

A new family of two stage symmetric two-step methods with vanished phase-lag and its derivatives for the numerical integration of the Schrödinger equation

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Abstract A family of two stage low computational cost symmetric two-step methods with vanished phase-lag and its derivatives is developed in this paper. More specifically we produce:

- a two-stage symmetric two-step eighth algebraic order method which has the phase-lag and its first, second and third derivatives vanished and
- a two-stage symmetric two-step sixth algebraic order method, which is P-stable and has the phase-lag and its first and second derivatives vanished.

The local truncation error, the interval of periodicity and the effect of the vanishing of the phase-lag and its derivatives on the efficiency of the obtained method are also studied in this paper.

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1 Introduction

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

$$p''(x) = f(x, p), \quad p(x_0) = p_0 \quad \text{and} \quad p'(x_0) = p'_0 \quad (1)$$

with solutions which are behaved periodically and/or oscillatory is the subject of this paper.

We specially give attention to problems with mathematical models which consist of systems of second order ordinary differential equations of the form (1) (i.e. systems of second order ordinary differential equations with not explicit appearance of the first derivative p').

The basic idea is the introduction of a two stage two-step family of methods with the following properties:

- maximum algebraic order
- vanished phase-lag and
- vanished derivatives of the phase-lag of maximum possible order
- investigation of the stability of the new family of methods

With this procedure we avoid the Runge–Kutta or Runge–Kutta–Nyström or Runge–Kutta type (multistage) multistep methods. With these methods and in order to achieve the same properties as mentioned above we need much more stages and/or steps (see [1]). The more stages and steps have a consequence of more computational cost. Our proposed method is of low computational cost since it has only two stages.

Our paper has the following form:

- The phase-lag analysis of symmetric multistep methods and the direct formula for the computation of their phase-lag are presented in Sect. 2.
- In Sect. 3 the development of the new two stages symmetric two step methods is presented. More specifically we present the production of a two stages symmetric two step method with vanished phase-lag and its first, second and third derivatives and the construction of a two stages symmetric two step P-stable method with vanished phase-lag and its first and second derivatives .
- The local truncation error is investigated in Sect. 4 using a scalar test problem. For this problem, asymptotic expressions of the local error and comparison of these asymptotic expressions with the asymptotic expressions of other methods are also given. Useful remarks for the local error for this scalar test problem are also given.
- In Sect. 5 the stability and interval of periodicity of the new obtained methods is studied using a scalar test equation with frequency different than the frequency of the scalar test equation used for the phase-lag analysis. We give special attention on the development of the P-stable method of the family.

- The procedure of the Local Error Estimation is investigated in Sect. 6.1. The Local Error Estimation is based on the 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 Sect. 7.

2 Phase-lag analysis for symmetric 2m-step methods

We consider the 2m-step methods

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

for the numerical approximation of the initial value problem (1).

The methodology which we use for the numerical solution of the initial value problem (1) is based on the following algorithm:

- We divide the area of integration $[a, b]$ into $2m$ equally spaced intervals i.e. $\{x_i\}_{i=-m}^m \in [a, b]$.
- We apply the symmetric 2m-step method (2) within the above defined intervals.
- The area of integration $[a, b]$ is defined based on the physical characteristics of the 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.

We call the multistep method given by (2), 2m-step method since the number of steps used for the integration is equal to $2m$.

Definition 1 If for the method (2) we have $c_{-i} = c_i$ and $b_{-i} = b_i$, $i = 0(1)m$, then the method is called symmetric 2m-step method

Remark 1 The multistep method (2) is associated with a linear operator which is given by:

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

where $y \in C^2$.

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

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

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

we obtain the following difference equation:

$$A_m(v) p_{n+m} + \cdots + A_1(v) p_{n+1} + A_0(v) p_n + A_1(v) p_{n-1} + \cdots + A_m(v) p_{n-m} = 0 \quad (5)$$

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

With the the difference equation (5) is associated a characteristic equation which is given by:

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

Definition 3 [3] We say that a symmetric $2m$ -step method with characteristic equation given by (6) has an interval of periodicity $(0, v_0^2)$ if, for all $v \in (0, v_0^2)$, the roots $\lambda_i, i = 1(1)2m$ of Eq. (6) satisfy:

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

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

Definition 4 (see [3]) P-stable is called a multistep method if its interval of periodicity is equal to $(0, \infty)$. The necessary and sufficient conditions in order a symmetric multistep method to be P-stable are

$$|\lambda_1| = |\lambda_2| = 1, \quad |\lambda_j| \leq 1, \quad j = 3(1)2m \forall v \quad (8)$$

Definition 5 Singularly almost P-stable is called a multistep method with interval of periodicity equal to $(0, \infty) - S$.¹

Definition 6 [4,5] For any symmetric multistep method which is associated to the characteristic equation (6) the phase-lag is the leading term in the expansion of

$$t = v - \theta(v) \quad (9)$$

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

Definition 7 [6] A method is called **phase-fitted** if the phase-lag is vanished (i.e. equal to zero).

Theorem 1 [4] The symmetric $2m$ -step method with associated characteristic equation given by (6) has phase-lag order q and phase-lag constant c given by

$$-cv^{q+2} + O(v^{q+4}) = \frac{2A_k(v) \cos(kv) + \cdots + 2A_j(v) \cos(jv) + \cdots + A_0(v)}{2k^2 A_k(v) + \cdots + 2j^2 A_j(v) + \cdots + 2A_1(v)} \quad (10)$$

¹ Where S is a set of distinct points.

