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Runge-Kutta Type Tenth Algebraic Order Method with Vanished Phase-Lag and its First, Second, Third, Fourth and Fifth Derivatives for the Numerical Solution of the Schrödinger Equation

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Abstract: A Runge-Kutta type tenth algebraic order two-step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives is produced in this paper. We also investigate the effect of elimination of the phase-lag and its derivatives on the efficiency of the obtained method.

Keywords: Phase-lag, derivative of the phase-lag, initial value problems, oscillating solution, symmetric, hybrid, multistep, Runge-Kutta type, Schrödinger equation

1 Introduction

The approximate solution of special second order initial value problems of the form :

$$q''(x) = f(x,q),\ q(x_0) = q_0 \ and \ q'(x_0) = q'_0 \qquad (1)$$

is studied in this paper. Special attention is given for the problems of the form (1) with solutions with periodical and/or oscillating behavior.

The special characteristic of the mathematical models of the form (1) is the consistent of systems of second order ordinary differential equations from which the first derivative q' does not appear explicitly.

We will investigate a family of Runge-Kutta type (4-stages) two-step method is introduced. With this family we avoid the many steps method since in these cases we need unstable methods (for problems with periodical and /or oscillating solutions), like Runge-Kutta or Runge-Kutta-Nystöm methods, for the first steps of the method. This creates serious computational problems since increase the computational time and the instabilities of the method. In order to achieve high algebraic order the numerical methods must have many steps or many stages or both of them. We note that many steps methods are proposed in some cases (see [50]). Additionally the new proposed family of methods has some more benefits like the very good behavior on the numerical solution of problems with periodical and /or oscillating solutions. The benefits are the result of important properties which this family has like the vanishing of the phase-lag and its derivatives.

The paper has the following form:

–In Section 2 we present the theory on the phase-lag analysis of symmetric multistep methods.
–The development of the new Runge-Kutta type tenth algebraic order two-step method with vanished phase-lag and its first, second, third, fourth and fifth derivatives is presented in Section 3.
–In Section 4 based on a model problem we study the local truncation error of the new method and using other similar methods of the literature we present the comparative local truncation error analysis.

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–The definition of the stability interval (interval of periodicity) of the produced method is presented in Section 5. For the investigation of the stability properties we use scalar test equation with frequency different than the frequency of the scalar test equation used for the phase-lag analysis
–In the Subsection 6.1 we present the Local Error estimation. This is based on methods with similar characteristics but with different algebraic order and
–The approximate solution of the coupled differential equations arising from the Schrödinger equation is presented in Section 6.2.
–Finally, in Section 7 we present some conclusions.

We note here that the numerical solution of the coupled differential equations arising from the Schrödinger equation is an important problem for the computational chemistry which is a part of information sciences.

2 Phase-lag Analysis for Symmetric $2m$-Step Methods

Consider the $2m$-Step methods

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

for the numerical solution of the initial value problem (1). We have the following:

1.In order to solve numerically the initial value problem (1) we divide the integration area $[a,b]$ into m equally spaced intervals i.e. $\{x_i\}_{i=-m}^{m} \in [a,b]$. Within these intervals we apply the method (2). The integration area is defined based on the physical characteristics of the specific problem.
2.We define the quantity h as $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$. This quantity is called stepsize of integration.
3.For the multistep method given by (2) the number of steps, which are used for the integration, is equal to $2m$. This is the reason that this is called $2m$-step method).

*Remark.*If $c_{-i} = c_i$ and $b_{-i} = b_i$, $i = 0(1)m$ then the method (2) is called symmetric $2m$-step method.

*Remark.*The linear operator, which is associated with the Multistep Method (2), is given by:

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

where $q \in C^2$.

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

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

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

the following difference equation is obtained :

$$A_m(v) q_{n+m} + \ldots + A_1(v) q_{n+1} + A_0(v) q_n + A_1(v) q_{n-1} + \ldots + A_m(v) q_{n-m} = 0 \tag{5}$$

where $v = \phi h$, h is the stepsize and $A_j(v)$ $j = 0(1)m$ are polynomials of v.

