**MATCH**
*Communications in Mathematical and in Computer Chemistry*

MATCH Commun. Math. Comput. Chem. **74** (2015) 609-644

ISSN 0340 - 6253

# Runge–Kutta Type Tenth Algebraic Order Two–Step Method with Vanished Phase–Lag and its First, Second and Third Derivatives

**Junyan Ma[a], Theodore E. Simos[1b]**

[a] *School of information engineering,Chang'an University, Xi'an, China,710064*
majy@chd.edu.cn

[b] *Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia*
*Laboratory of Computational Sciences, Department of Informatics and Telecommunications, Faculty of Economy, Management and Informatics, University of Peloponnese, GR-221 00 Tripolis, Greece*
tsimos.conf@gmail.com

## Abstract

In this paper we develop a new two-step tenth algebraic order Runge–Kutta type method. The vanishing of its phase–lag and its first, second and third derivatives is required for this method. The impact of the vanishing of the phase–lag and its first, second and third derivatives of the new obtained Runge–Kutta type two-step method on the effectiveness of the method is investigated in this paper. We will study (1) the construction of the method, (2) the its local truncation error (LTE) and the comparison of its LTE with LTE of other similar methods in the literature (comparative local truncation error analysis), (3) the stability (interval of periodicity) of the developed method. We mention that for the investigation of the stability of the new obtained method we will use a scalar test equation with frequency different than the frequency of the scalar test equation used for phase–lag analysis (stability analysis), (4) its efficiency with application on the resonance problem of the Schrödinger equation and on the coupled differential equations arising from the Schrödinger equation. It is will be shown the efficiency of this category

[1] Highly Cited Researcher, Active Member of the European Academy of Sciences and Arts
Active Member of the European Academy of Sciences Corresponding Member of European Academy of Arts, Sciences and Humanities

of methods on the approximate solution of the Schrödinger equation and related initial-value or boundary-value problems with solutions which have periodical and/or oscillating behavior. We note here that this method is an improvement of the recent developed method in [1]. We also introduce, for the first time in the literature, a new error estimation which is based on the number of derivatives which are vanished in a method. .

## 1. INTRODUCTION

In this paper we will investigate the improvement of the efficiency of a class of low computational cost high algebraic order two–step methods for the approximate solution of the Schrödinger equation and related problems. We will examine the efficiency of the new developed scheme on the numerical solution of both (1) the radial time independent Schrödinger equation and (2) the coupled differential equation arising from the Schrödinger equation. The numerical solution of this kind of problems are significantly important on Computational Chemistry (see [2] and references therein). The Schrödinger equation is an important part for most of the quantum chemical calculations. We note that the Schrödinger's equation can be solved only numerically for more than one particle. The Schrödinger equation offer us the possibility to compute important molecular properties (for example vibrational energy levels and wave functions of systems) and to give a detailed presentation of the molecule's electronic structure (see for more details in [3–6]).

In more details in this paper we improved the method developed for the first time in the literature in [1]. What we have improved is the number of derivatives of the phase–lag which will be vanished. In [1] we had vanished phase–lag and its first and second derivatives. In this paper we will have vanished phase–lag and its first, second and third derivatives. As we will prove in the analysis of the new method, this improvement optimizes the accuracy of the method. The method retains the benefits of the method developed in [1], i.e., we have a tenth order two–step method of only three stages. In this paper, for the first time in the literature, we introduce a new error estimation which is based on the number of derivatives which are vanished in a method.

We will study the numerical solution of special second order periodic and/or oscillatory initial value problems 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 for which the solutions have periodic and/or oscillating behavior.

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

In this section we will present the phase–lag analysis of symmetric multistep methods. The above mentioned analysis is based on the following algorithm:

- First we define the multistep finite difference method for the the approximate solution of the initial value problem (1). This method has the general form

$$\sum_{i=-m}^{m} c_i \, p_{n+i} = h^2 \sum_{i=-m}^{m} b_i \, f(x_{n+i}, p_{n+i}) \, . \tag{2}$$

- We define the area of integration, the integration interval and the stepsize of integration

  The above method can be used for the numerical integration of the initial value problem (1) following the procedure: (1) Let us consider that the integration of the initial value problem (1) is taken place within the interval $[a, b]$. (2) The interval $[a, b]$ is divided into $m$ equally spaced intervals i.e., $\{x_i\}_{i=-m}^{m} \in [a, b]$ . (3) Based on (2) we define the quantity $h$ by $h = |x_{i+1} - x_i|, \;\; i = 1 - m(1)m - 1$. This quantity is called **the stepsize of integration**.

- Definition of $2\,m$-step method and symmetric $2\,m$-step method,

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

  **Remark 2.** *The method (2) is called symmetric if and only if* $c_{-i} = c_i$ *and* $b_{-i} = b_i$, $i = 0(1)m$.

- Definition of the algebraic order $q$ of a Multistep Method (2)

  **Remark 3.** *The below mentioned linear operator*

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

  *is associated with the Multistep Method (2), where* $p \in C^2$.

**Definition 1.** [7] 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 $1, x, x^2, \ldots, x^{q+1}$.

- Definition of the scalar test equation, difference equation, characteristic equation of a symmetric $2\,m$-step method

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

  $$p'' = -\phi^2\, p$$

  we have the following difference equation:

  $$A_m(v)\, y_{n+m} + \cdots + A_1(v)\, y_{n+1} + A_0(v)\, y_n + A_1(v)\, y_{n-1} + \cdots + A_m(v)\, y_{n-m} = 0 \quad (4)$$

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

  The characteristic equation associated with (4) is given by:

  $$A_m(v)\, \lambda^m + \cdots + A_1(v)\, \lambda + A_0(v) + A_1(v)\, \lambda^{-1} + \cdots + A_m(v)\, \lambda^{-m} = 0\,. \quad (5)$$

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

  **Definition 2.** [8] *A symmetric $2\,m$-step method with characteristic equation given by (5) 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. (5) satisfy:*

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

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

  **Definition 3.** [9], [10] *For any method corresponding to the characteristic equation (5), the phase–lag is defined as the leading term in the expansion of*

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

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

  **Definition 4.** [11] *A method is called* **phase-fitted** *if its phase–lag is equal to zero.*

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

**Theorem 1.** [9] *The symmetric $2\,m$-step method with characteristic equation given by (5) has phase–lag order $q$ and phase–lag constant $c$ given by*

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

**Remark 4.** *The above mentioned formula can be used for a direct calculation of the the phase–lag of any symmetric $2\,m$-step method.*

**Remark 5.** *For the purpose of our paper , the symmetric two-step method has phase–lag order $q$ and phase–lag constant $c$ given by:*

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

## 3. THE NEW HIGH ALGEBRAIC ORDER RUNGE–KUTTA TWO–STEP METHOD WITH VANISHED PHASE–LAG AND ITS FIRST, SECOND AND THIRD DERIVATIVES

We consider the family of methods

$$\begin{aligned}
\widehat{p}_n &= p_n - a_0\,h^2\left(f_{n+1} - 2\,f_n + f_{n-1}\right) - 2\,a_1\,h^2\,f_n \\
\widetilde{p}_n &= p_n - a_2\,h^2\left(f_{n+1} - 2\,\widehat{f}_n + f_{n-1}\right) \\
p_{n+1} - 2\,p_n + p_{n-1} &= h^2\left[b_1\,(f_{n+1} + f_{n-1}) + b_0\,\widetilde{f}_n\right]
\end{aligned} \tag{6}$$

where $f_i = p''(x_i, p_i)\,, i = -2(1)2$ and $a_j$, $j = 0(1)2$ and $b_i$, $i = 0, 1$ are free parameters.

### 3.1. Construction of the Method

The family of methods (6), with:

$$b_1 = \frac{1}{12} \tag{7}$$

will be studied.

