase–lag and its first and second derivatives, is developed, for the first time in the literature, in this paper. The new four–stages method is developed based on the following steps:

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- Contentment of the necessary and sufficient conditions for P–stability.
- Contentment of the condition of the expunging of the phase–lag.
- Contentment of the junctures of the expunging of the first and second derivatives of the phase–lag.

The result of the above methodology is the development, for the first time in the literature, of a four–stages P–stable fourteen algebraic order symmetric two–step method with expunged phase–lag and its derivatives up to order two.

We present also a full numerical and theoretical analysis for the new algorithm which contains the following steps:

- the development of the new four–stages method,
- the achievement of its local truncation error (LTE),
- the foundation of the asymptotic form of the LTE of the new four–stages method,
- the foundation of the stability and interval of periodicity of the new four–stages method,
- the achievement of an embedded algorithm and the determination of the variable step technique for the changing of the step sizes,
- the evaluation of the computational efficiency of the new four–stages method with its 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 study leads to the conclusion that the new four–stages method is more efficient than the existed ones.

1 Introduction

A new four–stages P–stable two–step algorithm with eliminated phase–lag and its first and second derivatives is created, for the first time in the literature, in this paper.

The creation of the new proposed four–stages P–stable two–step algorithm follows the below mentioned levels:

- Level 1: Satisfaction of the property of the P–stability.
- Level 2: Satisfaction of the property for the elimination of the phase–lag.
- Level 3: Satisfaction of the properties for the elimination of the first and second derivatives of the phase–lag.

We will evaluate the effectiveness of the new four–stages algorithm by applying it to:

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

We mention here that the efficient numerical 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 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 [10–13]).

We will also create an embedded numerical algorithm which is based on an local truncation error control procedure and a variable–step method. This new embedded algorithm is based on the new created four–stages algorithm.

The problems which are investigated in this paper belong to the following category of special problems:

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

which have periodical and/or oscillating solutions.

The main classes of the numerical algorithms and their literature is presented below:

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

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

$$\text{or } x^i \exp(\omega x),\ i = 0, 1, 2, \ldots \tag{2}$$

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

– Numerical algorithms which have the property of evanescence (or vanishing or elimination) of the phase–lag and its derivatives.

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

- Multistep exponentially, trigonometrically and phase fitted schemes and multistep methods with minimal phase–lag: [1]– [8], [18]– [21], [25]– [28], [34], [38], [40], [44], [48]– [49], [53], [58], [60]– [61], [71]– [73], [79]– [82]. In this class of schemes, multistep algorithms are created. This class is divided into two subcategories:

  – Multistep algorithms 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 algorithms which have the property of evanescence (or vanishing or elimination) of the phase–lag and its derivatives.

- Symplectic integrators: [42]– [43], [51], [54], [57], [67]– [70], [76]. In this class of numerical algorithms, schemes for which the Hamiltonian energy of the system remains almost constant during the integration procedure, are obtained.

- Nonlinear algorithms: [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 algorithms: [14]– [17], [22]– [24], [35]– [37], [41]. In the category of numerical methods, numerical algorithms with constant coefficients are constructed.

2 Theory for the development of symmetric multistep schemes

In this section we present the theory for the creation of the general form of the symmetric multistep algorithms.

Since the multistep algorithms are finite difference methods, the methodology of the discretization of the integration domain is used for the numerical solution of the problems of the form (1). In this research, the integration domain $[a, b]$ is discretized by using the $2\,m$-step symmetric scheme of the form (3). We note that for these type of method the parameter m determines the number of the discretization points.

The following symbols are used:

- h determines the stepsize of the integration which is equivalent with the step length of the discretization. It is defined 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 denotes the n-th point on the discretized domain.
- φ_n denotes the approximation of the function $\varphi(x)$ at the point x_n. The approximation φ_n is determined using a numerical algorithm like the $2\,m$-step method (3) described below

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

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

The above family of schemes is used for the numerical 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*

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

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

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

If we apply the symmetric $2\,m$-step algorithm $\Delta\,(m)$ into the model equation

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

we obtain the difference equation:

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

and its associated characteristic equation:

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

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] *We call that a symmetric* $2\,m$*-step algorithm has an non zero interval of periodicity* $(0, v_0^2)$*, if its characteristic equation (9)has the following roots :*

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

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

Definition 5. *(see [15]) We call a symmetric multistep algorithm* **P-stable** *if its interval of periodicity is equal to* $(0, \infty)$.

Remark 3. *We call a symmetric multistep algorithm* **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. *We call a symmetric multistep algorithm 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 algorithm 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] We call a symmetric multistep algorithm 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*

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

Based on the Theorem 1, we obtain the following conclusion:

Conclusion 1. *For the family of symmetric two–step methods the phase-lag order* υ *and the phase-lag constant* ϖ *can be directly computed using the formula:*

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

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

3 A new four–stages P–stable symmetric symmetric method with expunged phase–lag and its first and second derivatives

The following family of four–stages algorithms is considered:

$$\begin{aligned}
\widehat{\varphi}_{n+1} &= \varphi_{n+1} - h^2 \left(c_1 \, f_{n+1} - c_0 \, f_n + c_1 \, f_{n-1} \right) \\
\tilde{\varphi}_{n+1} &= \varphi_{n+1} - h^2 \left(c_3 \, \widehat{f}_{n+1} - c_2 \, f_n + c_3 \, f_{n-1} \right) \\
\check{\varphi}_{n+1} &= \varphi_{n+1} - h^2 \left(c_5 \, \tilde{f}_{n+1} - c_4 \, f_n + c_5 \, f_{n-1} \right) \\
\varphi_{n+1} + a_1 \, \varphi_n + \varphi_{n-1} &= h^2 \left[b_1 \, \left(\check{f}_{n+1} + f_{n-1} \right) + b_0 \, f_n \right]
\end{aligned} \tag{16}$$

where $f_{n+i} = \varphi'' \left(x_{n+i}, \varphi_{n+i} \right), i = -1(1)1$, $\widehat{f}_{n+1} = \varphi'' \left(x_{n+1}, \widehat{q}_{n+1} \right)$, $\tilde{f}_{n+1} = \varphi'' \left(x_{n+1}, \tilde{\varphi}_{n+1} \right)$, $\check{f}_{n+1} = \varphi'' \left(x_{n+1}, \check{\varphi}_{n+1} \right)$ and a_1, b_i, $i = 0$, 1 and c_j, $i = 0 \, (1) \, 5$ are parameters.

Remark 4. *The new four–stages method is hybrid and consequently nonlinear with the the approximations to be based on the point x_{n+1}.*

We study the following specific case:

$$\begin{aligned}
b_0 \, = \, \frac{5}{6}, \, b_1 \, = \, \frac{1}{12}, \, c_2 \, = \, \frac{92605}{86919}, \\
c_3 \, = \, \frac{2347}{173838}, \, c_4 \, = \, \frac{4139}{84370}, \, c_5 \, = \, \frac{4139}{168740}.
\end{aligned} \tag{17}$$

Remark 5. *The parameters given by (17) reserves that the new four–stages method (16) will have algebraic order fourteen which is the maximum possible one.*

Application of the new four–stages method (16) with the constant coefficient given by (17) to the scalar test equation (7), leads to the difference equation (8) with $m = 1$ and to the corresponding characteristic equation (9) with $m = 1$ with:

$$\begin{aligned}
\Upsilon_1 \left(v \right) &= 1 + \frac{1}{12} \, v^2 + \frac{4139}{2024880} \, v^4 + \frac{2347}{85044960} \, v^6 + \frac{2347 \, c_1}{85044960} \, v^8 \\
\Upsilon_0 \left(v \right) &= a_1 + \frac{5}{6} \, v^2 - \frac{4139}{1012440} \, v^4 - \frac{18521}{8504496} \, v^6 - \frac{2347 \, c_0}{85044960} \, v^8
\end{aligned} \tag{18}$$

The layers for the development of the new four–stages algorithm are presented in the flowchart of Figure 1 (for construction of flowcharts in LaTeX one can see [90]):