Remark 2 The formula (10) must be used for the direct calculation of the phase-lag for any symmetric $2m$ -step multistep method.

Remark 3 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:

$$-cv^{q+2} + O(v^{q+4}) = \frac{2A_1(v)\cos(v) + A_0(v)}{2A_1(v)} \tag{11}$$

3 The new two stages family of symmetric two-step methods

Consider the hybrid family of two-step methods

$$\begin{aligned} \widehat{p}_{n+\frac{1}{2}} &= \frac{1}{2}(p_n + p_{n+1}) - h^2 \left[a_0 f_n + \left(\frac{1}{8} - a_0\right) f_{n+1} \right] \\ \widehat{p}_{n-\frac{1}{2}} &= \frac{1}{2}(p_n + p_{n-1}) - h^2 \left[a_0 f_n + \left(\frac{1}{8} - a_0\right) f_{n-1} \right] \\ p_{n+1} - 2p_n + p_{n-1} &= h^2 \left[b_1 (f_{n+1} + f_{n-1}) + b_0 f_n + b_2 \left(\widehat{f}_{n+\frac{1}{2}} + \widehat{f}_{n-\frac{1}{2}}\right) \right] \end{aligned} \tag{12}$$

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

Applying the method (12) to the scalar test equation (4), we obtain the difference equation (5) with:

$$\begin{aligned} A_1(v) &= 1 + v^2 \left(b_1 + b_2 \left(\frac{1}{2} + v^2 \left(\frac{1}{8} - a_0 \right) \right) \right) \\ A_0(v) &= -2 + v^2 \left(b_0 + b_2 (2v^2 a_0 + 1) \right) \end{aligned} \tag{13}$$

3.1 The two stages family of eight algebraic order symmetric two-step method with vanished phase-lag and its first, second and third derivatives

We request the above multistage method (12) to have eliminated the phase-lag and its first, second and third derivatives. Consequently, the following system of equations holds:

$$\text{Phase-lag (PL)} = \frac{T_0}{T_1} = 0 \tag{14}$$

$$\text{First derivative of the phase-lag} = \frac{\partial PL}{\partial v} = 0 \tag{15}$$

$$\text{Second derivative of the phase-lag} = \frac{\partial^2 PL}{\partial v^2} = 0 \quad (16)$$

$$\text{Third derivative of the phase-lag} = \frac{\partial^3 PL}{\partial v^3} = 0 \quad (17)$$

where

$$\begin{aligned} T_0 &= 8 \cos(v) v^4 b_2 a_0 - \cos(v) v^4 b_2 - 8 v^4 b_2 a_0 - 8 \cos(v) v^2 b_1 \\ &\quad - 4 \cos(v) b_2 v^2 - 4 v^2 b_0 - 4 b_2 v^2 - 8 \cos(v) + 8 \\ T_1 &= 8 v^4 b_2 a_0 - v^4 b_2 - 8 v^2 b_1 - 4 b_2 v^2 - 8 \end{aligned}$$

Solving the above system of Eqs. (14)–(17), we can find the coefficients of the new obtained two stages two-step method: a_0 , a_1 , b_0 , b_1 , b_2 . In Supplement Material A we give the above mentioned coefficients.

For some values of $|v|$ (for example when for some values of $|v|$ the denominators of the formulae of the coefficients are equal to zero). For these cases and other that the formulae of the coefficients are subject to heavy cancelations, Taylor series expansions should be used. In Supplement Material B we give the Taylor series expansions of the coefficients.

The behavior of the coefficients of the new two stage two-step method is presented in Fig. 1.

Based on the above coefficients, we can find the local truncation error of the new developed two stage two-step method (12) (mentioned as *TwoStageTwoStep8*) which is given by:

$$\begin{aligned} LTE_{TwoStageTwoStep8} &= \frac{59}{76204800} h^{10} \left(p_n^{(10)} + 4 \phi^2 p_n^{(8)} + 6 \phi^4 p_n^{(6)} \right. \\ &\quad \left. + 4 \phi^6 p_n^{(4)} + \phi^8 p_n^{(2)} \right) + O(h^{12}) \end{aligned} \quad (18)$$

3.2 The two stages family of sixth algebraic order P-stable symmetric two-step method with vanished phase-lag and its first, second and third derivatives

Requesting the above multistage method (12) to have vanished the phase-lag and its first and second derivatives we have to solve the systems of Eqs. (14)–(16). At the same time and in order the method to be P-stable (and using , we request the characteristic equation (6) with $m = 1$ to have as roots:

$$\lambda_1 = \exp(I \phi h) = \exp(I v), \quad \lambda_2 = \exp(-I \phi h) = \exp(-I v) \quad (19)$$

Solving the above system of equations we can find the coefficients of the new obtained two stages two-step P-stable method: a_0 , a_1 , b_0 , b_1 , b_2 . In Supplement Material C we give the above mentioned coefficients.

