

Multistep methods with vanished phase-lag and its first and second derivatives for the numerical integration of the Schrödinger equation

Ibraheem Alolyan · T. E. Simos

Received: 20 August 2010 / Accepted: 1 September 2010 / Published online: 17 September 2010
© Springer Science+Business Media, LLC 2010

Abstract A tenth algebraic order eight-step method is developed in this paper. For this method we require the phase-lag and its first and second derivatives to be vanished. A comparative error analysis and a comparative stability analysis are also presented in this paper. The new proposed method is applied for the numerical solution of the one-dimensional Schrödinger equation. The efficiency of the new methodology is proved via the theoretical analysis and the numerical applications. General conclusions about the importance of several properties on the construction of numerical algorithms for the approximate solution of the radial Schrödinger equation are also presented.

Keywords Numerical solution · Schrödinger equation · Multistep methods · Hybrid methods · Interval of periodicity · P-stability · Phase-lag · Phase-fitted

Highly Cited Researcher, Active Member of the European Academy of Sciences and Arts. Active Member of the European Academy of Sciences Corresponding Member of European Academy of Arts, Sciences and Humanities.

I. Alolyan · T. E. Simos
Department of Mathematics, College of Sciences, King Saud University, P. O. Box 2455,
Riyadh 11451, Saudi Arabia

T. E. Simos
Laboratory of Computational Sciences, Department of Computer Science and Technology,
Faculty of Sciences and Technology, University of Peloponnese, 221 00 Tripolis, Greece

T. E. Simos (✉)
10 Konitsis Street, Amfitheá—Paleon Faliron, 175 64 Athens, Greece
e-mail: tsimos.conf@gmail.com; tsimos@mail.ariadne-t.gr

1 Introduction

The radial Schrödinger equation can be written as:

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x). \quad (1)$$

Mathematical Models in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc. can be express via the above boundary value problem (see for example [1–4]).

For the above Eq. (1) we have the following definitions:

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

The boundary conditions are:

$$y(0) = 0 \quad (2)$$

and a second boundary condition, for large values of x , determined by physical considerations.

Large research on the construction of numerical methods for the solution of the Schrödinger equation has been done the last years. The aim and scope of this research is the construction of fast and reliable methods for the solution of the Schrödinger equation and related problems (see for example [5–40]).

More specifically the last years:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge–Kutta and Runge–Kutta Nyström type have been developed in [10–33].
- In [34–36] exponentially and trigonometrically fitted Runge–Kutta and Runge–Kutta Nyström methods are obtained.
- Multistep phase-fitted methods and multistep methods with minimal phase-lag are developed in [41–103].
- Symplectic integrators are studied in [104–118].
- Exponentially and trigonometrically multistep methods have been developed in [119–132].
- Review papers have been written in [133–135] and Proceedings of Conferences have been published in [136–139].

We can divide the numerical methods for the numerical solution of the Schrödinger equation and related problems into two main categories:

1. Methods with constant coefficients
2. Methods with coefficients depending on the frequency of the problem.¹

¹ When using a functional fitting algorithm for the solution of the radial Schrödinger equation, the fitted frequency is equal to: $\sqrt{[l(l+1)/x^2 + V(x) - k^2]}$.

The purpose of this paper is to develop a new tenth algebraic order eight-step method which has the phase-lag and its first and second derivative equal to zero. We study the local truncation error and the stability for several methods and a comparative error analysis and a comparative stability analysis are presented in this paper. We will apply the new proposed method to the numerical solution of the radial Schrödinger equation. The efficiency of the new methodology will be proved via theoretical analysis and numerical applications. We note here that general conclusions about the importance of several properties on the construction of numerical algorithms for the approximate solution of the radial Schrödinger equation are also presented in this paper.

More specifically, we will develop a family of implicit symmetric eight-step methods of tenth algebraic order. The development of the new family is based on the requirement of vanishing the phase-lag and its first and second derivatives. We will investigate the stability and the error of the methods of the new family. Finally, we will apply the new proposed method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. The paper is organized as follows. In Sect. 2 we present the theory of the new methodology. In Sect. 3 we present the development of the new family of methods. A comparative error analysis and its conclusions are presented in Sect. 4. In Sect. 5 we will investigate the stability properties of the new developed methods. In the same section a comparative stability analysis is also presented. In Sect. 6 the numerical results are presented. Remarks and conclusions are discussed in Sect. 7. Finally in the Appendices we present analytic expansions for the errors for several methods and the expansion of the characteristic equation in the special case $s = v$.

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$p'' = f(x, p) \quad (3)$$

consider a multistep method with m steps which can be used over the equally spaced intervals $\{x_i\}_{i=0}^m \in [a, b]$ and $h = |x_{i+1} - x_i|$, $i = 0(1)m - 1$.