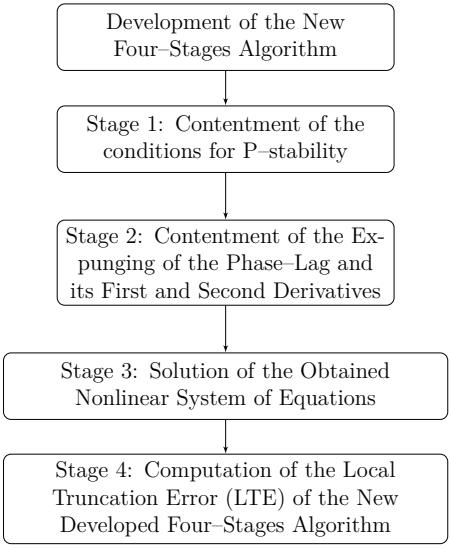

Figure 1. Production of the four–stages two–step symmetric algorithm

3.1 Contentment of the conditions for P–stability

In order to obtain the contentment of the conditions for the P–stability for the new four–stages method, the technique of Lambert and Watson [15] and Wang [83] is used:

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

$$\left(\mathrm{e}^{I\,v}\right)^2\ \Upsilon_0\left(v\right) + \mathrm{e}^{I\,v}\,\Upsilon_1\left(v\right) + \Upsilon_0\left(v\right) = 0 \tag{19}$$

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

$$\left(\mathrm{e}^{-I\,v}\right)^2\ \Upsilon_0\left(v\right) + \mathrm{e}^{-I\,v}\,\Upsilon_1\left(v\right) + \Upsilon_0\left(v\right) = 0 \tag{20}$$

Remark 6. *The conditions for P–stability (19) and (20) are produced using:*

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

3.2 Contentment of the expunging of the phase–lag and its first and second derivatives

The contentment of the expunging of the phase–lag and its first and second derivatives for the new four–stages algorithm (16) with coefficients mentioned in (17) leads to the system of equations:

$$\text{Phase}-\text{Lag(PL)} \;=\; \frac{1}{2}\,\frac{\Psi_0}{\Psi_3}=0 \tag{21}$$

$$\text{First Derivative of the Phase}-\text{Lag} \;=\; \frac{\Psi_1}{\Psi_3^2}=0 \tag{22}$$

$$\text{Second Derivative of the Phase}-\text{Lag} \;=\; \frac{\Psi_2}{\Psi_3^3}=0 \tag{23}$$

where $\Psi_j\,(v)\,,\; j=0(1)3$ are given in the Appendix A.

3.3 Solution of the obtained system of nonlinear equations which is defined by (19) - (23)

Solving the nonlinear system of equations produced by (19), (20), (21)–(23), the coefficients of the new four–stages method are determined:

$$\begin{aligned} a_1 \;&=\; \frac{\Psi_4}{340179840\,\cos(v)\,v+3061618560\,\sin(v)} \\ c_0 \;&=\; \frac{\Psi_5}{4694\,v^8\,(\cos(v)\,v+9\,\sin(v))} \\ c_1 \;&=\; -\frac{\Psi_6}{2347\,v^8\,(\cos(v)\,v+9\,\sin(v))} \end{aligned} \tag{24}$$

where $\Psi_j\,(v)\,,\; j=4(1)6$ are given in the Appendix B.

The probability, during the integration procedure, of impossibility of determination of the coefficients (24) - a reason, for example, can be that the denominators of (24) $\longrightarrow$ 0 for some values of $|v|$ - leads us to give the truncated Taylor series expansions of the coefficients developed in (24) in the Appendix C.

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

The development of the new four–stages algorithm is integrated (see Figure 1) with the determination of its local truncation error (LTE):

$$LTE_{NM4SPS2DV}=-\frac{53}{161653459968000}\,h^{16}\left(5\,\varphi_n^{(16)}+32\,\phi^6\,\varphi_n^{(10)}\right.$$

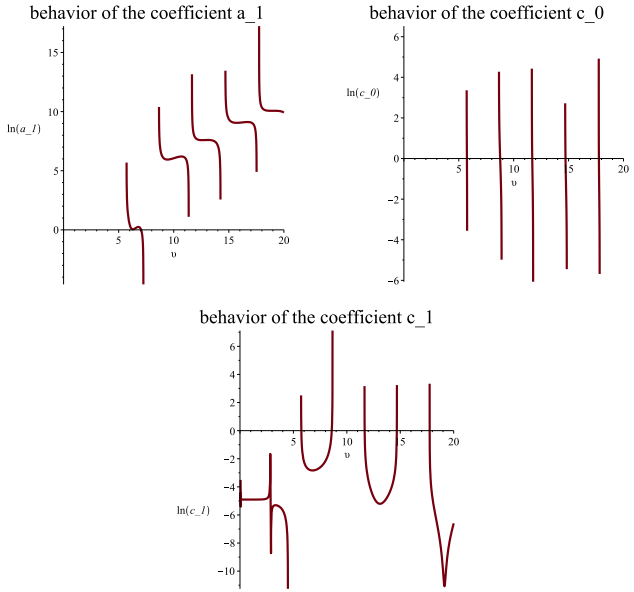

Figure 2. Behavior of the coefficients of the new four–stages method (16) given by (24) for several values of $v = \phi\, h$.

$$+30\,\phi^8\,\varphi_n^{(8)} - 3\,\phi^{16}\,\varphi_n\Big) + O\left(h^{18}\right). \tag{25}$$

We symbolize the new obtained four–stages method as $NM4SPS2DV$. The explanation of the abbreviation $NM4SPS2DV$ is: New Method of Four–Stages P–Stable with Vanished Phase–Lag and its Derivatives up to Order Two.

Remark 7. *The above determined LTE formula (25) is useful for*

- *the definition of the algebraic order of the new four–stages method*
- *for the construction of the asymptotic form of the local error for a specific test problem on which the evaluation of the efficiency of the new method will be based.*

4 Local truncation error and stability analysis of the new four–stages method

4.1 Comparative local truncation error analysis

In this section we will study the local truncation error of some four–stages schemes, based on the test model:

$$\varphi''(x) \;=\; (V(x) - V_c + \Gamma)\;\varphi(x) \tag{26}$$

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 8. *It is easy to see that the test model (26) is the radial time independent Schrödinger equation with potential* $V(x)$.

We will evaluate the following four–stages algorithms:

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

$$LTE_{CL} = -\frac{53}{32330691993600}\, h^{16}\, \varphi_n^{(16)} + O\left(h^{18}\right). \tag{27}$$

4.1.2 P–stable method with vanished phase–lag and its first and second derivatives developed in section 3

The formula of the Local Truncation Error for this four–stages algorithm is given by (25)

For the comparative error analysis, the following methodology is used:

- Step 1: We apply the LTE formulae given by (27) and (25) to the scalar model (26).
- Step 2: Step 1 leads to the new formulae of LTE.

Remark 9. *The technique which is used for the production of the new formulae of LTE consists of the substitution of the formulae of the derivatives of the function φ, which are obtained using the scalar model (26)), in the formulae given by (27) and (25). Some formulae of the derivatives of the function φ are given in the Appendix D.*

- Step 3: Step 2 leads to the new formulae of LTE for the four–stages algorithms which are under evaluation.

  Remark 10. *Observation of the new formulae of $LTE \longrightarrow$ 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 is given by:

$$LTE = h^p \sum_{j=0}^{k} \Phi_j \, \Gamma^j \tag{28}$$

  with Φ_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 four–stages method and k is the maximum possible power of Γ in the formulae of LTE.

- Step 4: Two set of values for the parameter Γ are investigated:

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

     Resultants:

$$\Gamma \approx 0 \Rightarrow \Gamma^i \approx 0, \, i = 1, 2, \ldots . \tag{29}$$

     which leads to:

$$LTE_{\Gamma=0} = h^k \, \Lambda_0 \tag{30}$$

     Remark 11. *The quantity Λ_0 is the same for all the four–stages methods of the same family, i.e. $LTE_{CL} = LTE_{NM4SPS2DV} = h^{16} \, \Lambda_0$. Λ_0 is given in the Appendix E.*

Theorem 2. *The formula (29) leads us to we conclusion that for* $\Gamma = V_c - E \approx 0$ *the asymptotic forms of the local truncation error of the classical method (constant coefficients - (27)) and the local truncation error of the four–stages method with vanished phase–lag and its first and second derivatives developed in Section 3 (with LTE given by (25), 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, $\Gamma >> 0 \vee \Gamma << 0 \Rightarrow |\Gamma| >> 0$.

   Resultants:

   The most accurate four–stages method is the one with asymptotic formula of LTE, given by (28), which contains the minimum power of Γ (i.e. minimum values for k) and the maximum value of p.

- The above leads us to the following asymptotic forms of the LTE formulae for the four–stages methods which are under evaluation.

