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ORIGINAL PAPER

A Runge–Kutta type implicit high algebraic order two-step method with vanished phase-lag and its first, second, third and fourth derivatives for the numerical solution of coupled differential equations arising from the Schrödinger equation

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Abstract A Runge–Kutta type (four stages) eighth algebraic order two-step method with phase-lag and its first, second, third and fourth derivatives equal to zero is produced in this paper. We also study the results of elimination of the phase-lag and its derivatives on the efficiency of the method. Our studies consist: (1) the construction of the method, (2) the determination of the local truncation error of the proposed method, (3) the investigation of the local truncation error analysis using the comparison with other similar methods of the literature, (4) the computation of the interval of periodicity (stability interval) of the developed method. For this calculation we use a scalar test equation with frequency different than the frequency of the scalar test equation used

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for the phase-lag analysis, (5) the definition of the error estimation based on methods with different algebraic orders and (6) the investigation of the effectiveness of the new obtained method studying the numerical solution of the coupled differential equations arising from the Schrödinger equation.

Keywords Schrödinger equation · Multistep methods · Interval of periodicity · Phase-lag · Phase-fitted · Derivatives of the phase-lag

Mathematics Subject Classification 65L05

1 Introduction

A new Runge–Kutta type two-step four stages method is developed in this paper. The highlights of the new method are the following:

1. The method is of two-step
2. The method is of eighth algebraic order
3. The method has vanished its phase-lag
4. The method has vanished its first, second, third and fourth derivatives of the phase-lag

In order to develop a high algebraic order finite difference method the following characteristics must hold: (1) the method must have many steps, (2) the method must have many stages or (3) the method must have many steps and many stages (see [52]). This specific procedure to produce high algebraic order finite difference methods has as result the following:

– increase the computational time and
– increase the instabilities of the method. The reason for this is that in order the multistep methods to be applied on a problem, they need at the beginning the application of unstable methods (for problems with periodical and/or oscillating solutions) like Runge–Kutta or Runge–Kutta–Nystöm methods.

The above creates serious computational difficulties. Consequently, if we apply the above mentioned multistep methods to problems with periodical and/or oscillating solutions, then computational cost is large and the accuracy is small. These problems are solved with the proposed family of methods since they are two-step methods.

The approximate solution of special second order initial value problems with periodical and/or oscillating solutions of the form:

$$y''(x) = f(x, y), \quad y(x_0) = q_0 \quad and \quad y'(x_0) = y'_0 \tag{1}$$

will be studied in this paper.

The above mentioned problems consist of systems of ordinary differential equations of second order in which the first derivative y' does not appear explicitly.

2 Phase-lag for symmetric multistep finite difference methods

For the numerical solution of the initial value problem (1) let us consider the multistep methods

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

We have the following remarks:

1. In order the above mentioned method (2) to be applied for the solution of the problem of the form (1), we have to follow the algorithm
   - We define the integration area: $[a, b]$
   - We divide the above integration are into m equally spaced intervals i.e. $\{x_i\}_{i=-m}^{m} \in [a, b]$.
2. The quantity h is called stepsize of integration and is given by $h = |x_{i+1} - x_i|$, $i = 1 - m(1)m - 1$.
3. The number of steps of the specific used multistep method (2) is equal to $2\,m$. Based on this, the specific method can be called $2\,m$-step method.

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

Remark 2 The linear operator

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

is associated with the multistep method (2), where $y \in C^2$.

Definition 1 [1] The multistep method (2) is called of algebraic 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 $2\,m$-step method, $[(i = -m(1)m]$, to the scalar test equation

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

the following difference equation is produced:

$$\begin{aligned} &A_m(v) \, y_{n+m} + \cdots + A_1(v) \, y_{n+1} + A_0(v) \, y_n \\ &+A_1(v) \, y_{n-1} + \cdots + A_m(v) \, y_{n-m} = 0 \end{aligned} \tag{5}$$

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

There is a characteristic equation associated with (5) which is given by:

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

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

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

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

Definition 3 [14,15] The symmetric multistep method with characteristic equation given by (6) has phase-lag which is equal to 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] **Phase-fitted** is called a method if its phase-lag is equal to zero.

