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Four–Stages Twelfth Algebraic Order Two–Step Method with Vanished Phase–Lag and its First and Second Derivatives for the Numerical Solution of the Schrödinger Equation

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Abstract

In this paper we introduce, for the fist time in the literature, a new four–stages symmetric two–step method of twelfth algebraic order. For the new family of methods we request the vanishing of the phase–lag and its first and second derivatives. We investigate how the vanishing of the phase–lag and its derivatives affect on the effectiveness of the finally produced new four–stages symmetric two-step method . We will study the following:

- the construction of the method,
- the computation of the local truncation error (LTE) of the new four–stages symmetric two–step method
- the analysis of the LTE when the produced method is applied to a test problem (which is the radial Schrödinger equation)

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- the comparison of the asymptotic formula of the LTE of the developed method (which is produced by the application of the new obtained four–stages symmetric two–step method to the test problem mentioned above) with the asymptotic formulae of the LTEs of other similar methods in the literature (comparative local truncation error analysis),
- the stability (interval of periodicity) of the new obtained four–stages symmetric two–step method . We mention that for the investigation of the stability of the new produced method we use a scalar test equation with frequency different than the frequency of the scalar test equation used for the phase–lag analysis (stability analysis),
- the examination of the effectiveness of the new obtained method applying it to two problems of the literature: (i) the resonance problem of the Schrödinger equation and (ii) the coupled differential equations arising from the Schrödinger equation.

Finally, it will be proved that this new introduced family of methods is very efficient for the numerical solution of the Schrödinger equation and related initial-value or boundary-value problems with periodical and /or oscillating solutions . We mention here that the proposed method is an improvement of the recent developed methods in [1], [2] and [3]. .

1. INTRODUCTION

In this paper we will present, for the first time in the literature, family of four–stages symmetric two–step method of twelfth algebraic order. These methods are developed for the efficient numerical solution of the Schrödinger equation and related problems . We will examine the effectiveness of the new obtained method applying it on the numerical solution of

1. the radial time independent Schrödinger equation and
2. the coupled differential equation arising from the Schrödinger equation.

We note that the efficient approximate solution of the Schrödinger equation and related problems is very important on Computational Chemistry (see [4] and references therein). The most of the quantum chemical calculations contain the Schrödinger equation as a very critical part of them . We also note that the Schrödinger's equation can be solved only numerically for more than one particle. Solving efficiently the Schrödinger equation we can

1. compute important molecular properties (for example vibrational energy levels and wave functions of systems) and
2. give a substantial presentation of the molecule's electronic structure (see for more details in [5–8]).

We will improve the methods developed for the first time in the literature in [1] and [2] by introducing, for the first time in the literature, a higher algebraic order family of methods . More specifically while the methods developed in [1] and [2] are of tenth algebraic order, the family of methods introduced in this paper is of twelfth algebraic order. At the same time we will also give the conditions in order to developed method to have vanished the phase–lag and its first and second derivatives.

We will study the numerical solution of special second order initial value problems with periodical and/or oscillating solution of the form:

$$p''(x) = f(x,p), \;\; p(x_0) = p_0 \;\; and \;\; p'(x_0) = p'_0 \,. \tag{1}$$

In more details, we will study the systems of ordinary differential equations of second order in which the first derivative p' does not appear explicitly and which have solutions with periodical and/or oscillating behavior.

2. PHASE–LAG ANALYSIS OF SYMMETRIC $2\,m$ MULTISTEP METHODS

The following algorithm describes the necessary steps for the phase–lag analysis of symmetric multistep methods :

1. Selection and presentation of the multistep finite difference method for the the approximate solution of the initial value problem (1). The method has the general form
$$\sum_{i=-m}^{m} c_i \, p_{n+i} = h^2 \sum_{i=-m}^{m} b_i \, f(x_{n+i}, p_{n+i}) \,. \tag{2}$$

2. Definition of the area of integration, which is called integration interval, and definition of the stepsize (step length) of integration

   The above presented multistep method can be used for the approximate integration of the initial value problem (1) following the procedure:

   - We consider as integration interval for the numerical solution of the initial value problem (1) the interval $[a,b]$.
   - The above mentioned integration interval $[a,b]$ is divided into m equally spaced intervals i.e., $\{x_i\}_{i=-m}^{m} \in [a,b]$.

- Based on above step we define the quantity h by $h = |x_{i+1} - x_i|, \quad i = 1 - m(1)m - 1$. This quantity is called **the stepsize of integration** or **the step length of integration** .

3. Definition of a subclass of $2\,m$-step methods which is called symmetric $2\,m$-step methods,

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

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

4. Definition of the algebraic order q of a Multistep Method presented by (2)

   Remark 2 *The Multistep Method (2) is associated with the following linear operator*

$$L(x) = \sum_{i=-m}^{m} c_i\, p(x + ih) - h^2 \sum_{i=-m}^{m} b_i\, p''(x + ih) \tag{3}$$

   where $p \in C^2$.

   Definition 2 [9] The multistep method (2) is called algebraic of order q if the associated linear operator L given by (3) vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{q+1}$.

5. Definition of the terms: scalar test equation, difference equation, characteristic equation for a symmetric $2\,m$-step method

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

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

   we have the following difference equation:

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

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

The difference equation (5) is associated with the following characteristic equation :

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

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

Definition 3 [10] *A symmetric $2\,m$-step method with characteristic equation given by (6) is said to have an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots $\lambda_i, i = 1(1)2\,m$ of Eq. (6) satisfy:*

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

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

Definition 4 [11], [12] *For any method corresponding to the characteristic equation (6), the phase–lag is defined as the leading term in the expansion of*

$$t = v - \theta(v)\,. \quad (8)$$

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

Definition 5 [13] *A method is called* **phase-fitted** *if its phase–lag is equal to zero.*

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

Theorem 1 [11] *The symmetric $2\,m$-step method with characteristic equation given by (6) has phase–lag order s and phase–lag constant c given by*

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

Remark 3 *The direct computation of the the phase–lag of any symmetric* $2\,m$*-step method can be done using the above mentioned formula .*

Remark 4 *A symmetric two-step method has phase–lag order* s *and phase–lag constant* c *given by:*

