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Hybrid High Algebraic Order Two–Step Method with Vanished Phase–Lag and Its First and Second Derivatives

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Abstract

A new two-step high algebraic order (tenth order) two-step hybrid (Runge-Kutta type) method is developed in this paper. For this new method we require the vanishing of its phase-lag and its first and second derivatives. We will study the effects of the vanishing of the phase-lag and its first and second derivatives of the specific proposed hybrid two-step method on the efficiency of the method. In more details in this paper we will investigate the following:

- the development of the method
- the local truncation error of the new method and its comparison with other methods in the literature (comparative local truncation error analysis)
- the stability (interval of periodicity) of the obtained method using frequency for the scalar test equation different than the frequency used in the scalar test equation for phase-lag analysis (stability analysis).
- the efficiency of the new produced method applying it on the resonance problem of the Schrödinger equation

We will prove that this kind of methods are efficient for the numerical solution of the Schrödinger equation and related initial-value or boundary-value problems with periodic and/or oscillating solutions.

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1 Introduction

The present paper studies the development of a high order numerical method for the numerical solution of the Schrödinger equation and related problems. We apply the new algorithm on the approximate solution of the radial time independent Schrödinger equation and on the numerical approximation of the coupled Schrödinger equations. It is very well known that the Schrödinger equation and its numerical solution is very important in Computational Chemistry (see [1] and references therein).

More specifically, in this paper we will obtain the first time in the literature a new two-step high algebraic order (tenth order) two-step hybrid (Runge-Kutta type) method. In the most well known cases in the literature multistep methods need many steps or stages in order to be high algebraic order. This has cost on the accuracy and/or on computational cost. This is solved with the new method since it has only three stages and is two-step. With the method presented in this paper, we give a methodology to obtain high algebraic order two-step methods (i.e. multistep methods with the fewer step (two)) which also have other important properties (vanished phase-lag and its derivatives).

The above mentioned method is developed for the numerical solution of special second order initial value problems of the form:

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

with periodical and/or oscillatory solution.

More specifically, systems of ordinary differential equations of second order in which the first derivative y' does not appear explicitly are the models of the above mentioned problems.

2 Phase-lag analysis of symmetric $2\,k$ multistep methods

For the the numerical solution of the initial value problem (1), finite difference methods of the form

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

can be used. In the above mentioned method the integration interval $[a, b]$ is divided into k equally spaced intervals i.e. $\{x_i\}_{i=-k}^{k} \in [a, b]$ and the stepsize of integration h is given by $h = |x_{i+1} - x_i|, \quad i = 1 - k(1)k - 1$. These methods are called multistep. For the specific multistep method the number of steps is equal to $2\,k$.

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

Remark 2. *The below mentioned linear operator*

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

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

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

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

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

we have the following difference equation:

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

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

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

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

Definition 2. [3] *A symmetric* $2\,k$*-step method with characteristic equation given by (6) is said to have an interval of periodicity* $(0, v_0^2)$ *if, for all* $v \in (0, v_0^2)$, *the roots* $\lambda_i, i = 1(1)2\,k$ *of Eq. (6) satisfy:*

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

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

Definition 3. [4], [5] *For any method corresponding to the characteristic equation (6) the phase-lag is defined as the leading term in the expansion of*

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

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

Definition 4. *[6] A method is called* **phase-fitted** *if its phase-lag is equal to zero*

Theorem 1. [4] *The symmetric* $2\,k$*-step method with characteristic equation given by (6) has phase-lag order* p *and phase-lag constant* c *given by*

$$-cv^{p+2} + O(v^{p+4}) = \frac{2\,A_k(v)\,\cos(k\,v) + ... + 2\,A_j(v)\,\cos(j\,v) + ... + A_0(v)}{2\,k^2\,A_k(v) + ... + 2\,j^2\,A_j(v) + ... + 2\,A_1(v)} \tag{9}$$

Remark 3. *We can use the above mentioned formula for a direct computation of the the phase-lag of any symmetric* $2\,k$*-step method.*

Remark 4. *For the purpose of our paper , the symmetric two-step method has phase-lag order* p *and phase-lag constant* c *given by:*

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

3 The new high algebraic order hybrid two–step method with vanished phase–lag and its first and second derivatives

Consider the family of methods

$$\begin{aligned} \widehat{y}_n &= y_n - a_0\,h^2\left(f_{n+1} - 2\,f_n + f_{n-1}\right) - 2\,a_1\,h^2\,f_n \\ \widetilde{y}_n &= y_n - a_2\,h^2\left(f_{n+1} - 2\,\widehat{f}_n + f_{n-1}\right) \\ y_{n+1} - 2\,y_n + y_{n-1} &= h^2\left[b_1\,(f_{n+1} + f_{n-1}) + b_0\,\widetilde{f}_n\right] \end{aligned} \tag{11}$$