The request the above method (6) with coefficient (7) to have vanished phase–lag and its first, second and third derivatives leads to the following equations:

$$\text{Phase}--\text{Lag(PL)} = \frac{1}{2}\frac{T_0}{1+v^2\left(\frac{1}{12}+b_0a_2v^2\left(-2\,a_0v^2+1\right)\right)} = 0 \tag{8}$$

$$\text{First Derivative of the Phase}--\text{Lag} = \frac{T_1}{\left(24\,v^6a_0a_2b_0-12\,v^4a_2b_0-v^2-12\right)^2} = 0 \tag{9}$$

$$\text{Second Derivative of the Phase}--\text{Lag} = \frac{T_2}{\left(24\,v^6a_0a_2b_0-12\,v^4b_0a_2-v^2-12\right)^3} = 0 \tag{10}$$

$$\text{Third Derivative of the Phase}--\text{Lag} = \frac{T_3}{\left(24\,v^6a_0a_2b_0-12\,v^4b_0a_2-v^2-12\right)^4} = 0 \tag{11}$$

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

We obtain the coefficients of the new proposed Runge–Kutta type method by solving the above system of equations (8)–(11):

$$a_0 = \frac{1}{4}\frac{T_4}{T_5} \quad , \quad a_1 = \frac{1}{2}\frac{T_6}{T_5}$$

$$a_2 = \frac{T_7}{T_8} \quad , \quad b_0 = \frac{1}{6}\frac{T_9}{T_{10}} \tag{12}$$

where

$$\begin{aligned}
T_4 &= -\left(\cos\left(v\right)\right)^2v^6+4\,\sin\left(v\right)\cos\left(v\right)v^5+2\,v^5\sin\left(v\right)\\
&- 27\,\left(\cos\left(v\right)\right)^2v^4-2\,v^6+198\,\sin\left(v\right)\cos\left(v\right)v^3+6\,\cos\left(v\right)v^4\\
&+ 90\,\sin\left(v\right)v^3+216\,\left(\cos\left(v\right)\right)^2v^2-51\,v^4\\
&+ 864\,\sin\left(v\right)\cos\left(v\right)v-288\,\cos\left(v\right)v^2-864\,\sin\left(v\right)v\\
&+ 1152\,\left(\cos\left(v\right)\right)^2+72\,v^2-2304\,\cos\left(v\right)+1152\\
T_5 &= v^3\Big(-\left(\cos\left(v\right)\right)^2v^5-33\,\left(\cos\left(v\right)\right)^2v^3-2\,v^5\\
&+ 72\,\sin\left(v\right)\cos\left(v\right)v^2+36\,\sin\left(v\right)v^2-342\,\left(\cos\left(v\right)\right)^2v\\
&- 21\,v^3+1260\,\sin\left(v\right)\cos\left(v\right)-468\,\cos\left(v\right)v-1260\,\sin\left(v\right)+810\,v\Big)\\
T_6 &= \sin\left(v\right)\left(\cos\left(v\right)\right)^2v^5+4\,\sin\left(v\right)\cos\left(v\right)v^5\\
&-3\,\left(\cos\left(v\right)\right)^3v^4+33\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2v^3\\
&- 5\,v^5\sin\left(v\right)+150\,\sin\left(v\right)\cos\left(v\right)v^3-36\,\left(\cos\left(v\right)\right)^3v^2\\
&+ 9\,\cos\left(v\right)v^4+252\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2v-183\,\sin\left(v\right)v^3\\
&- 6\,v^4-504\,\sin\left(v\right)\cos\left(v\right)v-576\,\left(\cos\left(v\right)\right)^3+108\,\cos\left(v\right)v^2\\
&+ 252\,\sin\left(v\right)v+1728\,\left(\cos\left(v\right)\right)^2-72\,v^2-1728\,\cos\left(v\right)+576
\end{aligned}$$

$$
\begin{aligned}
T_7 &= -\left(\cos\left(v\right)\right)^2 v^5 - 33\,\left(\cos\left(v\right)\right)^2 v^3 - 2\,v^5 \\
&+ 72\,\sin\left(v\right)\cos\left(v\right) v^2 + 36\,\sin\left(v\right) v^2 - 342\,\left(\cos\left(v\right)\right)^2 v \\
&- 21\,v^3 + 1260\,\sin\left(v\right)\cos\left(v\right) - 468\,\cos\left(v\right) v - 1260\,\sin\left(v\right) + 810\,v \\
T_8 &= v^2\Big(2\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2 v^4 - \left(\cos\left(v\right)\right)^2 v^5 \\
&+ 4\,\sin\left(v\right)\cos\left(v\right) v^4 + 18\,\left(\cos\left(v\right)\right)^3 v^3 \\
&+ 42\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2 v^2 - 12\,\sin\left(v\right) v^4 \\
&- 3\,\left(\cos\left(v\right)\right)^2 v^3 - 2\,v^5 + 318\,\sin\left(v\right)\cos\left(v\right) v^2 \\
&+ 792\,\left(\cos\left(v\right)\right)^3 v - 36\,\cos\left(v\right) v^3 - 1512\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2 \\
&- 360\,\sin\left(v\right) v^2 + 21\,v^3 + 3024\,\sin\left(v\right)\cos\left(v\right) - 2376\,\cos\left(v\right) v \\
&- 1512\,\sin\left(v\right) + 1584\,v\Big) \\
T_9 &= 2\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2 v^4 - \left(\cos\left(v\right)\right)^2 v^5 \\
&+ 4\,\sin\left(v\right)\cos\left(v\right) v^4 + 18\,\left(\cos\left(v\right)\right)^3 v^3 \\
&+ 42\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2 v^2 - 12\,\sin\left(v\right) v^4 \\
&- 3\left(\cos\left(v\right)\right)^2 v^3 - 2\,v^5 + 318\,\sin\left(v\right)\cos\left(v\right) v^2 \\
&+ 792\left(\cos\left(v\right)\right)^3 v - 36\,\cos\left(v\right) v^3 - 1512\,\sin\left(v\right)\left(\cos\left(v\right)\right)^2 \\
&- 360\,\sin\left(v\right) v^2 + 21\,v^3 + 3024\,\sin\left(v\right)\cos\left(v\right) - 2376\,\cos\left(v\right) v \\
&- 1512\,\sin\left(v\right) + 1584\,v \\
T_{10} &= v^2\Big(\left(\cos\left(v\right)\right)^2 v^3 + 4\,\sin\left(v\right)\cos\left(v\right) v^2 \\
&+ 2\,\sin\left(v\right) v^2 + 3\,\left(\cos\left(v\right)\right)^2 v + 2\,v^3 + 30\,\sin\left(v\right)\cos\left(v\right) \\
&- 18\,\cos\left(v\right) v - 30\,\sin\left(v\right) + 15\,v\Big).
\end{aligned}
$$

For the case of heavy cancelations for some values of $|v|$ of the above formulae given by (12), the following Taylor series expansions should be used :

$$
\begin{aligned}
a_0 &= -\frac{1}{112} - \frac{25\,v^2}{56448} - \frac{133307\,v^4}{5811886080} \\
&- \frac{69304247\,v^6}{57832737177600} - \frac{7704074170729\,v^8}{122820633131192156160} \\
&- \frac{424924254408836447\,v^{10}}{12937434211507256969612697600} - \frac{1781825884550821929679\,v^{12}}{10360297316575011374584823808000} \\
&- \frac{475883814081135716010310 1\,v^{14}}{52842489257244514015842402136227840 0} \\
&- \frac{3053068352774426857128516431557\,v^{16}}{64743886057718152440546491314957619036160 00}
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{5908623971672750260142672306424 31\, v^{18}}{2392934028693262914202598319000833599576473600 0} + \cdots \\
\\
a_1 &= \frac{1}{8} - \frac{25\, v^2}{4928} + \frac{85093\, v^4}{507386880} \\
&+ \frac{1699153\, v^6}{13127113359360} + \frac{6126671263123\, v^8}{53612181128694988800} \\
&+ \frac{11458816343172173\, v^{10}}{22589170845488861360947 20} + \frac{961505735415818479\, v^{12}}{3546942747660290230950297600} \\
&+ \frac{25138205340936738083492 3\, v^{14}}{17743204573555850249519732097024000} \\
&+ \frac{20967657861887833041499596908 23\, v^{16}}{28261220104559510985952833510497373388880000} \\
&+ \frac{17642642415193348130540829878243\, v^{18}}{45414551959326935914818118545564474802176 0000} + \cdots \\
\\
a_2 &= \frac{1}{300} + \frac{v^2}{22176} - \frac{31991\, v^4}{36324288000} \\
&- \frac{474931\, v^6}{4068320256000} - \frac{78835746827\, v^8}{11502931424624640000} \\
&- \frac{270050471413\, v^{10}}{979129522864049356800} - \frac{250414854231396079\, v^{12}}{24057212376769692696576000000} \\
&- \frac{2469764922808486124 87\, v^{14}}{68168516990814601225017753600 0000} \\
&- \frac{1257362677400429139703 81\, v^{16}}{10307079769011167705222684344320000000} \\
&- \frac{4735873548315110229469 37\, v^{18}}{11543929341292507829849406465638400000 00} + \cdots \\
\\
b_0 &= \frac{5}{6} - \frac{v^{10}}{95800320} - \frac{4751\, v^{12}}{10461394944000} \\
&- \frac{220139\, v^{14}}{10545086103552000} - \frac{2683501739\, v^{16}}{3312844250291896320000} \\
&- \frac{137691778121\, v^{18}}{4880584083199261409280000} + \cdots
\end{aligned}
\tag{13}
$$

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

We give for the new method (6) with the coefficients given by (12)–(13) the symbol: $NM2SH3DV$. The local truncation error of this method is given by:

$$
LTE_{NM2SH3DV} = -\frac{1}{95800320}\, h^{12} \left( 4\, p_n^{(12)} + 15\, \phi^2\, p_n^{(10)} + 20\, \phi^4\, p_n^{(8)} - \phi^{10}\, p_n^{(2)} \right) + O\left(h^{14}\right).
$$

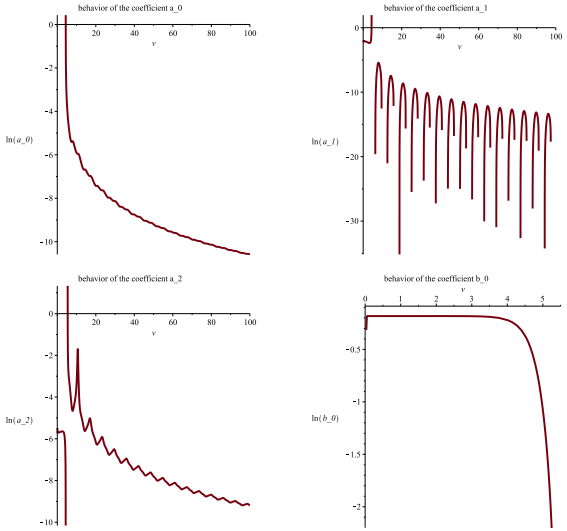


Figure 1: Behavior of the coefficients of the new proposed method given by (12) for several values of $v = \phi\, h$.

