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Hybrid Tenth Algebraic Order Method with Vanished Phase-Lag and its First, Second, Third and Fourth Derivatives for the Approximate Solution of the Schrödinger Equation

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Abstract: A hybrid tenth algebraic order two-step method with vanished phase-lag and its first, second, third and fourth derivatives is obtained in this paper. One more scope of this paper is to study the effect of vanishing of the phase-lag and its derivatives on the effectiveness of the produced method.

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

1 Introduction

In the present paper we will investigate the numerical solution of special second order initial value problems of the form:

$$p''(x) = f(x,p), \;\; p(x_0) = q_0 \textit{ and } p'(x_0) = p'_0 \qquad (1)$$

We are interested especially for the problems of (1) with periodical and/or oscillating solutions.

It is easy for one to see, from the model (1), that the main characteristic of the problems of our interest is that their mathematical expressions consist of systems of ordinary differential equations of second order in which the first derivative p' does not appear explicitly.

In this paper we will introduce a hybrid (4-stages) two-step tenth algebraic order method is introduced in this paper. In order to achieve high algebraic order the numerical methods must have many steps or many stages or both of them (see [3]). The above methodology (many steps and/or stages) creates serious computational difficulties since increase the computational time and instabilities of the method (due to the requirement the application of the method to be started using using unstable methods (for problems with periodical and /or oscillating solutions) like Runge-Kutta or Runge-Kutta-Nystöm methods). Therefore, the application of this type methods has serious problems on computational cost and on the accuracy. The above described problem is solved since the new method is of two-step. For the accuracy of the approximate solution of problems with periodical and /or oscillating solutions, the new obtained method has very critical properties which are the elimination of the phase-lag and its derivatives.

Our investigation involves:

–the development of the method,
–the definition of the local truncation error of the new method and based on this the comparative local truncation error analysis using other similar methods of the literature,
–the determination of the stability interval (interval of periodicity) of the obtained method using a scalar test

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equation with frequency different than the frequency of the scalar test equation used for the phase-lag analysis

– the determination of the Error Estimation based on methods with similar characteristics but with different algebraic order and

– the examination of the efficiency of the new developed method by applying it on the numerical solution of the coupled differential equations arising from the Schrödinger equation. We note here that this problem is a very important problem for the computational chemistry which is a part of information sciences.

2 Phase-lag for Symmetric $2k$ Multistep Methods

We use the multistep methods

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

in order to solve numerically the initial value problem (1). We have the following remarks:

1. The method (2) is applied within integration intervals. The integration interval is defined using the interval of interest for the solution of the problem (1), which is equal to $[a,b]$, after its division into k equally spaced subintervals i.e. $\{x_i\}_{i=-k}^{k} \in [a,b]$.
2. The quantity h, called stepsize of integration and is given by $h = |x_{i+1} - x_i|$, $i = 1-k(1)k-1$.
3. For the specific multistep method the number of steps, which are used for the integration, is equal to $2k$ (and for this reason can be called $2k$-step method).

Remark. We call a method (2) as symmetric multistep method if and only if $c_{-i} = c_i$ and $b_{-i} = b_i$, $i = 0(1)k$.

Remark. The linear operator

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

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

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

Applying the symmetric $2k$-step method, $(i = -k(1)k)$, to the scalar test equation

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

we obtain the following difference equation:

$$\begin{aligned} &A_k(v)\, p_{n+m} + \ldots + A_1(v)\, p_{n+1} + A_0(v)\, p_n \\ &\quad + A_1(v)\, p_{n-1} + \ldots + A_k(v)\, q_{n-k} = 0 \end{aligned} \tag{5}$$

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

The characteristic equation associated with (5) is give by :

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

Definition 2.[16] *We say that a symmetric $2k$-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 $\lambda_i, i = 1(1)2k$ of Eq. (6) satisfy:*

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

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 q, if the quantity $t = O(v^{q+1})$ as $v \to \infty$ is hold.