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

$$-cv^{q+2} + O(v^{q+4}) = \frac{2A_m(v)\cos(mv) + \cdots + 2A_j(v)\cos(jv) + \cdots + A_0(v)}{2m^2 A_m(v) + \cdots + 2j^2 A_j(v) + \cdots + 2A_1(v)}. \tag{9}$$

Remark 3 In order to calculate the phase-lag for any symmetric $2m$-step multistep method we use the formula (9).

Remark 4 In our study the investigated method is a symmetric two-step method with characteristic polynomials $A_j(v)\ j = 0, 1$. For this case the phase-lag of order q and the phase-lag constant c are given by:

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

3 The new high algebraic order four-stages two-step method with vanished phase-lag and its first, second, third and fourth derivatives

Let us consider the family of two-step four-stages hybrid methods

$$\begin{aligned}
\widehat{y}_{n+\frac{1}{2}} &= \frac{1}{52}\left(3y_{n+1} + 20y_n + 29y_{n-1}\right) \\
&\quad + \frac{h^2}{4992}\left(41f_{n+1} - 682f_n - 271f_{n-1}\right) \\
\widehat{y}_{n-\frac{1}{2}} &= \frac{1}{104}\left(5y_{n+1} + 146y_n - 47y_{n-1}\right) \\
&\quad + \frac{h^2}{4992}\left(-59f_{n+1} + 1438f_n + 253f_{n-1}\right)
\end{aligned}$$

$$\widetilde{y}_n = y_n - a_0\, h^2 \left(f_{n+1} - 4\, \widehat{f}_{n+\frac{1}{2}} + 6\, f_n - 4\, \widehat{f}_{n-\frac{1}{2}} + f_{n-1} \right)$$
$$y_{n+1} + a_1\, y_n + y_{n-1} = h^2 \left[b_1\, (f_{n+1} + f_{n-1}) + b_0\, \widetilde{f}_n + b_2 \left(\widehat{f}_{n+\frac{1}{2}} + \overline{f}_{n-\frac{1}{2}} \right) \right] \tag{11}$$

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.

We require the above mentioned Runge–Kutta type method (11) to have the phase-lag and its first, second, third and fourth derivatives equal to zero (vanishing). Therefore the following system of equations is obtained:

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

$$\text{First Derivative of the Phase-Lag} = \frac{\partial PL}{\partial v} = \frac{T_2}{T_3^2} = 0 \tag{13}$$

$$\text{Second Derivative of the Phase-Lag} = \frac{\partial^2 PL}{\partial v^2} = \frac{T_4}{T_3^3} = 0 \tag{14}$$

$$\text{Third Derivative of the Phase-Lag} = \frac{\partial^3 PL}{\partial v^3} = \frac{T_5}{T_3^4} = 0 \tag{15}$$

$$\text{Fourth Derivative of the Phase-Lag} = \frac{\partial^4 PL}{\partial v^4} = \frac{T_6}{T_3^5} = 0 \tag{16}$$

where $T_j,\ j = 0(1)6$ are given in the Supplementary Material A.

Solving the above mentioned system of Eqs. (12)–(16), we produce the coefficients of the new Runge–Kutta type method:

$$a_0 = \frac{C_0}{C_1}, a_1 = -2\frac{C_2}{C_3}, b_0 = 2\frac{C_4}{C_5},$$
$$b_1 = -\frac{1}{3}\frac{C_6}{C_5}, b_2 = \frac{C_7}{3\,C_5} \tag{17}$$

where $C_i, i = 0(1)7$ are given in the Supplementary Material B.

In the case that the formulae given by (17) are subject to heavy cancellations for some values of $|v|$ (for example in the case of values of $|v|$ for which the denominators are near to zero), the following Taylor series expansions should be used:

$$a_0 = -\frac{2}{10647} + \frac{157\, v^2}{1107288} + \frac{590687\, v^4}{86454832464} + \frac{43086809\, v^6}{157347795084480} - \frac{1036316339\, v^8}{717977988970482240} - \frac{39143150250741937\, v^{10}}{2932279545194567106739200} - \frac{94019173388684460139\, v^{12}}{15818123360961188836596247961600}$$