## 4. COMPARATIVE ERROR ANALYSIS

Our investigation on local truncation error analysis is based on the test problem:

$$p''(x) \;=\; (V(x) - V_c + G)\; p(x) \tag{14}$$

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
- $E$ is the energy.

We study the following methods :

### 4.1. Classical Method (i.e., Method (6) with Constant Coefficients)

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

### 4.2. Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in [1]

$$LTE_{ExplTwoStepPC} = -\frac{1}{23950080}\, h^{12} \left( p_n^{(12)} + 3\,\phi^2\, p_n^{(10)} + 3\,\phi^4\, p_n^{(8)} + \phi^6\, p_n^{(6)} \right) + O\left(h^{14}\right).$$

### 4.3. The New Proposed Method with Vanished Phase–Lag and Its First, Second and Third Derivatives Developed in Section 3

$$LTE_{NM2SH3DV} = -\frac{1}{95800320}\, h^{12} \left( 4\, p_n^{(12)} + 15\,\phi^2\, p_n^{(10)} + 20\,\phi^4\, p_n^{(8)} - \phi^{10}\, p_n^{(2)} \right) + O\left(h^{14}\right).$$

We follow the procedure

- As we mentioned in the beginning of this section, we base our study on the test problem (14). Based on this test problem we computer the derivatives which are necessary for the computation of the Local Truncation Errors. Some of the expressions of the derivatives used in these computations are presented in the Appendix B.

- The above computed expressions of the derivatives (some of which are presented in the Appendix B), are substituted in the formulae of the Local Truncation Error. Consequently, the resulting formulae of the Local Truncation Errors are dependent from the quantity $G$ and the energy $E$.

- We base our investigation on the two cases for the parameter $G$ :

  1. **The Energy and the potential are closed each other.** Consequently $G = V_c - E \approx 0$ i.e., the value of the parameter $G$ is approximately equal to zero.

**Remark 6.** *In the case $G = V_c - E \approx 0$, all the quantities in the expressions of the local truncation error with terms of several power of $G$ are approximately equal to zero.*

**Remark 7.** *In the case $G = V_c - E \approx 0$, only the terms of the expressions of the local truncation error for which the power to $G$ is equal to zero i.e., the terms which are free from $G$ are considered. The reason is the previous remark.*

In the case $G = V_c - E \approx 0$ (free from $G$ terms) the local truncation error for the classical method (constant coefficients), the local truncation error for the method with vanished the phase–lag and its first and second derivatives and the local truncation error for the method with vanished the phase–lag and its first, second and third 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.** Consequently $G >> 0$ or $G << 0$. Then $|G|$ is a large number. In these cases the best (more accurate) method is the method which has the minimum power of $G$ in the expressions of the local truncation error.

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

Based on the above procedure we obtain the following asymptotic expansions of the Local Truncation Errors:

### 4.4. Classical Method

$$LTE_{CL} = -\frac{1}{23950080} h^{12} \left( p(x)\ G^6 + \cdots \right) + O\left(h^{14}\right).$$

### 4.5. Method with Vanished Phase–Lag and Its First and Second Derivatives Developed in [1]

$$LTE_{ExplTwoStepPC} = -\frac{1}{5987520} h^{12} \left( \left( \frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x) \right) p(x)\ G^4 + \cdots \right) + O\left(h^{14}\right).$$

### 4.6. The New Proposed Method with Vanished Phase–Lag and Its First, Second and Third Derivatives Developed in Section 3

$$LTE_{NM2SH3DV} = -\frac{1}{23950080}\, h^{12} \left[ \left( 15 \left( \frac{\mathrm{d}}{\mathrm{d}x} g\left(x\right) \right)^{2} p\left(x\right) + 20\, g\left(x\right)\, p\left(x\right)\, \frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}} g\left(x\right) \right.\right.$$
$$\left.\left. +10 \left( \frac{\mathrm{d}^{3}}{\mathrm{d}x^{3}} g\left(x\right) \right) \frac{\mathrm{d}}{\mathrm{d}x} p\left(x\right) + 51 \left( \frac{\mathrm{d}^{4}}{\mathrm{d}x^{4}} g\left(x\right) \right) p\left(x\right) \right) G^{3} \right] + O\left(h^{14}\right).$$

From the above mentioned analysis we have the following theorem:

**Theorem 2.**

- *Classical Method (i.e., the method (6) with constant coefficients): For this method the error increases as the sixth power of $G$.*
- *High Algebraic Order Two–Step Method with Vanished Phase–lag and its First and Second Derivatives developed in* [1]*: For this method the error increases as the fourth power of $G$.*
- *High Algebraic Order Two–Step Method with Vanished Phase–lag and its First, Second and Third Derivatives developed in Section 3: For this method the error increases as the third power of $G$.*

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

## 5. STABILITY ANALYSIS

The stability analysis ia based on the scalar test equation:

$$p'' = -\omega^{2}\, p\,. \tag{15}$$

**Remark 8.** *The frequency of the scalar test equation of the phase–lag analysis ($\phi$) – studied above – is different with the frequency of the scalar test equation used for the stability analysis i.e., $\omega \neq \phi$.*

Application to the scalar test equation (15) leads to the following difference equation:

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

where

$$\begin{aligned} A_1(s,v) &= 1+b_1\,s^2+a_2\,b_0\,s^4-2\,a_0\,a_2\,b_0\,s^6 \\ A_0(s,v) &= -2+b_0\,s^2-2\,a_2\,b_0\,s^4+4\,a_2\,b_0\,s^6\,(a_0-a_1) \end{aligned} \tag{16}$$

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

Substituting the coefficients $a_i$, $i=0(1)2$ and $b_0$ into the formulae (16) we obtain:

$$A_1(s,v)=\frac{1}{12}\frac{T_{11}}{T_{12}}\quad,\quad A_0(s,v)\,=\,\frac{1}{6}\frac{T_{13}}{T_{12}}$$

where

$$\begin{aligned} T_{11} &= -42\,s^4v^6+15\,s^2v^8+1620\,s^4v^4+2\,s^6v^6 \\ &- 4\,s^4v^8+2\,s^2v^{10}+51\,s^6v^4-72\,s^6v^2 \\ &+ 12\,(\cos(v))^2\,v^{10}+36\,(\cos(v))^2\,v^8 \\ &+ 24\,\sin(v)\,v^9-216\,\cos(v)\,v^8 \\ &- 1152\,(\cos(v))^2\,s^6-360\,\sin(v)\,v^7+2304\,\cos(v)\,s^6 \\ &- 4\,\cos(v)\sin(v)\,s^6v^5+4\,\cos(v)\sin(v)\,s^2v^9 \\ &- 198\,\cos(v)\sin(v)\,s^6v^3+144\,\cos(v)\sin(v)\,s^4v^5 \\ &+ 30\,\cos(v)\sin(v)\,s^2v^7-864\,\cos(v)\sin(v)\,s^6v \\ &+ 2520\,\cos(v)\sin(v)\,s^4v^3+180\,v^8+24\,v^{10}-1152\,s^6 \\ &+ (\cos(v))^2\,s^6v^6-2\,(\cos(v))^2\,s^4v^8 \\ &+ (\cos(v))^2\,s^2v^{10}+27\,(\cos(v))^2\,s^6v^4 \\ &- 66\,(\cos(v))^2\,s^4v^6+3\,(\cos(v))^2\,s^2v^8 \\ &- 2\,\sin(v)\,s^6v^5+2\,\sin(v)\,s^2v^9+48\,\cos(v)\sin(v)\,v^9 \\ &- 6\,\cos(v)\,s^6v^4-18\,\cos(v)\,s^2v^8-216\,(\cos(v))^2\,s^6v^2 \\ &- 684\,(\cos(v))^2\,s^4v^4-90\,\sin(v)\,s^6v^3+72\,\sin(v)\,s^4v^5 \\ &- 30\,\sin(v)\,s^2v^7+360\,\cos(v)\sin(v)\,v^7+288\,\cos(v)\,s^6v^2 \\ &- 936\,\cos(v)\,s^4v^4+864\,\sin(v)\,s^6v-2520\,\sin(v)\,s^4v^3 \\ T_{12} &= v^7\Big((\cos(v))^2\,v^3+4\,\sin(v)\cos(v)\,v^2 \end{aligned}$$