4.1.3 Classical method

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

$$LTE_{CL} = \frac{53}{32330691993600}\,h^{16}\left(\varphi\left(x\right)\,\Gamma^{8} + \cdots\right) + O\left(h^{18}\right). \tag{31}$$

We note here that we present the leading term in the asymptotic form of the Local Truncation Error. Consequently, the symbol $\cdots$ means that there are also terms for $\Gamma^{j}\; j = 0\,(1)\,7$.

4.1.4 P–stable method with vanished phase–lag and its first and second derivatives developed in section 3

$$LTE_{NM4SPS2DV} = \frac{53}{505167062400}\,h^{16}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi\left(x\right)\varphi\left(x\right)\,\Gamma^{6} + \cdots\right) + O\left(h^{18}\right). \tag{32}$$

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 $\Gamma^{j}\; j = 0\,(1)\,5$.

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 eighth power of* Γ.
- *P–Stable Tenth Algebraic Order Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in Section 3: For this method the error increases as the sixth 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 four–stages method with vanished phase–lag and its derivatives up to order two is the most accurate one.

4.2 Stability analysis

The following scalar model is used:

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

Remark 12. *The observation of (7) and (33) leads to the conclusion that* $\omega \neq \phi$, *where* ϕ *is the frequency of the scalar model (7) (phase–lag analysis) and* ω *is the frequency of the scalar model (33) (stability analysis).*

Application of the new four–stages scheme (16) to the scalar model (33) leads to the difference equation:

$$\Omega_1(s,v)\,(\varphi_{n+1} + \varphi_{n-1}) + \Omega_0(s,v)\,\varphi_n = 0 \tag{34}$$

and the corresponding characteristic equation:

$$\Omega_1(s,v)\,\left(\lambda^2 + 1\right) + \Omega_0(s,v)\,\lambda = 0 \tag{35}$$

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

$$\begin{aligned} \Omega_1(s,v) &= 1 + s^2 b_1 + s^4 b_1 c_5 + s^6 b_1 c_3 c_5 + s^8 b_1 c_1 c_3 c_5 \\ \Omega_0(s,v) &= a_1 + s^2 b_0 - s^4 b_1 c_4 - s^6 b_1 c_2 c_5 - s^8 b_1 c_0 c_3 c_5, \end{aligned} \tag{36}$$

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

Remark 13. *Observing the formulae (36) and (18), we arrive to the conclusion that the formulae (36) are dependent on s and v, while the formulae (18) are dependent only on v.*

Substituting the coefficients b_j, $j = 0, 1$ and c_k, $k = 2(1)5$ given by (17) and the coefficients a_1 and c_k, $k = 0, 1$ given by (24) into the stability polynomials (36), we obtain the following formulae for the stability polynomials $\Omega_j(s, v)$, $j = 0, 1$:

$$\begin{aligned} \Omega_1(s, v) &= -\frac{\Psi_7(s, v)}{85044960\,\Psi_8(s, v)} \\ \Omega_0(s, v) &= -\frac{\Psi_9(s, v)}{170089920\,\Psi_8(s, v)} \end{aligned} \tag{37}$$

where $\Psi_j(s, v)$, $j = 7(1)9$ are given in the Appendix F.

Remark 14. *We note that the conditions and definitions of P–stability and singularly almost P–stability, which are given in Section 2, are given for problems with one frequency i.e. for problems in which the following relation is hold: $\omega = \phi$.*

In order the new proposed four–stages method (16) to satisfy the condition of a non zero interval of periodicity, the following relation for the of its characteristic equation (35) must hold:

$$|\lambda_{1,2}| \leq 1 \tag{38}$$

4.2.1 Flowchart for the construction of the $s - v$ domain for the new four–stages method

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

The result of the flowchart presented in Figure 3 leads to the $s - v$ domain which is constructed in Figure 4.

Remark 15. *Observation on the $s - v$ domain presented in Figure 4 leads to the following remarks:*

1. *The new produced four–stages P–stable method is stable within the shadowed area of the domain.*

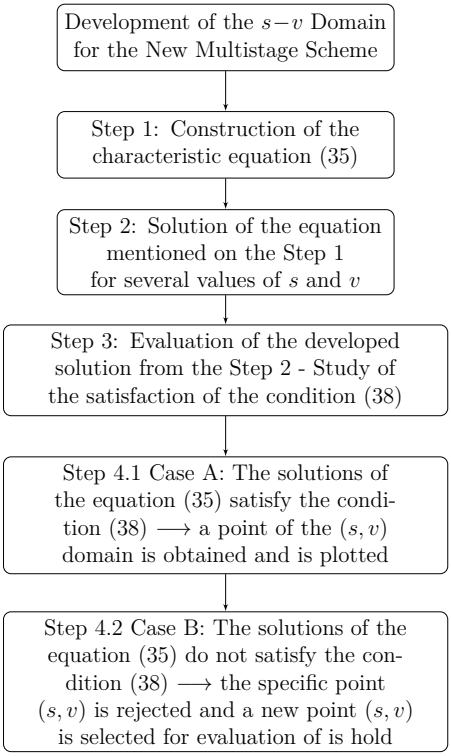

Figure 3. Procedure for the construction of the $s - v$ domain for the new four–stages scheme

2. *The new produced four–stages P–stable method is unstable within the white area of the domain.*

Remark 16. *The above observations leads to the following remarks on the applicability of the new produced four–stages P–stable method:*

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.*

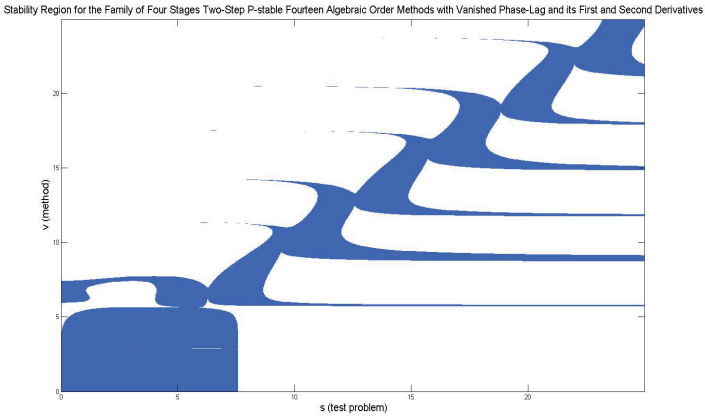

Figure 4. The plot of $s - v$ domain of the new produced four–stages P–stable method with eliminated phase–lag and its first and second derivatives.

The methodology for the determination of the interval of periodicity of the new produced four–stages P–stable method is as follows:

1. Substitution $s = v$ on the stability polynomials Ω_i, $i = 0, 1$ given by (37).

2. Evaluation of the produced area around the first diagonal of the $s-v$ domain defined in Figure 4.

The above methodology leads us to the conclusion that the interval of periodicity of the new produced four–stages P–stable method is equal to $(0, \infty)$.

We have the the following theorem:

Theorem 4. *The new four–stages P–stable method produced in Section 3:*

- *is of four stages*
- *is of fourteen algebraic order,*
- *has eliminated the phase–lag and its first and second derivatives 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 obtained four–stages method is based on its application to the numerical solution of:

1. The one–dimensional time–independent Schrödinger equation and
2. The systems of coupled differential equations of the Schrödinger type.

5.1 Radial or one–dimensional time independent Schrödinger equation

The one–dimensional time–independent Schrödinger equation is given by:

$$\varphi''(r) = [l(l+1)/r^2 + V(r) - k^2]\,\varphi(r), \tag{39}$$

where

1. The function $\Theta(r) = l(l+1)/r^2 + V(r)$ determines *the effective potential*, for which we have that: $\Theta(r) \to 0$ as $r \to \infty$.
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*.

The problem (39) is a boundary value one and consequently the boundary conditions are:

$$\varphi(0) = 0$$

and another condition at the end point of the integration area which is determined for large values of r from the physical considerations and characteristics of the specific problem.

The new obtained four–stages method has its coefficients a_1, c_0, c_1 dependent from the quantity $v = \phi\, h$, where ϕ is the frequency of the specific problem. Consequently, in order the coefficients of the new four–stages algorithm to be computed during the integration, it is necessary the determination of the frequency ϕ for the specific problem. In our numerical evaluations and for (39) 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

As we mentioned above the model of the radial time–independent Schrödinger equation (39) consists the potential $V(r)$. Therefore, the computation of the the values of the potential $V(r)$ requires the formula of the function of the potential $V(r)$. For our numerical evaluation the Wood–Saxon potential is used. The formula of the Wood–Saxon potential is given by:

$$V(r) = \frac{\Psi_0}{1+\xi} - \frac{\Psi_0\,\xi}{a\,(1+\xi)^2} \tag{40}$$

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 plot of the Wood–Saxon potential for several values of r.