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

3. THE NEW TWELFTH ALGEBRAIC ORDER FOUR–STAGES SYMMETRIC TWO–STEP METHOD WITH VANISHED PHASE–LAG AND ITS FIRST AND SECOND DERIVATIVES

Let us consider the family of methods

$$\begin{aligned}
\widehat{p}_n &= p_n - a_0\,h^2\left(f_{n+1} - 2\,f_n + f_{n-1}\right) - 2\,a_1\,h^2\,f_n \\
\tilde{p}_n &= p_n - a_2\,h^2\left(f_{n+1} - 2\,\widehat{f}_n + f_{n-1}\right) \\
\bar{p}_n &= p_n - a_3\,h^2\left(f_{n+1} - 2\,\tilde{f}_n + f_{n-1}\right) \\
p_{n+1} + a_4\,p_n + p_{n-1} &= h^2\left[b_1\,\left(f_{n+1} + f_{n-1}\right) + b_0\,\bar{f}_n\right]
\end{aligned} \tag{11}$$

where $f_i = p''\left(x_i, p_i\right), i = -2(1)2$, $\widehat{f}_n = p''\left(x_n, \widehat{p}_n\right)$, $\tilde{f}_n = p''\left(x_n, \tilde{p}_n\right)$, $\bar{f}_n = p''\left(x_n, \bar{p}_n\right)$ and a_j, $j = 0(1)4$ and b_i, $i = 0, 1$ are free parameters.

3.1. Development of the Method

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

$$a_0 \,=\, -\frac{27}{3200},\; a_1 \,=\, \frac{3}{32},\; a_2 \,=\, -\frac{10}{693},\; a_4 \,=\, -2\,. \tag{12}$$

Requiring the above symmetric four–stages two-step method (11) with coefficient (12) to have vanished phase–lag and its first and second derivatives, the following system of equations is obtained :

$$\text{Phase}--\text{Lag(PL)} \,=\, \frac{T_0}{T_1} = 0 \tag{13}$$

$$\text{First Derivative of the Phase} - -\text{Lag} \;=\; \frac{T_2}{T_1^2} = 0 \tag{14}$$

$$\text{Second Derivative of the Phase} - -\text{Lag} \;=\; \frac{T_3}{T_1^3} \tag{15}$$

where T_j, $j = 0(1)3$ are given in the Appendix A.

Solving the above system of equations (13)–(15), we obtain the coefficients of the new proposed four–stages symmetric two–step method :

$$a_3 \;=\; 2310\,\frac{T_4}{T_5} \quad , \quad b_0 \;=\; -24\,\frac{T_6}{T_7}$$

$$b_1 \;=\; -12\,\frac{T_8}{T_7} \tag{16}$$

where T_j, $j = 4(1)8$ are given in the Appendix B.

For the above mentioned formulae given by (16) and in the case of heavy cancelations for some values of $|v|$, the Taylor series expansions given in the Appendix C should be used .

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

We present the new method (11) with the coefficients given by (16) and their Taylor series expansions given in Appendix C with the symbol: $NM4SH2DV$. The local truncation error of this method is given by:

$$LTE_{NM4SH2DV} = \frac{307}{186810624000}\,h^{14}\left(p_n^{(14)} - 15\,\phi^8\,p_n^{(6)} - 24\,\phi^{10}\,p_n^{(4)} - 10\phi^{12}\,p_n^{(2)}\right) + O\left(h^{16}\right). \tag{17}$$

4. COMPARATIVE ERROR ANALYSIS

For the investigation on the local truncation error analysis we use the the test problem:

$$p''(x) \;=\; (V(x) - V_c + G)\;p(x) \tag{18}$$

where

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

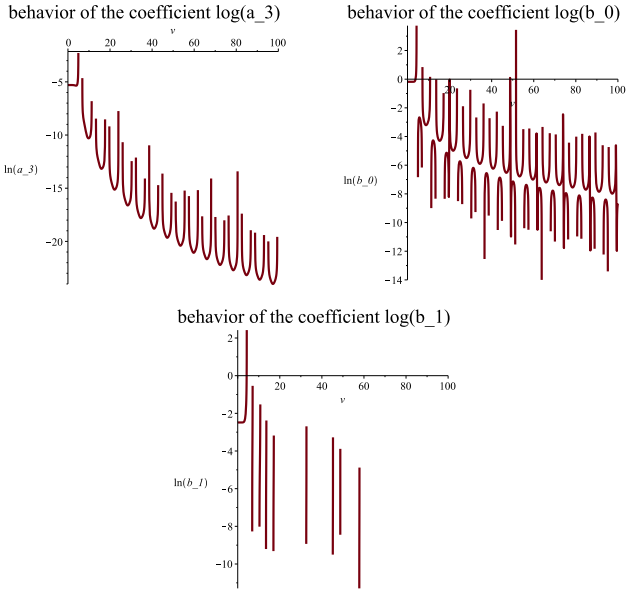

Figure 1: Behavior of the coefficients of the new obtained method given by (16) for several values of $v = \phi\, h$.

- E is the energy.

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

We study the following methods :

4.1. Classical Method (i.e., Method (11) with Constant Coefficients)

$$LTE_{CL} = \frac{307}{186810624000}\, h^{14}\, p_n^{(14)} + O\left(h^{16}\right). \tag{19}$$

4.2. Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in Section 3

$$LTE_{NM4SH2DV} = \frac{307}{186810624000}\, h^{14} \left(p_n^{(14)} - 15\,\phi^8\, p_n^{(6)} - 24\,\phi^{10}\, p_n^{(4)} - 10\phi^{12}\, p_n^{(2)} \right) + O\left(h^{16}\right). \tag{20}$$

We use the following procedure

- In order to calculate the formulae of the Local Truncation Errors which are based on the the test problem (18) which we use for our error analysis, the calculation of the derivatives of the function which are included in the formulae of the Local Truncation Errors is necessary . Some of the expressions of the above mentioned derivatives which are used in these formulae are presented in the Appendix D.
- The above calculated expressions of the derivatives (some of which are presented in the Appendix D), are then substituted in the formulae of the Local Truncation Error given in (19) and (20). As a result of the substitution we have that the new formulae of the Local Truncation Errors are dependent from the quantity G and the energy E.
- We base our study on the two cases for the parameter G :

  1. **The Potential and the Energy are closed each other.** Consequently $G = V_c - E \approx 0$ i.e., the value of the parameter G is approximately equal to zero. We note here that the general form of the Local Truncation Errors is given by:

$$LTE = h^{14} \sum_{k=0}^{j} B_k \, G^k \tag{21}$$

  where B_k are constant numbers (classical case) or polynomials of v and $G = V_c - E$ (frequency dependent cases).