$$
\begin{aligned}
&-\frac{11372461693281782110 3\, v^{14}}{10281780184624772437875611750400 0}\\
&+\frac{36651352989939160754555070 7\, v^{16}}{22156750997841670314362875593237381120 00}\\
&+\frac{19650488117650172404549698066 7\, v^{18}}{12097586044821551991642130073907610091520000}+\cdots\\
a_1 = &-2+\frac{157\, v^{10}}{204422400}+\frac{47563\, v^{12}}{736656560640}+\frac{48493\, v^{14}}{191530705766400}\\
&-\frac{14204527\, v^{16}}{89636370298675200}-\frac{231159834331\, v^{18}}{16640095782246064128000}+\cdots\\
b_0 = &\frac{13}{30}-\frac{157\, v^4}{212940}-\frac{180137\, v^6}{30694023360}+\frac{363877\, v^8}{591144153600}\\
&-\frac{13398973909\, v^{10}}{130719706685568000}+\frac{9936070831\, v^{12}}{86667165532531584000}\\
&+\frac{24264863264944987\, v^{14}}{79119495420634473412608000}+\frac{10558982561489\, v^{16}}{770644435915270844928000}\\
&+\frac{485800042795331629003\, v^{18}}{10333259284320208258001525145600 00}+\cdots\\
b_1 = &\frac{1}{60}-\frac{157\, v^4}{1277640}-\frac{2066021\, v^6}{184164140160}-\frac{25084351\, v^8}{95765352883200}\\
&+\frac{436520401\, v^{10}}{24509945003544000}+\frac{2463906123857\, v^{12}}{1040005986390379008000}\\
&+\frac{66668435065236689\, v^{14}}{47471697252380684047564800 0}+\frac{125226903741859\, v^{16}}{50862532770407875765248000}\\
&-\frac{1203054206829187705 57\, v^{18}}{33817939475957045208004991385600 0}+\cdots\\
b_2 = &\frac{4}{15}+\frac{157\, v^4}{319410}+\frac{81451\, v^6}{5755129380}-\frac{1680923\, v^8}{855047793600}\\
&-\frac{2720580749\, v^{10}}{19607956002835200}-\frac{290279697863\, v^{12}}{65000374149398688000}\\
&+\frac{55199831330671\, v^{14}}{74174526956844818824320 0}+\frac{350653779619001\, v^{16}}{12715633192601968941312000}\\
&+\frac{1200828519750605415419\, v^{18}}{58124583474301171451258578944000 0}+\cdots
\end{aligned}
\tag{18}
$$

The behavior of the coefficients of the proposed method is presented in Fig. 1.

In the following we present the local truncation error of the new developed Runge–Kutta type method (11) (mentioned as $ExpTwoStepRKT10$) with the coefficients given by (17)–(18):