The equation :

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

is called characteristic equation and is associated with (5).

Definition 2.[16] *We say that a symmetric $2m$-step method with characteristic equation given by (6) has an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots $\lambda_i, i = 1(1)2m$ of Eq. (6) satisfy:*

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

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

Definition 3.[14], [15] *For any symmetric multistep method which is associated to the characteristic equation (6) the phase-lag is the leading term in the expansion of*

$$t = v - \theta(v) \tag{8}$$

The order of phase-lag is p, if the quantity $t = O(v^{p+1})$ as $v \to \infty$ is hold.

Definition 4.*[2] If for a method the phase-lag is vanished (i.e. equal to zero), then this method is called* **phase-fitted**.

Theorem 1.[14] *The symmetric $2k$-step method with associated characteristic equation given by (6) has phase-lag order p and phase-lag constant c given by*

$$-cv^{p+2} + O(v^{p+4}) = \frac{P_0}{P_1} \tag{9}$$

where
$P_0 = 2A_m(v)\cos(mv) + \ldots + 2A_j(v)\cos(jv) + \ldots + A_0(v)$
and $P_1 = 2m^2 A_m(v) + \ldots + 2j^2 A_j(v) + \ldots + 2A_1(v)$.

*Remark.*For the direct calculation of the phase-lag for any symmetric $2m$-step multistep method we use the formula (9).

*Remark.*In our study we use symmetric two-step methods. Considering that their characteristic polynomials are given by $A_j(v)\ j=0,1$, the phase-lag of order p with phase-lag constant c are given by:

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

3 The New Proposed Tenth Algebraic Order Runge-Kutta Type Two-Step Method with Vanished Phase-Lag and Its First, Second, Third, Fourth and Fifth Derivatives

Consider the hybrid family of two-step methods

$$\begin{aligned}
\widehat{q}_{n+\frac{1}{2}} &= \left(\frac{3}{52}q_{n+1}+a_0\,q_n+\frac{29}{52}q_{n-1}\right)\\
&+\frac{h^2}{4992}\left(41\,f_{n+1}-682\,f_n-271\,f_{n-1}\right)\\
\widehat{q}_{n-\frac{1}{2}} &= \frac{1}{104}\left(5\,q_{n+1}+146\,q_n-47\,q_{n-1}\right)\\
&+\frac{h^2}{4992}\left(-59\,f_{n+1}+1438\,f_n+253\,f_{n-1}\right)\\
\widetilde{q}_n &= q_n-a_1h^2\left(f_{n+1}\right.\\
&\left.-4\,\widehat{f}_{n+\frac{1}{2}}+6\,f_n-4\,\widehat{f}_{n-\frac{1}{2}}+f_{n-1}\right)\\
q_{n+1}+a_2\,q_n+q_{n-1} &= h^2\left[b_1\,(f_{n+1}+f_{n-1})\right.\\
&\left.+b_0\,\widetilde{f}_n+b_2\left(\widehat{f}_{n+\frac{1}{2}}+\overline{f}_{n-\frac{1}{2}}\right)\right]
\end{aligned} \tag{11}$$

where $f_i=q''(x_i,q_i),i=-1\left(\frac{1}{2}\right)1$ and $a_i,\ i=0(1)2\ b_j\ j=0(1)2$ are free parameters.

We require the above Runge-Kutta type method (11) to have vanished the phase-lag and its first, second, third, fourth and fifth derivatives. Therefore, the following system of equations is produced :

$$\text{Phase}-\text{Lag(PL)}=\frac{1}{2}\frac{T_0}{T_1}=0 \tag{12}$$

$$\text{First Derivative of the Phase}-\text{Lag}=\frac{\partial PL}{\partial v}=0 \tag{13}$$

$$\text{Second Derivative of the Phase}-\text{Lag}=\frac{\partial^2 PL}{\partial v^2}=0 \tag{14}$$