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

3.1 Development of the Method

We will investigate the family of methods (11), with:

$$b_0 = \frac{5}{6},\ b_1 = \frac{1}{12} \tag{12}$$

In order the above mentioned method (11) with coefficients (12) to have vanished phase-lag and its first and second derivatives the following equations must hold:

$$\mathrm{Phase-Lag(PL)} = \frac{1}{2}\frac{T_0}{1+v^2\left(\frac{1}{12}+\frac{5}{6}\,a_2v^2\left(-2\,a_0v^2+1\right)\right)} = 0 \tag{13}$$

$$\mathrm{First\ Derivative\ of\ the\ Phase-Lag} = \frac{T_1}{\left(20\,v^6a_0a_2-10\,v^4a_2-v^2-12\right)^2} = 0 \tag{14}$$

$$\mathrm{Second\ Derivative\ of\ the\ Phase-Lag} = \frac{T_2}{\left(20\,v^6a_0a_2-10\,v^4a_2-v^2-12\right)^3} = 0 \tag{15}$$

where

$$\begin{aligned}
T_0 &= 2\left(1+v^2\left(1/12+5/6\,a_2v^2\left(-2\,a_0v^2+1\right)\right)\right)\cos(v)\\
&\quad -2+v^2\left(5/6+5/6\,a_2v^2\left(4\,a_0v^2-4\,a_1v^2-2\right)\right)\\
T_1 &= -400\sin(v)\,v^{12}{a_0}^2{a_2}^2+400\sin(v)\,v^{10}a_0{a_2}^2-400\,v^9a_1{a_2}^2\\
&\quad +40\sin(v)\,v^8a_0a_2-100\sin(v)\,v^8{a_2}^2+480\sin(v)\,v^6a_0a_2+480\,v^7a_0a_2\\
&\quad -80\,v^7a_1a_2-20\sin(v)\,v^6a_2-1440\,v^5a_1a_2-240\sin(v)\,v^4a_2\\
&\quad -120\,v^5a_2-\sin(v)\,v^4-24\sin(v)\,v^2-144\sin(v)+144\,v\\
T_2 &= -1728-60\cos(v)\,v^{10}a_0a_2-1440\cos(v)\,v^8a_0a_2\\
&\quad -8640\cos(v)\,v^6a_0a_2+86400\,v^4a_1a_2+240\,v^8a_1a_2\\
&\quad +4000\,v^{12}a_1{a_2}^3+300\cos(v)\,v^{10}{a_2}^2+8160\,v^6a_1a_2\\
&\quad +4320\cos(v)\,v^4a_2+1200\,v^{10}a_1{a_2}^2+1000\cos(v)\,v^{12}{a_2}^3\\
&\quad -72000\,v^6a_0a_2+3600\cos(v)\,v^8{a_2}^2+30\cos(v)\,v^8a_2+720\cos(v)\,v^6a_2\\
&\quad -48000\,v^{12}{a_0}^2{a_2}^2+21600\,v^{10}a_0{a_2}^2-1440\,v^8a_0a_2\\
&\quad -3600\,v^8{a_2}^2+120\,v^6a_2+17280\,v^4a_2+36\cos(v)\,v^4+\cos(v)\,v^6+432\,v^2\\
&\quad +1728\cos(v)+1200\cos(v)\,v^{14}{a_0}^2{a_2}^2-6000\cos(v)\,v^{14}a_0{a_2}^3
\end{aligned}$$

$$+14400\cos(v)v^{12}{a_0}^2{a_2}^2-1200\cos(v)v^{12}a_0{a_2}^2-14400\cos(v)v^{10}a_0{a_2}^2$$
$$+24000v^{14}a_0a_1{a_2}^3+8000v^{12}a_0a_1{a_2}^2+201600v^{10}a_0a_1{a_2}^2$$
$$-8000\cos(v)v^{18}{a_0}^3{a_2}^3+12000\cos(v)v^{16}{a_0}^2{a_2}^3+432\cos(v)v^2$$

Solving the above system of equations (13)-(15), the coefficients of the new proposed hybrid method are obtained :

$$a_0=\frac{1}{4}\frac{T_3}{T_4},\ a_1=\frac{1}{2}\frac{T_5}{T_6}$$
$$a_2=-\frac{1}{5}\frac{T_7}{T_8} \tag{16}$$

where

$$T_3=-(\cos(v))^2v^4+7\sin(v)\cos(v)v^3+11\cos(v)v^4$$
$$+5v^3\sin(v)-16(\cos(v))^2v^2+2v^4+216\cos(v)v\sin(v)$$
$$+8\cos(v)v^2-216v\sin(v)+288(\cos(v))^2+8v^2-576\cos(v)+288$$
$$T_4=v^3\Big(-(\cos(v))^2v^3+5\sin(v)\cos(v)v^2$$
$$+5\cos(v)v^3+25\sin(v)v^2-18(\cos(v))^2v$$
$$+2v^3+126\sin(v)\cos(v)-18\cos(v)v-126\sin(v)+36v\Big)$$
$$T_5=(\cos(v)-1)\Big(3\cos(v)v^4+15v^3\sin(v)$$
$$-4(\cos(v))^2v^2+6v^4-16\cos(v)v^2-144(\cos(v))^2$$
$$+20v^2+288\cos(v)-144\Big)$$
$$T_6=v^3\Big(-(\cos(v))^2v^3+5\sin(v)\cos(v)v^2$$
$$+5\cos(v)v^3+25\sin(v)v^2-18(\cos(v))^2v$$
$$+2v^3+126\sin(v)\cos(v)-18\cos(v)v-126\sin(v)+36v\Big)$$
$$T_7=-(\cos(v))^2v^3+5\sin(v)\cos(v)v^2+5\cos(v)v^3$$
$$+25\sin(v)v^2-18(\cos(v))^2v+2v^3+126\sin(v)\cos(v)$$
$$-18\cos(v)v-126\sin(v)+36v$$
$$T_8=v^4\Big(-(\cos(v))^2v+3\sin(v)\cos(v)$$
$$-\cos(v)v-3\sin(v)+2v\Big)$$

