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A low computational cost eight algebraic order hybrid method with vanished phase-lag and its first, second, third and fourth derivatives for the approximate solution of the Schrödinger equation

Hang Ning[1] · **T. E. Simos[2,3,4]**

Abstract A low computational cost eighth algebraic order hybrid two-step method with vanished phase-lag and its first, second, third and fourth derivatives is developed in this paper. We also investigate the local truncation error, the stability and the result of the elimination of the phase-lag and its derivatives on the effectiveness of the produced method.

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✉ T. E. Simos
  tsimos.conf@gmail.com

  Hang Ning
  ninghang@chd.edu.cn

1 School of information engineering, Chang'an University, Xi'an 710064, China

2 Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia

3 Laboratory of Computational Sciences, Department of Informatics and Telecommunications, Faculty of Economy, Management and Informatics, University of Peloponnese, 221 00 Tripolis, Greece

4 10 Konitsis Street, Amfithea - Paleon Faliron, 175 64 Athens, Greece

1 Introduction

In this paper we study the numerical solution of special second order initial value problems of the form:

$$y''(x) = f(x, y), \quad y(x_0) = y_0 \ and \ y'(x_0) = y'_0 \tag{1}$$

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

A characteristic of the problems of the form (1) is that the models of such problems consist of systems of second order ordinary differential equations from which the first derivative y' does not appear explicitly.

Our basic idea is to introduce a hybrid method (multistage) with low number of stages which has very important properties: (1) high algebraic order (2) vanished phase-lag and (3) vanished derivatives of the phase-lag. More specifically in this paper we introduce a two-step three stage method of eighth algebraic order with vanished phase-lag and its first, second, third and fourth derivatives. With this procedure we avoid the Runge–Kutta or Runge–Kutta–Nyström or Hybrid multistep methods which in order to achieve the abo0ve mentioned properties need much more stages and/or steps (see [52]) and therefore much more computational cost. The method is of low computational cost since it is of only three stages.

The paper has the following form: The basic theory on the phase-lag analysis and the direct formula for the computation of the phase0-lag of symmetric multistep methods are presented in Sect. 2. In Sect. 3 we present the construction of the new hybrid eighth algebraic order two-step method with vanished phase-lag and its first, second, third and fourth derivatives. The error is studied in Sect. 4. More specifically, in this section the local truncation error (LTE) of the new method is investigated using a model problem. A comparative LTE analysis is also presented using other similar methods of the literature. In Sect. 5 we study the stability of the new proposed method. More precisely, in this section we define the stability area and the interval of periodicity of the new produced method using a scalar test equation with frequency different than the frequency of the scalar test equation used for the phase-lag analysis. The procedure of the Local Error estimation is presented in Sect. 6.1. The Local Error Estimation is based on similar methods with different algebraic order. The numerical solution of the coupled differential equations arising from the Schrödinger equation is presented in Sect. 6.2. Finally, conclusions are presented in Section.

Remark 1 It is noted that the approximate 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 Theory of the phase-lag analysis for symmetric $2k$-step methods

Let us consider the $2k$-Step methods

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

for the approximate solution of the initial value problem (1). The numerical solution of the initial value problem (1) is based on the division of the are of integration $[a, b]$ into $2k$ equally spaced intervals i.e. $\{x_i\}_{i=-k}^k \in [a, b]$. The procedure we use continues with the application of the method (2) within these intervals. The are of integration $[a, b]$ is defined based on the physical properties of the specific problem. The quantity h is defined as $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$ and is called stepsize of integration. The multistep method given by (2) is called $2k$-step method since the number of steps, which are used for the integration, is equal to $2k$.

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

Remark 3 The linear operator, which is associated with the Multistep Method (2), is given by:

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

where $y \in C^2$.

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 $1, x, x^2, \ldots, x^{m+1}$.