  Remark 5 *In the case $G = V_c - E \approx 0$, all the terms of the expressions of the local truncation error with terms of several power of G are approximately equal to zero, i.e., $G^k \approx 0$, $k = 1, 2, 3, \cdots$.*

  Remark 6 *In the case $G = V_c - E \approx 0$, we take into account only the terms of the expressions of the local truncation error for which the power of G is equal to zero (i.e., the terms of G^0) i.e., the terms which are free from G are considered. The reason is the previous remark .*

  In the case $G = V_c - E \approx 0$ the local truncation error is equal to the non zero terms of the expressions of the local truncation errors (i.e. the local truncation error is equal to the expressions with free from G terms). For this reason the

local truncation error for the classical method (constant coefficients) and the local truncation error for the method with vanished the phase–lag and its first and second derivatives are the same since the expressions which are free from G in the local truncation errors in this case are the same. Therefore, for these values of G, the methods are of comparable accuracy.

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

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

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

4.4. Classical Method

$$LTE_{CL} = \frac{307}{186810624000} h^{14} \left(p(x)\ G^7 + \cdots \right) + O\left(h^{16}\right). \tag{22}$$

4.5. Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in Section 3

$$LTE_{NM4SH2DV} = \frac{307}{2335132800} h^{14} \left(\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x) \right) p(x)\ G^5 + \cdots \right) + O\left(h^{16}\right). \tag{23}$$

From the above mentioned analysis we have the following theorem:

Theorem 2

- *Classical Method (i.e., the method (11) with constant coefficients): For this method the error increases as the seventh power of G.*
- *High Algebraic Order Two–Step Method with Vanished Phase–lag and its First and Second Derivatives developed in Section 3: For this method the error increases as the fifth power of G.*

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

5. STABILITY ANALYSIS

The study of the stability properties of the new obtained method is based on the scalar test equation:

$$p'' = -\omega^2 \, p \, . \tag{24}$$

Remark 7 *The frequency of the scalar test equation of the phase–lag analysis* (ϕ) *– studied above – is different with the frequency of the scalar test equation used for the stability analysis* (ω) *i.e.,* $\omega \neq \phi$.

If we apply the four–stages symmetric two–step method produced in this paper to the scalar test equation (24) we obtain the following difference equation:

$$A_1 \, (s, v) \; (p_{n+1} + p_{n-1}) + A_0 \, (s, v) \; p_n = 0 \tag{25}$$

where

$$\begin{aligned} A_1 \, (s, v) &= 1 + b_1 \, s^2 + a_3 \, b_0 \, s^4 - 2 \, a_2 \, a_3 \, b_0 \, s^6 + 4 \, a_0 \, a_2 \, a_3 \, b_0 \, s^8 \\ A_0 \, (s, v) &= -2 + b_0 \, s^2 - 2 \, a_3 \, b_0 \, s^4 + 4 \, a_2 \, a_3 \, b_0 \, s^6 + 8 \, a_2 \, a_3 \, b_0 \; (a_1 - a_0) \; s^8 \end{aligned} \tag{26}$$

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

Substituting the coefficients b_j, $j = 0, 1$, a_i, $i = 0(1)4$ and b_0 given by (12) and (16) into the formulae (26) we obtain:

$$A_1 \, (s, v) = \frac{T_9}{T_{10}} \quad , \quad A_0 \, (s, v) \; = \; 2 \, \frac{T_{11}}{T_{10}} \tag{27}$$

where

$$\begin{aligned} T_9 &= -324 \, \cos (v) \sin (v) \, s^2 v^6 - 4800 \, \cos (v) \sin (v) \, s^2 v^4 + 110880 \, \cos (v) \sin (v) \, s^2 v^2 \\ &+ 55440 \, \sin (v) \cos (v) \, v^4 - 166320 \, \cos (v) \sin (v) \, s^4 + 55440 \, \cos (v) \, s^4 v \end{aligned}$$