For some values of $|v|$ (for example when for some values of $|v|$ the denominators of the formulae of the coefficients are equal to zero). For these cases and other that the

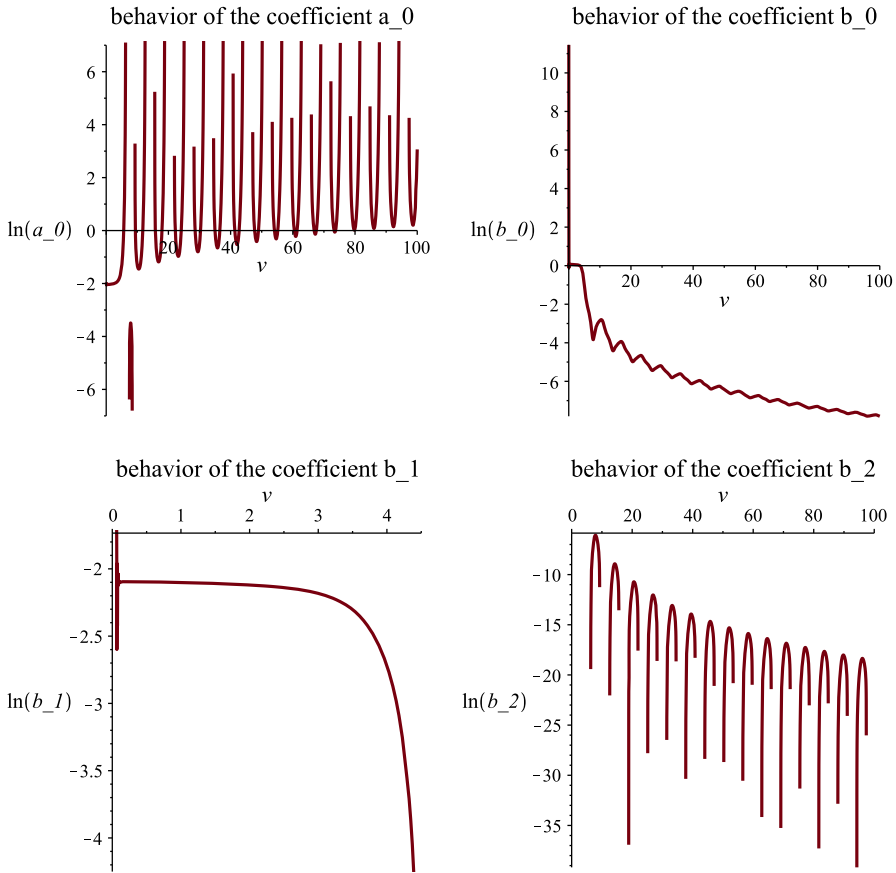


Fig. 1 Behavior of the coefficients of the new obtained hight algebraic two stage two-step method for several values of $v = \phi h$

formulae of the coefficients are subject to heavy cancelations, Taylor series expansions should be used. In Supplement Material D we give the Taylor series expansions of the coefficients.

The behavior of the coefficients of the new two stage two-step P-stable method is shown in Fig. 2.

Substituting the above coefficients, we obtain the local truncation error of the new developed P-stable two stage two-step method (12) with coefficients determined in Sect. 3.2 (mentioned as *TwoStageTwoStep6*) which is given by:

$$\begin{aligned}
 LTE_{TwoStageTwoStep6} = & \frac{43}{205632} h^8 \left(p_n^{(8)} + 3\phi^2 p_n^{(6)} \right. \\
 & \left. + 3\phi^4 p_n^{(4)} + \phi^6 p_n^{(2)} \right) + O\left(h^{10}\right) \quad (20)
 \end{aligned}$$

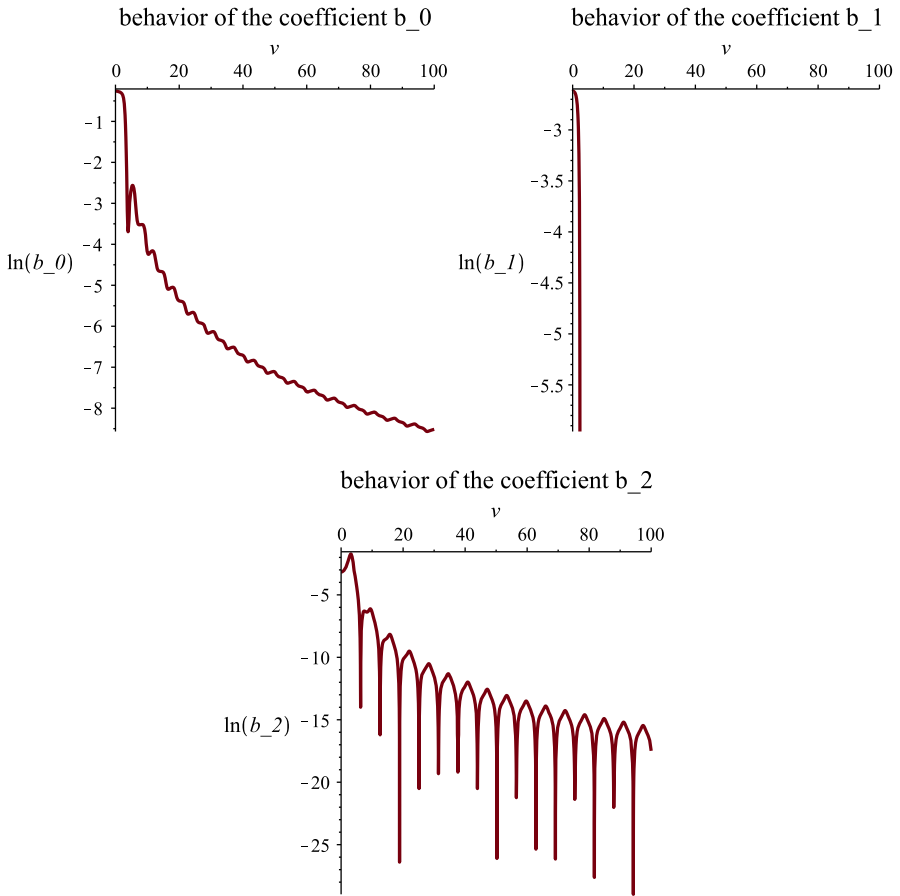


Fig. 2 Behavior of the coefficients of the new P-stable two stage two-step method for several values of $v = \phi h$