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

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

leads to the following difference equation:

$$A_k(v)\, y_{n+k} + \cdots + A_1(v)\, y_{n+1} + A_0(v)\, y_n + A_1(v)\, y_{n-1} + \cdots + A_k(v)\, y_{n-k} = 0 \tag{5}$$

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

The associated characteristic equation to the difference Eq. (5) is given by:

$$A_k(v)\, \lambda^k + \cdots + A_1(v)\, \lambda + A_0(v) + A_1(v)\, \lambda^{-1} + \cdots + A_k(v)\, \lambda^{-k} = 0. \tag{6}$$

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 λ_i, $i = 1(1)2m$ of Eq. (6) satisfy:

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

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

Definition 3 [14,15] For any symmetric multistep method which is associated to the characteristic Eq. (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] A method is called **phase-fitted** if the phase-lag is vanished (i.e. equal to zero).

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

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

where $P_0 = 2\,A_k(v)\,\cos(k\,v) + \cdots + 2\,A_j(v)\,\cos(j\,v) + \cdots + A_0(v)$ *and* $P_1 = 2\,k^2\,A_k(v) + \cdots + 2\,j^2\,A_j(v) + \cdots + 2\,A_1(v)$.

Remark 4 The formula (9) must be used for the direct calculation of the phase-lag for any symmetric $2\,k$-step multistep method.

Remark 5 In our investigation we use symmetric two-step methods. Assuming that their characteristic polynomials are given by $A_j(v)\ j = 0, 1$, the phase-lag of order q with phase-lag constant c are given by:

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

3 The low computational cost new proposed eighth algebraic order hybrid two-step method with vanished phase-lag and its first, second, third and fourth derivatives

Consider the hybrid family of two-step methods

$$\widehat{y}_{n+\frac{1}{2}} = \frac{1}{52}\left(3\,y_{n+1} + 20\,y_n + 29\,y_{n-1}\right)$$
$$+ \frac{h^2}{4992}\left(41\,f_{n+1} - 682\,f_n - 271\,f_{n-1}\right)$$
$$\widehat{y}_{n-\frac{1}{2}} = \frac{1}{104}\left(5\,y_{n+1} + 146\,y_n - 47\,y_{n-1}\right)$$
$$+ h^2\left(-\frac{59}{4992}\,f_{n+1} + a_0\,f_n + \frac{253}{4992}\,f_{n-1}\right)$$
$$y_{n+1} + a_1\,y_n + y_{n-1} = h^2\left[b_1\,(f_{n+1} + f_{n-1}) + b_0\,f_n + b_2\left(\widehat{f}_{n+\frac{1}{2}} + \overline{f}_{n-\frac{1}{2}}\right)\right] \tag{11}$$

where $f_i = y''(x_i, y_i)$, $i = -1\left(\frac{1}{2}\right)1$ 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:

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

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

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

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

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

where

$$
\begin{aligned}
T_0 = T_0 &= 2\left(1 + v^2\left(b_1 + b_2\left(\frac{11}{104} + \frac{3\,v^2}{832}\right)\right)\right)\cos(v) \\
&\quad + a_1 + v^2\left(b_0 + b_2\left(\frac{93}{52} + \frac{341\,v^2}{2496} - v^2 a_0\right)\right) \\
T_1 &= 1 + v^2\left(b_1 + b_2\left(\frac{11}{104} + \frac{3\,v^2}{832}\right)\right)
\end{aligned}
$$

Solving the above system of Eqs. (12)–(16), we obtain the coefficients of the new developed low cost hybrid method: a_0, a_1, b_0, b_1, b_2. For the cases that the formulae of the coefficients are subject to heavy cancelations 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), Taylor series expansions should be used.