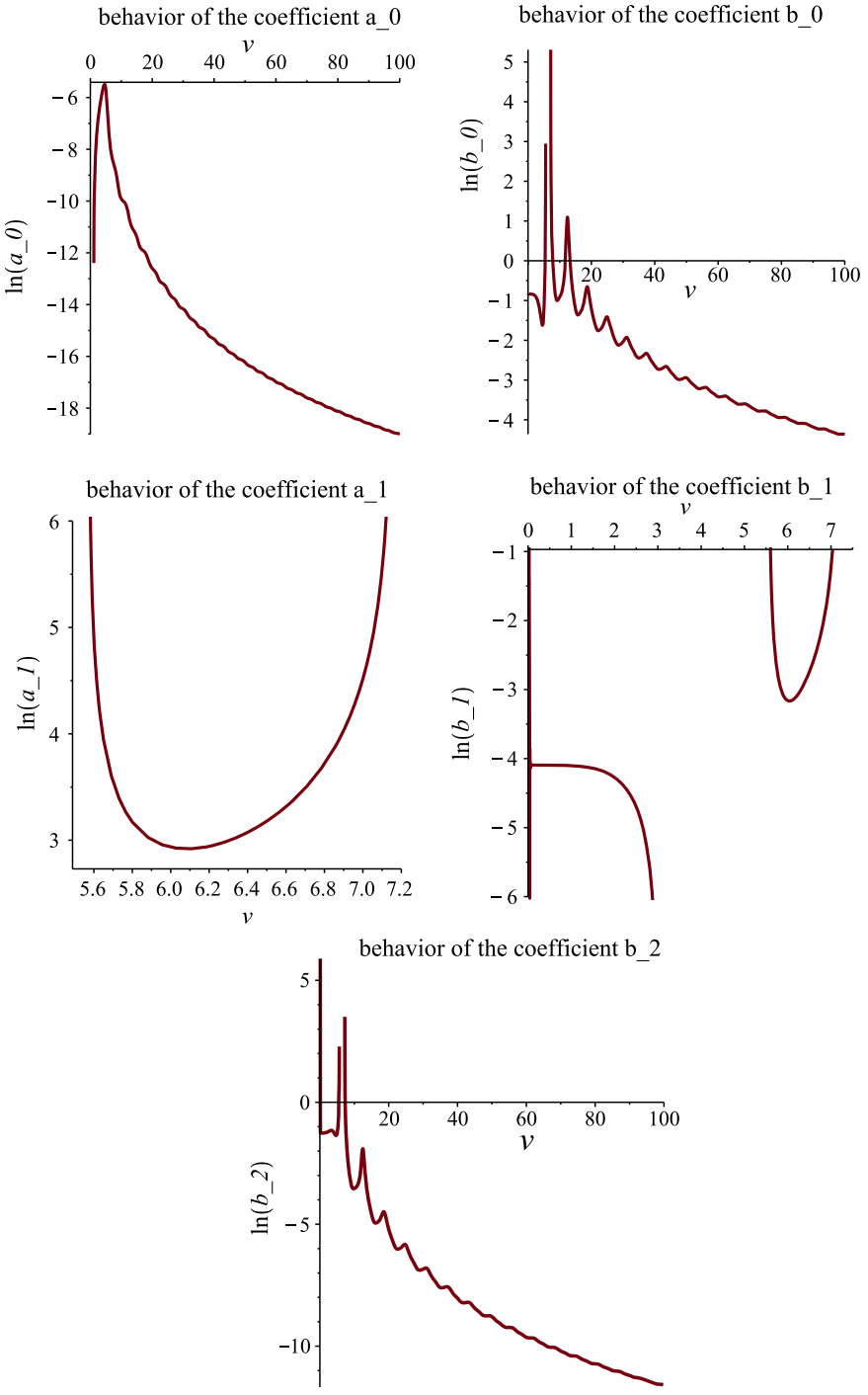

Fig. 1 Behavior of the coefficients of the new proposed method given by (17) for several values of $v = \phi h$

$$LTE_{ExpTwoStepRKT10} = \frac{157}{204422400} h^{10} \left(y_n^{(10)} + 5\phi^2 y_n^{(8)} + 10\phi^4 y_n^{(6)} + 10\phi^6 y_n^{(4)} + 5\phi^8 y_n^{(2)} + \phi^{10} y_n \right) + O\left(h^{12}\right) \quad (19)$$

4 Comparative local truncation error analysis

In order to study the asymptotic behavior of the local truncation error we consider the following test problem

$$y''(x) = (V(x) - V_c + G)\ y(x) \quad (20)$$

where

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

$$LTE_{CL} = \frac{157}{204422400} h^{10} y_n^{(10)} + O\left(h^{14}\right) \quad (21)$$

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

$$LTE_{ExpTwoStepRKT10} = \frac{157}{204422400} h^{10} \left(y_n^{(10)} + 5\phi^2 y_n^{(8)} + 10\phi^4 y_n^{(6)} + 10\phi^6 y_n^{(4)} + 5\phi^8 y_n^{(2)} + \phi^{10} y_n \right) + O\left(h^{12}\right) \quad (22)$$

The investigation is based on the following procedure:

- In order to calculate the formulae of the local truncation errors (*LTE*) we have to compute the derivatives of the function y which consists of *LTE*. We present the expressions of these derivatives, which are based on the test problem (20), in the Supplementary Material C.
- Based on the previous step new formulae, which are dependent on the energy E and parameter G [(see (20)], of the local truncation errors are produced.