If the above formulae given by (16) are subject to heavy cancellations for some values of $|v|$ (i.e. if for some values of $|v|$ the denominators T_4, T_6 and T_8 become equal to zero) then the following Taylor series expansions should be used :

$$
\begin{aligned}
a_0 \;=\; & -\frac{1}{112} - \frac{5\,v^2}{14112} - \frac{24229\,v^4}{1695133440} - \frac{2275439\,v^6}{3915758246400} \\
& - \frac{6318217679\,v^8}{266537832315955200} - \frac{2613882395959\,v^{10}}{2699618183157063168000} \\
& - \frac{13343835818812619\,v^{12}}{337249261607259484849766400} - \frac{8522252256417086767\,v^{14}}{527001566740991071472590848000} \\
& - \frac{12092119012662287495717 63\,v^{16}}{18294690748912147929028120059248640000} \\
& - \frac{11417117652980864911043324 3\,v^{18}}{42260735629987061716054957336864358400000} \\
& + \ldots \\
a_1 \;=\; & \frac{1}{8} - \frac{5\,v^2}{1232} + \frac{13991\,v^4}{147987840} - \frac{257\,v^6}{3155556096} \\
& + \frac{2494780423\,v^8}{69807527511321600} + \frac{146040173101\,v^{10}}{1225540952988762009 60} \\
& + \frac{1475700332690009\,v^{12}}{2944239585460201851863040 0} + \frac{213102124861569883\,v^{14}}{1042849661170003495929888768 00} \\
& + \frac{1334356040520857950590 37\,v^{16}}{1597155541571695454121502544855040000} \\
& + \frac{5039543844159315371152 13\,v^{18}}{1475771720412246599608268351446056960 00} + \ldots \\
a_2 \;=\; & \frac{1}{300} + \frac{v^2}{27720} - \frac{227\,v^4}{504504000} - \frac{593\,v^6}{12713500800} \\
& - \frac{6343\,v^8}{3072364162560} - \frac{19737049\,v^{10}}{265605881853312000} \\
& - \frac{70569265127\,v^{12}}{2900416229838167040000 0} - \frac{139568743260 61\,v^{14}}{1849189371495621778022400 00} \\
& - \frac{22513737506177\,v^{16}}{9957173538822578804736000000} \\
& - \frac{3782807166869\,v^{18}}{5722754475996976870932480000 0} + \ldots
\end{aligned}
\tag{17}
$$

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

The local truncation error of the new obtained hybrid method (11) (mentioned as *ExpTwoStepPC*) with the coefficients given by (16) - (17) is given by:

$$
LTE_{ExplTwoStepPC} = -\frac{1}{23950080}\,h^{12}\left(q_n^{(12)} + 3\,\phi^2\,q_n^{(10)} + 3\,\phi^4\,q_n^{(8)} + \phi^6\,q_n^{(6)}\right) + O\left(h^{14}\right) \tag{18}
$$

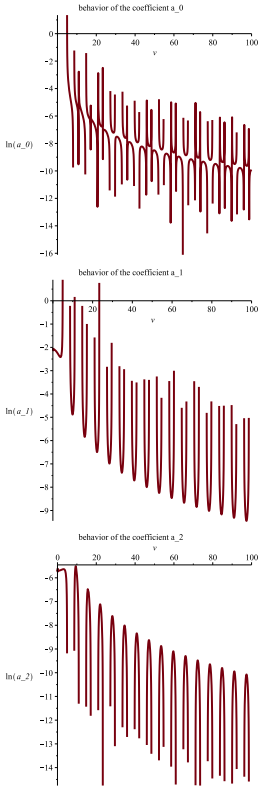

Figure 1: Behavior of the coefficients of the new proposed method given by (16) for several values of $v = \phi\, h$.

4 Comparative error analysis

In this section we will study the local truncation error analysis considering the test problem:

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

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.

The methods mentioned below are investigated :

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

$$LTE_{CL} = -\frac{1}{23950080}\, h^{12}\, q_n^{(12)} + O\left(h^{14}\right) \tag{20}$$

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

$$LTE_{ExplTwoStepPC} = -\frac{1}{23950080}\, h^{12} \left(q_n^{(12)} + 3\,\phi^2\, q_n^{(10)} + 3\,\phi^4\, q_n^{(8)} + \phi^6\, q_n^{(6)} \right) + O\left(h^{14}\right) \tag{21}$$

The procedure contains the following stages

- Based on the test problem (19), the derivatives which appear in the formulae of the Local Truncation Errors are computed. The expressions of some derivatives are presented in the Appendix.