$$\text{Third Derivative of the Phase}-\text{Lag}=\frac{\partial^3 PL}{\partial v^3}=0 \tag{15}$$

$$\text{Fourth Derivative of the Phase}-\text{Lag}=\frac{\partial^4 PL}{\partial v^4}=0 \tag{16}$$

$$\text{Fifrh Derivative of the Phase}-\text{Lag}=\frac{\partial^5 PL}{\partial v^5}=0 \tag{17}$$

where

$$\begin{aligned}
T_0 &= 2\left(1+v^2\left(b_1+b_0a_1v^2\left(\frac{15}{26}-\frac{3v^2}{208}\right)+b_2\left(\frac{11}{104}+\frac{3v^2}{832}\right)\right)\right.\\
&\left.\cos(v)+a_2+v^2\left(b_0\left(1+a_1v^2\left(-4a_0+\frac{63v^2}{104}+\frac{5}{13}\right)\right)\right.\right.\\
&\left.\left.+b_2\left(a_0-\frac{63v^2}{416}+\frac{73}{52}\right)\right)\right)\\
T_1 &= 1+v^2\left(b_1+b_0a_1v^2\left(\frac{15}{26}-\frac{3v^2}{208}\right)+b_2\left(\frac{11}{104}+\frac{3v^2}{832}\right)\right)
\end{aligned}$$

If we solve the above system of equations (12)-(17), we produce the coefficients of the new obtained Runke-Kutta type method : a_0,a_1,a_2,b_0,b_1,b_2. There are cases that the formulae of the coefficients are subject to heavy cancellations for some values of $|v|$ (for example when for some values of $|v|$ the denominators of the formulae of the coefficients are equal to zero). For these cases Taylor series expansions should be used.

In Figure 1 we present the behavior of the coefficients of the new method.

The local truncation error of the new developed Runge-Kutta type method (11) (mentioned as $ExpTwoStepRKT10$) is given by:

$$\begin{aligned}
LTE_{ExpTwoStepRKT10} &= -\frac{8641}{67060224000}h^{12}\left(q_n^{(12)}\right.\\
&+6\phi^2q_n^{(10)}+15\phi^4q_n^{(8)}+20\phi^6q_n^{(6)}\\
&\left.+15\phi^8q_n^{(4)}+6\phi^{10}q_n^{(2)}+\phi^{12}q_n\right)+O\left(h^{14}\right)
\end{aligned} \tag{18}$$

4 Comparative Local Truncation Error Analysis

In order to study the behavior of the Local Truncation Error we consider the test problem

$$q''(x)=(V(x)-V_c+G)\,q(x) \tag{19}$$

where (1) $V(x)$ is a potential function, (2) V_c is the constant value approximation of the potential on the specific point x, (3) $G=V_c-E$ and (4) E is the energy.

We will investigate the local truncation error of the following methods:

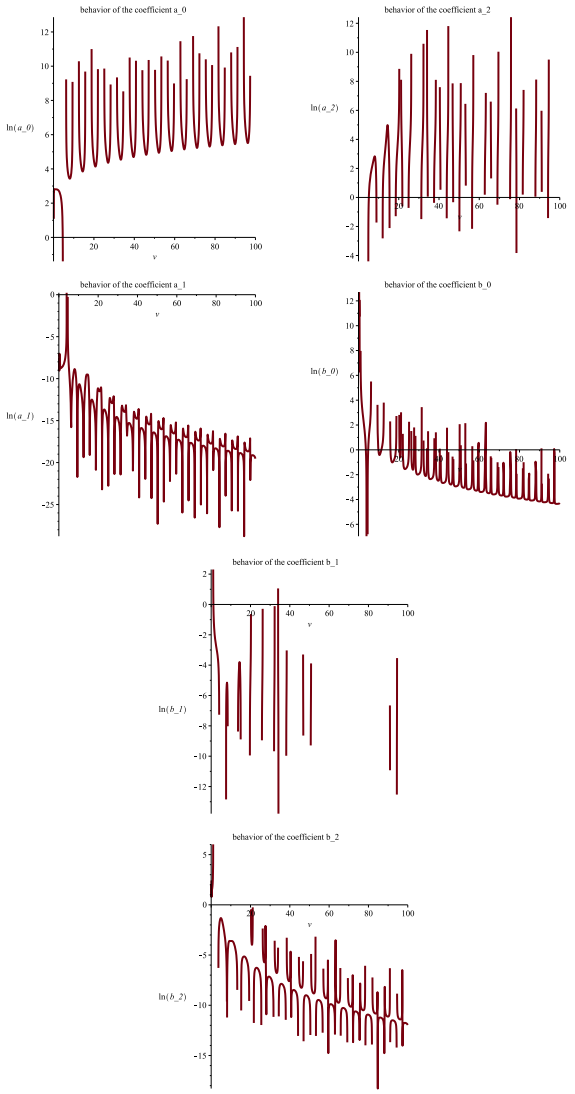

Fig. 1: Behavior of the coefficients of the new proposed method for several values of $v = \phi h$.

4.1 Classical Method (i.e. the method (11) with constant coefficients)

$$LTE_{CL} = -\frac{8641}{67060224000} h^{12} q_n^{(12)} + O\left(h^{14}\right) \qquad (20)$$

4.2 The New Proposed Method with Vanished Phase-Lag and its First, Second, Third, Fourth and Fifth Derivatives Produced in Section 3

$$LTE_{ExpTwoStepRKT10} = -\frac{8641}{67060224000} h^{12} \left(q_n^{(12)} + 6\phi^2 q_n^{(10)} + 15\phi^4 q_n^{(8)} + 20\phi^6 q_n^{(6)} + 15\phi^8 q_n^{(4)} + 6\phi^{10} q_n^{(2)} + \phi^{12} q_n \right) + O\left(h^{14}\right) \qquad (21)$$

The Local Error Analysis is based on the following procedure :

- It is easy to see that the formulae of the Local Truncation Errors consists of derivatives of the function q. Consequently we calculate the expressions of these derivatives which are based on the test problem (19). We present some of the expressions of the derivatives of the function q in the Appendix.
- Based on the above step of the algorithm, new formulae of the Local Truncation Errors are produced which are based on the expressions of the derivatives of the function q given in the Appendix. It is easy to see that these new formulae of the Local Truncation Errors are dependent on the quantity G and energy E.
- Consequently, the above mentioned formulae of the Local Truncation Errors leads to expressions of the Local Truncation Error which contain the parameter G (see (19)). Our investigation is based on two cases for the parameter G :
  1. First Case: $V_c - E = G \approx 0$. The physical meaning of this case is that the Energy and the Potential are closed each other. Consequently, all the terms of $G^n n \geq 1$ are approximately equal to zero. Therefore, approximately equal to zero are all the terms in the formulae of the local truncation error which contain powers of G (i.e. which contain $G^n n \geq 1$). Consequently, in this case the expression of the local truncation error is equal with the term which contain only the power of G^0 i.e. which contain free from G terms. Due to the fact that the free from G term of the expression of the local truncation error for the classical method (constant coefficients) is equal with the free from G term of the expression of the local truncation error for the methods with vanished the phase-lag and its first, second, third, fourth and fifth derivatives, the asymptotic behavior of the local truncation error for the classical method and the asymptotic behavior of the local truncation error for the methods with vanished the phase-lag and its first, second, third, fourth and fifth derivatives is the same. Consequently, for these values of G, the methods are of comparable accuracy.

2.$G >> 0$ or $G << 0$. Therefore, $|G|$ is a large number. It is easy to see that the most accurate methods are the methods with expressions of the local truncation error which contain minimum power of G.

–Finally the asymptotic expressions of the Local Truncation Errors are presented.