Definition 4.[2] *If for a method the phase-lag is 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 q and phase-lag constant c given by*

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

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

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

Remark. Since in our investigation we study the symmetric two-step methods, with characteristic polynomials $A_j(v)$ $j = 0, 1$, the phase-lag of order q with phase-lag constant c is given by:

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

3 The New Tenth Algebraic Order Hybrid Two-Step Method with Vanished Phase-Lag and Its First, Second, Third and Fourth Derivatives

We consider the family of two-step methods

$$\begin{aligned}
\widehat{p}_{n+\frac{1}{2}} &= \frac{1}{52}\left(3\,p_{n+1}+20\,p_n+29\,p_{n-1}\right) \\
&+\frac{h^2}{4992}\left(41\,f_{n+1}-682\,f_n-271\,f_{n-1}\right) \\
\widehat{p}_{n-\frac{1}{2}} &= \frac{1}{104}\left(5\,p_{n+1}+146\,p_n-47\,p_{n-1}\right) \\
&+\frac{h^2}{4992}\left(-59\,f_{n+1}+1438\,f_n+253\,f_{n-1}\right) \\
\widetilde{p}_n &= p_n-a_0\,h^2\Big(f_{n+1} \\
&-4\,\widehat{f}_{n+\frac{1}{2}}+6\,f_n-4\,\widehat{f}_{n-\frac{1}{2}}+f_{n-1}\Big) \\
\overline{p}_n &= p_n-a_1\,h^2\Big(f_{n+1} \\
&-4\,\widehat{f}_{n+\frac{1}{2}}+6\,\widetilde{f}_n-4\,\widehat{f}_{n-\frac{1}{2}}+f_{n-1}\Big) \\
p_{n+1}-2\,p_n+p_{n-1} &= h^2\Big[b_1\,\left(f_{n+1}+f_{n-1}\right) \\
&+b_0\,\widetilde{f}_n+b_2\left(\widehat{f}_{n+\frac{1}{2}}+\overline{f}_{n-\frac{1}{2}}\right)\Big] \qquad (11)
\end{aligned}$$

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

Requesting the above hybrid method (11) to have vanished the phase-lag and its first, second, third and fourth derivatives, the following system of equations is obtained :

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

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

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

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

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

where

$$\begin{aligned}
T_0 &= 2\left(1+v^2\left(b_1+b_0a_1v^2\left(\frac{15}{26}-\frac{3\,v^2}{208}\right.\right.\right. \\
&\left.\left.\left.+6\,a_0v^2\left(\frac{15}{26}-\frac{3\,v^2}{208}\right)\right)+b_2\left(\frac{11}{104}+\frac{3\,v^2}{832}\right)\right)\right) \\
&\cos(v)-2+v^2\left(b_0\left(1+a_1v^2\left(-\frac{15}{13}+\frac{63\,v^2}{104}\right.\right.\right. \\
&\left.\left.\left.+6\,a_0v^2\left(-\frac{15}{13}+\frac{63\,v^2}{104}\right)\right)\right)+b_2\left(\frac{93}{52}-\frac{63\,v^2}{416}\right)\right) \\
T_1 &= 1+v^2\left(b_1+b_0a_1v^2\left(\frac{15}{26}-\frac{3\,v^2}{208}\right.\right. \\
&\left.\left.+6\,a_0v^2\left(\frac{15}{26}-\frac{3\,v^2}{208}\right)\right)+b_2\left(\frac{11}{104}+\frac{3\,v^2}{832}\right)\right)
\end{aligned}$$

Solving the above system of equations (12)-(16), we can obtain the coefficients of the new proposed hybrid method : a_0, a_1, b_0, b_1, b_2. For the case that the formulae are subject to heavy cancellations for some values of $|v|$ then 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 obtained hybrid method (11) (mentioned as $ExpTwoStepHY10$) is given by:

$$\begin{aligned}
LTE_{ExpTwoStepHY10} &= -\frac{47563}{3683282803200}\,h^{12}\Big(p_n^{(12)} \\
&+5\,\phi^2\,p_n^{(10)}+10\,\phi^4\,p_n^{(8)}+10\,\phi^6\,p_n^{(6)} \\
&+5\,\phi^8\,p_n^{(4)}+\phi^{10}\,p_n^{(2)}\Big)+O\left(h^{14}\right) \qquad (17)
\end{aligned}$$

4 Comparative Error Analysis

Let us consider the test problem

$$p''(x) = \left(V(x)-V_c+G\right)\,p(x) \qquad (18)$$

where

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

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

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

$$LTE_{CL} = -\frac{47563}{3683282803200}\,h^{12}\,p_n^{(12)}+O\left(h^{14}\right) \qquad (19)$$