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

The LTE of the new cost method (11) (mentioned as $ExpTwoStepLCH8$) is given by:

$$
\begin{aligned}
LTE_{ExpTwoStepLCH8} &= \frac{59}{76204800}\,h^{10}\left(y_n^{(10)} + 5\,\phi^2\,y_n^{(8)} + 10\,\phi^4\,y_n^{(6)} + 10\,\phi^6\,y_n^{(4)}\right. \\
&\quad \left. + 5\,\phi^8\,y_n^{(2)} + \phi^{10}\,y_n\right) + O\left(h^{14}\right)
\end{aligned}
\tag{17}
$$

4 Local truncation error analysis

In this section we will investigate the behavior of the Local Truncation Error. We will use the test problem

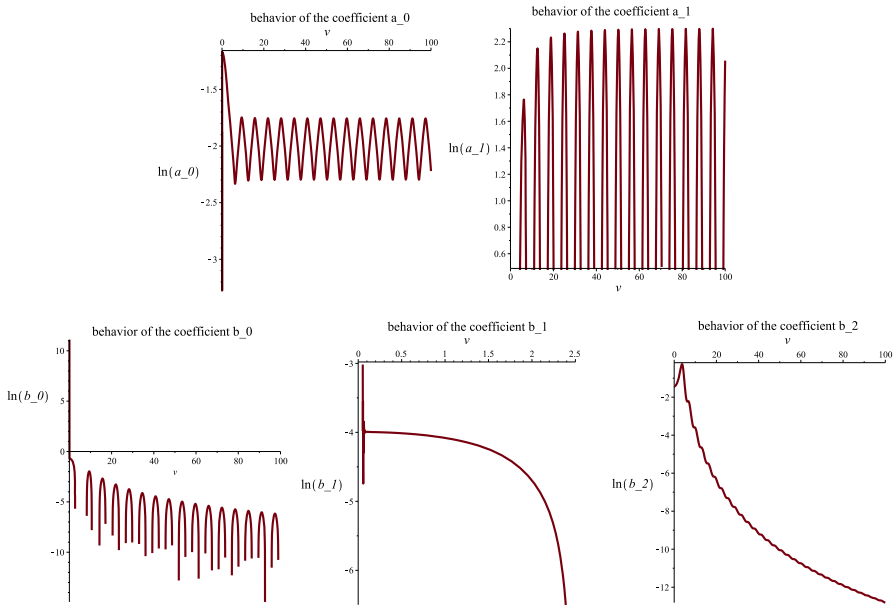$$y''(x) = (V(x) - V_c + G)\,y(x) \tag{18}$$

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

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 study the LTE of the following methods:

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

$$LTE_{CL} = \frac{59}{76204800} h^{10} y_n^{(10)} + O\left(h^{14}\right) \qquad (19)$$

4.2 The new proposed method with vanished phase-lag and its first, second, third and fourth derivatives produced in Sect. 3

$$LTE_{ExpTwoStepLCH8} = \frac{59}{76204800} h^{10} \left(y_n^{(10)} + 5\phi^2 y_n^{(8)} + 10\phi^4 y_n^{(6)} \right.$$
$$\left. + 10\phi^6 y_n^{(4)} + 5\phi^8 y_n^{(2)} + \phi^{10} y_n \right) + O\left(h^{14}\right) \quad (20)$$

Below we describe our analysis:

– Since the formulae of the LTE consist of the derivatives of the function y, we compute the expressions of these derivatives based on the test problem (18). Some of the expressions of the derivatives of the function y are given in the "Appendix".

– The new formulae of the LTE are based on the expressions of the derivatives of the function y given in the "Appendix" and are dependent on the quantity G and energy E.
– Our study is based on two cases for the parameter G:
   1. First case: $V_c - E = G \approx 0$. This means that the Energy and the Potential are closed each other. Therefore, all the terms of $G^n\ n \geq 1$ are approximately equal to zero. Consequently, all the terms in the formulae of the LTE which contain $G^n\ n \geq 1$ are approximately equal to zero. Therefore, for this case the LTE is equal with the term which contain only the power of G^0 i.e. which contain free from G terms. Since the free from G term of the LTE formula for the classical method (constant coefficients) is equal with the free from G term of the local truncation error formula for the methods with vanished the phase-lag and its first, second, third and fourth derivatives, the asymptotic behavior of the LTE for the classical method and the asymptotic behavior of the LTE for the methods with vanished the phase-lag and its first, second, third and fourth derivatives is the same. Consequently, for these values of G, the methods are of comparable accuracy.
   2. $G >> 0$ or $G << 0$. Consequently, $|G|$ is a large number. Therefore, the most accurate methods are the methods with formula of the LTE which contain minimum power of G.
– Finally the asymptotic expressions of the LTEs are presented.