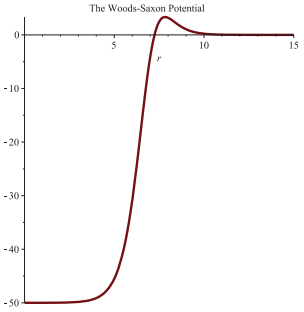

Figure 5. Plot of the Woods–Saxon potential for several values of r.

Based on the Woods–Saxon potential and the methodology introduced in [20], [21] and [19], the following values of the frequency ϕ are used during the integration procedure:

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

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, $v = \phi\, h = \sqrt{-50 + E}\, h$.

Remark 17. *We note here that 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 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

As we mentioned above the numerical solution of the problem (39):

- with $l = 0$ and
- using the Woods-Saxon potential (40)

is the first problem where the new proposed four–stages two–step method will be evaluated.

From theoretical point of view the integration interval of the above problem is equal to $[0, \infty)$. In order to solve the problem (39) numerically, it is necessary the interval $[0, \infty)$ to be approximated by a finite one. For the purposed of our numerical tests, we approximate the the interval $[0, \infty)$ by the interval $[0, 15]$. We will apply the numerical solution of the problem (39) under the above conditions, to a wide range of energies: $E \in [1, 1000]$.

The faster elimination of the potential $V(r)$ then the term $\frac{l(l+1)}{r^2}$, leads to a new form for the equation (39):

$$\varphi''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) \varphi(r) = 0 \tag{41}$$

when $r \to \infty$. The solutions of the model (41) 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 $n_l(k\,r)$ represent the spherical Bessel and Neumann functions respectively (see [84]).

Therefore, the asymptotic form of the solution of the model (39) (i.e. in the case where $r \to \infty$) is given by:

$$\varphi(r) \approx A\,kr\,j_l(kr) - B\,kr\,n_l(kr)$$

$$\approx \quad AC \left[\sin\left(kr - \frac{l\pi}{2} \right) + \tan\delta_l \cos\left(kr - \frac{l\pi}{2} \right) \right]$$

where δ_l is the phase shift and A, B, $AC \in \mathbb{R}$. The phase shift is computed based on the direct formula:

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

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 $S(r) = k\, r\, j_l(k\, r)$ and $C(r) = -k\, r\, n_l(k\, r)$. The problem described above is an initial–value one. Therefore, it is necessary to compute the values of φ_j, $j = 0, 1$ before starting the application of a two–step scheme. The value φ_0 is determined by the initial condition of the problem. The value φ_1 is computed using the high order Runge–Kutta–Nyström methods (see [22] and [23]). The values φ_i, $i = 0, 1$ are the basis in order to compute the phase shift δ_l at the point r_2 of the asymptotic region. We note that φ_j is the approximation of the function φ at the point x_j.

The numerical solution of the above problem leads to two possible results:

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

In our numerical tests we chosen the second problem, which is known as **the resonance problem**.

The boundary conditions are:

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

For comparison purposes we use the following methods for the computation of the the positive eigenenergies of the resonance problem:

- **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 NM4SPS2DV**: the Four–Stages Fourteen Algebraic Order P–stable Symmetric Two–Step method with vanished phase-lag and its first and second derivatives developed in Section 3.

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

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

In order to define the quantity Err, two values of the specific eigenenergy are used:

1. The computed eigenenergies determined as $E_{calculated}$ which are computed using each of the numerical methods under evaluation.

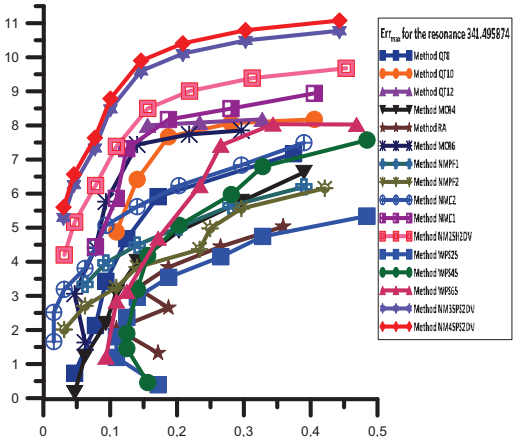

Figure 6. Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

2. The accurate eigenenergies (or as also called **reference values** for the eigenenergies) determined as $E_{accurate}$ which 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 all the numerical methods under evaluation and for several values of CPU time (in seconds).
- the needed CPU time (in seconds) (as mentioned above).

We use the symbols E_2 and E_3 for the eigenenergies in our numerical tests 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 therefore the newly obtained method can show its efficiency more effectively.

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

Figures 6 and 7 lead us to the following conclusions:

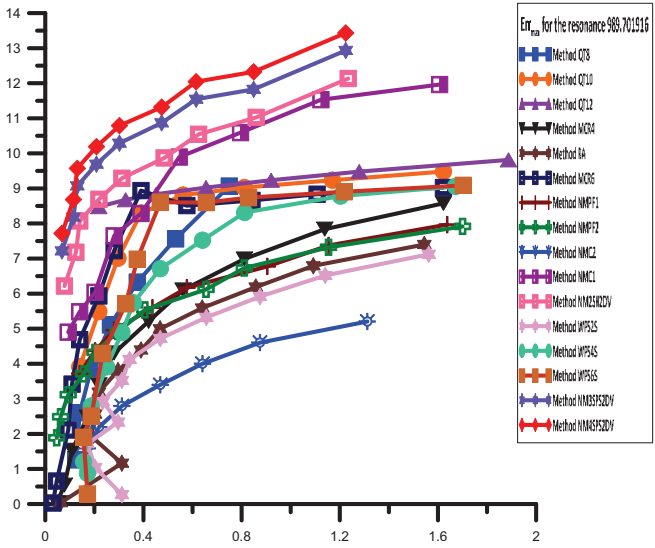

Figure 7. Accuracy (Digits) for several values of *CPU* Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

- **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 NM4SPS2DV**, is the most efficient one.

5.2 Error estimation

The second of our tests is the numerical solution of systems of coupled differential equations arising from the Schrödinger equation.

We will use variable–step schemes in order to solve this problem.

Definition 9. *Variable–step method is called the numerical algorithm with a step length or a stepsize which is changing during the integration procedure.*

Definition 10. *We call Local Truncation Error Estimation Procedure (LTERRESTPRO) a methodology which uses a variable–step method for changing the stepsize during the integration.*

For the bibliography on the development of numerical methods of constant or variable step length for the numerical solution of the Schrödinger equation and related problems one can see [14]– [83] and references therein.

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

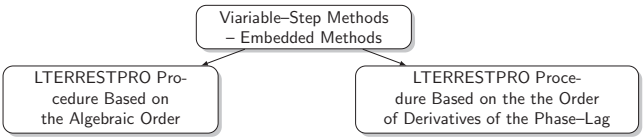

Figure 8. Categories of LTERRESTPRO Procedures used for the Development of Embedded Methods for the Problems with Oscillatory and/or Periodical Solutions

The estimation of the local truncation error (LTE) in the lower order solution φ_{n+1}^{L} is necessary for the procedure of changing of the stepsize during the integration. We use for this the following relation:

$$LTE = \mid \varphi_{n+1}^{H} - \varphi_{n+1}^{L} \mid \tag{42}$$

where φ_{n+1}^{L} and φ_{n+1}^{H} are

- **LTERRESTPRO Procedure which is based on the algebraic order of the numerical schemes**. For this procedure, φ_{n+1}^{L} denotes the numerical method with the lower algebraic order solution and φ_{n+1}^{H} denotes the numerical method with the higher algebraic order solution.
- **LTERRESTPRO Procedure 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 vanished for the numerical methods which belong in this procedure are p and s respectively, where $p < s$. For this procedure φ_{n+1}^{L} denotes the numerical method with vanished all the derivatives of the phase–lag until the order p and φ_{n+1}^{H} denotes the numerical method with vanished all the derivative of the phase–lag until the order s.