$$
\begin{aligned}
&+ \; 2\sin(v)\,v^2 + 3\,(\cos(v))^2\,v + 2\,v^3 + 30\sin(v)\cos(v) \\
&- \; 18\cos(v)\,v - 30\sin(v) + 15\,v\Big) \\
T_{13} \;&= \; 1584\,s^2v^6 + 42\,s^4v^6 + 21\,s^2v^8 - 1620\,s^4v^4 - 2\,s^6v^6 + 4\,s^4v^8 \\
&- \; 2\,s^2v^{10} - 39\,s^6v^4 + 216\,s^6v^2 - 12\,(\cos(v))^2\,v^{10} \\
&- \; 36\,(\cos(v))^2\,v^8 - 24\sin(v)\,v^9 \\
&+ \; 216\cos(v)\,v^8 - 2304\,(\cos(v))^2\,s^6 + 360\sin(v)\,v^7 \\
&+ \; 1152\cos(v)\,s^6 - 4\cos(v)\sin(v)\,s^6v^5 \\
&+ \; 4\cos(v)\sin(v)\,s^2v^9 - 102\cos(v)\sin(v)\,s^6v^3 \\
&- \; 144\cos(v)\sin(v)\,s^4v^5 + 318\cos(v)\sin(v)\,s^2v^7 \\
&+ \; 1872\cos(v)\sin(v)\,s^6v - 2520\cos(v)\sin(v)\,s^4v^3 \\
&- \; 180\,v^8 - 24\,v^{10} - (\cos(v))^2\,s^6v^6 \\
&+ \; 2\,(\cos(v))^2\,s^4v^8 - (\cos(v))^2\,s^2v^{10} \\
&- \; 27\,(\cos(v))^2\,s^6v^4 + 66\,(\cos(v))^2\,s^4v^6 \\
&- \; 3\,(\cos(v))^2\,s^2v^8 + 12\sin(v)\,s^6v^5 - 12\sin(v)\,s^2v^9 \\
&- \; 48\cos(v)\sin(v)\,v^9 - 12\cos(v)\,s^6v^4 \\
&- \; 36\cos(v)\,s^2v^8 + 216\,(\cos(v))^2\,s^6v^2 \\
&+ \; 684\,(\cos(v))^2\,s^4v^4 + 456\sin(v)\,s^6v^3 \\
&- \; 72\sin(v)\,s^4v^5 - 360\sin(v)\,s^2v^7 - 360\cos(v)\sin(v)\,v^7 \\
&- \; 504\cos(v)\,s^6v^2 + 936\cos(v)\,s^4v^4 \\
&- \; 1368\sin(v)\,s^6v + 2520\sin(v)\,s^4v^3 + 3024\cos(v)\sin(v)\,s^2v^5 \\
&- \; 2\,(\cos(v))^2\sin(v)\,s^6v^5 + 2\,(\cos(v))^2\sin(v)\,s^2v^9 \\
&- \; 66\,(\cos(v))^2\sin(v)\,s^6v^3 + 42\,(\cos(v))^2\sin(v)\,s^2v^7 \\
&- \; 504\,(\cos(v))^2\sin(v)\,s^6v - 1512\,(\cos(v))^2\sin(v)\,s^2v^5 \\
&- \; 1512\sin(v)\,s^2v^5 + 1152\,(\cos(v))^3\,s^6 + 72\,(\cos(v))^3\,s^6v^2 \\
&+ \; 18\,(\cos(v))^3\,s^2v^8 + 792\,(\cos(v))^3\,s^2v^6 \\
&- \; 2376\cos(v)\,s^2v^6 + 6\,(\cos(v))^3\,s^6v^4\,.
\end{aligned}
$$

**Definition 5.** *(see* [8]*) A multistep method is called P-stable if its interval of periodicity is equal to* $(0, \infty)$.

**Definition 6.** *A multistep method is called singularly almost P-stable if its interval of periodicity is equal to* $(0,\infty)-S$ [2]. *We use the term singularly almost P-stable method only 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.

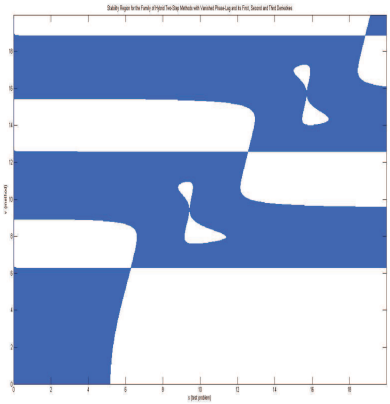

Figure 2: $s-v$ plane of the new developed two-step tenth algebraic order method with vanished phase–lag and its first, second and third derivatives.

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

- *The shadowed area denotes where the method is stable,*
- *The white area denotes the region where the method is unstable.*

**Remark 10.** *In the cases of problems for which the mathematical models request only one frequency per differential equation in the model, the observation of* **the surroundings of the first diagonal of the** $s-v$ **plane** *is required. 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. There are many problems in Sciences, Engineering and Technology for which their mathematical models*

[2] where $S$ is a set of distinct points

*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 remark, we investigate the case where the frequency of the scalar test equation used for the stability analysis is equal with the frequency of the scalar test equation used for the phase–lag analysis , i.e., we investigate the case where $s = v$ (i.e., on the the $s - v$ plane see the surroundings of the first diagonal). Based on the above mentioned study we found that the interval of periodicity in the case $s = v$ is equal to: $(0, 26)$.

Based on the above we have the following theorem:

**Theorem 3.** *The method obtained in section 3:*

- *is of tenth algebraic order,*
- *has the phase–lag and its first, second and third derivatives equal to zero*
- *has an interval of periodicity equals to:* $(0, 26)$*, 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

We will study the effectiveness of the new obtained numerical scheme. This will be possible by investigating :

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

### 6.1. Radial Time–Independent Schrödinger Equation

The radial time independent Schrödinger equation is given by :

$$p''(r) = [l(l+1)/r^2 + V(r) - k^2]\, p(r). \tag{17}$$

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*.

Since the problem (17) is a boundary value one, the boundary conditions must be defined. For the initial point we have the boundary condition :

$$p(0) = 0$$

and another boundary condition, for large values of $r$, determined by physical considerations.

The new obtained method has coefficients which are frequency dependent. Therefore, the parameter $\phi$ of the coefficients of the method ($v = \phi\, h$) must be defined. The parameter $\phi$ for the radial Schrödinger equation and for the case $l = 0$ is given by :

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

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

### 6.1.1. Woods–Saxon Potential

We use for our numerical tests the well known Woods-Saxon potential which is written as :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{18}$$

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.

Using the methodology proposed by Ixaru et al. [12], we approximate the potential in some critical points. Based on these approximations we define the value of the parameter $\phi$.

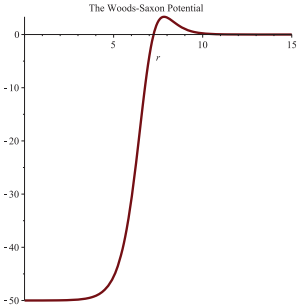


Figure 3: The Woods-Saxon potential.

We choose $\phi$ as follows (see for details [13] and [14]) :

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

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

### 6.1.2. Radial Schrödinger Equation – The Resonance Problem

Our first numerical experiment consists of the numerical solution of the radial time independent Schrödinger equation (17) with the Woods-Saxon potential (18).

Since the above mentioned problem has an infinite interval of integration i.e., $r \in \left(0, \infty\right)$, it is necessary to approximate this interval by a finite one. Consequently, we will use the integration interval $r \in [0, 15]$. We will solve the above problem in a domain of energies equal to: $E \in [1, 1000]$.

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

$$p''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) p(r) = 0 \tag{19}$$

In (19) the differential equation 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. Thus, the solution of equation (17) (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 $\delta_l$ is the phase shift that may 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 $C(r) = -krn_l(kr)$. Since in our test, the problem is treated as an initial–value problem, we need $p_j\,,\ j = 0, 1$ before starting a two-step method. From the initial condition, we obtain $p_0$. The value $p_1$ is obtained by using high order Runge–Kutta–Nyström methods (see [15] and [16]). With these starting values, we evaluate at $r_2$ of the asymptotic region the phase shift $\delta_l$.