The following asymptotic expansions of the LTEs are obtained based on the analysis presented above:

4.3 Classical method

$$LTE_{CL} = \frac{59}{4762800} h^{10} \left(y(x)\, G^5 + \cdots \right) + O\left(h^{12}\right) \tag{21}$$

4.4 The new proposed method with vanished phase-lag and its first, second, third, fourth and fifth derivatives produced in Sect. 3

$$LTE_{ExpTwoStepLCH8}$$
$$= \frac{59}{76204800} h^{10} \left(\left(\frac{d^4}{dx^4} g(x) \right) y(x)\, G^2 + \cdots \right) + O\left(h^{12}\right) \tag{22}$$

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 fifth power of G.*
– *Low Cost Eighth Algebraic Order Two-Step Method with Vanished Phase-lag and its First, Second, Third and Fourth Derivatives developed in Sect. 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 LOw Cost Eighth 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

In this section we will investigate the stability properties of the new obtained hybrid method.

Let us consider the following scalar test equation:

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

Remark 6 The frequency of the scalar test equation for the stability analysis (ω) is different from the frequency of the scalar test equation used for the phase-lag analysis (ϕ) i.e. $\omega \neq \phi$.

Applying the new produced hybrid method to the scalar test Eq. (23) the following difference equation is obtained:

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

where

$$A_1(s, v) = 1 + s^2 \left(b_1 + \frac{11 b_2}{104} \right) + \frac{3 b_2}{832} s^4$$

$$A_0(s, v) = a_1 + s^2 \left(b_0 + \frac{93 b_2}{52} \right) - s^4 \left(a_0 b_2 - \frac{341}{2496} b_2 \right) \tag{25}$$

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

We have the following definitions:

Definition 5 (see [16]) A multistep method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Definition 6 A multistep method with interval of periodicity equal to $(0, \infty) - S$ [1] is called singularly almost P-stable .

Remark 7 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 Fig. 2.

Remark 8 Based on the $s-v$ region presented in Fig. 2: (1) The method is stable within the shadowed area, (2) The method is unstable within the white area.