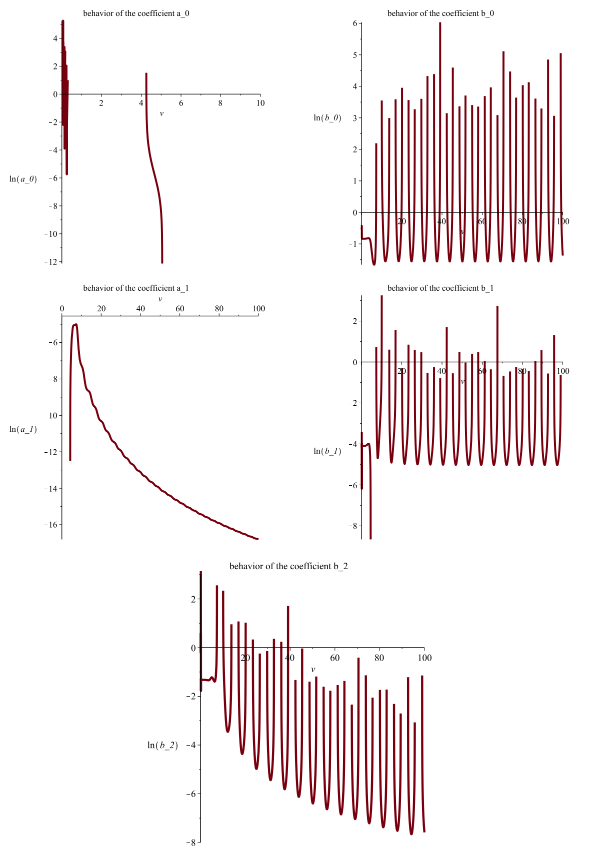

Fig. 1: Behavior of the coefficients of the new proposed method for several values of $v = \phi\, h$.

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

$$LTE_{ExpTwoStepHY10} = -\frac{47563}{3683282803200}\, h^{12} \left(p_n^{(12)} + 5\,\phi^2\, p_n^{(10)} + 10\,\phi^4\, p_n^{(8)} + 10\,\phi^6\, p_n^{(6)} + 5\,\phi^8\, p_n^{(4)} + \phi^{10}\, p_n^{(2)} \right) + O\left(h^{14}\right) \quad (20)$$

We follow the below mentioned procedure :

– Since the formulae of the Local Truncation Errors consists of derivatives of the function p, we the expressions of these derivatives based on the test problem (18). In Appendix we present some of these expressions.
– We produce new formulae of the Local Truncation Errors which are based on the above expressions of the derivatives given in the above step. We note here that the new obtained formulae are dependent on the energy E.
– The previous step of the algorithm leads to expressions of the Local Truncation Error which contain the parameter G (see (18)). We proceed our study taking into account two cases for the parameter G :
  1. Case where $V_c - E = G \approx 0$. Is the case where the Energy and the potential are closed each other. Consequently, the terms in the formulae of the local truncation error which contain powers of G (i.e. which contain $G^n\, n \geq 1$) are approximately equal to zero. Therefore, the expression of the local truncation error is equal with the term which contain only the power of G^0 i.e. which is free from G. Consequently, the local truncation error for the classical method (constant coefficients) - which contains only free from g terms - is equal with the local truncation error of the methods with vanished the phase-lag and its first, second, third and fourth derivatives. This is due to the fact that the expressions of the terms of the local truncation errors which are free from G are the same in this case. Therefore, for these values of G, the methods are of comparable accuracy.
  2. $G >> 0$ or $G << 0$. Then $|G|$ is a large number. The most accurate methods are the methods with expressions of the local truncation error which contain minimum power of G.
– Finally we present the asymptotic expressions of the Local Truncation Errors.

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

4.3 Classical Method

$$LTE_{CL} = -\frac{47563}{3683282803200}\, h^{12} \left(p\,(x)\, G^6 + \cdots \right) + O\left(h^{14}\right) \quad (21)$$

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

$$LTE_{ExpTwoStepHY10} = -\frac{47563}{230205175200}\, h^{12} \left(\frac{d^4}{dx^4}\, g\,(x)\; p\,(x) \right) G^3 + \cdots + O\left(h^{14}\right) \quad (22)$$

From the above equations 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.*

–Eighth 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 Tenth Algebraic Order Method with Vanished Phase-Lag and its First, Second, Third and Fourth Derivatives is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

5 Stability Analysis

Let us consider the scalar test equation for the investigation of the stability of the new proposed hybrid method :

$$p'' = -\omega^2 p. \tag{23}$$

As one can see the above scalar test equation has frequency which is different than the frequency of the scalar test equation for the phase-lag analysis (ϕ) which is investigated above i.e. $\omega \neq \phi$.