The following asymptotic expansions of the Local Truncation Errors are obtained based on the analysis presented above :

4.3 Classical Method

$$LTE_{CL} = -\frac{8641}{67060224000} h^{12} \left(q(x)\, G^6 + \cdots \right) + O\left(h^{14}\right) \tag{22}$$

4.4 The New Proposed Method with Vanished Phase-Lag and its First, Second, Third, Fourth and Fifth Derivatives Produced in Section 3

$$\begin{aligned} LTE_{ExpTwoStepRKT10} = & -\frac{8641}{4191264000} h^{12} \\ & \left(2\frac{\mathrm{d}^5}{\mathrm{d}x^5} g(x) \frac{\mathrm{d}}{\mathrm{d}x} q(x) + 5\frac{\mathrm{d}^6}{\mathrm{d}x^6} g(x)\, q(x) \right. \\ & +10\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g(x)\right)^2 q(x) + 15\frac{\mathrm{d}^3}{\mathrm{d}x^3} g(x) \frac{\mathrm{d}}{\mathrm{d}x} g(x)\, q(x) \\ & \left. +6\frac{\mathrm{d}^4}{\mathrm{d}x^4} g(x)\, g(x)\, q(x) \right) G^2 + \cdots + O\left(h^{14}\right) \end{aligned} \tag{23}$$

From the above 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 sixth power of G.*

–Tenth Algebraic Order Two-Step Method with Vanished Phase-lag and its First, Second, Third, Fourth and Fifth Derivatives developed in Section 3: For this method the error increases as the Second power of G.

So, for the approximate integration of the time independent radial Schrödinger equation the New Obtained Tenth Algebraic Order Method with Vanished Phase-Lag and its First, Second, Third, Fourth and Fifth Derivatives is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

5 Stability Analysis

In order to study the stability properties of the new proposed Runge-Kutta type method we consider the following scalar test equation :

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

It is easy to see that the above scalar test equation has frequency (ω) which is different than the frequency of the scalar test equation for the phase-lag analysis (ϕ) which was studied above i.e. $\omega \neq \phi$.

If we apply the new proposed Runge-Kutta type method to the scalar test equation (24) we have following difference equation:

$$A_1(s,v)\left(q_{n+1} + q_{n-1}\right) + A_0(s,v)\, q_n = 0 \tag{25}$$

where

$$\begin{aligned} A_1(s,v) &= 1 + s^2 b_1 + \frac{15 b_0 a_1 s^4}{26} \\ &\quad - \frac{3 s^6 b_0 a_1}{208} + \frac{11 b_2 s^2}{104} + \frac{3 s^4 b_2}{832} \\ A_0(s,v) &= a_2 + s^2 b_0 - 4 s^4 b_0 a_1 a_0 + \frac{63 s^6 b_0 a_1}{104} \\ &\quad + \frac{5 b_0 a_1 s^4}{13} + s^2 b_2 a_0 - \frac{63 s^4 b_2}{416} + \frac{73 b_2 s^2}{52} \end{aligned} \tag{26}$$

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

Based on the above and on the Section 2 we have the following definitions:

Definition 5.*(see [16]) We call P-stable a multistep method with interval of periodicity equal to* $(0,\infty)$.

Definition 6.*We call singularly almost P-stable a multistep method with interval of periodicity equal to* $(0,\infty) - S$ [1].

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

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

*Remark.*The following conclusions are extracted based on the $s - v$ region presented in Figure 2 : (1) The method is stable within the shadowed area, (2) The method is unstable within the white area.