- Using the expressions of the derivatives presented in the Appendix, we substitute them in the formulae of the Local Truncation Error. Therefore, we produce formulae of the local truncation errors which are dependent on the energy E.

- The study is based on the two cases for the parameter G (which will appear in the expressions of the Local Truncation Error obtained from the above mentioned stage of the algorithm for the comparative local truncation error analysis) :

  1. The energy and the potential are closed each other. Consequently $G = V_c - E \approx 0$ i.e. the value of the parameter G is approximately equal to zero. Therefore, all the terms in the expressions of the local truncation error with several powers of G are approximately equal to zero (the expression of the Local Truncation Error can be written as: $LTE = C_0 + C_1\, G + C_2\, G^2 + C_3\, G^3 + \ldots + C_n\, G^n$. In the case that $G \approx 0$ the terms $C_1\, G$, $C_2\, G^2$, $C_3\, G^3$, $\ldots$, $C_n\, G^n$ are ≈ 0. Therefore only the term C_0 exists). As a result of the above remarks, we consider only the terms of the expressions of the local truncation error for which the power to G is equal to zero i.e. the terms which are free from G. In this case (free from G terms) the local truncation error for the classical method (constant coefficients) and the methods with vanishing phase-lag and its derivatives are the same since the expressions free from G of the local truncation errors in

both cases mentioned above are the same. Therefore, for these values of G, the methods are of comparable accuracy.

2. $G >> 0$ or $G << 0$. Then $|G|$ is a large number. In these cases we wish to have expressions of the local truncation error with terms with minimum power of G.

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

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

4.3 Classical Method

$$LTE_{CL} = -\frac{1}{23950080}\, h^{12} \left(y\left(x\right)\, G^{6} + \cdots \right) + O\left(h^{14}\right) \tag{22}$$

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

$$LTE_{ExplTwoStepPC} = -\frac{1}{5987520}\, h^{12} \left(\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} g\left(x\right) \right) y\left(x\right)\, G^{4} + \cdots \right) + O\left(h^{14}\right) \tag{23}$$

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.*
- *High Algebraic Order Two-Step Method with Vanished Phase-lag and its First and Second Derivatives developed in Section 3: For this method the error increases as the fourth power of G.*

So, for the approximate integration of the time independent radial Schrödinger equation the New Obtained High Algebraic Order Method with Vanished Phase-Lag and its First and Second 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 investigate the stability of the new obtained method, we apply it to the scalar test equation:

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

where $\omega \neq \phi$, i.e. the frequency of the scalar test equation of the phase-lag analysis (ϕ) - studied above - is different with the frequency of the scalar test equation used for the stability analysis, which will be studied here.

The application to the scalar test equation (24) leads to the following difference equation:

$$A_1(s,v) \; (y_{n+1} + y_{n-1}) + A_0(s,v) \; y_n = 0 \tag{25}$$

where

$$\begin{aligned} A_1(s,v) &= \frac{1}{12} \frac{T_9}{v^7 \left((\cos(v))^2 v - 3 \sin(v) \cos(v) + \cos(v) v + 3 \sin(v) - 2 v \right)} \\ A_0(s,v) &= \frac{1}{6} \frac{T_{10}}{v^7 \left((\cos(v))^2 v - 3 \sin(v) \cos(v) + \cos(v) v + 3 \sin(v) - 2 v \right)} \end{aligned} \tag{26}$$

where

$$\begin{aligned} T_9 \; = \; & -288 \, (\cos(v))^2 \, s^6 + 576 \cos(v) \, s^6 + 72 \, s^4 v^4 \\ & -2 \, s^6 v^4 + 4 \, s^4 v^6 - 2 \, s^2 v^8 - 8 \, s^6 v^2 + 12 \, (\cos(v))^2 \, v^8 \\ & +12 \cos(v) \, v^8 + 36 \sin(v) \, v^7 - 288 \, s^6 - 24 \, v^8 \\ & -7 \sin(v) \cos(v) \, s^6 v^3 + 10 \sin(v) \cos(v) \, s^4 v^5 \\ & -3 \sin(v) \cos(v) \, s^2 v^7 - 216 \sin(v) \cos(v) \, s^6 v \\ & +252 \sin(v) \cos(v) \, s^4 v^3 - 8 \cos(v) \, s^6 v^2 \\ & +50 \sin(v) \, s^4 v^5 - 36 \sin(v) \cos(v) \, v^7 + 10 \cos(v) \, s^4 v^6 \\ & -36 \cos(v) \, s^4 v^4 - 5 \sin(v) \, s^6 v^3 - 2 \\ & (\cos(v))^2 \, s^4 v^6 + 3 \sin(v) \, s^2 v^7 \\ & + (\cos(v))^2 \, s^2 v^8 - 36 \, (\cos(v))^2 \, s^4 v^4 \\ & -252 \sin(v) \, s^4 v^3 - 11 \cos(v) \, s^6 v^4 \\ & +16 \, (\cos(v))^2 \, s^6 v^2 + (\cos(v))^2 \, s^6 v^4 \\ & + \cos(v) \, s^2 v^8 + 216 \sin(v) \, s^6 \, v \\ T_{10} \; = \; & -576 \, (\cos(v))^2 \, s^6 + 288 \cos(v) \, s^6 \end{aligned}$$