– Our investigation is proceeded taking into account two cases for the parameter G:
  1. First case: $V_c - E = G \approx 0$. By definition this case means that the energy and the potential are closed each other. Consequently in this case $G \approx 0$ and therefore all the terms in the formulae of the local truncation error which contain powers of G (i.e. which contain G^j $j \geq 1$) are approximately equal to zero. Consequently, the only non zero expression in the formulae of the local truncation error is the expression which contain only the power of G^0 i.e. which is free from G. Therefore, 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. The reason for this is that the expressions of the terms of the local truncation errors which are free from G are the same in both cases of methods (the classical and this with vanished phase-lag and its derivatives). Therefore, for these values of G, the methods are of comparable accuracy.
  2. Second case: $G >> 0$ or $G << 0$. Then $|G|$ is a large number. It is easy to see that the most accurate methods are those 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

$$LTE_{CL} = \frac{157}{204422400} h^{10} \left(y(x)\ G^5 + \cdots \right) + O\left(h^{12}\right) \tag{23}$$

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

$$LTE_{ExpTwoStepRKT10} = \frac{157}{12776400} h^{10} \left(\frac{\mathrm{d}^4}{\mathrm{d}x^4} g(x)\, y(x) \right) G^2 + \cdots + O\left(h^{12}\right) \tag{24}$$

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 fifth power of G.*
– *Eighth algebraic order two-step method with vanished phase-lag and its first, second and third 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 proposed 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

For our investigation on the stability of the new proposed methods, we consider the scalar test equation:

$$y'' = -\omega^2 y. \tag{25}$$

with frequencies $\omega \neq \phi$. We note that ϕ was the frequency for the scalar test equation for the phase-lag analysis (see Eq. (4)).

If we apply the proposed method (11) with the coefficients given by (17) to the scalar test Eq. (25), we obtain the following difference equation:

$$A_1(s, v)\ (y_{n+1} + y_{n-1}) + A_0(s, v)\ y_n = 0 \tag{26}$$

where

$$\begin{aligned} A_1(s, v) &= 1 + s^2 b_1 + \frac{15\, b_0 a_0 s^4}{26} - \frac{3\, s^6 b_0 a_0}{208} + \frac{11\, b_2 s^2}{104} + \frac{3\, s^4 b_2}{832} \\ A_0(s, v) &= a_1 + s^2 b_0 - \frac{15\, b_0 a_0 s^4}{13} + \frac{63\, s^6 b_0 a_0}{104} + \frac{93\, b_2 s^2}{52} - \frac{63\, s^4 b_2}{416} \end{aligned} \tag{27}$$

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

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

Definition 6 A multistep method is called singularly almost P-stable id its interval of periodicity is equal to $(0, \infty) - S$ [1]. The term singularly almost P-stable method is applicable only in the cases where $\omega = \phi$ 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 5 We can see two area in the s–v region presented in Fig. 2:

- The method is stable within the shadowed area,
- The method is unstable within the white area.

Remark 6 The models which describe many real problems in Sciences, Engineering and Technology the corresponding models consist only one frequency. Consequently, studying the stability in these cases we are interested only for the case where the

[1] where S is a set of distinct points

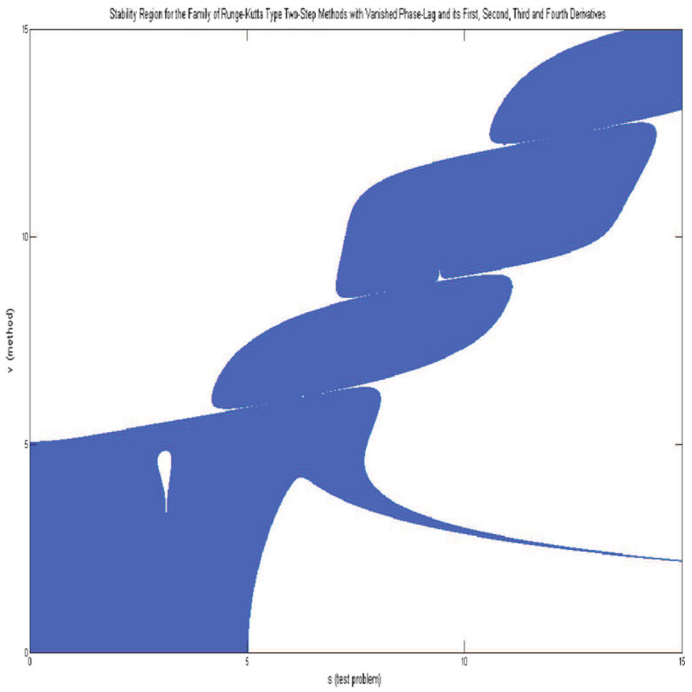

Fig. 2 *s–v* plane of the new obtained two-step high order method with vanished phase-lag and its first, second, third and fourth derivatives

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. for the case where $\omega = \phi$. For 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 $s = v$. An example of such problem is the Schrödinger equation.