[1] where S is a set of distinct points

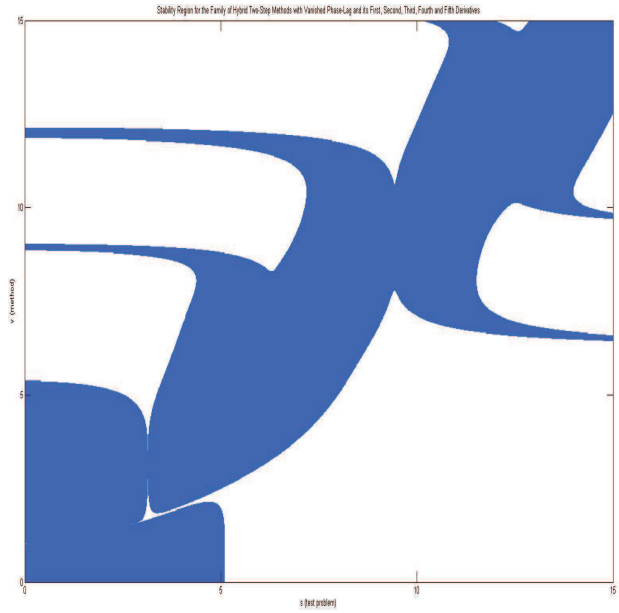

Fig. 2: $s-v$ plane of the new obtained two-step high order method with vanished phase-lag and its first, second, third and fourth derivatives

*Remark.*The mathematical models of many real problems in Sciences, Engineering and Technology (for example the Schrödinger equation) consist only one frequency in the their model. Consequently, in these specific cases we are interested for the investigation of the stability of the proposed methods under the condition that the frequency of the scalar test equation for the stability analysis is equal with the frequency of the scalar test equation for the phase-lag analysis i.e. under the condition that $\omega = \phi$. Thefore, for these specific cases the study of the $s-v$ plane is limited on the **the surroundings of the first diagonal of the** $s-v$ **plane** i.e. on the areas where $s = v$.

Based on the above remark, we investigated the specific case where the frequency of the scalar test equation used for the the stability analysis is equal with the frequency of the scalar test equation used for phase-lag analysis , i.e. we study the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s-v$ plane). For this case : the new produced method has interval of periodicity equal to: $(0,\infty)$, i.e. is P-stable.

The above investigation leads to the following theorem:

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

–is of tenth algebraic order,
–has the phase-lag and its first, second, third, fourth and fifth derivatives equal to zero
–has an interval of periodicity equals to: $(0,\infty)$*, i.e. is P-stable 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

6.1 Error Estimation

The estimation of the local truncation error (LTE) on the approximate solution of systems of differential equations was the subject of large research the last decades. This can be verified from the existing literature. The subject of this research was the development of new techniques for the local error estimation (see for example [1]-[54]).

In our numerical tests we base our methodology for the local truncation error estimation on the algebraic order of the methods. The result of this methodology is an embedded pair of multistep methods. More precisely our technique is based on the fact that the maximum algebraic order of a multistep method produces highly accurate approximate solutions for oscillatory and/or periodical problems.

The local truncation error in y^L_{n+1} is estimated by

$$LTE = | y^H_{n+1} - y^L_{n+1} | \tag{27}$$

y^L_{n+1} denotes the lower order solution and we use for this the method developed in [54], which is of eight algebraic order and y^H_{n+1} denotes the higher order solution and we use for this the method obtained in this paper, which is of tenth algebraic order.

The estimated step length for the $(n+1)^{st}$ step, which would give a local error equal to *acc*, is given by

$$h_{n+1} = h_n \left(\frac{acc}{LTE} \right)^{\frac{1}{p}} \tag{28}$$

where p is the algebraic order of the method, h_n is the step length used for the n^{th} step and *acc* is the requested accuracy of the local error.

*Remark.*Our technique for the local truncation error estimation is based on the lower algebraic order solution y^L_{n+1}. In our tests we use the well know procedure of performing local extrapolation. Consequently, if the estimation of the local error is less than *acc*, we accept at each point the higher algebraic order solution y^H_{n+1} while the local error is controlled in lower algebraic order solution y^L_{n+1}.

6.2 Coupled differential equations

There are lot of problems in

1.quantum chemistry,

2.material science,
3.theoretical physics,
4.atomic physics,
5.physical chemistry,
6.theoretical chemistry and
7.chemical physics

for which their models can be transferred in a coupled differential equations of the Schrödinger type.

We write the close-coupling differential equations of the Schrödinger type as:

$$\left[\frac{d^2}{dx^2}+k_i^2-\frac{l_i(l_i+1)}{x^2}-V_{ii}\right]y_{ij}=\sum_{m=1}^{N}V_{im}y_{mj} \qquad (29)$$

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

The case in which all channels are open is considered for our numerical tests. Therefore, the following boundary conditions are hold (see for details [56]):

$$y_{ij}=0 \ at \ x=0 \qquad (30)$$

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

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

*Remark.*The obtained method can also be used for the case of closed channels.