$$
\begin{aligned}
&-72\,s^4v^4+14\,s^6v^4-4\,s^4v^6-10\,s^2v^8+48\,s^6v^2\\
&-12\,(\cos(v))^2\,v^8-12\,\cos(v)\,v^8-36\,\sin(v)\,v^7+24\,v^8\\
&+8\,(\cos(v))^3\,s^6v^2-23\,\sin(v)\cos(v)\,s^6v^3\\
&-10\,\sin(v)\cos(v)\,s^4v^5-15\,\sin(v)\cos(v)\,s^2v^7\\
&+216\,\sin(v)\cos(v)\,s^6v-252\,\sin(v)\cos(v)\,s^4v^3\\
&+288\,(\cos(v))^3\,s^6-64\,\cos(v)\,s^6v^2\\
&-50\,\sin(v)\,s^4v^5+36\,\sin(v)\cos(v)\,v^7-10\,\cos(v)\,s^4v^6\\
&+36\,\cos(v)\,s^4v^4+35\,\sin(v)\,s^6v^3+2\,(\cos(v))^2\,s^4v^6\\
&+15\,\sin(v)\,s^2v^7+5\,(\cos(v))^2\,s^2v^8\\
&+36\,(\cos(v))^2\,s^4v^4+252\,\sin(v)\,s^4v^3\\
&+5\,\cos(v)\,s^6v^4+8\,(\cos(v))^2\,s^6v^2\\
&-7\,(\cos(v))^2\,s^6v^4+5\,\cos(v)\,s^2v^8-216\,\sin(v)\,s^6v
\end{aligned}
$$

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

Based on the analysis presented in Section 2, we have the following definitions:

Definition 5. *(see [3]) 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* $(0,\infty)-S$ [2]. *The term singularly almost P-stable method is used only in the cases when the frequency of the scalar test equation for the phase-lag analysis is equal to the frequency of the scalar test equation for the stability analysis, i.e.* $\omega=\phi$.

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

Remark 5. *On the* $s-v$ *region:*

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

Remark 6. *There are a lot of real problems in sciences and engineering for which their mathematical models require the frequencies* s *and* v *to be equal. Therefore, it is necessary*

[2] where S is a set of distinct points

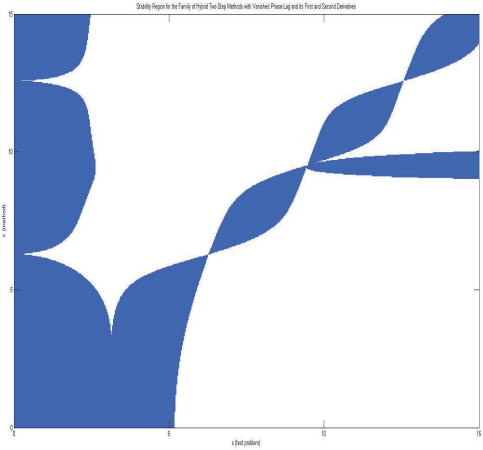

Figure 2: $s - v$ plane of the new obtained two-step high order method with vanishing phase-lag and its first and second derivatives

to observe **the surroundings of the first diagonal of the $s - v$ plane**. *These are the cases of the mathematical models which have only one frequency per differential equation in the model. For these problems we have to examine the case where 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. See for example the time independent Schrödinger equation and the coupled equations arising from the Schrödinger equation.*

Based on the above remark, we study the case where 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, i.e. we investigate the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s - v$ plane). The above mentioned study leads to the conclusion that the new obtained 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 method obtained in section 3:*

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

The efficiency of the new proposed numerical scheme will be investigated in this section, studying:

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

6.1 Radial time–independent Schrödinger equation

The radial time independent Schrödinger equation can be written as :

$$y''(r) = [l(l+1)/r^2 + V(r) - k^2]\, y(r). \tag{27}$$

where

1. The function $W(r) = l(l+1)/r^2 + V(r)$ is called *the effective potential*. This satisfies $W(x) \to 0$ as $x \to \infty$,
2. The quantity k^2 is a real number denoting *the energy*,
3. The quantity l is a given integer representing the *angular momentum*,
4. V is a given function which denotes the *potential*.

This is a boundary value problem which has the following boundary conditions :

$$y(0) = 0 \tag{28}$$

and another boundary condition, for large values of r, determined by physical properties and characteristics of the specific problem.