$$
\begin{aligned}
&+ \; 27\cos(v)\,s^8v + 887040\cos(v)\,s^2v + 55440\,(\cos(v))^2\,s^4v + 4800\sin(v)\,s^2v^4 \\
&- \; 54\,s^8v - 6096\,(\cos(v))^2\,s^2v^5 - 1008\cos(v)\,s^2v^7 - 149280\,(\cos(v))^2\,s^2v^3 \\
&+ \; 216\,s^2v^7 - 3200\,s^6v - 6096\,s^2v^5 - 110880\,s^4v + 183360\,s^2v^3 \\
&- \; 443520\,s^2v - 443520\,(\cos(v))^2\,s^2v + 405\cos(v)\sin(v)\,v^8 - 81\cos(v)\sin(v)\,s^8 \\
&+ \; 81\sin(v)\,s^8 - 4905\sin(v)\,v^8 + 3200\cos(v)\,v^7 + 1600\cos(v)\,s^6v \\
&+ \; 12192\cos(v)\,s^2v^5 + 1600\,(\cos(v))^2\,s^6v - 110880\,v^5 + 55440\,(\cos(v))^2\,v^5 \\
&+ \; 55440\cos(v)\,v^5 - 55440\sin(v)\,v^4 - 110880\sin(v)\,s^2v^2 + 81\,(\cos(v))^2\,v^9 \\
&+ \; 981\cos(v)\,v^9 + 3200\,(\cos(v))^2\,v^7 + 27\,(\cos(v))^2\,s^8v - 108\,(\cos(v))^2\,s^2v^7 \\
&- \; 6400\,v^7 + 8424\sin(v)\,s^2v^6 - 162\,v^9 - 34080\cos(v)\,s^2v^3 + 4800\sin(v)\,s^6 \\
&- \; 9600\sin(v)\,v^6 + 166320\sin(v)\,s^4 - 4800\cos(v)\sin(v)\,s^6 \\
&+ \; 9600\cos(v)\sin(v)\,v^6 \\
T_{10} \;=\; & v^4\Big(81\,(\cos(v))^2\,v^5 + 405\sin(v)\cos(v)\,v^4 + 981\cos(v)\,v^5 \\
&- \; 4905\sin(v)\,v^4 + 3200\,(\cos(v))^2\,v^3 - 162\,v^5 + 9600\sin(v)\cos(v)\,v^2 \\
&+ \; 3200\cos(v)\,v^3 - 9600\sin(v)\,v^2 + 55440\,(\cos(v))^2\,v \\
&- \; 6400\,v^3 + 55440\sin(v)\cos(v) + 55440\cos(v)\,v - 55440\sin(v) - 110880\,v\Big) \\
T_{11} \;=\; & -4176\cos(v)\sin(v)\,s^2v^6 + 4800\cos(v)\sin(v)\,s^2v^4 - 110880\cos(v)\sin(v)\,s^2v^2 \\
&- \; 55440\sin(v)\cos(v)\,v^4 + 166320\cos(v)\sin(v)\,s^4 - 55440\cos(v)\,s^4v - 327\cos(v)\,s^8v \\
&+ \; 443520\cos(v)\,s^2v - 55440\,(\cos(v))^2\,s^4v - 4800\sin(v)\,s^2v^4 + 654\,s^8v \\
&+ \; 38400\,(\cos(v))^3\,s^2v^3 + 443520\,(\cos(v))^3\,s^2v + 1296\,(\cos(v))^3\,s^2v^5 \\
&- \; 12192\,(\cos(v))^2\,s^2v^5 + 1308\cos(v)\,s^2v^7 + 34080\,(\cos(v))^2\,s^2v^3 \\
&- \; 816\,s^2v^7 + 3200\,s^6v - 9600\,s^2v^5 + 110880\,s^4v - 221760\,s^2v^3 - 887040\,(\cos(v))^2\,s^2v \\
&- \; 405\cos(v)\sin(v)\,v^8 + 981\cos(v)\sin(v)\,s^8 - 981\sin(v)\,s^8 \\
&+ \; 4905\sin(v)\,v^8 - 3200\cos(v)\,v^7 - 1600\cos(v)\,s^6v + 20496\cos(v)\,s^2v^5 \\
&- \; 1600\,(\cos(v))^2\,s^6v + 110880\,v^5 - 55440\,(\cos(v))^2\,v^5 - 55440\cos(v)\,v^5 \\
&+ \; 55440\sin(v)\,v^4 + 110880\sin(v)\,s^2v^2 - 81\,(\cos(v))^2\,v^9 - 981\cos(v)\,v^9 \\
&- \; 3200\,(\cos(v))^2\,v^7 - 327\,(\cos(v))^2\,s^8v + 408\,(\cos(v))^2\,s^2v^7 \\
&+ \; 6400\,v^7 - 3924\sin(v)\,s^2v^6 + 162\,v^9 + 149280\cos(v)\,s^2v^3 - 4800\sin(v)\,s^6 \\
&+ \; 9600\sin(v)\,v^6 - 166320\sin(v)\,s^4 + 4800\cos(v)\sin(v)\,s^6 - 9600\cos(v)\sin(v)\,v^6\,.
\end{aligned}
$$

Definition 6 *(see* [10]*) A multistep method is called P-stable if its interval of periodicity is equal to* $(0, \infty)$.

Definition 7 *A multistep method is called singularly almost P-stable if its interval of periodicity is equal to* $(0, \infty) - S$ [2].

Remark 8 *The term singularly almost P-stable method is used in the cases when the frequency of the scalar test equation for the phase–lag analysis is equal with the frequency of the scalar test equation for the stability analysis, i.e.,* $\omega = \phi$.

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

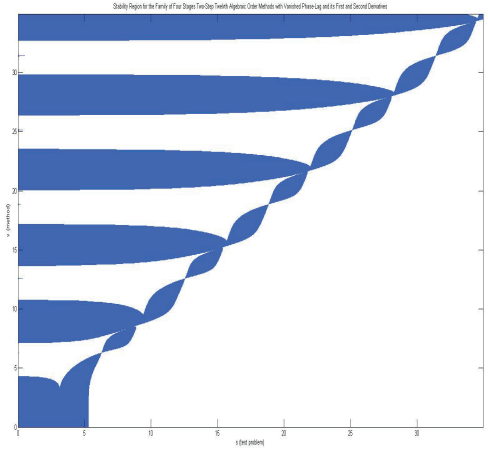

Figure 2: $s-v$ plane of the new obtained symmetric four–stages two–step twelfth algebraic order method with vanished phase–lag and its first and second derivatives.

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

1. *The shadowed area denotes where the method is stable,*

2. *The white area denotes the region where the method is unstable.*

Remark 10 *The observation of* **the surroundings of the first diagonal of the** $s - v$ **plane** *is requested in the cases of problems for which the models require only one frequency*

[2] where S is a set of distinct points

per differential equation in the specific model. This is because in these cases the frequency of the scalar test equation used for the phase–lag analysis is equal with the frequency of the scalar test equation used for the stability analysis. One can find many problems in Sciences, Engineering and Technology for which their mathematical models are of the form described above (for example the time independent Schrödinger equation and the coupled equations arising from the Schrödinger equation).

Based on the above investigation , we study the case where the frequency of the scalar test equation used for the phase–lag analysis is equal with the frequency of the scalar test equation used for the stability analysis , i.e., we study the case where $s = v$ (equivalent with $\omega = \phi$) (i.e., on the the $s - v$ plane see the surroundings of the first diagonal). Based on the above mentioned investigation we found that the interval of periodicity in the case $s = v$ is equal to: $(0, 29)$.