For our evaluation methodology we use the first LTERRESTPRO procedure for the estimation of the local truncation error. Consequently, we use:

As φ_{n+1}^{L} we use the tenth algebraic order method developed in [6] and as φ_{n+1}^{H} we use the fourteenth algebraic order method developed in Section 3.

Using the Local Truncation Error Control Procedure $LTERRESTPRO$, in Figure 9 we present the variable–step technique used in our paper.Notifications:

- h_n is denoted as the step length which is used during the n^{th} step of the integration technique and
- acc is denoted as the requested accuracy for the local truncation error LTE which is defined by the user.

Remark 18. *We use the methodology of* **local extrapolation**, *i.e. the local truncation error estimation is based on the lower order solution φ_{n+1}^{L} while the approximation of the solution at each point of the integration domain is done via the higher order solution φ_{n+1}^{H}.*

5.3 The system of coupled differential equations arising from the Schrödinger equation

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

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

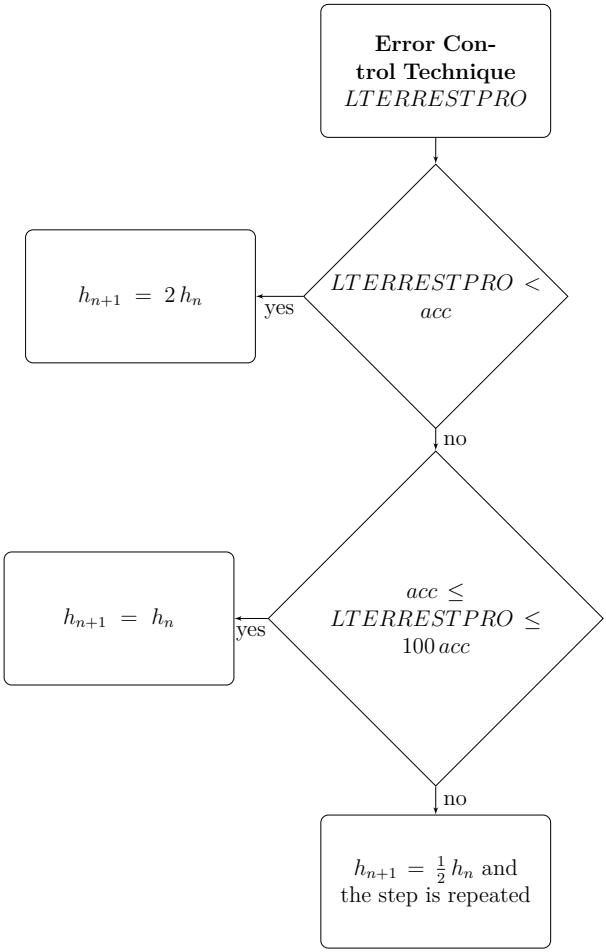

Figure 9. Flowchart for the Local Truncation Error Control Technique $LTERRESTPRO$. The parameter acc is defined by the user

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

Models of problems which are expressed with systems of differential equations of the above form, can be found in several scientific disciplines like: quantum chemistry, material science, theoretical physics, quantum physics, atomic physics, physical chemistry, chemical physics, quantum chemistry, electronics, etc.

Since the above problem is a boundary value one, the boundary conditions, are given

by (see for details [29]):

$$\varphi_{ij} = 0 \; at \; x = 0$$
$$\varphi_{ij} \sim k_i \, x j_{l_i} \left(k_i x\right) \delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} \, k_i \, x \, n_{li} \left(k_i x\right) \tag{43}$$

Remark 19. *The four–stages scheme produced in this and the associated embedded method can be applied effectively to both open and close channels problem.*

The analysis presented in [29] leads to the new formulae of the asymptotic condition (43):

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

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

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

The specific problem which we solve in our numerical tests is the rotational excitation of a diatomic molecule by neutral particle impact. This problem can be found in several 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. In the above mentioned problem one can finds the close–coupling Schrödinger equations (see [9], [10–13], [85] - [89]). Using the determinations:

- 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 have:

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

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 determines the angular momentum of the quantum numbers (j,l) and j'' and l'' determine the quantum numbers.

The following potential V is used during our numerical experiments (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 consequently, 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 determined from formulae described by Bernstein et al. [30] and $\hat{\mathbf{k}}_{j'j}$ determines a unit vector parallel to the wave vector $\mathbf{k}_{j'j}$ and $P_i,\ i=0,2$ determine the Legendre polynomials (see for details [31]). We note also that $V_0(x)$ and $V_2(x)$ determine the potential functions defined by the user. Based on the above achievements, we obtain the following new formulae of the boundary conditions:

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

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

where S matrix. For K matrix of (43) the following formula is used:

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

Based on the methodology fully described in [29], we use the four–stages two–step method and the embedded pair both obtained in this paper in order to solve numerically the above mentioned problem.

We use the following parameters for the $\mathbf{S}$ matrix for our numerical tests:

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

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

Based on the study fully presented in [29] we chose the following for our test:

- $J = 6$ and
- $j = 0$ for the excitation of the rotator state to levels up to $j' = 2, 4$ and 6.

The above values obtain systems of **four, nine and sixteen coupled differential equations of the Schrödinger type**, respectively. Following the theory and the methodology fully described in [31] and [29], the potential is considered infinite for x less than x_0. Therefore, the boundary condition (44) can be written now as

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

For our numerical test and for comparison purposes we use the following methods:

- 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 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 VI**.
- 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 VII**.

In Table 2 we present:

[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

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	0.896	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 VII	4	0.896	0.01	1.2×10^{-8}
	9	0.896	0.39	1.9×10^{-8}
	16	0.896	7.12	2.2×10^{-8}

- the real time of computation requested by the numerical algorithms I-VII mentioned 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,

- the maximum error on 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.

6 Conclusions

A new P–stable four–stages fourteen algebraic order two–step method with eliminated phase–lag and its first and second derivatives was created in this paper.

The creation was done using the following levels:

1. 1st Level: Satisfaction of the P–stability properties (based on the requirements first introduced by Lambert and Watson [15] and Wang [83]).
2. 2nd Level: Satisfaction of the property of the elimination of the phase–lag.
3. 3rd Level: Satisfaction of the properties of the elimination of the first and second derivatives of the phase–lag.

We note here that the above methodology for the creation of P–stable numerical methods was first introduced by Medvedev and Simos [6].

We have also analyzed the new created four–stages two–step method using the following levels:

- 1st Level: Computation of the local truncation error (LTE).
- 2nd Level: Computation of the asymptotic form of the LTE
- 3rd Level: Comparison of the asymptotic form of the LTE of the new four–stages two–step method with the asymptotic forms of the LTE of similar methods.
- 4th Level: Investigation of the stability and the interval of periodicity properties of the new four–stages two–step method.
- 5th Level: Evaluation of the computational efficiency of the four–stages two–step method.

The theoretical, computational and numerical achievements presented in this paper lead to the conclusion that the new four–stages two–step method is more effective for the numerical solution of the Schrödinger equation than other well known and recently obtained methods of the literature.

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Appendix A: Formulae for the $\Upsilon_i(v)$, $i = 0(1)3$

$$
\begin{aligned}
\Psi_0 &= 4694\cos(v)\,v^8\,c_1 - 2347\,v^8\,c_0 \\
&+ 4694\cos(v)\,v^6 - 185210\,v^6 \\
&+ 347676\cos(v)\,v^4 - 347676\,v^4 \\
&+ 14174160\cos(v)\,v^2 + 70870800\,v^2 \\
&+ 170089920\cos(v) + 85044960\,a_1 \\
\Psi_1 &= 6027204351168000\,v - 2863208668320\sin(v)\,v^6 \\
&- 79794794439360\sin(v)\,v^4 - 63486403764\sin(v)\,v^8 \\
&- 1205440870233600\sin(v)\,v^2 - 31380540408\,v^9 \\
&- 5508409\sin(v)\,v^{12} - 815995572\sin(v)\,v^{10} \\
&- 2957863708800\,v^7 - 7232645221401600\sin(v) \\
&- 62037576881280\,v^5 - 59136183025920\,v^3 + 434687870\,v^{13}c_1 \\
&- 815995572\,v^{11}c_0 + 1631991144\,v^{11}c_1 - 49900130280\,v^9c_0 \\
&- 399201042240\sin(v)\,v^8c_1 - 815995572\sin(v)\,v^{12}c_1 \\
&- 33266753520\sin(v)\,v^{10}c_1 - 798402084480\,v^7a_1c_1 \\
&- 798402084480\,v^7c_0 - 5508409\,v^{13}c_0 \\
&- 11016818\sin(v)\,v^{14}c_1 - 5508409\sin(v)\,v^{16}{c_1}^2 \\
&- 499001302800\,v^9c_1 - 602720435116800\,va_1 \\
&- 598801563360\,v^5a_1 - 29568091512960\,v^3a_1 \\
\Psi_2 &= -615100023548290215936000\cos(v) - 2304728831776020249600\,v^6
\end{aligned}
$$