Since the proposed method in this paper belongs to the category of the frequency dependent methods, it is necessary the parameter ϕ of the coefficients of the method ($v = \phi\, h$) to be determined. For the category of problems of the radial Schrödinger equation, the parameter ϕ (for $l = 0$) is given by :

$$\phi = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{29}$$

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

6.1.1 Woods–Saxon potential

The well known Woods-Saxon potential is used for our numerical experiments. The model of the Woods-Saxon potential is given by :

$$V(r) = \frac{u_0}{1+q} - \frac{u_0\, q}{a\,(1+q)^2} \tag{30}$$

with $q = \exp\left[\frac{r-X_0}{a}\right]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

The behavior of Woods-Saxon potential is shown in Figure 3.

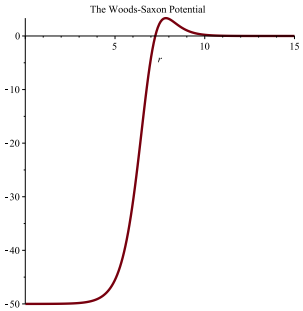

Figure 3: The Woods-Saxon potential.

We use the approximation of the potential using some critical points on the description of the potential. We use these critical points in order to determine the value of the parameter ϕ (see for details [7]).

For the purpose of our tests, we choose ϕ as follows (we use the methodology presented in [8] and [9]) :

$$\phi = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{31}$$

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

6.1.2 Radial Schrödinger equation – the resonance problem

The first numerical test for the efficiency of the obtained new high order hybrid is the numerical solution of the radial time independent Schrödinger equation (27) with the Woods-Saxon potential (30).

In order to proceed with the numerical solution of the above mentioned problem, it is necessary to approximate the true interval of integration, which is equal to $r \in \left(0, \infty\right)$, by a finite one. We use the integration interval $r \in [0, 15]$. The domain of energies in which we will solve the above problem is equal to: $E \in [1, 1000]$.

For r greater than some value R and for the case of positive energies, $E = k^2$, the radial Schrödinger equation effectively reduces to

$$y''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) y(r) = 0 \tag{32}$$

The reason for this is faster decrease of the potential than the term $\frac{l(l+1)}{r^2}$.

In the above mathematical model, the differential equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus, the solution of equation (27) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} y(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{33}$$

where δ_l is the phase shift that may be calculated from the formula

$$\tan\delta_l = \frac{y(r_2)\, S(r_1) - y(r_1)\, S(r_2)}{y(r_1)\, C(r_1) - y(r_2)\, C(r_2)} \tag{34}$$

for distinct r_1 and r_2 points in the asymptotic region (we choose r_1 as the right-hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need $y_j, \quad j = 0, 1$ before starting a two-step method. From the initial condition, we obtain y_0. The value y_1 is obtained by using high order Runge-Kutta-Nyström methods(see [10]

and [11]). With these starting values, we evaluate at r_2 of the asymptotic region the phase shift δ_l.

For the case of positive energies we have the problem known as resonance problem. Two forms for this problem:

- finding the phase-shift δ_l or
- finding those E, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$.

We actually solve the latter problem, known as **the resonance problem**.

The boundary conditions for this problem are:

$$y(0) = 0,\ y(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{35}$$

We compute the approximate positive eigenenergies of the Woods-Saxon resonance problem using:

- The eighth order multi-step method developed by Quinlan and Tremaine [12], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [12], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [12], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [13], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [14], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [15], which is indicated as **Method MCR6**
- The classical form of the Two-Step Hybrid Method developed in Section 3, which is indicated as **Method NMCL** [3].

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

- The Phase-Fitted Method (Case 1) developed in [2], which is indicated as **Method NMPF1**
- The Phase-Fitted Method (Case 2) developed in [2], which is indicated as **Method NMPF2**
- The Method developed in [16] (Case 2), which is indicated as **Method NMC2**
- The Method developed in [16] (Case 1), which is indicated as **Method NMC1**
- The New Obtained Two-Step Hybrid Method developed in Section 3, which is indicated as **Method NM2SH2DV**

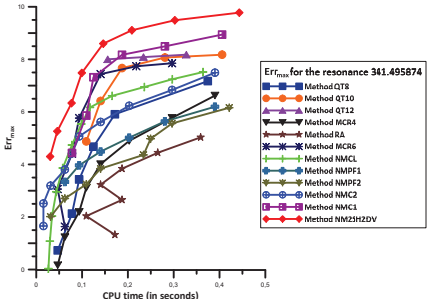

Figure 4: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

We defined some reference values using the well known two-step method of Chawla and Rao [15] with small step size for the integration. We then compared the numerically calculated eigenenergies with these reference values. In Figures 4 and 5, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{36}$$

of the eigenenergies $E_2 = 341.495874$ and $E_3 = 989.701916$ respectively, for several values of CPU time (in seconds). We note that the CPU time (in seconds) counts the computational cost for each method.