Application of the new hybrid method to the scalar test equation (23) leads to the following difference equation:

$$A_1(s,v)\,(p_{n+1} + p_{n-1}) + A_0(s,v)\,p_n = 0 \tag{24}$$

where

$$\begin{aligned} A_1(s,v) &= 1 + s^2 b_1 + \frac{15\,b_0 a_1 s^4}{26} - \frac{3\,s^6 b_0 a_1}{208} \\ &+ \frac{45\,b_0 a_1 s^6 a_0}{13} - \frac{9\,s^8 b_0 a_1 a_0}{104} + \frac{11\,b_2 s^2}{104} + \frac{3\,s^4 b_2}{832} \\ A_0(s,v) &= -2 + s^2 b_0 - \frac{15\,b_0 a_1 s^4}{13} + \frac{63\,s^6 b_0 a_1}{104} \\ &- \frac{90\,b_0 a_1 s^6 a_0}{13} + \frac{189\,s^8 b_0 a_1 a_0}{52} + \frac{93\,b_2 s^2}{52} - \frac{63\,s^4 b_2}{416} \end{aligned}$$

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

We have the following definitions (see for more details within Section 2 of the present paper):

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]. *This 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.*

[1] where S is a set of distinct points

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

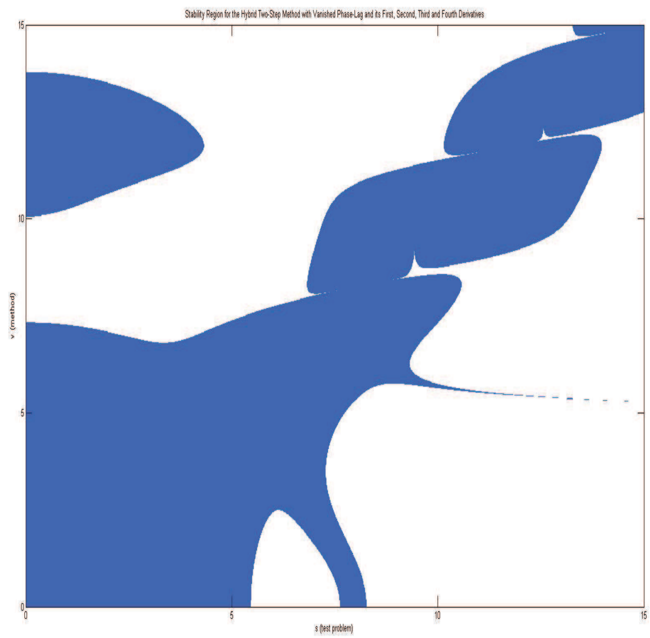

Fig. 2: $s - v$ plane of the new obtained two-step high order method with vanished phase-lag and its first, second, third and fourth derivatives

*Remark.*From the $s - v$ region presented in Figure 2 we can have the following conclusions : (1) The method is stable within the shadowed area, (2) The method is unstable within the white area.

*Remark.*In many real problems in Sciences, Engineering and Technology the corresponding models consist only one frequency. Therefore, in these cases we are interested for the study 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 $\omega = \phi$. For these cases the investigation 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 $s = v$. An example is the Schrödinger equation.

Based on the above remark, we studied the 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 investigate the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s - v$ plane). Consequently, we extract the following result: the new obtained 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 proposed method developed in section 3:*

- *is of tenth algebraic order,*
- *has the phase-lag and its first, second, third and fourth 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

In the literature many techniques have been proposed the last decades for the estimation of the local truncation error (LTE) on the numerical solution of systems of differential equations (see for example [1]-[53]).

Our methodology for the local error estimation technique is based on the algebraic order of the methods and on an embedded pair of multistep methods. More specifically our methodology is based on the fact that the maximum algebraic order of a multistep method produces highly accurate approximate solutions for problems with oscillatory and/or periodical behavior.

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

$$LTE = | y_{n+1}^H - y_{n+1}^L | \tag{25}$$

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

$$h_{n+1} = h_n \left(\frac{acc}{LTE} \right)^{\frac{1}{q}} \tag{26}$$

where q 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.*The local truncation error estimate is based on the lower algebraic order solution y_{n+1}^L. However, if the estimation of the local error is less than acc, we adopt the widely used procedure of performing local extrapolation. Thus, although an estimation of the local error is controlled in lower algebraic order solution y_{n+1}^L, it is the higher algebraic order solution y_{n+1}^H which is accepted at each point.