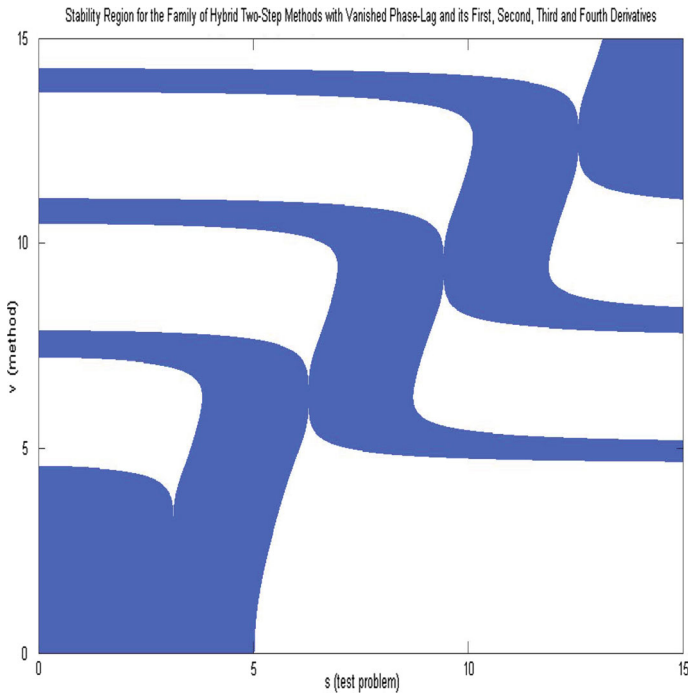[1] where S is a set of distinct points

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

Remark 9 Since the models of many real problems in Sciences, Engineering and Technology (for example the Schrödinger equation) consist only one frequency in the their model, we are interested for the study of the stability of the proposed methods 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 i.e. when $\omega = \phi$. Consequently, in these 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 studied the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s-v$ plane). For our obtained method the interval of periodicity is equal to: $(0, \infty)$, i.e. is P-stable.

The above investigation leads to the following theorem:

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

– *is of eighth 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*
– *is low computational cost since has only 3 stages.*

6 Numerical results

6.1 Error estimation

In order to approximate the solution of a problem using variable-step algorithms, an error estimation procedure is necessary. Much research has been done the last decades on the estimation of the LTE for the numerical solution of systems of differential equations (see for example [1–56]).

In the literature there are several methodologies for the local error estimation. One of the most useful is the one which is based on the algebraic order of the methods. The results of the methodologies for the local error estimation is an embedded pair. Our embedded pair of multistep methods is based on the algebraic order and on the fact that the maximum algebraic order of a multistep method produces highly accurate numerical solutions for oscillatory and/or periodical problems.

The LTE in y_{n+1}^L is estimated by

$$LTE = \mid y_{n+1}^H - y_{n+1}^L \mid \tag{26}$$

y_{n+1}^L denotes the lower order solution and we use for this the method developed in [57], which is of sixth algebraic order and y_{n+1}^H denotes the higher order solution and we use for this the method obtained in this paper, which is of eighth algebraic order.

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

$$h_{n+1} = h_n \left(\frac{acc}{LTE} \right)^{\frac{1}{p}} \tag{27}$$

where p is the algebraic order of the method, h_n is the step length used for the nth step and acc is the requested accuracy of the local error.

Remark 10 Our technique for the LTE estimation is based on the lower algebraic order solution y_{n+1}^L. The procedure of performing local extrapolation is used in our numerical tests. Therefore, we accept at each point the higher algebraic order solution y_{n+1}^H while the local error is controlled in lower algebraic order solution y_{n+1}^L for an estimation of the local error less than acc.

6.2 Coupled differential equations

There are lot of problems in

– quantum chemistry,
– material science,
– theoretical physics,
– atomic physics,
– physical chemistry,

– theoretical chemistry and
– 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:

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{28}$$

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

We will investigate the case in which all channels are open. Therefore, we have the following boundary conditions: (see for details [59]):

$$y_{ij} = 0 \ at \ x = 0 \tag{29}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x) \delta_{ij} + \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x) \tag{30}$$

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

Remark 11 We note here that the new obtained low cost method can also be used for the case of closed channels.

The detailed analysis presented in [59] is our guideline for our application. 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 (30) as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K'} \tag{31}$$

Remark 12 The detailed presentation of the problem can be found in [59]. In the same paper the well know Iterative Numerov method of Allison is also described.

The mathematical model of the real problem of rotational excitation of a diatomic molecule by neutral particle impact can be transferred into 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 [59], 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

$$\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2}\right] y_{j'l'}^{Jjl}(x)$$

$$= \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} < j'l'; \quad J \mid V \mid j''l''; \quad J > y_{j''l''}^{Jjl}(x) \qquad (32)$$

where

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

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 [59], 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. [60] 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 [61]). The boundary conditions are

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

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

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

where the scattering S matrix is related to the K matrix of (30) by the relation

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

In order to compute the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles, an algorithm which includes a numerical method for step-by-step integration from the initial value to matching points is needed. We use an algorithm which is based on the similar algorithm which has been produced for the numerical tests of [59].