4 Local truncation error analysis

In order to investigate the behavior of the Local Truncation Error, we use the scalar test problem

$$p''(x) = (V(x) - V_c + G) p(x) \quad (21)$$

where

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

We will investigate the behavior of the local truncation error for the following methods.

4.1 Classical method (i.e. the method (12) with constant coefficients)

$$LTE_{CL} = \frac{59}{76204800} h^{10} p_n^{(10)} + O(h^{12}) \tag{22}$$

4.2 The new obtained two stage two-step method with vanished phase-lag and its first, second and third derivatives produced in Sect. 3.1

$$LTE_{TwoStageTwoStep8} = \frac{59}{76204800} h^{10} \left(p_n^{(10)} + 4\phi^2 p_n^{(8)} + 6\phi^4 p_n^{(6)} + 4\phi^6 p_n^{(4)} + \phi^8 p_n^{(2)} \right) + O(h^{12}) \tag{23}$$

4.3 Classical method for the P-stable version of the method

$$LTE_{CL2} = \frac{43}{205632} h^8 p_n^{(8)} + O(h^{10}) \tag{24}$$

4.4 The new obtained two stage two-step P-stable method with vanished phase-lag and its first and second derivatives produced in Sect. 3.2

$$LTE_{TwoStageTwoStep6} = \frac{43}{205632} h^8 \left(p_n^{(8)} + 3\phi^2 p_n^{(6)} + 3\phi^4 p_n^{(4)} + \phi^6 p_n^{(2)} \right) + O(h^{10}) \tag{25}$$

Our Local Truncation Error analysis is given below:

- We have to apply the local truncation error formulae on the scalar test problem (21). In order to do this, we have to calculate the derivatives of the function p based on the problem (21). Some of the expressions of these calculations are given in the “Appendix”.
- Since the new formulae of the Local Truncation Errors are computed based on the previous step, they are dependent on the quantities G and energy E .
- Our investigation studies two cases for the quantity G :
 1. First Case: $V_c - E = G \approx 0$: This is the case in which the Energy is closed to the Potential. Consequently, all the terms of $G^n, n \geq 1$ are approximately equal to zero. Therefore, all the terms in the formulae of the local truncation error which contain $G^n, n \geq 1$ are approximately equal to zero. Consequently, the formulae of the local truncation error consist only the terms with G^0 i.e. which consist with the terms which are free from G . We can observe that for the above mentioned methods the free from G terms are the same. Therefore, for this case the asymptotic behavior of the local truncation error formula for the classical method and the asymptotic behavior of the local truncation error

formula for the method with vanished the phase-lag and its first, second and third derivatives is the same. Consequently, in this case and for these values of G , the methods mentioned above are of comparable accuracy.

2. $G \gg 0$ or $G \ll 0$. Consequently, $|G|$ is a large number. For this case, the most accurate numerical methods are the methods with local truncation error formula which contain minimum power of G .
- Finally the asymptotic expressions of the Local Truncation Errors are presented.

Based on the above algorithm we found the following asymptotic expansions of the Local Truncation Errors:

4.5 Classical method

$$LTE_{CL} = \frac{59}{4762800} h^{10} \left(y(x) G^5 + \dots \right) + O(h^{12}) \quad (26)$$

4.6 The new obtained two stage two-step method with vanished phase-lag and its first, second and third derivatives produced in Sect. 3.1

$$\begin{aligned} LTE_{TwoStageTwoStep8} = & -\frac{59}{19051200} h^{10} \left[\left(4 \left(\frac{d^2}{dx^2} g(x) \right) g(x) p(x) \right. \right. \\ & + 3 \left(\frac{d}{dx} g(x) \right)^2 p(x) + 7 \left(\frac{d^4}{dx^4} g(x) \right) p(x) \\ & \left. \left. + 2 \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} p(x) \right) \right) G^2 + \dots \right] + O(h^{12}) \end{aligned} \quad (27)$$

4.7 Classical method for the P-stable version of the method

$$LTE_{CL2} = \frac{43}{205632} h^8 G^4 + \dots + O(h^{10}) \quad (28)$$

4.8 The new obtained two stage two-step P-stable method with vanished phase-lag and its first and second derivatives produced in Sect. 3.2

$$LTE_{TwoStageTwoStep6} = \frac{43}{51408} h^8 \left[\left(\frac{d^2}{dx^2} g(x) \right) p(x) G^2 + \dots \right] + O(h^{10}) \quad (29)$$

The above analysis leads to the following theorem:

Theorem 2 1. Eighth Order Symmetric Two-step Methods

- Classical Method (i.e. the method (12) with constant coefficients): For this method the error increases as the fifth power of G .
- Two Stage Two-Step Eighth Algebraic Order Method with Vanished Phase-lag and its First, Second and Third Derivatives developed in Sect. 3.1: For this method the error increases as the Second power of G .