Based on the above we have the following theorem:

Theorem 3 *The method developed in section 3:*

- *is of four stages*
- *is of twelfth algebraic order,*
- *has the phase–lag and its first and second derivatives equal to zero*
- *has an interval of periodicity equals to:* $(0, 29)$*, when the frequency of the scalar test equation used for the phase–lag analysis is equal with the frequency of the scalar test equation used for the stability analysis*

6. NUMERICAL RESULTS

The study of the efficiency of the new obtained method is presented in this section. More specifically, we will study the application of the new developed method on two problems :

- the numerical solution of the radial time–independent Schrödinger equation and
- the numerical solution of coupled differential equations of the Schrödinger type

6.1. Radial Time–Independent Schrödinger Equation

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

$$p''(r) = [l(l+1)/r^2 + V(r) - k^2]\, p(r). \tag{28}$$

where

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

The problem (28)) belongs to the boundary value problems category and consequently we must define the boundary conditions . The value of the function p on the initial point of integration (which is called the initial value) gives us the first boundary condition :

$$p(0) = 0$$

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

Our new developed methods belongs in the category of methods with frequency dependent coefficients. Consequently, we must define the parameter ϕ of the coefficients of the new produced method ($v = \phi\, h$), in order to be possible to determine the coefficients. For the radial Schrödinger equation and for the case $l = 0$ the parameter ϕ is defined by the relation :

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

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

6.1.1. Woods–Saxon Potential

Since in the model of radial Schrödinger equation the definition of a potential is requested, we define for our numerical tests as potential, the well known Woods–Saxon potential.

The model of Wood–Saxon potential is given by :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{29}$$

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

In Figure 3 we present the behavior of the Woods–Saxon potential .

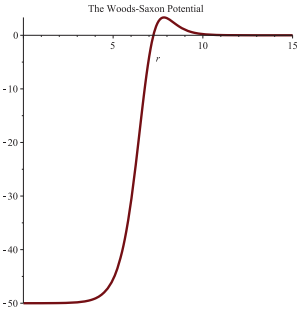

Figure 3: The Woods–Saxon potential.

During the integration we use, for the Woods–Saxon potential, approximate values in some critical points. This methodology proposed by Ixaru et al. ([14] [16]). Use these approximations we can define the value of the parameter ϕ.

We choose ϕ as follows (see for details [15] and [16]) :

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

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

6.1.2. Radial Schrödinger Equation – The Resonance Problem

The first numerical test which we will solve using the new developed method is the numerical solution of the radial time independent Schrödinger equation (28) using as potential the Woods-Saxon potential (29) .

Since the interval of integration of the above mentioned problem is equal to $(0,\infty)$ i.e. is an infinite interval of integration i.e., it is necessary to be approximated with a finite one, in order to be possible to be solved numerically . Therefore, for our numerical test we will use the integration interval $r \in [0,15]$ which is a finite one . For our numerical test we will use the domain of energies : $E \in [1,1000]$.

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

$$p''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) p(r) = 0 \tag{30}$$

The above reduced model (30) has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively.

Therefore, the solution of equation (28) (when $r \to \infty$), has the asymptotic form

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

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

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

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. As we mentioned above in our numerical test, the problem is treated as an initial–value problem, and therefore we need p_j , $j = 0(1)4$ in order to be possible the application of our new six–step method. The value p_0 is obtained from the initial condition . The values p_i, $i = 1(1)4$ are obtained by using high order Runge–Kutta–Nyström methods (see [17] and [18]). With these starting (initial) values, we evaluate at r_2 of the asymptotic region the phase shift δ_l.

In the case of positive energies the problem described above is called resonance problem . This problem can be occurred with two forms :

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

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

The boundary conditions for this problem are:

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

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

- the eighth order multi–step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT8**;
- the tenth order multi–step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10**;
- the twelfth order multi–step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT12**;
- the fourth algebraic order method of Chawla and Rao with minimal phase–lag [20], which is indicated as **Method MCR4**;
- the exponentially–fitted method of Raptis and Allison [21], which is indicated as **Method RA** ;
- the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase–lag [22], which is indicated as **Method MCR6**;
- the Phase-Fitted Method (Case 1) developed in [9], which is indicated as **Method NMPF1**;
- the Phase-Fitted Method (Case 2) developed in [9], which is indicated as **Method NMPF2**;
- the Method developed in [23] (Case 2), which is indicated as **Method NMC2**;

- the method developed in [23] (Case 1), which is indicated as **Method NMC1**;
- the Two-Step Hybrid Method developed in [1], which is indicated as **Method NM2SH2DV**;
- the new obtained Four Stages Symmetric Two–Step method developed in Section 3, which is indicated as **Method NM4SH2DV**

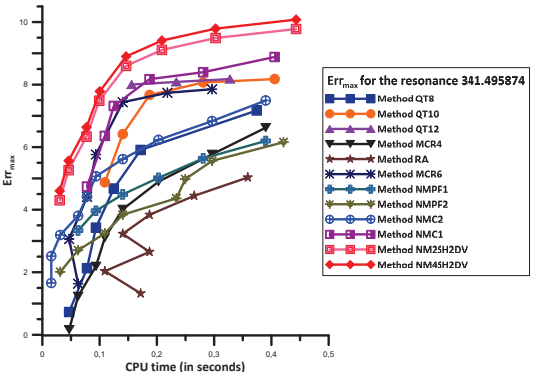

Figure 4: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

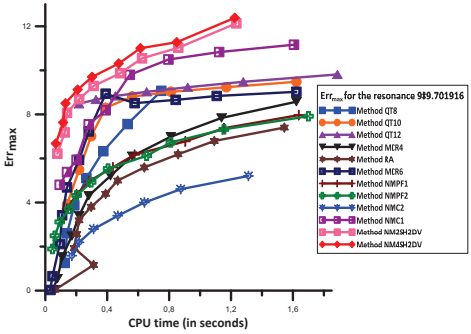

Figure 5: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

Using the well known two-step method of Chawla and Rao [22] with small step size for the integration, we compute the reference values . The procedure which we follow consists of the numerical computation of the eigenenergies and after that the comparison of the numerically computed eigenenergies with the reference values. In Figures 4 and 5, we present the maximum absolute error $Err_{max} = |\log_{10}(Err)|$ where

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

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

6.1.3 Remarks on the Numerical Results for the Radial Schrödinger Equation

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

1. The tenth algebraic order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase–lag [20], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase–lag [22], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.

2. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10**

3. The Phase-Fitted Method (Case 1) developed in [9], which is indicated as **Method NMPF1** is more efficient than the exponentially-fitted method of Raptis and Allison [21] and the Phase-Fitted Method (Case 2) developed in [9], which is indicated as **Method NMPF2**

4. The Method developed in [23] (Case 2), which is indicated as **Method NMC2** is more efficient than the exponentially-fitted method of Raptis and Allison [21], which is indicated as **Method MRA** and the Phase-Fitted Method (Case 2) developed in [9], which is indicated as **Method NMPF2** and the Phase-Fitted Method (Case 1) developed in [9], which is indicated as **Method NMPF1**

5. The Method developed in [23] (Case 1), which is indicated as **Method NMC1**, is more efficient than all the other methods mentioned above.

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

7. Finally, the new Four–Stages Twelfth Algebraic Order Method developed in Section 3, which is indicated as **Method NM4SH2DV**, is the most efficient one.

6.2. Error Estimation

We will study the numerical solution of couple differential equations arising from the Schrödinger equation. In order to achieve this, we will use a variable–step algorithm . In order to apply the variable–step schemes on the numerical solution of systems of differential equations, it is necessary to define the estimation of the local truncation error (LTE) . Several methodologies and several algorithms of variable–step form for the numerical solution of systems of differential equations which have been developed over the last decades can be found in the literature (see for example [9]– [70]).

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

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

2. the fact that in the case of use of a multistep method with the maximum possible algebraic order, a better numerical solution for the problems with oscillatory or periodical solution is obtained .

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

obtained in the present paper - which is of twelfth algebraic order has vanished the phase-lag and its first and second derivatives. Based on the above, the local truncation error in y_{n+1}^L is estimated by

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

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

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

where q is the algebraic order of the method.

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

6.3. Coupled Differential Equations

Mathematical models consisting of coupled differential equations of the Schrödinger type can be found in many problems within

- quantum chemistry,
- material science,
- theoretical physics,
- atomic physics,
- physical chemistry and chemical physics,
- etc.

The close-coupling differential equations of the Schrödinger type can be written as :

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

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

The case in which all channels are open will be studied in this paper . Therefore, we have the following boundary conditions (see for details [24]):

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

$$p_{ij} \sim k_i \, x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} \, k_i \, x \, n_{li}(k_i x) \tag{31}$$

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

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

Defining a matrix K' and diagonal matrices M, N by (see for detailed analysis in [24]):

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

we find that the asymptotic condition (31) can be written as:

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

The close–coupling differential equations of the Schrödinger type express the mathematical model of the rotational excitation of a diatomic molecule by neutral particle impact which is an important real problem in quantum chemistry, theoretical physics, material science, atomic physics and molecular physics . In this mathematical model we have the following notations:

- The entrance channel is denoted (see for details in [24]) by the quantum numbers (j, l),
- The exit channels are denoted by (j', l'), and
- the total angular momentum by $J = j + l = j' + l'$.

The above notations leads to

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

where

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

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

The potential V is given by (see for details [24]):

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

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

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

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [25] 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 [26]). The boundary conditions are given by

$$p^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \tag{32}$$

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

where the relation of scattering S matrix with K matrix of (31) is given by

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

In order to compute the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles, we use an algorithm which consists of the numerical method for step-by-step integration from the initial value to matching points . We use for our numerical tests an algorithm which is analogous with the algorithm developed for the numerical tests of [24].

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

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

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

As is described in [24], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of **four, nine and sixteen coupled**

differential equations, respectively. Following the procedure obtained by Bernstein [26] and Allison [24] the potential is considered infinite for values of x less than some x_0. The wave functions then zero in this region and effectively the boundary condition (32) may be written as

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

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

- the Iterative Numerov method of Allison [24] which is indicated as **Method I**[3],
- the variable–step method of Raptis and Cash [27] which is indicated as **Method II**,
- the embedded Runge–Kutta Dormand and Prince method 5(4) [18] which is indicated as **Method III**,
- the embedded Runge–Kutta method ERK4(2) developed in Simos [28] 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 new developed embedded two–step method which is indicated as **Method VII** .

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

[3]We note here that Iterative Numerov method developed by Allison [24] 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 VII. acc=10^{-6}. Note that hmax is the maximum stepsize.

Method	N	hmax	RTC	MErr
Method I	4	0.014	3.25	1.2×10^{-3}
	9	0.014	23.51	5.7×10^{-2}
	16	0.014	99.15	6.8×10^{-1}
Method II	4	0.056	1.55	8.9×10^{-4}
	9	0.056	8.43	7.4×10^{-3}
	16	0.056	43.32	8.6×10^{-2}
Method III	4	0.007	45.15	9.0×10^{0}
	9			
	16			
Method IV	4	0.112	0.39	1.1×10^{-5}
	9	0.112	3.48	2.8×10^{-4}
	16	0.112	19.31	1.3×10^{-3}
Method V	4	0.448	0.20	1.1×10^{-6}
	9	0.448	2.07	5.7×10^{-6}
	16	0.448	11.18	8.7×10^{-6}
Method VI	4	0.448	0.15	3.2×10^{-7}
	9	0.448	1.40	4.3×10^{-7}
	16	0.448	10.13	5.6×10^{-7}
Method VII	4	0.448	0.08	6.4×10^{-8}
	9	0.448	1.04	7.6×10^{-8}
	16	0.448	9.12	8.5×10^{-8}

7. CONCLUSIONS

A family of twelfth algebraic order symmetric two–step methods, introduced for the first time in the literature, is studied in this paper. More specifically, we studied:

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

The theoretical analysis and numerical results given above, leads us to the conclusion that the new developed method is of high efficiency for the numerical solution of the radial Schrödinger equation and of the coupled differential equations arising from the Schrödinger equation .