Based on the above remark, for the new proposed method we investigated 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). The result of this investigation is the following: for the case $s = v$ the new proposed method has interval of periodicity equal to: $(0, \infty)$, i.e. is P-stable.

The above study leads to the following theorem:

Theorem 3 *The proposed method developed in Sect.* 3:

- *is of eighth algebraic order,*
- *has vanished the phase-lag and its first, second, third and fourth derivatives*
- *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 last decades many methodologies have been proposed in the literature for the estimation of the local truncation error (LTE) on the numerical solution of systems of differential equations (see for example [1–57]).

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

For the local error estimation, we use as lower order solution y_{n+1}^L the method developed in [58], which is of sixth algebraic order. As higher order solution y_{n+1}^H we use the method obtained in this paper - which is of eighth algebraic order. Now, the local truncation error in y_{n+1}^L is estimated by

$$LTE = \mid y_{n+1}^H - y_{n+1}^L \mid \tag{28}$$

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

$$h_{n+1} = h_n \left(\frac{acc}{LTE}\right)^{\frac{1}{q}} \tag{29}$$

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 7 The lower algebraic order solution y_{n+1}^L is the basis for the local truncation error estimate. Considering that the estimation of the local error is less than acc, we use the well known 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

The mathematical models of many problems can be transferred into a coupled differential equations of the Schrödinger type. Problems of this kind can be found in

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

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

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii}\right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{30}$$

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

For our numerical tests we consider the case in which all channels are open. So we have the following boundary conditions (see for details [59]):

$$y_{ij} = 0 \; at \; x = 0 \tag{31}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{li}(k_i x) \tag{32}$$

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

Remark 8 The produced method can also be used for the case of closed channels.

Our investigation is based on the detailed analysis obtained in [59]. 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 (32) as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N}\mathbf{K}' \tag{33}$$

Remark 9 Detailed description on the problem one can find in [59]. 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 [59].

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 [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

$$\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l'+1)}{x^2}\right] y_{j'l'}^{Jjl}(x)$$
$$= \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} < j'l'; J \mid V \mid j''l''; J > y_{j''l''}^{Jjl}(x) \tag{34}$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}\left[E + \frac{\hbar^2}{2I}\left\{j(j+1) - j'(j'+1)\right\}\right] \tag{35}$$

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

$$V(x, \hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}), \tag{36}$$

and the coupling matrix element may then be written as

$$< j'l'; J \mid V \mid j''l''; J >= \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x) \tag{37}$$

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

$$y^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \tag{38}$$

$$y^{Jjl}_{j'l'}(x) \sim \delta_{jj'}\delta_{ll'}\exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l')\exp[i(k_{j'j}x - 1/2l'\pi)] \tag{39}$$

where the scattering S matrix is related to the K matrix of (32) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1} \tag{40}$$

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 [59].

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

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

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

Table 1 Coupled differential equations

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	0.14	3.4×10^{-7}
	9	0.448	1.37	5.8×10^{-7}
	16	0.448	9.58	8.2×10^{-7}

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

than some x_0. The wave functions then zero in this region and effectively the boundary condition (38) may be written as

$$y_{j'l'}^{Jjl}(x_0) = 0 \tag{41}$$

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 [62] 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 [63] 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 1. 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 eighth algebraic order two-step methods was investigated in this paper. The main subjects was:

1. the study of the vanishing of the phase-lag and its first, second, third and fourth derivatives
2. the investigation of the comparative local truncation error analysis
3. the study of the stability of the proposed method using 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 effectiveness of the new produced method on the numerical solution of the coupled Schrödinger equations.

Based on the above mentioned results, it is easy to see the efficiency of the new obtained 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).

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