2. Sixth Order Symmetric Two-step Methods

- Classical Method: For this method the error increases as the fourth power of G .
- Two Stage Two-Step P -stable Sixth Algebraic Order Method with Vanished Phase-lag and its First and Second Derivatives developed in Sect. 3.2: For this method the error increases as the Second power of G .

So, for the numerical solution of the time independent one-dimensional Schrödinger equation the new developed Two Stage Two-Step Eighth Algebraic Order Method with Vanished Phase-lag and its First, Second and Third Derivatives is the most efficient from theoretical point of view, especially for large values of $|G| = |V_c - E|$.

5 Stability analysis

The interval of periodicity and stability of the new proposed two stage two-step method is studied in this section. In order to investigate the stability of a symmetric multistep method, we consider the scalar test equation:

$$p'' = -\omega^2 p. \tag{30}$$

Remark 4 We note here that the frequency used in the scalar test equation for the stability analysis (ω) is not equal to the frequency of the scalar test equation used for the phase-lag analysis (ϕ) i.e. $\omega \neq \phi$.

If we apply the new two stage two-step method to the scalar test Eq. (30) we obtain the following difference equation:

$$A_1(s, v) (p_{n+1} + p_{n-1}) + A_0(s, v) p_n = 0 \tag{31}$$

where for the method developed in the Sect. 3.1 we have

$$A_1(s, v) = \frac{T_{13}}{T_{14}}, \quad A_0(s, v) = -2 \frac{T_{15}}{T_{14}} \tag{32}$$

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

$$\begin{aligned} T_{13} = & (\cos(v))^2 s^4 v^3 - 2 (\cos(v))^2 s^2 v^5 + (\cos(v))^2 v^7 - 8 \cos(v) \sin(v) s^4 v^2 \\ & + 8 \cos(v) \sin(v) s^2 v^4 - 21 (\cos(v))^2 s^4 v - 6 (\cos(v))^2 s^2 v^3 \\ & + 3 (\cos(v))^2 v^5 - 4 \sin(v) s^4 v^2 + 4 \sin(v) s^2 v^4 + 2 s^4 v^3 \end{aligned}$$

$$\begin{aligned}
& -4s^2v^5 + 2v^7 + 12 \cos(v) \sin(v) s^4 + 60 \cos(v) \sin(v) s^2v^2 \\
& + 12 \cos(v) s^4v - 36 \cos(v) s^2v^3 - 12 \sin(v) s^4 \\
& - 60 \sin(v) s^2v^2 + 9s^4v + 42s^2v^3 - 3v^5 \\
T_{14} = & v^5 \left((\cos(v))^2 v^2 + 3 (\cos(v))^2 + 2v^2 - 3 \right) \\
T_{15} = & 3 (\cos(v))^2 v^5 + 12 (\cos(v))^2 \sin(v) s^4 + 12 (\cos(v))^3 s^4v \\
& - 36 (\cos(v))^3 s^2v^3 + (\cos(v))^2 v^7 + 8 \cos(v) \sin(v) s^4v^2 \\
& - 8 \cos(v) \sin(v) s^2v^4 - 24 \sin(v) s^4v^2 + (\cos(v))^2 s^4v^3 \\
& - 2 (\cos(v))^2 s^2v^5 - 12 \cos(v) \sin(v) s^4 - 21 (\cos(v))^2 s^4v \\
& + 2s^4v^3 - 4s^2v^5 - 6 (\cos(v))^2 s^2v^3 + 24 \sin(v) s^2v^4 - 3v^5 \\
& + 4 (\cos(v))^2 \sin(v) s^4v^2 - 4 (\cos(v))^2 \sin(v) s^2v^4 \\
& + 60 (\cos(v))^2 \sin(v) s^2v^2 - 60 \cos(v) \sin(v) s^2v^2 \\
& + 33s^4v - 30s^2v^3 + 2v^7 - 24 \cos(v) s^4v + 72 \cos(v) s^2v^3
\end{aligned}$$

while for the method developed in the Sect. 3.2 we have

$$A_1(s, v) = \frac{T_{16}}{T_{17}}, \quad A_0(s, v) = 2 \frac{T_{18}}{T_{17}} \quad (33)$$

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

$$\begin{aligned}
T_{16} = & 24 (\cos(v))^2 s^4v - 48 (\cos(v))^2 s^2v^3 + 24 (\cos(v))^2 v^5 \\
& - 72 \cos(v) \sin(v) s^4 + 48 \cos(v) \sin(v) s^2v^2 + 24 \cos(v) \sin(v) v^4 \\
& + 24 \cos(v) s^4v - 23 \cos(v) s^2v^3 - \cos(v) v^5 - 192 (\cos(v))^2 s^2v \\
& + 72 \sin(v) s^4 - 173 \sin(v) s^2v^2 + \sin(v) v^4 - 48s^4v \\
& + 96s^2v^3 - 48v^5 + 184 \cos(v) s^2v + 8s^2v \\
T_{17} = & v^4 \left(24 (\cos(v))^2 v + 24 \cos(v) \sin(v) - \cos(v) v + \sin(v) - 48v \right) \\
T_{18} = & (\cos(v))^2 s^4v + 23 (\cos(v))^2 s^2v^3 - 24 (\cos(v))^2 v^5 \\
& + 192 (\cos(v))^3 s^2v - 3 \cos(v) \sin(v) s^4 + 127 \cos(v) \sin(v) s^2v^2 \\
& - 24 \cos(v) \sin(v) v^4 + \cos(v) s^4v - 2 \cos(v) s^2v^3 + \cos(v) v^5 \\
& - 184 (\cos(v))^2 s^2v + 3 \sin(v) s^4 - 2 \sin(v) s^2v^2 \\
& - \sin(v) v^4 - 2s^4v - 46s^2v^3 + 48v^5 - 8 \cos(v) s^2v
\end{aligned}$$

Remark 5 The terms P-stable and singularly almost P-stable method is hold in the cases $\omega = \phi$ i.e. only 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 two stage two-step method produced in the Sect. 3.1 is shown in Fig. 3.