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

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

$$
\begin{aligned}
T_0 &= 27\cos(v)\,v^8 b_0 a_3 - 327\,v^8 b_0 a_3 + 1600\cos(v)\,b_0 a_3 v^6 \\
&- 1600\,b_0 a_3 v^6 + 55440\cos(v)\,b_0 a_3 v^4 - 55440\,b_0 a_3 v^4 \\
&+ 55440\cos(v)\,v^2 b_1 + 27720\,v^2 b_0 + 55440\cos(v) - 55440 \\
T_1 &= 27\,v^8 b_0 a_3 + 1600\,b_0 a_3 v^6 + 55440\,b_0 a_3 v^4 + 55440\,v^2 b_1 + 55440 \\
T_2 &= -2993760\sin(v)\,v^{10} a_3 b_0 b_1 - 177408000\sin(v)\,v^8 a_3 b_0 b_1 \\
&- 6147187200\sin(v)\,v^6 a_3 b_0 b_1 - 6147187200\sin(v)\,b_0 a_3 v^4 \\
&- 86400\sin(v)\,v^{14} {a_3}^2 {b_0}^2 - 5553760\sin(v)\,v^{12} {a_3}^2 {b_0}^2 \\
&- 177408000\sin(v)\,v^{10} {a_3}^2 {b_0}^2 - 3073593600\sin(v)\,v^8 {a_3}^2 {b_0}^2
\end{aligned}
$$

$$
\begin{aligned}
&- \ 2993760\,\sin(v)\,v^8a_3b_0 - 177408000\,\sin(v)\,v^6a_3b_0 - 108773280\,v^9a_3b_0b_1\\
&- \ 354816000\,v^7a_3b_0b_1 - 6147187200\,v^5a_3b_0b_1\\
&- \ 729\,\sin(v)\,v^{16}{a_3}^2{b_0}^2 + 3073593600\,vb_0 + 6147187200\,vb_1\\
&- \ 6147187200\,\sin(v)\,v^2b_1 - 3073593600\,v^5a_3{b_0}^2 - 3073593600\,\sin(v)\,v^4{b_1}^2\\
&- \ 177408000\,v^7a_3{b_0}^2 - 960000\,v^{13}{a_3}^2{b_0}^2 - 66528000\,v^{11}{a_3}^2{b_0}^2\\
&- \ 4490640\,v^9a_3{b_0}^2 - 133056000\,v^7a_3b_0 - 3073593600\,\sin(v)\\
T_3 \ &= \ 340800058368000\,b_1 + 170400029184000\,b_0 - 170400029184000\,\cos(v)\\
&- \ 248961081600\,\cos(v)\,v^8b_0a_3 - 14753249280000\,\cos(v)\,b_0a_3v^6\\
&- \ 511200087552000\,\cos(v)\,b_0a_3v^4 - 121247280\,\cos(v)\,v^{16}{a_3}^2{b_0}^2\\
&- \ 14370048000\,\cos(v)\,v^{14}{a_3}^2{b_0}^2 - 923701363200\,\cos(v)\,v^{12}{a_3}^2{b_0}^2\\
&- \ 29506498560000\,\cos(v)\,v^{10}{a_3}^2{b_0}^2 - 51636372480000\,b_0a_3v^6\\
&- \ 511200087552000\,\cos(v)\,v^2b_1 - 1022400175104000\,v^2{b_1}^2 - 19683\,\cos(v)\,v^{24}{a_3}^3{b_0}^3\\
&- \ 340800058368000\,v^6a_3b_0{b_1}^2 - 170400029184000\,v^6a_3{b_0}^2b_1\\
&- \ 59012997120000\,v^8a_3b_0{b_1}^2 - 29506498560000\,\cos(v)\,v^8a_3b_0b_1\\
&- \ 1022400175104000\,\cos(v)\,v^6a_3b_0b_1 - 511200087552000\,\cos(v)\,v^8a_3b_0{b_1}^2\\
&- \ 497922163200\,\cos(v)\,v^{10}a_3b_0b_1 - 245887488000000\,v^6a_3b_0b_1\\
&- \ 4089600700416000\,v^4a_3b_0b_1 - 78893000524800\,v^8a_3b_0b_1\\
&+ \ 1022400175104000\,v^8{a_3}^2{b_0}^2b_1 - 29506498560000\,v^8a_3{b_0}^2b_1\\
&- \ 674740281600\,\cos(v)\,v^{16}{a_3}^3{b_0}^3 - 511200087552000\,\cos(v)\,v^{10}{a_3}^2{b_0}^2b_1\\
&- \ 14753249280000\,\cos(v)\,v^{10}a_3b_0{b_1}^2 - 29506498560000\,\cos(v)\,v^{12}{a_3}^2{b_0}^2b_1\\
&- \ 248961081600\,\cos(v)\,v^{12}a_3b_0{b_1}^2 - 14370048000\,\cos(v)\,v^{16}{a_3}^2{b_0}^2b_1\\
&- \ 923701363200\,\cos(v)\,v^{14}{a_3}^2{b_0}^2b_1 - 121247280\,\cos(v)\,v^{18}{a_3}^2{b_0}^2b_1\\
&- \ 30151953216000\,v^{10}a_3b_0{b_1}^2 - 1244805408000\,v^{10}a_3{b_0}^2b_1\\
&+ \ 88519495680000\,v^{10}{a_3}^2{b_0}^2b_1 - 27184334284800\,v^{12}{a_3}^2{b_0}^2b_1\\
&+ \ 129330432000\,v^{14}{a_3}^2{b_0}^2b_1 + 20558149920\,v^{16}{a_3}^2{b_0}^2b_1\\
&- \ 18466048000\,\cos(v)\,v^{18}{a_3}^3{b_0}^3 - 3499200\,\cos(v)\,v^{22}{a_3}^3{b_0}^3\\
&- \ 328607280\,\cos(v)\,v^{20}{a_3}^3{b_0}^3 - 511200087552000\,\cos(v)\,v^8{a_3}^2{b_0}^2\\
&- \ 170400029184000\,\cos(v)\,v^6{b_1}^3 - 511200087552000\,\cos(v)\,v^4{b_1}^2
\end{aligned}
$$

$$
\begin{aligned}
&+ \; 511200087552000\, v^8 {a_3}^2 {b_0}^3 - 511200087552000\, v^2 b_0 b_1 \\
&+ \; 64665216000\, v^{14} {a_3}^2 {b_0}^3 + 44259747840000\, v^{10} {a_3}^2 {b_0}^3 \\
&- \; 170400029184000\, \cos(v)\, v^{12} {a_3}^3 {b_0}^3 + 7445280000\, v^{18} {a_3}^3 {b_0}^3 \\
&- \; 11064936960000\, v^{14} {a_3}^3 {b_0}^3 + 848730960\, v^{16} {a_3}^2 {b_0}^3 \\
&+ \; 2083160217600\, v^{12} {a_3}^2 {b_0}^3 - 159667200000\, v^{16} {a_3}^3 {b_0}^3 \\
&+ \; 77760000\, v^{20} {a_3}^3 {b_0}^3 - 2044800350208000\, v^4 a_3 {b_0}^2 \\
&- \; 122943744000000\, v^6 a_3 {b_0}^2 - 33194810880000\, v^{10} {a_3}^2 {b_0}^2 \\
&+ \; 32332608000\, v^{14} {a_3}^2 {b_0}^2 + 372556800000\, v^{12} {a_3}^2 {b_0}^2 \\
&- \; 3485455142400\, v^8 a_3 {b_0}^2 - 14753249280000\, \cos(v)\, v^{14} {a_3}^3 {b_0}^3 .
\end{aligned}
$$