$$- \; 33295113411815974118400\, v^{4} - 143233541199203264409600\, v^{2}$$

$$- \; 53304062970357239040\, v^{8} - 12928235923\, \cos\left(v\right) v^{18}$$

$$- \; 512583352956908513280000\, a_{1} + 421422460419280320\, v^{10}$$

$$+ \; 220950385012728\, v^{14} + 29255400239322096\, v^{12}$$

$$+ \; 4243754583657388800\, v^{8} a_{1} c_{1} - 475300513369627545600\, v^{6} a_{1} c_{1}$$

$$+ \; 1040944661713756800\, v^{10} a_{1} c_{1} - 12928235923\, \cos\left(v\right) v^{24} {c_{1}}^{3}$$

$$- \; 45876483175002480\, v^{12} c_{0} - 14351287847755098240\, v^{10} c_{1}$$

$$+ \; 2076425259161853600\, v^{12} c_{1} + 94569538910945616\, v^{14} c_{1}$$

$$- \; 117115605767160\, \cos\left(v\right) v^{18} {c_{1}}^{2} - 1405387269205920\, \cos\left(v\right) v^{16} {c_{1}}^{2}$$

$$- \; 5745424822452\, \cos\left(v\right) v^{18} c_{1} - 38784707769\, \cos\left(v\right) v^{22} {c_{1}}^{2}$$

$$- \; 2872712411226\, \cos\left(v\right) v^{20} {c_{1}}^{2} - 38784707769\, \cos\left(v\right) v^{20} c_{1}$$

$$+ \; 38784707769\, v^{20} c_{0} c_{1} - 475300513369627545600\, v^{6} c_{0}$$

$$- \; 2872712411226\, \cos\left(v\right) v^{16} - 447007768902324\, \cos\left(v\right) v^{16} c_{1}$$

$$- \; 20159852233641120\, \cos\left(v\right) v^{14} c_{1} - 2872712411226\, v^{16} c_{0}$$

$$+ \; 8198092403701200\, v^{16} {c_{1}}^{2} + 9837710884441440\, v^{10} a_{1}$$

$$- \; 425553114736008\, v^{14} c_{0} + 512583352956908513280000$$

$$+ \; 9575708037420\, v^{18} c_{0} c_{1} + 1020212430890\, v^{18}\, c_{1}$$

$$+ \; 819809240370120\, v^{16} c_{0} c_{1} - 329892163135164\, \cos\left(v\right) v^{14}$$

$$- \; 24007788523551672\, \cos\left(v\right) v^{12} - 1204342384201276320\, \cos\left(v\right) v^{10}$$

$$- \; 55168809587546054400\, v^{8} c_{0} - 594125641712034432000\, v^{8} c_{1}$$

$$+ \quad 889546964873364\, v^{16} c_1 + 37016968351902739200\, v^6 a_1$$

$$+ \quad 936850195542381120\, v^8 a_1 - 12928235923\, v^{18} c_0$$

$$- \quad 3060637292670\, v^{20} {c_1}^2 - 19151416074840\, v^{18} {c_1}^2$$

$$- \quad 50925055003888665600\, \cos(v)\, v^8 c_1$$

$$- \quad 561835147647533760\, \cos(v)\, v^{12} c_1$$

$$- \quad 8487509167314777600\, \cos(v)\, v^{10} c_1$$

$$+ \quad 16864647230471040\, v^{14} a_1 {c_1}^2$$

$$+ \quad 16864647230471040\, v^{14} c_0 c_1 + 24828508422637920\, v^{12} a_1 c_1$$

$$- \quad 2392797873552166080\, v^{10} c_0 + 688356159979065177600\, v^4 a_1$$

$$+ \quad 5270732343934644787200\, v^2 a_1$$

$$- \quad 42391524755918257920\, \cos(v)\, v^8$$

$$- \quad 1035540006778525248000\, \cos(v)\, v^6$$

$$- \quad 16586509563916746854400\, \cos(v)\, v^4$$

$$- \quad 153775005887072553984000\, \cos(v)\, v^2$$

$$\Psi_3 \quad = \quad 2347\, v^8\, c_1 + 2347\, v^6 + 173838\, v^4 + 7087080\, v^2 + 85044960.$$

Appendix B: Formulae for the $\Upsilon_j(v)$, $j = 4(1)6$

$$\Psi_4 \quad = \quad 185210\, \cos(v)\, v^7 + 2347\, v^7 \cos(2\, v)$$

$$+ \quad 555630\, \sin(v)\, v^6 - 7041\, v^6 \sin(2\, v)$$

$$- \quad 7041\, v^7 + 695352\, \cos(v)\, v^5 + 347676\, v^5 \cos(2\, v)$$

$$
\begin{aligned}
&+ \; 3476760\,\sin(v)\,v^4 - 1738380\,v^4\sin(2\,v) \\
&- \; 1043028\,v^5 - 212612400\,\cos(v)\,v^3 \\
&+ \; 21261240\,v^3\cos(2\,v) - 1488286800\,\sin(v)\,v^2 \\
&- \; 148828680\,v^2\sin(2\,v) - 63783720\,v^3 \\
&+ \; 340179840\,v\cos(2\,v) - 3061618560\,\sin(2\,v) \\
&- \; 1020539520\,v \\
\Psi_5 \;&= \; 2347\,(\cos(v))^2\,v^7 + 30511\,\cos(v)\sin(v)\,v^6 \\
&- \; 277815\,\cos(v)\,v^7 - 680359680\,v \\
&+ \; 235020\,(\cos(v))^2\,v^5 - 3055965\,\sin(v)\,v^6 \\
&- \; 4694\,v^7 + 3824436\,\cos(v)\sin(v)\,v^4 \\
&+ \; 4097364\,\cos(v)\,v^5 + 10135608\,(\cos(v))^2\,v^3 \\
&- \; 4519788\,\sin(v)\,v^4 - 695352\,v^5 \\
&+ \; 191351160\,\cos(v)\sin(v)\,v^2 + 46561032\,\cos(v)\,v^3 \\
&+ \; 531531000\,\sin(v)\,v^2 - 42522480\,v^3 \\
&+ \; 2381258880\,\cos(v)\sin(v) - 1700899200\,\cos(v)\,v \\
\Psi_6 \;&= \; 2347\,\cos(v)\,v^7 + 11735\,\sin(v)\,v^6 \\
&+ \; 202002\,\cos(v)\,v^5 + 173838\,\sin(v)\,v^4 \\
&- \; 1111260\,v^5 + 9868488\,\cos(v)\,v^3 - 2781408\,v^3 \\
&- \; 21261240\,\sin(v)\,v^2 + 170089920\,\cos(v)\,v \\
&- \; 595314720\,\sin(v) + 425224800\,v.
\end{aligned}
$$

Appendix C: Truncated Taylor Series Expansion Formulae for the coefficients of the new proposed multistage scheme given by (24)

$$
\begin{aligned}
a_1 &= -2 - \frac{53\,v^{16}}{53884486656000} - \frac{4578089\,v^{18}}{90028044925378560000} + \cdots \\
c_0 &= -\frac{592847}{422460} + \frac{53\,v^6}{69705900} \\
&- \frac{10499317\,v^8}{46009611648000} - \frac{925328737\,v^{10}}{50066822856960000} \\
&- \frac{32980634809\,v^{12}}{14161758465254400000} - \frac{468157795613\,v^{14}}{1628602223504256000000} \\
&- \frac{1025325640556311\,v^{16}}{2872854322261507584000000} \\
&- \frac{756845475622778557\,v^{18}}{17064754674233355048960000000} + \cdots \\
c_1 &= \frac{6253}{844920} + \frac{53\,v^6}{139411800} + \frac{5898883\,v^8}{92019223296000} \\
&+ \frac{1177910291\,v^{10}}{137683762856640000} + \frac{107298199231\,v^{12}}{99132309256780800000} \\
&+ \frac{140054628697\,v^{14}}{1036383233139072000000} \\
&+ \frac{1932493783626253\,v^{16}}{1149141728904603033600000000} \\
&+ \frac{178413063067461767\,v^{18}}{8532377337116677524480000000} + \cdots
\end{aligned}
$$