Our application is based on the detailed analysis obtained in [56]. We define a matrix K' and diagonal matrices M, N as:

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

Based on the above we can write the asymptotic condition (31) as:

$$\mathbf{y}\sim\mathbf{M}+\mathbf{NK}'$$

*Remark.*We can find detailed description on the problem in [56]. There, one the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation is described. This is the well know Iterative Numerov method of Allison [56].

The rotational excitation of a diatomic molecule by neutral particle impact is a real problem for which its mathematical model can be transferred to close-coupling differential equations of the Schrödinger type. This problem occurs frequently in quantum chemistry, theoretical physics, material science, atomic physics and molecular physics. Denoting, as in [56], 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

$$\left[\frac{d^2}{dx^2}+k_{j'j}^2-\frac{l'(l'+1)}{x^2}\right]y^{Jjl}_{j'l'}(x)=$$
$$\frac{2\mu}{\hbar^2}\sum_{j''}\sum_{l''}<j'l';J\mid V\mid j''l'';J>y^{Jjl}_{j''l''}(x) \qquad (32)$$

where

$$k_{j'j}=\frac{2\mu}{\hbar^2}[E+\frac{\hbar^2}{2I}\{j(j+1)-j'(j'+1)\}] \qquad (33)$$

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.

As analyzed in [56], the potential V can be expanded as

$$V(x,\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj})=V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj})+V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}), \qquad (34)$$

and the coupling matrix element may then be written as

$$<j'l';J\mid V\mid j''l'';J>=\delta_{j'j''}\delta_{l'l''}V_0(x)+f_2(j'l',j''l'';J)V_2(x) \qquad (35)$$

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [57] 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 [58]). The boundary conditions are

$$y^{Jjl}_{j'l'}(x)=0 \text{ at } x=0 \qquad (36)$$

$$y^{Jjl}_{j'l'}(x)\sim\delta_{jj'}\delta_{ll'}\exp[-i(k_{jj}x-1/2l\pi)]$$
$$-\left(\frac{k_i}{k_j}\right)^{1/2}S^J(jl;j'l')\exp[i(k_{j'j}x-1/2l'\pi)] \qquad (37)$$

where the scattering S matrix is related to the K matrix of (31) by the relation

$$\mathbf{S}=(\mathbf{I}+\mathbf{iK})(\mathbf{I}-\mathbf{iK})^{-1} \qquad (38)$$

An algorithm which must include a numerical method for step-by-step integration from the initial value to matching points is needed in order to compute the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles. We use an algorithm which is based on the similar algorithm which has been produced for the numerical tests of [56].

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

$$\frac{2\mu}{\hbar^2}=1000.0,\ \frac{\mu}{I}=2.351,\ E=1.1,$$
$$V_0(x)=\frac{1}{x^{12}}-2\frac{1}{x^6},\ V_2(x)=0.2283V_0(x).$$

As is described in [56], we take $J=6$ and consider excitation of the rotator from the $j=0$ state to levels up

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}. We 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	0.10	1.5×10^{-8}
	9	0.448	1.24	6.8×10^{-8}
	16	0.448	9.03	5.9×10^{-8}

to $j' = 2,4$ and 6 giving sets of **four, nine and sixteen coupled differential equations**, respectively. Following the procedure obtained by Bernstein [58] and Allison [56] 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 (36) may be written as

$$y^{Jjl}_{j'l'}(x_0) = 0 \tag{39}$$

For the numerical solution of this problem we have used the most well known methods for the above problem:

–the Iterative Numerov method of Allison [56] which is indicated as **Method I**,
–the variable-step method of Raptis and Cash [55] which is indicated as **Method II**,
–the embedded Runge-Kutta Dormand and Prince method 5(4) [49] which is indicated as **Method III**,
–the embedded Runge-Kutta method ERK4(2) developed in Simos [59] which is indicated as **Method IV**,
–the new developed embedded two-step method which is indicated as **Method V**

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 is presented in Table. In the same table 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.