We call the problem as resonance problem in the case of positive energies. We have two forms for this problem:

- finding the phase-shift $\delta_l$ 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 [17], which is indicated as **Method QT8**;
- the tenth order multi–step method developed by Quinlan and Tremaine [17], which is indicated as **Method QT10**;

- the twelfth order multi–step method developed by Quinlan and Tremaine [17], which is indicated as **Method QT12**;
- the fourth algebraic order method of Chawla and Rao with minimal phase–lag [18], which is indicated as **Method MCR4**;
- the exponentially–fitted method of Raptis and Allison [19], which is indicated as **Method MRA** ;
- the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase–lag [20], which is indicated as **Method MCR6**;
- the classical form of the Two-Step Hybrid Method developed in Section 3, which is indicated as **Method NMCL** [3];
- the Phase-Fitted Method (Case 1) developed in [7], which is indicated as **Method NMPF1**;
- the Phase-Fitted Method (Case 2) developed in [7], which is indicated as **Method NMPF2**;
- the Method developed in [21] (Case 2), which is indicated as **Method NMC2**;
- the method developed in [21] (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 Two-Step Runge–Kutta type method developed in Section 3, which is indicated as **Method NM2SH3DV**.

The reference values are determined using the well known two-step method of Chawla and Rao [20] with small step size for the integration. We calculated numerically the eigenenergies and we compared the computed values with the reference values. In Figures 4 and 5, we present the maximum absolute error $Err_{max} = |\log_{10}(Err)|$ where

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

[3] with the term classical we mean the method of Section 3 with constant coefficients

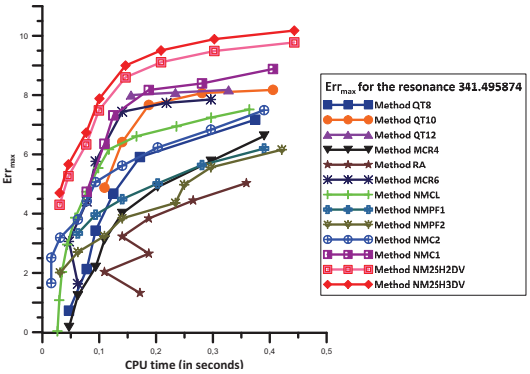


Figure 4: Accuracy (Digits) for several values of $CPU$ Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

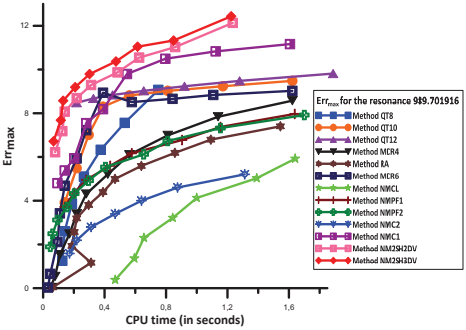


Figure 5: Accuracy (Digits) for several values of $CPU$ Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0.

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 classical form of the Two-Step Hybrid Method developed in Section 3, which is indicated as **Method NMCL** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase–lag [18], which is indicated as **Method MCR4**, the exponentially-fitted method of Raptis and Allison [19], which is indicated as **Method MRA**, the Phase-Fitted Method (Case 1) developed in [7], which is indicated as **Method NMPF1**, the Phase-Fitted Method (Case 2) developed in [7], which is indicated as **Method NMPF2**, the Method developed in [21] (Case 2), which is indicated as **Method NMC2** and the eighth order multi-step method developed by Quinlan and Tremaine [17], which is indicated as **Method QT8**.

2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [17], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase–lag [18], 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 [17], 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 [20], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.

3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [17], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [17], which is indicated as **Method QT10**

4. The Phase-Fitted Method (Case 1) developed in [7], which is indicated as **Method NMPF1** is more efficient than the exponentially-fitted method of Raptis and Allison [19] and the Phase-Fitted Method (Case 2) developed in [7], which is indicated as **Method NMPF2**

5. The Method developed in [21] (Case 2), which is indicated as **Method NMC2** is more efficient than the exponentially-fitted method of Raptis and Allison [19] and the Phase-Fitted Method (Case 2) developed in [7], which is indicated as **Method NMPF2** and the Phase-Fitted Method (Case 1) developed in [7], which is indicated as **Method NMPF1**

6. The Method developed in [21] (Case 1), which is indicated as **Method NMC1**, is more efficient than all the other methods mentioned above.

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

8. Finally, the New Obtained Two-Step Runge–Kutta type Method developed in Section 3, which is indicated as **Method NM2SH3DV**, is the most efficient one.

### 6.2. Error Estimation

The estimation of the local truncation error (LTE) is necessary in order to produce variable-step schemes. Several schemes of this form have been developed the last decades for the numerical solution of systems of differential equations (see for example [7]– [64]).

Our scheme for variable step integration consists a local error estimation technique which is based on an embedded pair of multistep methods and on the fact that when the algebraic order is maximal then we have better numerical solution for the problems with oscillatory or periodical behavior.

We use as lower order solution $y_{n+1}^L$, for the purpose of local error estimation, the method developed in [64] - which is of eight algebraic order. As higher order solution $y_{n+1}^H$ we use the method obtained in the present paper - which is of tenth algebraic order. Now, the local truncation error in $y_{n+1}^L$ is estimated by

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

For a required local error of $acc$ and for a step size used for the $n^{th}$ step equal to $h_n$, the estimated step size for the $(n+1)^{st}$ step, which would give a local error equal to $acc$, 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.

Our local truncation error estimate is based on the lower order solution $y_{n+1}^L$. However, for an error estimate which is less than *acc*, we adopt the widely used procedure of performing local extrapolation. Thus, although the control of an estimation of the local error is taken place in lower order solution $y_{n+1}^L$, it is the higher order solution $y_{n+1}^H$ which is accepted at each point.

### 6.3. Coupled Differential Equations

The mathematical models of many problems in

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

consist of coupled differential equations of the Schrödinger type.

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

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

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

We will study the case in which all channels are open. Consequently, the following boundary conditions are hold (see for details [22]):

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

$$p_{ij} \sim k_i\, x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}\, k_i\, x\, n_{li}(k_i x) \tag{20}$$

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

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

Defining a matrix $K'$ and diagonal matrices $M$, $N$ by (see for detailed analysis in [22]):

$$K'_{ij} \;=\; \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij}$$

$$M_{ij} = k_i x j_{l_i}(k_i x)\delta_{ij}$$
$$N_{ij} = k_i x n_{l_i}(k_i x)\delta_{ij}$$

we find that the asymptotic condition (20) can be written as:

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

The rotational excitation of a diatomic molecule by neutral particle impact is a real problem in quantum chemistry, theoretical physics, material science, atomic physics and molecular physics with its mathematical model to be expressed with close–coupling differential equations of the Schrödinger type. Denoting, as in [22], the entrance channel by the quantum numbers $(j, l)$, the exit channels by $(j', l')$, and the total angular momentum by $J = j + l = j' + l'$, we find that

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

where

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

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

The potential $V$ can be be written as (see for details [22]):

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

and consequently, the coupling matrix 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. [23] 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 [24]). The boundary conditions are

$$p_{j'l'}^{Jjl}(x) = 0 \text{ at } x = 0 \tag{21}$$

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

where the relation of scattering S matrix with $K$ matrix of (20) is given by

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

The numerical method for step-by-step integration from the initial value to matching points is included in the algorithm which is used for the calculation of the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles. The algorithm used in our numerical tests is based on an analogous algorithm which has been developed for the numerical tests of [22].

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

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

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

As is described in [1], 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 [24] and Allison [22] 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 (21) may be written as

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

For the approximate solution of the above mentioned problem we have used the following methods:

- the Iterative Numerov method of Allison [22] which is indicated as **Method I**[4],
- the variable-step method of Raptis and Cash [25] which is indicated as **Method II**,
- the embedded Runge–Kutta Dormand and Prince method 5(4) [16] which is indicated as **Method III**,
- the embedded Runge–Kutta method ERK4(2) developed in Simos [26] 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 which is indicated as **Method VI**.

[4]We note here that Iterative Numerov method developed by Allison [22] 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 V. $acc$=$10^{-6}$. Note that hmax is the maximum stepsize.

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

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

## 7. CONCLUSIONS

A family of tenth algebraic order two-step methods is studied in this paper. More specifically, we investigated: (1) the procedure of vanishing of the phase–lag and its first, second and third derivatives, (2) the comparative error analysis, (3) the stability analysis and (4) the computational behavior of the new produced method and its effectiveness on the numerical solution of the radial Schrödinger equation and of the coupled Schrödinger equations both of which are of high importance for chemistry.

From the analysis and numerical results presented above, it is easy to see the efficiency of the new developed method for the approximate solution of the radial Schrödinger equation and of the coupled Schrödinger equations.