Appendix D: Expressions for the Derivatives of φ_n

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

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

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

$$+ \quad \left(\frac{d}{dx}\varphi(x)\right)\frac{d^2}{dx^2}\Xi(x) + 22\,(\Xi(x)+\Gamma)^2\,\varphi(x)$$

$$+ \quad \frac{d^2}{dx^2}\Xi(x) + 28\,(\Xi(x)+\Gamma)\,\varphi(x)\left(\frac{d}{dx}\Xi(x)\right)^2$$

$$+ \quad 12\,(\Xi(x)+\Gamma)^2\left(\frac{d}{dx}\varphi(x)\right)\frac{d}{dx}\Xi(x) + (\Xi(x)+\Gamma)^4\,\varphi(x)$$

$$\ldots$$

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

$$\begin{aligned}
\Lambda_0 \;=\; & \frac{2173\,(\Xi(x))^2\,\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^4}{57733378560} + \frac{110399\,(\Xi(x))^4\,\varphi(x)\,\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)}{16165345996800} \\
+ \; & \frac{689\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)\right)\varphi(x)\,\frac{\mathrm{d}^9}{\mathrm{d}x^9}\Xi(x)}{177641164800} + \frac{53\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)\right)\varphi(x)\,\frac{\mathrm{d}^8}{\mathrm{d}x^8}\Xi(x)}{8074598400} \\
+ \; & \frac{23479\,(\Xi(x))^3\,\varphi(x)\,\frac{\mathrm{d}^8}{\mathrm{d}x^8}\Xi(x)}{4041336499200} + \frac{793781\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^3\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{2020668249600} \\
+ \; & \frac{63017\,(\Xi(x))^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{288666892800} \\
+ \; & \frac{622697\,(\Xi(x))^2\,\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{2020668249600} \\
+ \; & \frac{346037\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}^7}{\mathrm{d}x^7}\Xi(x)\right)\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{4041336499200} \\
+ \; & \frac{11819\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{91848556800} \\
+ \; & \frac{20087\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^3\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{72166723200} \\
+ \; & \frac{65243\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{91848556800}
\end{aligned}$$

$$+\frac{23797\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^8}{\mathrm{d}x^8}\Xi(x)\right)\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)}{673556083200}$$

$$+\frac{97997\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^7}{\mathrm{d}x^7}\Xi(x)\right)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{1010334124800}$$

$$+\frac{26129\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)\right)\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{144333446400}$$

$$+\frac{583\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{2385676800}$$

$$+\frac{2491\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}^9}{\mathrm{d}x^9}\Xi(x)\right)\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)}{168389020800}$$

$$+\frac{170713\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}^8}{\mathrm{d}x^8}\Xi(x)\right)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{4041336499200}$$

$$+\frac{53\left(\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)\right)^2\varphi(x)}{10766131200}+\frac{53\,(\Xi(x))^6\,\varphi(x)\,\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{128296396800}$$

$$+\frac{26977\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\frac{\mathrm{d}^7}{\mathrm{d}x^7}\Xi(x)}{367394227200}+\frac{53\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\varphi(x)\,\frac{\mathrm{d}^{10}}{\mathrm{d}x^{10}}\Xi(x)}{29606860800}$$

$$+\frac{265\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^3\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{1049697792}+\frac{371\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\frac{\mathrm{d}^{10}}{\mathrm{d}x^{10}}\Xi(x)}{104969779200}$$

$$+\frac{164353\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)\right)\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{288666892800}$$

$$+\frac{3551\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)}{9868953600}+\frac{53\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\frac{\mathrm{d}^7}{\mathrm{d}x^7}\Xi(x)}{1284595200}$$

$$+\frac{1007\left(\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)\right)\varphi(x)\,\frac{\mathrm{d}^7}{\mathrm{d}x^7}\Xi(x)}{113044377600}+\frac{1641569\,(\Xi(x))^2\,\varphi(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^3}{8082672998400}$$

$$+\frac{169441\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)\right)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{144333446400}$$

$$+\frac{8533\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\varphi(x)\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)\right)^2}{44410291200}+\frac{53\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^5\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)}{2624244480}$$

$$+\frac{53\left(\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)}{1009324800}$$

$$+\frac{11183\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{11102572800}$$

$$+\frac{438787\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\varphi(x)\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)\right)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{577333785600}$$

$$+\frac{265\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2\varphi(x)\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)}{2368548864}+\frac{624181\left(\Xi(x)\right)^2\varphi(x)\left(\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)\right)^2}{4041336499200}$$

$$+\frac{16271\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\varphi(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{15395567616}$$

$$+\frac{2491\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\varphi(x)\left(\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{9542707200}$$

$$+\frac{371\left(\Xi(x)\right)^4\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{28866689280}$$

$$+\frac{168169\left(\Xi(x)\right)^3\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)}{2020668249600}$$

$$+\frac{33443\left(\Xi(x)\right)^3\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)}{288666892800}$$

$$+\frac{31747\left(\Xi(x)\right)^3\varphi(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{202066824960}$$

$$+\frac{270883\,\Xi(x)\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2}{367394227200}$$

$$+\frac{14893\left(\Xi(x)\right)^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2}{52484889600}$$

$$+\frac{232511\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)^2\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{288666892800}$$

$$+\frac{6307\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)\right)^2}{7401715200}$$

$$+\frac{1277989\,(\Xi(x))^2\,\varphi(x)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)}{8082672998400}$$

$$+\frac{87821\,(\Xi(x))^2\,\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\frac{\mathrm{d}^7}{\mathrm{d}x^7}\Xi(x)}{1347112166400}$$

$$+\frac{5353\,(\Xi(x))^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)}{64148198400}$$

$$+\frac{176543\,(\Xi(x))^2\,\varphi(x)\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)\right)\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)}{673556083200}$$

$$+\frac{53\,(\Xi(x))^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{198806400}$$

$$+\frac{35351\,(\Xi(x))^2\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)}{192444595200}$$

$$+\frac{8851\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\frac{\mathrm{d}^5}{\mathrm{d}x^5}\Xi(x)}{32074099200}$$

$$+\frac{61427\,\Xi(x)\,\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^2\frac{\mathrm{d}^6}{\mathrm{d}x^6}\Xi(x)}{310872038400}$$

$$+\frac{5671\,\Xi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)\right)^2\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)}{9020840400}$$

$$+\frac{2809\,(\Xi(x))^3\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Xi(x)\right)\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{28866689280}$$

$$+\frac{2173\,(\Xi(x))^3\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\frac{\mathrm{d}^4}{\mathrm{d}x^4}\Xi(x)}{36083361600}$$

$$+\frac{38213\,(\Xi(x))^4\,\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\frac{\mathrm{d}^3}{\mathrm{d}x^3}\Xi(x)}{1154667571200}$$

$$+\frac{4717\left(\Xi\left(x\right)\right)^{2}\varphi\left(x\right)\frac{\mathrm{d}^{10}}{\mathrm{d}x^{10}}\Xi\left(x\right)}{2694224332800}+\frac{371\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi\left(x\right)\right)^{3}\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)}{1850428800}$$

$$+\frac{2491\,\Xi\left(x\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}^{11}}{\mathrm{d}x^{11}}\Xi\left(x\right)}{4041336499200}+\frac{53\left(\Xi\left(x\right)\right)^{8}\varphi\left(x\right)}{32330691993600}$$

$$+\frac{53\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)\varphi\left(x\right)\frac{\mathrm{d}^{11}}{\mathrm{d}x^{11}}\Xi\left(x\right)}{85530931200}+\frac{522739\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)^{2}\varphi\left(x\right)\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi\left(x\right)\right)^{2}}{1154667571200}$$

$$+\frac{65773\,\Xi\left(x\right)\varphi\left(x\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)\left(\frac{\mathrm{d}^{5}}{\mathrm{d}x^{5}}\Xi\left(x\right)\right)\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi\left(x\right)}{80826729984}$$

$$+\frac{371\left(\Xi\left(x\right)\right)^{5}\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi\left(x\right)}{288666892800}$$

$$+\frac{901\left(\Xi\left(x\right)\right)^{3}\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}^{7}}{\mathrm{d}x^{7}}\Xi\left(x\right)}{126291765600}+\frac{1961\left(\Xi\left(x\right)\right)^{4}\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}^{5}}{\mathrm{d}x^{5}}\Xi\left(x\right)}{384889190400}$$