Appendix B: Formulae for the T_j, $j = 4(1)8$

$$
\begin{aligned}
T_4 &= -(\cos(v))^2 v + 3\sin(v)\cos(v) - \cos(v)\, v - 3\sin(v) + 2v \\
T_5 &= v\Big(-34\,(\cos(v))^2 v^6 + 348\sin(v)\cos(v)\, v^5 - 108\,(\cos(v))^3 v^4 - 109\cos(v)\, v^6 \\
&+ 327\, v^5 \sin(v) + 1016\,(\cos(v))^2 v^4 + 68\, v^6 - 400\sin(v)\cos(v)\, v^3 - 3200\,(\cos(v))^3 v^2 \\
&- 1708\cos(v)\, v^4 + 400\, v^3 \sin(v) - 2840\,(\cos(v))^2 v^2 + 800\, v^4 + 9240\sin(v)\cos(v)\, v \\
&- 36960\,(\cos(v))^3 - 12440\cos(v)\, v^2 - 9240\, v\sin(v) \\
&+ 73920\,(\cos(v))^2 + 18480\, v^2 - 36960\cos(v)\Big) \\
T_6 &= -34\,(\cos(v))^2 v^6 + 348\sin(v)\cos(v)\, v^5 - 108\,(\cos(v))^3 v^4 \\
&- 109\cos(v)\, v^6 + 327\, v^5 \sin(v) + 1016\,(\cos(v))^2 v^4 + 68\, v^6 - 400\sin(v)\cos(v)\, v^3 \\
&- 3200\,(\cos(v))^3 v^2 - 1708\cos(v)\, v^4 + 400\, v^3 \sin(v) - 2840\,(\cos(v))^2 v^2 \\
&+ 800\, v^4 + 9240\sin(v)\cos(v)\, v - 36960\,(\cos(v))^3 - 12440\cos(v)\, v^2 \\
&- 9240\, v\sin(v) + 73920\,(\cos(v))^2 + 18480\, v^2 - 36960\cos(v) \\
T_7 &= v^3\Big(81\,(\cos(v))^2 v^5 + 405\sin(v)\cos(v)\, v^4 + 981\cos(v)\, v^5 \\
&- 4905\sin(v)\, v^4 + 3200\,(\cos(v))^2 v^3 - 162\, v^5 + 9600\sin(v)\cos(v)\, v^2 \\
&+ 3200\cos(v)\, v^3 - 9600\sin(v)\, v^2 + 55440\,(\cos(v))^2 v \\
&- 6400\, v^3 + 55440\sin(v)\cos(v) + 55440\cos(v)\, v - 55440\sin(v) - 110880\, v\Big) \\
T_8 &= 9\,(\cos(v))^2 v^6 + 27\sin(v)\cos(v)\, v^5 + 84\cos(v)\, v^6 + 508\,(\cos(v))^2 v^4
\end{aligned}
$$

$$- \quad 702\,v^5\sin(v) - 18\,v^6 + 400\,\sin(v)\cos(v)\,v^3 - 1016\,\cos(v)\,v^4 + 12440\,(\cos(v))^2\,v^2$$

$$- \quad 400\,v^3\sin(v) + 508\,v^4 - 9240\,\sin(v)\cos(v)\,v + 2840\,\cos(v)\,v^2 + 36960\,(\cos(v))^2 + 9240\,v\sin(v)$$

$$- \quad 15280\,v^2 - 73920\,\cos(v) + 36960\,.$$

Appendix C: Taylor Series Expansion Formulae for the coefficients of the new obtained method given by (16)

$$\begin{aligned} a_3 &= \frac{1}{200} - \frac{307\,v^8}{10378368000} + \frac{196451\,v^{10}}{108972864000000} \\ &- \frac{332581\,v^{12}}{13693965981696000} + \frac{91937711\,v^{14}}{1707466383342720000000} \\ &+ \frac{2548739647\,v^{16}}{14342717620078848000000} - \frac{6709218476060123\,v^{18}}{3170038922563923048038400000000} + \cdots \end{aligned}$$

$$\begin{aligned} b_0 &= \frac{5}{6} - \frac{307\,v^{10}}{3891888000} + \frac{4229\,v^{12}}{313841848320} + \frac{28458503\,v^{14}}{1232456938352640000} \\ &+ \frac{3741611063\,v^{16}}{393400254722162688000} + \frac{1348174591\,v^{18}}{1835867855370092544000} + \cdots \end{aligned}$$

$$\begin{aligned} b_1 &= \frac{1}{12} + \frac{307\,v^{10}}{7783776000} + \frac{4643\,v^{12}}{3138418483200} + \frac{11793247\,v^{14}}{246491387670528000} \\ &+ \frac{227673443\,v^{16}}{157360101888865075200} - \frac{701821793\,v^{18}}{3671735710740185088000} + \cdots . \end{aligned}$$

Appendix D: Formulae for the Derivatives of p_n

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

$$p_n^{(2)} = (V(x) - V_c + G)\,p(x)$$

$$p_n^{(3)} = \left(\frac{d}{dx}g(x)\right)p(x) + (g(x) + G)\,\frac{d}{dx}p(x)$$

$$p_n^{(4)} = \left(\frac{d^2}{dx^2}g(x)\right)p(x) + 2\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}p(x) + (g(x) + G)^2\,p(x)$$

$$p_n^{(5)} = \left(\frac{d^3}{dx^3}g(x)\right)p(x) + 3\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}p(x)$$

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

$$+ \quad 12\left(g\left(x\right)+G\right)^{2}\left(\frac{d}{dx}p\left(x\right)\right)\frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^{4}p\left(x\right)$$

...

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