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 Derivatives of $T_j$, $j = 0(1)3$

$$
\begin{aligned}
T_0 &= 2\left(1+v^2\left(\frac{1}{12}+b_0a_2v^2\left(-2\,a_0v^2+1\right)\right)\right)\cos(v)-2\\
&+ v^2b_0\left(1+a_2v^2\left(4\,a_0v^2-4\,a_1v^2-2\right)\right)\\
T_1 &= -576\sin(v)\,v^{12}{a_0}^2{a_2}^2{b_0}^2+576\sin(v)\,v^{10}a_0{a_2}^2{b_0}^2\\
&- 576\,v^9a_1{a_2}^2{b_0}^2-144\sin(v)\,v^8{a_2}^2{b_0}^2+48\sin(v)\,v^8a_0a_2b_0\\
&+ 576\,v^7a_0a_2{b_0}^2+576\sin(v)\,v^6a_0a_2b_0+96\,v^7a_0a_2b_0\\
&- 96\,v^7a_1a_2b_0-24\sin(v)\,v^6a_2b_0-1728\,v^5a_1a_2b_0\\
&- 144\,v^5a_2{b_0}^2-288\sin(v)\,v^4b_0a_2-24\,v^5a_2b_0-\sin(v)\,v^4\\
&- 24\sin(v)\,v^2+144\,vb_0-144\sin(v)+24\,v\\
T_2 &= -288-13824\cos(v)\,v^{18}{a_0}^3{a_2}^3{b_0}^3+36\cos(v)\,v^4\\
&+ 432\cos(v)\,v^2+1728\cos(v)+72\,v^2-10368\cos(v)\,v^{14}a_0{a_2}^3{b_0}^3\\
&+ \cos(v)\,v^6-20736\cos(v)\,v^{10}a_0{a_2}^2{b_0}^2-1728\cos(v)\,v^{12}a_0{a_2}^2{b_0}^2\\
&+ 20736\cos(v)\,v^{12}{a_0}^2{a_2}^2{b_0}^2+1728\cos(v)\,v^{14}{a_0}^2{a_2}^2{b_0}^2\\
&- 10368\cos(v)\,v^6a_0a_2b_0-1728\cos(v)\,v^8a_0a_2b_0-72\cos(v)\,v^{10}a_0a_2b_0\\
&+ 290304\,v^{10}a_0a_1{a_2}^2{b_0}^2+11520\,v^{12}a_0a_1{a_2}^2{b_0}^2\\
&+ 41472\,v^{14}a_0a_1{a_2}^3{b_0}^3+432\,v^2b_0+20736\cos(v)\,v^{16}{a_0}^2{a_2}^3{b_0}^3\\
&+ 3456\,v^4b_0a_2+24\,v^6a_2b_0-864\,v^8{a_2}^2{b_0}^2+20736\,v^4{a_2}{b_0}^2\\
&- 5184\,v^8{a_2}^2{b_0}^3+144\,v^6a_2{b_0}^2+5184\cos(v)\,v^4b_0a_2\\
&+ 36\cos(v)\,v^8a_2b_0+864\cos(v)\,v^6a_2b_0-1728\,b_0+432\cos(v)\,v^{10}{a_2}^2{b_0}^2\\
&+ 5184\cos(v)\,v^8{a_2}^2{b_0}^2-86400\,v^6a_0a_2{b_0}^2+1728\cos(v)\,v^{12}{a_2}^3{b_0}^3\\
&- 1728\,v^8a_0a_2{b_0}^2+288\,v^8a_1a_2b_0+6912\,v^{12}a_1{a_2}^3{b_0}^3\\
&+ 31104\,v^{10}a_0{a_2}^2{b_0}^3+1728\,v^{10}a_1{a_2}^2{b_0}^2
\end{aligned}
$$

$$
\begin{aligned}
&+ \; 5184\, v^{10} a_0 {a_2}^2 {b_0}^2 - 288\, v^8 a_0 a_2 b_0 + 103680\, v^4 a_1 a_2 b_0 \\
&- \; 69120\, v^{12} {a_0}^2 {a_2}^2 {b_0}^3 - 14400\, v^6 a_0 a_2 b_0 + 9792\, v^6 a_1 a_2 b_0 - 11520\, v^{12} {a_0}^2 {a_2}^2 {b_0}^2 \\
T_3 \; &= \; -3456\, v + 6912 \sin(v)\, v^2 + 864 \sin(v)\, v^4 \\
&+ \; 20736 \sin(v) + 288\, v^3 + 9953280\, v^7 a_1 {a_2}^2 {b_0}^2 \\
&+ \; 864 \sin(v)\, v^{12} {a_2}^2 {b_0}^2 - 165888 \sin(v)\, v^6 a_0 a_2 b_0 + 497664 \sin(v)\, v^{12} {a_0}^2 {a_2}^2 {b_0}^2 \\
&- \; 497664 \sin(v)\, v^{10} a_0 {a_2}^2 {b_0}^2 - 41472 \sin(v)\, v^8 a_0 a_2 b_0 \\
&+ \; 20736 \sin(v)\, v^6 a_2 b_0 + 82944 \sin(v)\, v^4 b_0 a_2 + 82944\, v^5 a_2 {b_0}^2 \\
&+ \; 13824\, v^5 a_2 b_0 - 207360\, b_0 a_2 v^3 - 41472\, v^{11} {a_2}^3 {b_0}^3 \\
&- \; 248832\, v^{11} {a_2}^3 {b_0}^4 + 1161216\, v^5 a_0 a_2 b_0 - 497664\, v^5 a_1 a_2 b_0 \\
&+ \; 497664\, v^9 a_1 {a_2}^2 {b_0}^2 - 27648\, v^7 a_1 a_2 b_0 + 124416 \sin(v)\, v^8 {a_2}^2 {b_0}^2 \\
&+ \; 20736 \sin(v)\, v^{10} {a_2}^2 {b_0}^2 - 4976640\, v^3 a_1 a_2 b_0 \\
&+ \; 414720\, v^7 {a_2}^2 {b_0}^2 + 3456\, v^9 {a_2}^2 {b_0}^2 + 20736\, v^9 {a_2}^2 {b_0}^3 \\
&+ \; 2488320\, v^7 {a_2}^2 {b_0}^3 + 82944 \sin(v)\, v^{12} {a_2}^3 {b_0}^3 - 1244160\, v^3 a_2 {b_0}^2 \\
&+ \; 6912 \sin(v)\, v^{14} {a_2}^3 {b_0}^3 + 20736 \sin(v)\, v^{16} {a_2}^4 {b_0}^4 \\
&+ \; 6967296\, v^5 a_0 a_2 {b_0}^2 + 1728\, v^3 b_0 + 48 \sin(v)\, v^{10} a_2 b_0 \\
&+ \; 1728 \sin(v)\, v^8 a_2 b_0 + 9953280\, v^{17} {a_0}^3 {a_2}^3 {b_0}^4 + 1658880\, v^{17} {a_0}^3 {a_2}^3 {b_0}^3 \\
&- \; 5971968\, v^{15} {a_0}^2 {a_2}^3 {b_0}^4 - 995328\, v^{15} {a_0}^2 {a_2}^3 {b_0}^3 \\
&+ \; 1990656\, v^{13} a_0 {a_2}^3 {b_0}^4 + 829440\, v^{13} {a_0}^2 {a_2}^2 {b_0}^3 \\
&+ \; 331776\, v^{13} a_0 {a_2}^3 {b_0}^3 + 138240\, v^{13} {a_0}^2 {a_2}^2 {b_0}^2 \\
&+ \; 34836480\, v^{11} {a_0}^2 {a_2}^2 {b_0}^3 - 995328\, v^{11} a_1 {a_2}^3 {b_0}^3 \\
&- \; 20736\, v b_0 + \sin(v)\, v^8 + 48 \sin(v)\, v^6 + 5806080\, v^{11} {a_0}^2 {a_2}^2 {b_0}^2 \\
&- \; 248832\, v^{11} a_0 {a_2}^2 {b_0}^3 - 41472\, v^{11} a_0 {a_2}^2 {b_0}^2 \\
&+ \; 6912\, v^{11} a_1 {a_2}^2 {b_0}^2 - 16920576\, v^9 a_0 {a_2}^2 {b_0}^3 \\
&- \; 96 \sin(v)\, v^{12} a_0 a_2 b_0 - 82944 \sin(v)\, v^{12} a_0 {a_2}^2 {b_0}^2 \\
&- \; 3456 \sin(v)\, v^{14} a_0 {a_2}^2 {b_0}^2 + 82944 \sin(v)\, v^{14} {a_0}^2 {a_2}^2 {b_0}^2 \\
&- \; 497664 \sin(v)\, v^{14} a_0 {a_2}^3 {b_0}^3 + 3456 \sin(v)\, v^{16} {a_0}^2 {a_2}^2 {b_0}^2 \\
&- \; 41472 \sin(v)\, v^{16} a_0 {a_2}^3 {b_0}^3 + 995328 \sin(v)\, v^{16} {a_0}^2 {a_2}^3 {b_0}^3 \\
&+ \; 82944 \sin(v)\, v^{18} {a_0}^2 {a_2}^3 {b_0}^3 - 165888 \sin(v)\, v^{18} a_0 {a_2}^4 {b_0}^4
\end{aligned}
$$