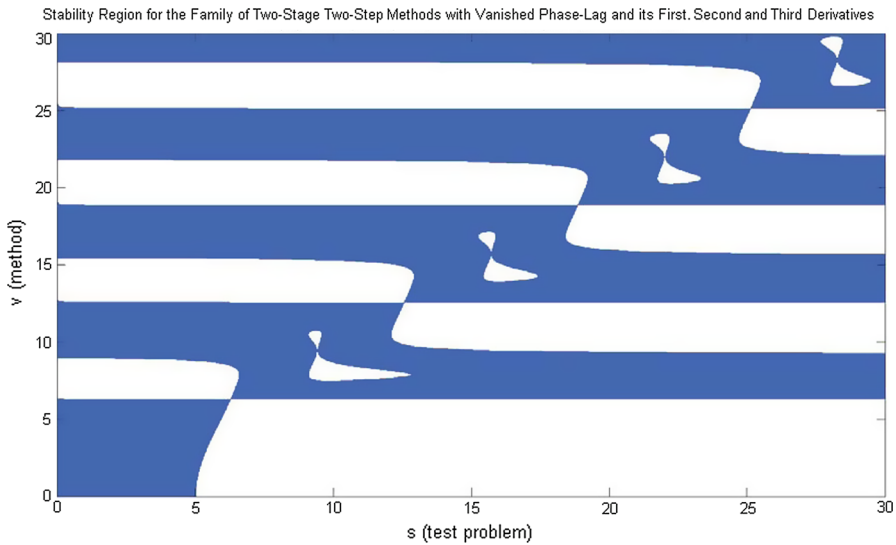


Fig. 3 $s-v$ plane of the new produced two stage two-step eighth algebraic order method with vanished phase-lag and its first, second and third derivatives

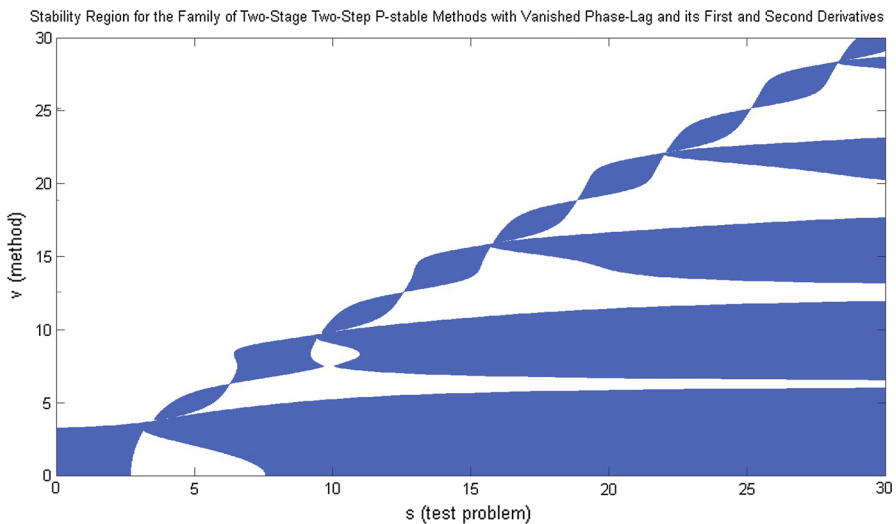


Fig. 4 $s-v$ plane of the new obtained two stage two-step P-stable sixth algebraic order method with vanished phase-lag and its first and second derivatives

The $s-v$ plane for the P-stable two stage two-step method obtained in the Sect. 3.2 is shown in Fig. 4.

Remark 6 The $s-v$ region presented in Figs. 3 and 4 leads to the following remarks: (1) The method is stable within the shadowed area, (2) The method is unstable within the white area.

Remark 7 Based on the fact that the most of the mathematical models of many real problems in Sciences, Engineering and Technology (for example the Schrödinger equation) consist only one frequency in the their model, it is of our interest the investigation of the stability of the obtained method 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 $\omega = \phi$ or $s = v$ (note that: $s = \omega h$ and $v = \phi h$). In these cases the investigation of the $s-v$ plane is limited on the **the surroundings of the first diagonal of the $s-v$ plane** i.e. on the areas where $s = v$.

In the case $s = v$ the characteristic equation for the method developed in Sect. 3.2 is given by:

$$4 \frac{(48 (\cos (v))^2 + 25 \sin (v) v - 46 \cos (v) - 2) (2 \lambda \cos (v) - \lambda^2 - 1)}{v (24 (\cos (v))^2 v + 24 \cos (v) \sin (v) - \cos (v) v + \sin (v) - 48 v)} = 0 \quad (34)$$

It is obvious from the above equation, that the roots of this equation are: $\lambda_1 = \exp(i v)$, $\lambda_2 = \exp(-i v)$ (where $i = \sqrt{-1}$) i.e. $|\lambda_1| = |\lambda_2| = 1$ and the method is P-stable.