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

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

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

Table 1 Coupled differential equations

Method	N	h_{max}	RTC	M_{Err}
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	0.08	1.1×10^{-7}
	9	0.448	1.19	2.3×10^{-7}
	16	0.448	8.52	3.6×10^{-7}

Real time of computation (in seconds) (RTC) and maximum absolute error (M_{Err}) 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

As is described in [59], 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 [61] and Allison [59] 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

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

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 [59] which is indicated as **Method I**,
– the variable-step method of Raptis and Cash [58] which is indicated as **Method II**,
– the embedded Runge–Kutta Dormand and Prince method 5(4) [51] which is indicated as **Method III**,
– the embedded Runge–Kutta method ERK4(2) developed in Simos [62] which is indicated as **Method IV**,
– the new obtained low cost 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 low computational cost eighth algebraic order hybrid two-step methods was studied in the present paper. More specifically:

1. we investigated the vanishing of the phase-lag and its first, second, third and fourth derivatives
2. we investigated the comparative LTE analysis
3. we studied the stability properties of the new low cost 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 investigated the computational behavior of the new produced method and its efficiency on the numerical solution of the coupled differential equations arising from 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).

Conflict of interest　The authors declare that they have no conflict of interest.

Ethical standard Consent to submit has been received explicitly from all co-authors, as well as from the responsible authorities—tacitly or explicitly—at the institute/organization where the work has been carried out, before the work is submitted.

8 Appendix: Formulae of the derivatives of q_n

Formulae of the derivatives which presented in the formulae of the LTEs:

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

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

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

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

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

$$+ 6 \left(g\left(x\right) + G\right) \left(\frac{d}{dx} y\left(x\right)\right) \frac{d}{dx} g\left(x\right) + \left(g\left(x\right) + G\right)^3 y\left(x\right)$$

$$y_n^{(7)} = \left(\frac{d^5}{dx^5} g\left(x\right)\right) y\left(x\right) + 5 \left(\frac{d^4}{dx^4} g\left(x\right)\right) \frac{d}{dx} y\left(x\right)$$

$$+ 11 \left(g\left(x\right) + G\right) y\left(x\right) \frac{d^3}{dx^3} g\left(x\right) + 15 \left(\frac{d}{dx} g\left(x\right)\right) y\left(x\right) \frac{d^2}{dx^2} g\left(x\right)$$

$$+ 13 \left(g\left(x\right) + G\right) \left(\frac{d}{dx} y\left(x\right)\right) \frac{d^2}{dx^2} g\left(x\right)$$

$$+ 10 \left(\frac{d}{dx} g\left(x\right)\right)^2 \frac{d}{dx} y\left(x\right) + 9 \left(g\left(x\right) + G\right)^2 y\left(x\right) \frac{d}{dx} g\left(x\right)$$

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

$$y_n^{(8)} = \left(\frac{d^6}{dx^6} g\left(x\right)\right) y\left(x\right) + 6 \left(\frac{d^5}{dx^5} g\left(x\right)\right) \frac{d}{dx} y\left(x\right)$$

$$+ 16 \left(g\left(x\right) + G\right) y\left(x\right) \frac{d^4}{dx^4} g\left(x\right) + 26 \left(\frac{d}{dx} g\left(x\right)\right) y\left(x\right) \frac{d^3}{dx^3} g\left(x\right)$$

$$+ 24 \left(g\left(x\right) + G\right) \left(\frac{d}{dx} y\left(x\right)\right) \frac{d^3}{dx^3} g\left(x\right)$$

$$+ 15 \left(\frac{d^2}{dx^2} g\left(x\right)\right)^2 y\left(x\right) + 48 \left(\frac{d}{dx} g\left(x\right)\right) \left(\frac{d}{dx} y\left(x\right)\right) \frac{d^2}{dx^2} g\left(x\right)$$

$$+ 22 \left(g\left(x\right) + G\right)^2 y\left(x\right) \frac{d^2}{dx^2} g\left(x\right) + 28 \left(g\left(x\right) + G\right) y\left(x\right) \left(\frac{d}{dx} g\left(x\right)\right)^2$$

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

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