7 Conclusions

A family of Runge-Kutta type tenth algebraic order two-step methods was investigated in the present paper. More specifically :

1.we investigated the elimination of the phase-lag and its first, second, third, fourth and fifth derivatives
2.we studied the comparative local truncation error analysis
3.we investigated the stability properties of the new proposed method using a scalar test equation with frequency different than the frequency used by the scalar test equation for the phase-lag analysis
4.we studied the computational behavior of the new produced method and its efficiency on the numerical solution of the Schrödinger equation.

As a conclusion of this study it is easy to see that the new obtained method is much more efficient than known ones for the approximate solution of the Schrödinger equation related problems..

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

Appendix: Formulae of the derivatives of q_n

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

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

$$q_n^{(3)} = \left(\frac{d}{dx}g(x)\right) q(x) + (g(x)+G)\frac{d}{dx}q(x)$$

$$q_n^{(4)} = \left(\frac{d^2}{dx^2}g(x)\right) q(x) + 2\left(\frac{d}{dx}g(x)\right)\frac{d}{dx}q(x) + (g(x)+G)^2 q(x)$$

$$q_n^{(5)} = \left(\frac{d^3}{dx^3}g(x)\right) q(x) + 3\left(\frac{d^2}{dx^2}g(x)\right)\frac{d}{dx}q(x) + 4(g(x)+G)\, q(x)\frac{d}{dx}g(x) + (g(x)+G)^2\frac{d}{dx}q(x)$$

$$q_n^{(6)} = \left(\frac{d^4}{dx^4}g(x)\right) q(x) + 4\left(\frac{d^3}{dx^3}g(x)\right)\frac{d}{dx}q(x) + 7(g(x)+G)\, q(x)\frac{d^2}{dx^2}g(x) + 4\left(\frac{d}{dx}g(x)\right)^2 q(x) + 6(g(x)+G)\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}g(x) + (g(x)+G)^3 q(x)$$

$$q_n^{(7)} = \left(\frac{d^5}{dx^5}g(x)\right)q(x) + 5\left(\frac{d^4}{dx^4}g(x)\right)\frac{d}{dx}q(x) + 11\left(g(x)+G\right)q(x)\frac{d^3}{dx^3}g(x) + 15\left(\frac{d}{dx}g(x)\right)q(x)\frac{d^2}{dx^2}g(x) + 13\left(g(x)+G\right)\left(\frac{d}{dx}q(x)\right)\frac{d^2}{dx^2}g(x) + 10\left(\frac{d}{dx}g(x)\right)^2\frac{d}{dx}q(x) + 9\left(g(x)+G\right)^2 q(x)\frac{d}{dx}g(x) + \left(g(x)+G\right)^3\frac{d}{dx}q(x)$$

$$q_n^{(8)} = \left(\frac{d^6}{dx^6}g(x)\right)q(x) + 6\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}q(x) + 16\left(g(x)+G\right)q(x)\frac{d^4}{dx^4}g(x) + 26\left(\frac{d}{dx}g(x)\right)q(x)\frac{d^3}{dx^3}g(x) + 24\left(g(x)+G\right)\left(\frac{d}{dx}q(x)\right)\frac{d^3}{dx^3}g(x) + 15\left(\frac{d^2}{dx^2}g(x)\right)^2 q(x) + 48\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}q(x)\right)\frac{d^2}{dx^2}g(x) + 22\left(g(x)+G\right)^2 q(x)\frac{d^2}{dx^2}g(x) + 28\left(g(x)+G\right)q(x)\left(\frac{d}{dx}g(x)\right)^2 + 12\left(g(x)+G\right)^2\left(\frac{d}{dx}q(x)\right)\frac{d}{dx}g(x) + \left(g(x)+G\right)^4 q(x)\ldots$$

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