The above remark leads to the following result:

- For the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s-v$ plane), the interval of periodicity for the new obtained method in Sect. 3.1 is equal to: $(0, 23)$.
- For the case where $s = v$ (i.e. see the surroundings of the first diagonal of the $s-v$ plane), the interval of periodicity for the new produced method in Sect. 3.2 is equal to: $(0, \infty)$, i.e. the method is P-stable.

The above investigation leads to the following theorem:

Theorem 3 For the obtained methods in Sect. 3 we have the following conclusions:

1. Two-Stage Symmetric Two-Step Method obtained in Sect. 3.1
 - is of eighth algebraic order;
 - has the phase-lag and its first, second and third derivatives equal to zero
 - has an interval of periodicity equals to: $(0, 23)$, 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 of low computational cost since has only 3 stages.
2. Two-Stage Symmetric Two-Step Method obtained in Sect. 3.2
 - is of sixth 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
 - is of low computational cost since has only 3 stages.

6 Numerical results

6.1 Error estimation

The numerical solution of a problem using variable-step procedure, requests an error estimation scheme. Much investigation has been done the last decades on the estimation of the local truncation error (LTE) for the approximate solution of systems of differential equations (see for example [1–65]).

Our methodology for the local error estimation will be based on the algebraic order of the methods (there are several other methodologies which will be used in other papers when we will develop the appropriate numerical methods). The methodology of the local error estimation leads to an embedded pair. In this paper we develop an embedded pair which is based on the algebraic order of the participant symmetric multistep methods and on the fact that the maximum algebraic order of a symmetric multistep method obtains highly accurate approximate solutions of problems with oscillatory and/or periodical solution.

The local truncation error in y_{n+1}^L is estimated by

$$LTE = \left| y_{n+1}^H - y_{n+1}^L \right| \quad (35)$$

y_{n+1}^L denotes the lower algebraic order solution and we use for this the symmetric two-stages two-step P-stable method of sixth algebraic order developed in Sect. 3.2 and y_{n+1}^H denotes the higher order solution and we use for this symmetric two-stages two-step method of eighth algebraic order obtained in Sect. 3.1.

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

$$h_{n+1} = h_n \left(\frac{acc}{LTE} \right)^{\frac{1}{q}} \quad (36)$$

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 8 We use the local extrapolation technique. With this procedure we accept at each point the higher algebraic order solution y_{n+1}^H , as approximation, while the local error is controlled using the 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 which are expressed with mathematical models which contain coupled differential equations of the Schrödinger type.

The close-coupling differential equations of the Schrödinger type can be written as:

$$\left[\frac{d^2}{dx^2} + k_i^2 - \frac{l_i(l_i + 1)}{x^2} - V_{ii} \right] y_{ij} = \sum_{m=1}^N V_{im} y_{mj} \quad (37)$$

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 [58]):

$$y_{ij} = 0 \quad \text{at} \quad x = 0 \quad (38)$$

$$y_{ij} \sim k_i x j_{l_i}(k_i x) \delta_{ij} + \left(\frac{k_i}{k_j} \right)^{1/2} K_{ij} k_i x n_{l_i}(k_i x) \quad (39)$$

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

Remark 9 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 [58] is our guideline for our application. We define a matrix K' and diagonal matrices M, N as:

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

Based on the above we can write the asymptotic condition (39) as:

$$\mathbf{y} \sim \mathbf{M} + \mathbf{N} \mathbf{K}' \quad (40)$$

Remark 10 The detailed description of the problem can be found in [58]. The Iterative Numerov method of Allison is also described in the same paper.

The model of the real problem of rotational excitation of a diatomic molecule by neutral particle impact can be expressed by 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 [58], 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

$$\begin{aligned} &\left[\frac{d^2}{dx^2} + k_{j'j}^2 - \frac{l'(l' + 1)}{x^2} \right] y_{j'l'}^{Jjl}(x) \\ &= \frac{2\mu}{\hbar^2} \sum_{j''} \sum_{l''} \langle j'l'; J | V | j''l''; J \rangle y_{j''l''}^{Jjl}(x) \end{aligned} \quad (41)$$

where

$$k_{j'j} = \frac{2\mu}{\hbar^2} \left[E + \frac{\hbar^2}{2I} \{j(j+1) - j'(j'+1)\} \right] \quad (42)$$

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 [58], the potential V can be expanded as

$$V(x, \hat{\mathbf{k}}_{j'j}, \hat{\mathbf{k}}_{jj}) = V_0(x)P_0(\hat{\mathbf{k}}_{j'j}, \hat{\mathbf{k}}_{jj}) + V_2(x)P_2(\hat{\mathbf{k}}_{j'j}, \hat{\mathbf{k}}_{jj}), \tag{43}$$

and the coupling matrix element may then be written as

$$\langle j'l'; J | V | j''l''; J \rangle = \delta_{j'j''} \delta_{l'l''} V_0(x) + f_2(j'l', j''l''; J) V_2(x) \tag{44}$$

where the f_2 coefficients can be obtained from formulas given by Bernstein et al. [59] 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 [60]). The boundary conditions are

$$y_{j'l'}^{Jjl}(x) = 0 \text{ at } x = 0 \tag{45}$$

$$y_{j'l'}^{Jjl}(x) \sim \delta_{jj'} \delta_{ll'} \exp[-i(k_{jj}x - 1/2l\pi)] - \left(\frac{k_i}{k_j}\right)^{1/2} S^J(jl; j'l') \exp[i(k_{j'j}x - 1/2l'\pi)] \tag{46}$$

where the scattering S matrix is related to the K matrix of (39) by the relation

$$\mathbf{S} = (\mathbf{I} + i\mathbf{K})(\mathbf{I} - i\mathbf{K})^{-1} \tag{47}$$