6.2 Coupled differential equations

In many problems in

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

their mathematical model can be transferred a coupled differential equations of the Schrödinger type.

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

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{27}$$

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

For our numerical tests we consider the case in which all channels are open. So we have the following boundary conditions (see for details [55]):

$$y_{ij} = 0 \ at \ x = 0 \tag{28}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x) \tag{29}$$

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

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

Our investigation is based on the detailed analysis obtained in [55]. 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 (29) as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}'$$

*Remark.*Detailed description on the problem one can find in [55]. There is described one the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation. This is the Iterative Numerov method of Allison [55].

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 [55], 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

$$\left[\frac{d^2}{dx^2} + k^2_{j'j} - \frac{l'(l'+1)}{x^2}\right] y^{Jjl}_{j'l'}(x) =$$

$$\frac{2\mu}{\hbar^2}\sum_{j''}\sum_{l''} < j'l';J \mid V \mid j''l'';J > y^{Jjl}_{j''l''}(x) \qquad (30)$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}] \qquad (31)$$

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 [55], the potential V can be expanded as

$$V(x,\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}), \qquad (32)$$

and the coupling matrix element may then be written as

$$< j'l';J \mid V \mid j''l'';J >= \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l',j''l'';J)V_2(x) \qquad (33)$$

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [56] 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 [57]). The boundary conditions are

$$y^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \qquad (34)$$

$$y^{Jjl}_{j'l'}(x) \sim \delta_{jj'}\delta_{ll'}\exp[-i(k_{jj}x - 1/2l\pi)]$$

$$-\left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl;j'l')\exp[i(k_{j'j}x - 1/2l'\pi)] \qquad (35)$$

where the scattering S matrix is related to the K matrix of (29) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1} \qquad (36)$$

In order to compute the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles we need an algorithm which must include a numerical method for step-by-step integration from the initial value to matching points. The specific algorithm is based on an similar algorithm which has been obtained for the numerical tests of [55].

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

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

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

Table 1: Coupled Differential Equations. Real time of computation (in seconds) (RTC) and maximum absolute error (MErr) to calculate $\mid S \mid^2$ 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	0.16	1.2×10^{-7}
	9	0.448	1.47	4.6×10^{-7}
	16	0.448	10.08	6.5×10^{-7}

As is described in [55], 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 [57] and Allison [55] 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 (34) may be written as

$$y^{Jjl}_{j'l'}(x_0) = 0 \qquad (37)$$

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 [55] which is indicated as **Method I**,
- the variable-step method of Raptis and Cash [54] 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 [58] which is indicated as **Method IV**,
- the new developed embedded two-step method which is indicated as **Method V**

In Table 3 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

In the present paper, we studied a family of tenth algebraic order two-step methods. The main subjects of this investigation was:

1. the study of the elimination of the phase-lag and its first, second and third derivatives
2. the comparative local truncation error analysis
3. the stability analysis with a scalar test equation which uses a frequency different than the frequency used by the scalar test equation for the phase-lag analysis
4. the computational behavior of the new obtained method and its effectiveness on the numerical solution of the coupled Schrödinger equations.

Based on the above mentioned results, it is easy for one to see the efficiency of the new produced method for the numerical 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 p_n

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

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

$$
\begin{aligned}
p_n^{(7)} &= \left(\frac{d^5}{dx^5} g(x)\right) p(x) + 5 \left(\frac{d^4}{dx^4} g(x)\right) \frac{d}{dx} p(x) \\
&\quad + 11 (g(x)+G) p(x) \frac{d^3}{dx^3} g(x) + 15 \left(\frac{d}{dx} g(x)\right) p(x) \\
&\quad \frac{d^2}{dx^2} g(x) + 13 (g(x)+G) \left(\frac{d}{dx} p(x)\right) \frac{d^2}{dx^2} g(x) \\
&\quad + 10 \left(\frac{d}{dx} g(x)\right)^2 \frac{d}{dx} p(x) + 9 (g(x)+G)^2 p(x) \\
&\quad \frac{d}{dx} g(x) + (g(x)+G)^3 \frac{d}{dx} p(x)
\end{aligned}
$$

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

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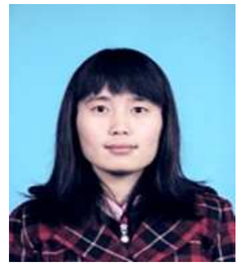

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