$$+\frac{25387\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)\varphi\left(x\right)\left(\frac{\mathrm{d}^{6}}{\mathrm{d}x^{6}}\Xi\left(x\right)\right)\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi\left(x\right)}{128296396800}$$

$$+\frac{1007\left(\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi\left(x\right)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}^{9}}{\mathrm{d}x^{9}}\Xi\left(x\right)}{88820582400}$$

$$+\frac{371\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi\left(x\right)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}^{8}}{\mathrm{d}x^{8}}\Xi\left(x\right)}{14803430400}+\frac{4823\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi\left(x\right)\right)^{2}\varphi\left(x\right)\frac{\mathrm{d}^{4}}{\mathrm{d}x^{4}}\Xi\left(x\right)}{22205145600}$$

$$+\frac{54007\,\Xi\left(x\right)\varphi\left(x\right)\left(\frac{\mathrm{d}^{5}}{\mathrm{d}x^{5}}\Xi\left(x\right)\right)^{2}}{734788454400}+\frac{12137\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)\varphi\left(x\right)\left(\frac{\mathrm{d}^{7}}{\mathrm{d}x^{7}}\Xi\left(x\right)\right)\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi\left(x\right)}{107768973312}$$

$$+\frac{2491\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)^{2}\varphi\left(x\right)\frac{\mathrm{d}^{8}}{\mathrm{d}x^{8}}\Xi\left(x\right)}{104969779200}$$

$$+\frac{148771\,\Xi\left(x\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)\left(\frac{\mathrm{d}^{4}}{\mathrm{d}x^{4}}\Xi\left(x\right)\right)\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi\left(x\right)}{144333446400}$$

$$+\frac{1643\left(\Xi\left(x\right)\right)^{2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}^{9}}{\mathrm{d}x^{9}}\Xi\left(x\right)}{449037388800}$$

$$+\frac{1007\left(\Xi\left(x\right)\right)^{5}\varphi\left(x\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)\right)^{2}}{577333785600}+\frac{53\left(\Xi\left(x\right)\right)^{6}\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi\left(x\right)\right)\frac{\mathrm{d}}{\mathrm{d}x}\Xi\left(x\right)}{577333785600}$$

$$+ \frac{371\left(\Xi(x)\right)^{3}\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^{3}}{28866689280} + \frac{53\left(\Xi(x)\right)^{5}\varphi(x)\frac{\mathrm{d}^{4}}{\mathrm{d}x^{4}}\Xi(x)}{18041680800}$$

$$+ \frac{39167\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^{4}\varphi(x)\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi(x)}{288666892800} + \frac{53\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi(x)\right)^{3}}{106913664}$$

$$+ \frac{298867\left(\Xi(x)\right)^{2}\varphi(x)\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi(x)\right)\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi(x)}{310872038400}$$

$$+ \frac{2334809\,\Xi(x)\varphi(x)\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi(x)\right)\left(\frac{\mathrm{d}^{4}}{\mathrm{d}x^{4}}\Xi(x)\right)\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)}{2020668249600}$$

$$+ \frac{7897\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)^{3}\varphi(x)\frac{\mathrm{d}^{5}}{\mathrm{d}x^{5}}\Xi(x)}{52484889600} + \frac{48707\left(\Xi(x)\right)^{3}\varphi(x)\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi(x)\right)^{2}}{505167062400}$$

$$+ \frac{53\left(\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi(x)\right)^{4}\varphi(x)}{526344192} + \frac{1219\,\Xi(x)\varphi(x)\frac{\mathrm{d}^{12}}{\mathrm{d}x^{12}}\Xi(x)}{8082672998400}$$

$$+ \frac{53\left(\frac{\mathrm{d}^{14}}{\mathrm{d}x^{14}}\Xi(x)\right)\varphi(x)}{32330691993600} + \frac{53\left(\frac{\mathrm{d}^{13}}{\mathrm{d}x^{13}}\Xi(x)\right)\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)}{2309335142400}$$

$$+ \frac{16589\left(\Xi(x)\right)^{4}\varphi(x)\left(\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi(x)\right)^{2}}{769778380800}$$

$$+ \frac{67363\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^{6}}{\mathrm{d}x^{6}}\Xi(x)\right)\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi(x)}{192444595200}$$

$$+ \frac{53\left(\frac{\mathrm{d}}{\mathrm{d}x}\Xi(x)\right)\left(\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x)\right)\left(\frac{\mathrm{d}^{4}}{\mathrm{d}x^{4}}\Xi(x)\right)^{2}}{159045120}$$

$$+ \frac{29839\left(\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}}\Xi(x)\right)\varphi(x)\left(\frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}}\Xi(x)\right)\frac{\mathrm{d}^{5}}{\mathrm{d}x^{5}}\Xi(x)}{88820582400}$$

at every point $x = x_n$.

Appendix F: Formulae for the $\Psi_j(v)$, $j = 7(1)9$

$$\begin{aligned}\Psi_7(s,v) &= 2347\cos(v)\,s^8v^7 - 2347\cos(v)\,s^6v^9\\ &+ 11735\sin(v)\,s^8v^6 - 21123\sin(v)\,s^6v^8\end{aligned}$$

$$
\begin{aligned}
&+ \quad 202002\cos(v)s^8v^5 - 173838\cos(v)s^4v^9 \\
&+ \quad 173838\sin(v)s^8v^4 - 1564542\sin(v)s^4v^8 \\
&- \quad 1111260\,s^8v^5 + 9868488\cos(v)s^8v^3 - 7087080\cos(v)s^2v^9 \\
&- \quad 21261240\sin(v)s^8v^2 + 425224800\,s^8v \\
&- \quad 63783720\sin(v)s^2v^8 - 2781408\,s^8v^3 \\
&+ \quad 170089920\cos(v)s^8v - 85044960\cos(v)v^9 \\
&- \quad 595314720\sin(v)s^8 - 765404640\sin(v)v^8 \\
\Psi_8(s,v) &= v^8(\cos(v)v + 9\sin(v)) \\
\Psi_9(s,v) &= 680359680\,v^9 - 695352\,s^8v^5 \\
&- \quad 42522480\,s^8v^3 - 680359680\,s^8v - 4694\,s^8v^7 \\
&- \quad 92605\cos(v)v^{15} - 277815\sin(v)v^{14} \\
&- \quad 347676\cos(v)v^{13} - 1738380\sin(v)v^{12} \\
&+ \quad 106306200\cos(v)v^{11} + 744143400\sin(v)v^{10} \\
&+ \quad 30511\sin(v)\cos(v)s^8v^6 - 277815\cos(v)s^8v^7 \\
&+ \quad 3824436\sin(v)\cos(v)s^8v^4 + 191351160\sin(v)\cos(v)s^8v^2 \\
&+ \quad 370420\cos(v)s^6v^9 - 3055965\sin(v)s^8v^6 \\
&+ \quad 3333780\sin(v)s^6v^8 + 4097364\cos(v)s^8v^5 \\
&+ \quad 695352\cos(v)s^4v^9 - 4519788\sin(v)s^8v^4 \\
&+ \quad 6258168\sin(v)s^4v^8 + 46561032\cos(v)s^8v^3 \\
&- \quad 141741600\cos(v)s^2v^9 + 531531000\sin(v)s^8v^2
\end{aligned}
$$

$$
\begin{aligned}
&- \ 1275674400 \sin(v) s^2 v^8 + 235020 (\cos(v))^2 s^8 v^5 \\
&- \ 1700899200 \cos(v) s^8 v + 2347 (\cos(v))^2 s^8 v^7 \\
&+ \ 10135608 (\cos(v))^2 s^8 v^3 + 2381258880 \sin(v) \cos(v) s^8 \\
&+ \ 695352 v^{13} - 340179840 (\cos(v))^2 v^9 \\
&+ \ 42522480 v^{11} + 4694 v^{15} \\
&+ \ 7041 \cos(v) \sin(v) v^{14} + 1738380 \cos(v) \sin(v) v^{12} \\
&+ \ 148828680 \cos(v) \sin(v) v^{10} + 3061618560 \cos(v) \sin(v) v^8 \\
&- \ 2347 (\cos(v))^2 v^{15} - 347676 (\cos(v))^2 v^{13} \\
&- \ 21261240 (\cos(v))^2 v^{11}.
\end{aligned}
$$

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