$$
\begin{aligned}
&- \; 663552\,\sin(v)\,v^{18}{a_0}^3{a_2}^3{b_0}^3 - 55296\,\sin(v)\,v^{20}{a_0}^3{a_2}^3{b_0}^3 \\
&+ \; 497664\,\sin(v)\,v^{20}{a_0}^2{a_2}^4{b_0}^4 - 663552\,\sin(v)\,v^{22}{a_0}^3{a_2}^4{b_0}^4 \\
&+ \; 331776\,\sin(v)\,v^{24}{a_0}^4{a_2}^4{b_0}^4 - 69672960\,v^9 a_0 a_1 {a_2}^2 {b_0}^2 \\
&- \; 5640192\,v^{11} a_0 a_1 {a_2}^2 {b_0}^2 - 138240\,v^{13} a_0 a_1 {a_2}^2 {b_0}^2 \\
&- \; 663552\,v^{15} a_0 a_1 {a_2}^3 {b_0}^3 - 55738368\,v^{15} {a_0}^2 a_1 {a_2}^3 {b_0}^3 \\
&- \; 1658880\,v^{17} {a_0}^2 a_1 {a_2}^3 {b_0}^3 - 1990656\,v^{17} a_0 a_1 {a_2}^4 {b_0}^4 \\
&- \; 3981312\,v^{19} {a_0}^2 a_1 {a_2}^4 {b_0}^4 - 3456\,\sin(v)\,v^{10} a_0 a_2 b_0 \\
&- \; 2820096\,v^9 a_0 {a_2}^2 {b_0}^2 + 3456\,v^9 a_0 a_2 {b_0}^2 + 576\,v^9 a_0 a_2 b_0 - 576\,v^9 a_1 a_2 b_0\,.
\end{aligned}
$$

## Appendix B: Formulae for the Derivatives of $p_n$

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

$$
\begin{aligned}
p_n^{(2)} &= (V(x) - V_c + G)\; p(x) \\
p_n^{(3)} &= \left(\frac{d}{dx} g(x)\right) p(x) + (g(x) + G)\,\frac{d}{dx} p(x) \\
p_n^{(4)} &= \left(\frac{d^2}{dx^2} g(x)\right) p(x) + 2\left(\frac{d}{dx} g(x)\right)\frac{d}{dx} p(x) + (g(x) + G)^2\, p(x) \\
p_n^{(5)} &= \left(\frac{d^3}{dx^3} g(x)\right) p(x) + 3\left(\frac{d^2}{dx^2} g(x)\right)\frac{d}{dx} p(x) \\
&+ \; 4\,(g(x) + G)\, p(x)\,\frac{d}{dx} g(x) + (g(x) + G)^2\,\frac{d}{dx} p(x) \\
p_n^{(6)} &= \left(\frac{d^4}{dx^4} g(x)\right) p(x) + 4\left(\frac{d^3}{dx^3} g(x)\right)\frac{d}{dx} p(x) \\
&+ \; 7\,(g(x) + G)\, p(x)\,\frac{d^2}{dx^2} g(x) + 4\left(\frac{d}{dx} g(x)\right)^2 p(x) \\
&+ \; 6\,(g(x) + G)\left(\frac{d}{dx} p(x)\right)\frac{d}{dx} g(x) + (g(x) + G)^3\, p(x) \\
p_n^{(7)} &= \left(\frac{d^5}{dx^5} g(x)\right) p(x) + 5\left(\frac{d^4}{dx^4} g(x)\right)\frac{d}{dx} p(x)
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad 11\left(g\left(x\right)+G\right)p\left(x\right)\frac{d^{3}}{dx^{3}}g\left(x\right)+15\left(\frac{d}{dx}g\left(x\right)\right)p\left(x\right)\\
&+ \quad \frac{d^{2}}{dx^{2}}g\left(x\right)+13\left(g\left(x\right)+G\right)\left(\frac{d}{dx}p\left(x\right)\right)\frac{d^{2}}{dx^{2}}g\left(x\right)\\
&+ \quad 10\left(\frac{d}{dx}g\left(x\right)\right)^{2}\frac{d}{dx}p\left(x\right)+9\left(g\left(x\right)+G\right)^{2}p\left(x\right)\\
&+ \quad \frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^{3}\frac{d}{dx}p\left(x\right)\\
p_{n}^{(8)} &= \quad \left(\frac{d^{6}}{dx^{6}}g\left(x\right)\right)p\left(x\right)+6\left(\frac{d^{5}}{dx^{5}}g\left(x\right)\right)\frac{d}{dx}p\left(x\right)\\
&+ \quad 16\left(g\left(x\right)+G\right)p\left(x\right)\frac{d^{4}}{dx^{4}}g\left(x\right)+26\left(\frac{d}{dx}g\left(x\right)\right)p\left(x\right)\\
&+ \quad \frac{d^{3}}{dx^{3}}g\left(x\right)+24\left(g\left(x\right)+G\right)\left(\frac{d}{dx}p\left(x\right)\right)\frac{d^{3}}{dx^{3}}g\left(x\right)\\
&+ \quad 15\left(\frac{d^{2}}{dx^{2}}g\left(x\right)\right)^{2}p\left(x\right)+48\left(\frac{d}{dx}g\left(x\right)\right)\\
&+ \quad \left(\frac{d}{dx}p\left(x\right)\right)\frac{d^{2}}{dx^{2}}g\left(x\right)+22\left(g\left(x\right)+G\right)^{2}p\left(x\right)\\
&+ \quad \frac{d^{2}}{dx^{2}}g\left(x\right)+28\left(g\left(x\right)+G\right)p\left(x\right)\left(\frac{d}{dx}g\left(x\right)\right)^{2}\\
&+ \quad 12\left(g\left(x\right)+G\right)^{2}\left(\frac{d}{dx}p\left(x\right)\right)\frac{d}{dx}g\left(x\right)+\left(g\left(x\right)+G\right)^{4}p\left(x\right)\\
&\ldots
\end{aligned}
$$

# References


[1] F. Hui, T. E. Simos, Hybrid high algebraic order two–step method with vanished phase–lag and its first and second derivatives, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 619–648.

[2] R. Vujasin, M. Senčanski, J. Radić–Perić, M. Perić, A comparison of various variational approaches for solving the one–dimensional vibrational Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 363–378.

[3] C. J. Cramer, *Essentials of Computational Chemistry*, Wiley, Chichester, 2004.

[4] F. Jensen, *Introduction to Computational Chemistry*, Wiley, Chichester, 2007.

[5] A. R. Leach, *Molecular Modelling – Principles and Applications*, Pearson, Essex, 2001.

[6] P. Atkins, R. Friedman, *Molecular Quantum Mechanics*, Oxford Univ. Press, Oxford, 2011.

[7] Z. A. Anastassi, T. E. Simos, A parametric symmetric linear four–step method for the efficient integration of the Schrödinger equation and related oscillatory problems, *J. Comp. Appl. Math.* **236** (2012) 3880–3889.

[8] J. D. Lambert, I. A. Watson, Symmetric multistep methods for periodic initial values problems, *J. Inst. Math. Appl.* **18** (1976) 189–202.

[9] T. E. Simos, P. S. Williams, A finite–difference method for the numerical solution of the Schrödinger equation, *J. Comp. Appl. Math.* **79** (1997) 189–205.

[10] R. M. Thomas, Phase properties of high order almost $P$-stable formulae, *BIT* **24** (1984) 225–238.

[11] A. D. Raptis, T. E. Simos, A four–step phase–fitted method for the numerical integration of second order initial–value problem, *BIT* **31** (1991) 160–168.

[12] L. G. Ixaru, M. Rizea, Comparison of some four–step methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.* **38** (1985) 329–337.

[13] L. G. Ixaru, M. Micu, *Topics in Theoretical Physics*, Central Institute of Physics, Bucharest, 1978.

[14] L. G. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies, *Comput. Phys. Commun.* **19** (1980) 23–27.

[15] J. R. Dormand, M. E. A. El–Mikkawy, P. J. Prince, Families of Runge–Kutta–Nyström formulae, *IMA J. Numer. Anal.* **7** (1987) 235–250.

[16] J. R. Dormand, P. J. Prince, A family of embedded Runge–Kutta formulae, *J. Comput. Appl. Math.* **6** (1980) 19–26.

[17] G. D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits, *Astronom. J.* **100** (1990) 1694–1700.