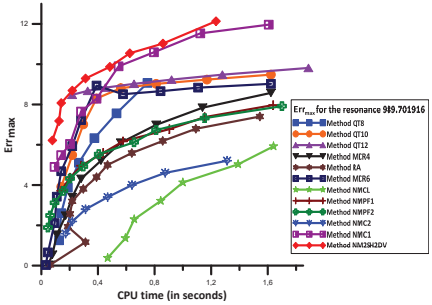

Figure 5: Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is less than 0

6.1.3 Remarks on the numerical results for the radial Schrödinger equation

From the numerical tests mentioned above, we have the following :

1. The classical form of the Two-Step Hybrid Method developed in Section 3, which is indicated as **Method NMCL** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [13], which is indicated as **Method MCR4**, the exponentially-fitted method of Raptis and Allison [14], which is indicated as **Method MRA**, the Phase-Fitted Method (Case 1) developed in [2], which is indicated as **Method NMPF1**, the Phase-Fitted Method (Case 2) developed in [2], which is indicated as **Method NMPF2**, the Method developed in [16] (Case 2), which is indicated as **Method NMC2** and the eighth order multi-step method developed by Quinlan and Tremaine [12], which is indicated as **Method QT8**.

2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [12], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [13], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [12], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [15], which is indicated as **Method MCR6** for large CPU time and less efficient than

the **Method MCR6** for small CPU time.

3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [12], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [12], which is indicated as **Method QT10**

4. The Phase-Fitted Method (Case 1) developed in [2], which is indicated as **Method NMPF1** is more efficient than the exponentially-fitted method of Raptis and Allison [14] and the Phase-Fitted Method (Case 2) developed in [2], which is indicated as **Method NMPF2**

5. The Method developed in [16] (Case 2), which is indicated as **Method NMC2** is more efficient than the exponentially-fitted method of Raptis and Allison [14] and the Phase-Fitted Method (Case 2) developed in [2], which is indicated as **Method NMPF2** and the Phase-Fitted Method (Case 1) developed in [2], which is indicated as **Method NMPF1**

6. The Method developed in [16] (Case 1), which is indicated as **Method NMC1**, is the more efficient than all the other methods mentioned above.

7. The New Obtained Method developed in Section 3, which is indicated as **Method NM2SH2DV**, is the most efficient one.

6.2 Error estimation

Last decades many methods have been proposed for the estimation of the local truncation error (LTE) in the numerical solution of systems of differential equations (see for example [2]- [60]).

In the present paper we base our local error estimation technique on an embedded pair of multistep methods and on the fact that when the algebraic order is maximal then we have better approximation for the solution for the problems with oscillatory or periodical behavior.

We use as lower order solution y_{n+1}^{L}, for the purpose of local error estimation, the method developed in [60] - which is of eight algebraic order. As higher-order solution y_{n+1}^{H} we use the method developed in this paper - which is of tenth algebraic order. Now,

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

$$LTE = \mid y^H_{n+1} - y^L_{n+1} \mid \tag{37}$$

If the local error of acc is requested and the step size used for the n^{th} step is h_n, the estimated step size for the $(n+1)^{st}$ step, which would give a local error equal to acc, must be

$$h_{n+1} = h_n \left(\frac{acc}{LTE}\right)^{\frac{1}{q}} \tag{38}$$

where q is the algebraic order of the method.

We mention that the local truncation error estimate is based on the lower order solution y^L_{n+1}. However, if the error estimate is less than acc, we adopt the widely used procedure of performing local extrapolation. Thus, although an estimate of the local error is controlled in lower order solution y^L_{n+1}, it is the higher-order solution y^H_{n+1} which is accepted at each point.

6.3 Coupled differential equations

There are many problems in quantum chemistry, material science, theoretical physics, atomic physics, physical chemistry and chemical physics which can be transformed to the solution of coupled differential equations of the Schrödinger type

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

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i+1)}{x^2} - V_{ii}\right] y_{ij} = \sum_{m=1}^{N} V_{im} y_{mj} \tag{39}$$

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

In the present illustrations we investigate the case in which all channels are open. So we have the following boundary conditions (see for details [17]):

$$y_{ij} = 0 \; at \; x = 0 \tag{40}$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x)\delta_{ij} + \left(\frac{k_i}{k_j}\right)^{1/2} K_{ij} k_i x n_{li}(k_i x) \tag{41}$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions, respectively. The present method can also be used for problems involving closed channels.

Based on the detailed analysis developed in [17] and defining a matrix K' and diagonal matrices M, N by:

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

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

we find that the asymptotic condition (41) may be written as:

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

One of the most well-known methods for the numerical solution of the coupled differential equations arising from the Schrödinger equation is the Iterative Numerov method of Allison [17].

A real problem in quantum chemistry, theoretical physics, material science, atomic physics and molecular physics which can be transformed to close-coupling differential equations of the Schrödinger type is the rotational excitation of a diatomic molecule by neutral particle impact. Denoting, as in [17], 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

$$\left[\frac{d^2}{dx^2} + k^2_{j'j} - \frac{l'(l'+1)}{x^2}\right] y^{Jjl}_{j'l'}(x) = \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} < j'l'; J \mid V \mid j''l''; J > y^{Jjl}_{j''l''}(x) \qquad (42)$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2}[E + \frac{\hbar^2}{2I}\{j(j+1) - j'(j'+1)\}] \qquad (43)$$

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.