An numerical scheme which includes a numerical method for step-by-step integration from the initial value to matching points is needed in order to compute the cross sections for rotational excitation of molecular hydrogen by impact of various heavy particles. For the purpose of our numerical tests we will use a scheme which is based on the similar algorithm which has been produced for the numerical tests of [58].

For numerical purposes we choose the \mathbf{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 [58], 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 [60] and Allison [58] 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 (45) may be written as

$$y_{j'l'}^{Jjl}(x_0) = 0 \tag{48}$$

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 [58] which is indicated as **Method I**,
- the variable-step method of Raptis and Cash [61] which is indicated as **Method II**,
- the embedded Runge–Kutta Dormand and Prince method 5(4) [53] which is indicated as **Method III**,
- the embedded Runge–Kutta method ERK4(2) developed in Simos [62] which is indicated as **Method IV**,
- the embedded symmetric two-step method developed in [63] which is indicated as **Method V**,
- the new developed low cost embedded symmetric two-step method which is indicated as **Method VI**.

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.

Table 1 Coupled differential equations

	Method	N	hmax	RTC	MErr
Real time of computation (in seconds) (RTC) and maximum absolute error (MErr) to calculate $ S ^2$ for the variable-step methods Method I–Method V. $acc = 10^{-6}$. We note that hmax is the maximum stepsize	Method 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}
	Method VI	4	0.448	0.07	2.8×10^{-7}
		9	0.448	1.14	4.3×10^{-7}
		16	0.448	8.39	7.1×10^{-7}

7 Conclusions

In this paper we developed a family of low computational cost two-stages symmetric two-step methods. The analysis of the new family of methods consists of:

1. We presented the development of the following methods
 - The first method is of eighth algebraic order and has the phase-lag and its first, second and third derivatives vanished.
 - The second method is of sixth algebraic order, is P-stable and has the phase-lag and its first and second derivatives vanished.
2. We studied the comparative local truncation error analysis.
3. We investigated the stability properties of the new family of methods using a scalar test equation with frequency different than the frequency used by the scalar test equation for the phase-lag analysis.
4. We finally studied the computational efficiency of the new family of methods applying it on the approximate solution of the coupled differential equations arising from the Schrödinger equation.

As a conclusion of this research we can see that the new family of methods produces an embedded pair which is much more efficient than known ones for the numerical solution of the Schrödinger equation and 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).

Compliance with ethical standards

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

Informed consent 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.

Appendix: Formulae of the derivatives of q_n

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

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

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

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

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

$$\begin{aligned}
y_n^{(6)} &= \left(\frac{d^4}{dx^4} g(x) \right) y(x) + 4 \left(\frac{d^3}{dx^3} g(x) \right) \frac{d}{dx} y(x) + 7 (g(x) + G) y(x) \frac{d^2}{dx^2} g(x) \\
&\quad + 4 \left(\frac{d}{dx} g(x) \right)^2 y(x) + 6 (g(x) + G) \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + (g(x) + G)^3 y(x) \\
y_n^{(7)} &= \left(\frac{d^5}{dx^5} g(x) \right) y(x) + 5 \left(\frac{d^4}{dx^4} g(x) \right) \frac{d}{dx} y(x) + 11 (g(x) + G) y(x) \frac{d^3}{dx^3} g(x) \\
&\quad + 15 \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^2}{dx^2} g(x) + 13 (g(x) + G) \left(\frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x) \\
&\quad + 10 \left(\frac{d}{dx} g(x) \right)^2 \frac{d}{dx} y(x) + 9 (g(x) + G)^2 y(x) \frac{d}{dx} g(x) + (g(x) + G)^3 \frac{d}{dx} y(x) \\
y_n^{(8)} &= \left(\frac{d^6}{dx^6} g(x) \right) y(x) + 6 \left(\frac{d^5}{dx^5} g(x) \right) \frac{d}{dx} y(x) + 16 (g(x) + G) y(x) \frac{d^4}{dx^4} g(x) \\
&\quad + 26 \left(\frac{d}{dx} g(x) \right) y(x) \frac{d^3}{dx^3} g(x) + 24 (g(x) + G) \left(\frac{d}{dx} y(x) \right) \frac{d^3}{dx^3} g(x) \\
&\quad + 15 \left(\frac{d^2}{dx^2} g(x) \right)^2 y(x) + 48 \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \frac{d^2}{dx^2} g(x) \\
&\quad + 22 (g(x) + G)^2 y(x) \frac{d^2}{dx^2} g(x) + 28 (g(x) + G) y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
&\quad + 12 (g(x) + G)^2 \left(\frac{d}{dx} y(x) \right) \frac{d}{dx} g(x) + (g(x) + G)^4 y(x) \dots
\end{aligned}$$

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