[18] M. M. Chawla, P. S. Rao, An Noumerov–type method with minimal phase–lag for the integration of second order periodic initial–value problems. II. Explicit method, *J. Comput. Appl. Math.* **15** (1986) 329–337.

[19] A. D. Raptis, A. C. Allison, Exponential–fitting methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.* **14** (1978) 1–5.

[20] M. M. Chawla, P. S. Rao, An explicit sixth–order method with phase–lag of order eight for $y'' = f(t, y)$, *J. Comput. Appl. Math.* **17** (1987) 363—368.

[21] T. E. Simos, On the explicit four–step methods with vanished phase–lag and its first derivative, *Appl. Math. Inf. Sci.* **8** (2014) 447–458.

[22] A. C. Allison, The numerical solution of coupled differential equations arising from the Schrödinger equation, *J. Comput. Phys.* **6** (1970) 378–391.

[23] R. B. Bernstein, A. Dalgarno, H. Massey , I. C. Percival, Thermal scattering of atoms by homonuclear diatomic molecules, *Proc. Roy. Soc. Ser. A* **274** (1963) 427–442.

[24] R. B. Bernstein, Quantum mechanical (phase shift) analysis of differential elastic scattering of molecular beams, *J. Chem. Phys.* **33** (1960) 795–804.

[25] A. D. Raptis, J. R. Cash, A variable step method for the numerical integration of the one–dimensional Schrödinger equation, *Comput. Phys. Commun.* **36** (1985) 113–119.

[26] T. E. Simos, Exponentially fitted Runge–Kutta methods for the numerical solution of the Schrödinger equation and related problems, *Comput. Mater. Sci.* **18** (2000) 315–332.

[27] G. A. Panopoulos, T. E. Simos, A new optimized symmetric embedded predictor–corrector method (EPCM) for initial–value problems with oscillatory solutions, *Appl. Math. Inf. Sci.* **8** (2014) 703–713.

[28] J. M. Franco, M. Palacios, High–order $P$-stable multistep methods, *J. Comput. Appl. Math.* **30** (1990) 1–10.

[29] J. D.Lambert, *Numerical Methods for Ordinary Differential Systems. The Initial Value Problem*, Wiley, New York, 1991, pp. 104–107.

[30] E. Stiefel, D. G. Bettis, Stabilization of Cowell's method, *Numer. Math.* **13** (1969) 154–175.

[31] G. A. Panopoulos, Z. A. Anastassi, T. E. Simos, Two new optimized eight–step symmetric methods for the efficient solution of the Schrödinger equation and related problems, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 773–785.

[32] T. E. Simos, G. Psihoyios, Preface, in: *Selected Papers of the International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)*, *J. Comput. Appl. Math.* **175** (2005) IX–IX.

[33] T. Lyche, Chebyshevian multistep methods for ordinary differential eqations, *Numer. Math.* **19** (1972) 65–75.

[34] A. Konguetsof, T. E. Simos, A generator of hybrid symmetric four–step methods for the numerical solution of the Schrödinger equation, *J. Comput. Appl. Math.* **158** (2003) 93–106.

[35] Z. Kalogiratou, T. Monovasilis, T. E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation, *J. Comput. Appl. Math.* **158** (2003) 83–92.

[36] Z. Kalogiratou, T. E. Simos, Newton–Cotes formulae for long–time integration, *J. Comput. Appl. Math.* **158** (2003) 75–82.

[37] G. Psihoyios, T. E. Simos, Trigonometrically fitted predictor–corrector methods for IVPs with oscillating solutions, *J. Comput. Appl. Math.* **158** (2003) 135–144.

[38] T. E. Simos, I. T. Famelis, C. Tsitouras, Zero dissipative, explicit Numerov–type methods for second order IVPs with oscillating solutions, *Numer. Algor.* **34** (2003) 27–40.

[39] T. E. Simos, Dissipative trigonometrically–fitted methods for linear second-order IVPs with oscillating solution, *Appl. Math. Lett.* **17** (2004) 601–607.

[40] K. Tselios, T. E. Simos, Runge–Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics, *J. Comput. Appl. Math.* **175** (2005) 173–181.

[41] D. P. Sakas, T. E. Simos, Multiderivative methods of eighth algrebraic order with minimal phase–lag for the numerical solution of the radial Schrödinger equation, *J. Comput. Appl. Math.* **175** (2005) 161–172.

[42] G. Psihoyios, T. E. Simos, A fourth algebraic order trigonometrically fitted predictor–corrector scheme for IVPs with oscillating solutions, *J. Comput. Appl. Math.* **175** (2005) 137–147.

[43] Z. A. Anastassi, T. E. Simos, An optimized Runge–Kutta method for the solution of orbital problems, *J. Comput. Appl. Math.* **175** (2005) 1–9.

[44] T. E. Simos, Closed Newton–Cotes trigonometrically–fitted formulae of high order for long–time integration of orbital problems, *Appl. Math. Lett.* **22** (2009) 1616–1621.

[45] S. Stavroyiannis, T. E. Simos, Optimization as a function of the phase–lag order of nonlinear explicit two–step $P$-stable method for linear periodic IVPs, *Appl. Numer. Math.* **59** (2009) 2467–2474.

[46] T. E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation, *Acta Appl. Math.* **110** (2010) 1331–1352.

[47] T. E. Simos, New stable closed Newton–Cotes trigonometrically fitted formulae for long–time integration, *Abstract Appl. Anal.* (2012) #182536.

[48] T. E. Simos, Optimizing a hybrid two–step method for the numerical solution of the Schrödinger equation and related problems with respect to phase–lag, *J. Appl. Math.* (2012) #420387.

[49] Z. A. Anastassi, T. E. Simos, A parametric symmetric linear four–step method for the efficient integration of the Schrödinger equation and related oscillatory problems, *J. Comput. Appl. Math.* **236** (2012) 3880–3889.

[50] D. F. Papadopoulos, T. E. Simos, A modified Runge–Kutta–Nyström method by using phase lag properties for the numerical solution of orbital problems, *Appl. Math. Inf. Sci.* **7** (2013) 433–437.

[51] T. Monovasilis, Z. Kalogiratou, T. E. Simos, Exponentially fitted symplectic Runge–Kutta–Nyström methods, *Appl. Math. Inf. Sci.* **7** (2013) 81–85.

[52] G. A. Panopoulos, T. E. Simos, An optimized symmetric 8-step semi–embedded predictor–corrector method for IVPs with oscillating solutions, *Appl. Math. Inf. Sci.* **7** (2013) 73–80.

[53] D. F. Papadopoulos, T. E Simos, The use of phase lag and amplification error derivatives for the construction of a modified Runge–Kutta–Nyström method, *Abstract Appl. Anal.* (2013) #910624.

[54] I. Alolyan, Z. A. Anastassi, T. E. Simos, A new family of symmetric linear four–step methods for the efficient integration of the Schrödinger equation and related oscillatory problems, *Appl. Math. Comput.* **218** (2012) 5370–5382.

[55] I. Alolyan, T. E. Simos, A family of high–order multistep methods with vanished phase–lag and its derivatives for the numerical solution of the Schrödinger equation, *Comput. Math. Appl.* **62** (2011) 3756–3774.

[56] C. Tsitouras, I. T. Famelis, T. E. Simos, On modified Runge–Kutta trees and methods, *Comput. Math. Appl.* **62** (2011) 2101–2111.

[57] A. A. Kosti, Z. A. Anastassi, T. E. Simos, Construction of an optimized explicit Runge–Kutta–Nyström method for the numerical solution of oscillatory initial value problems, *Comput. Math. Appl.* **61** (2011) 3381–3390.

[58] Z. Kalogiratou, T. Monovasilis, T. E. Simos, New modified Runge–Kutta–Nyström methods for the numerical integration of the Schrödinger equation, *Comput. Math. Appl.* **60** (2010) 1639–1647.

[59] T. Monovasilis, Z. Kalogiratou, T. E. Simos, A family of trigonometrically fitted partitioned Runge–Kutta symplectic methods, *Appl. Math. Comput.* **209** (2009) 91–96.

[60] T. E. Simos, High order closed Newton–Cotes trigonometrically–fitted formulae for the numerical solution of the Schrödinger equation, *Appl. Math. Comput.* **209** (2009) 137–151.

[61] A. Konguetsof, T. E. Simos, An exponentially–fitted and trigonometrically–fitted method for the numerical solution of periodic initial–value problems, *Comput. Math. Appl.* **45** (2003) 547–554.

[62] D. F. Papadopoulos, Z. A. Anastassi, T. E. Simos, An optimized Runge–Kutta–Nyström method for the numerical solution of the Schrödinger equation and related problems, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 551–566.

[63] Z. A. Anastassi, T. E. Simos, Trigonometrically fitted six–step symmetric methods for the efficient solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 733–752.

[64] T. E. Simos, A new Numerov–type method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **46** (2009) 981–1007.