Following the analysis of [17], the potential V can be expanded as

$$V(x, \hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}\hat{\mathbf{k}}_{jj}), \qquad (44)$$

and the coupling matrix element may then be written as

$$< j'l'; J \mid V \mid j''l''; J >= \delta_{j'j''}\delta_{l'l''}V_0(x) + f_2(j'l', j''l''; J)V_2(x) \qquad (45)$$

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [18] 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 [19]). The boundary conditions are

$$y^{Jjl}_{j'l'}(x) = 0 \text{ at } x = 0 \qquad (46)$$

$$y^{Jjl}_{j'l'}(x) \sim \delta_{jj'}\delta_{ll'} \exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp[i(k_{j'j}x - 1/2l'\pi)] \qquad (47)$$

where the scattering S matrix is related to the K matrix of (41) by the relation

$$\mathbf{S} = (\mathbf{I} + \mathbf{iK})(\mathbf{I} - \mathbf{iK})^{-1} \tag{48}$$

To calculate the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles an algorithm in which the numerical method for step-by-step integration from the initial value to matching points is included. This algorithm is based on an analogous algorithm which has been developed for the numerical applications of [17].

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

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

As is described in [1], we take $J = 6$ and consider excitation of the rotator from the $j = 0$ state to levels up to $j' = 2, 4$ and 6 giving sets of **four, nine and sixteen coupled differential equations**, respectively. Following the procedure obtained by Bernstein [19] and Allison [17] 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 (46) may be written as

$$y^{Jjl}_{j'l'}(x_0) = 0 \tag{49}$$

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 [17] which is indicated as **Method I**,
- the variable-step method of Raptis and Cash [20] which is indicated as **Method II**,
- the embedded Runge-Kutta Dormand and Prince method 5(4) [11] which is indicated as **Method III**,
- the embedded Runge-Kutta method ERK4(2) developed in Simos [21] which is indicated as **Method IV**,
- the new developed embedded two-step method which is indicated as **Method V**

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	0.20	1.1×10^{-6}
	9	0.448	2.07	5.7×10^{-6}
	16	0.448	11.18	8.7×10^{-6}

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 this paper, we investigated a family of high algebraic order two-step methods. The main subjects of this study was:

- the investigation of the vanishing of the phase-lag and its first and second derivatives
- the comparative error analysis
- the stability analysis.
- the computational behavior of the new produced method and its effectiveness on the numerical solution of the radial Schrödinger equation and of the coupled Schrödinger equations both of which are of high importance for Chemistry.

Based on the above mentioned results, it is easy to see the efficiency of the new obtained method for the numerical solution of the radial Schrödinger equation and of the coupled Schrödinger equations.

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

Appendix: Formulae of the derivatives of y_n

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

$$
\begin{aligned}
y_n^{(2)} &= (V(x) - V_c + G)\, y(x) \\
y_n^{(3)} &= \left(\frac{d}{dx} g(x)\right) y(x) + (g(x) + G) \frac{d}{dx} y(x) \\
y_n^{(4)} &= \left(\frac{d^2}{dx^2} g(x)\right) y(x) + 2 \left(\frac{d}{dx} g(x)\right) \frac{d}{dx} y(x) \\
&\quad + (g(x) + G)^2 y(x) \\
y_n^{(5)} &= \left(\frac{d^3}{dx^3} g(x)\right) y(x) + 3 \left(\frac{d^2}{dx^2} g(x)\right) \frac{d}{dx} y(x) \\
&\quad + 4\, (g(x) + G)\, y(x) \frac{d}{dx} g(x) + (g(x) + G)^2 \frac{d}{dx} y(x) \\
y_n^{(6)} &= \left(\frac{d^4}{dx^4} g(x)\right) y(x) + 4 \left(\frac{d^3}{dx^3} g(x)\right) \frac{d}{dx} y(x) \\
&\quad + 7\, (g(x) + G)\, y(x) \frac{d^2}{dx^2} g(x) + 4 \left(\frac{d}{dx} g(x)\right)^2 y(x) \\
&\quad + 6\, (g(x) + G) \left(\frac{d}{dx} y(x)\right) \frac{d}{dx} g(x) \\
&\quad + (g(x) + G)^3 y(x) \\
y_n^{(7)} &= \left(\frac{d^5}{dx^5} g(x)\right) y(x) + 5 \left(\frac{d^4}{dx^4} g(x)\right) \frac{d}{dx} y(x) \\
&\quad + 11\, (g(x) + G)\, y(x) \frac{d^3}{dx^3} g(x) + 15 \left(\frac{d}{dx} g(x)\right) y(x) \\
&\quad \frac{d^2}{dx^2} g(x) + 13\, (g(x) + G) \left(\frac{d}{dx} y(x)\right) \frac{d^2}{dx^2} g(x) \\
&\quad + 10 \left(\frac{d}{dx} g(x)\right)^2 \frac{d}{dx} y(x) + 9\, (g(x) + G)^2 y(x) \\
&\quad \frac{d}{dx} g(x) + (g(x) + G)^3 \frac{d}{dx} y(x)
\end{aligned}
$$

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

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