If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}$, $i = 0(1)\lfloor \frac{m}{2} \rfloor$.

When a symmetric $2k$ -step method, that is for $i = -k(1)k$, is applied to the scalar test equation

$$p'' = -\omega^2 p \quad (4)$$

a difference equation of the form

$$\begin{aligned} A_k(v) p_{n+k} + \cdots + A_1(v) p_{n+1} + A_0(v) p_n \\ + A_1(v) p_{n-1} + \cdots + A_k(v) p_{n-k} = 0 \end{aligned} \quad (5)$$

is obtained, where $v = \omega h$, h is the step length and $A_0(v), A_1(v), \dots, A_k(v)$ are polynomials of v .

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

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

Theorem 1 [140] *The symmetric 2k-step method with characteristic equation given by (6) has phase-lag order r and phase-lag constant c given by*

$$-c v^{r+2} + O(v^{r+4}) = \frac{2 A_k(v) \cos(k v) + \dots + 2 A_j(v) \cos(j v) + \dots + A_0(v)}{2 k^2 A_k(v) + \dots + 2 j^2 A_j(v) + \dots + 2 A_1(v)} \tag{7}$$

The formula proposed from the above theorem gives us a direct method to calculate the phase-lag of any symmetric 2k-step method.

Remark 1 The First and Second Derivatives of the phase-lag for the multistep methods are computed based on the above direct formula (7).

3 The new family of eight-step methods

3.1 Development of the new methods

We introduce the following family of methods to integrate $p'' = f(x, p)$:

$$\sum_{i=1}^4 a_i (p_{n+i} + p_{n-i}) + a_0 p_n = h^2 \left[\sum_{i=1}^4 b_i (p''_{n+i} + p''_{n-i}) + b_0 p''_n \right] \tag{8}$$

where $a_4 = 1$.

In order to develop the new method we apply the following procedure:

1. General requirements for the new proposed method

We require the above method to have:

- the maximum algebraic order and
- three free parameters,

The satisfaction of the above two requirement leads to the following relations:

$$\begin{aligned} b_0 &= 30 b_4 + 16 b_3 + 6 b_2 - \frac{95}{6} \\ b_1 &= -16 b_4 - 9 b_3 - 4 b_2 + \frac{125}{12} \end{aligned} \tag{9}$$

2. Computation of the difference equation and the associated characteristic equation

Now we apply the above method to the scalar test Eq. (4) and we get the following difference equation:

$$\sum_{i=0}^4 A_i(v) (p_{n+i} + p_{n-i}) = 0 \quad (10)$$

where $v = \omega h$, h is the step length and $A_i(v)$, $i = 0(1)4$ are polynomials of v . The characteristic equation associated with (10) can be written as:

$$\sum_{i=0}^4 A_i(v) (\lambda^i + \lambda^{-i}) = 0 \quad (11)$$

where

$$\begin{aligned} A_0 &= v^2 \left(30 b_4 + 16 b_3 + 6 b_2 - \frac{95}{6} \right) \\ A_1 &= -1 + v^2 \left(-16 b_4 - 9 b_3 - 4 b_2 + \frac{125}{12} \right) \\ A_2 &= 2 + v^2 b_2 \\ A_3 &= -2 + v^2 b_3 \\ A_4 &= 1 + v^2 b_4 \end{aligned} \quad (12)$$

3. Computation of the corresponding phase-lag

We apply now the direct formula for the computation of the phase-lag (7) for $k = 4$ and for A_j , $j = 0, 1, \dots, 4$ given by (12). This leads to the following equation:

$$\begin{aligned} phl &= \frac{T_0}{T_1} \\ T_0 &= 2 \left(1 + v^2 b_4 \right) \cos(4v) + 2 \left(-2 + v^2 b_3 \right) \cos(3v) \\ &\quad + 2 \left(2 + v^2 b_2 \right) \cos(2v) + 2 \left(-1 + v^2 \left(-16 b_4 - 9 b_3 \right. \right. \\ &\quad \left. \left. - 4 b_2 + \frac{125}{12} \right) \right) \cos(v) + v^2 \left(30 b_4 + 16 b_3 + 6 b_2 - \frac{95}{6} \right) \\ T_1 &= 10 + 32 v^2 b_4 + 18 v^2 b_3 + 8 v^2 b_2 + 2 v^2 \left(-16 b_4 \right. \\ &\quad \left. - 9 b_3 - 4 b_2 + \frac{125}{12} \right) \end{aligned} \quad (13)$$

4. Computation of the corresponding first derivative of the phase-lag

The phase-lag's first derivative is given by:

$$p'hl = \left[-\frac{1}{5} \left(-4608 v b_4 - 2304 v b_3 - 576 v b_2 + 4608 v \cos(v) b_4 \right. \right.$$

$$\begin{aligned}
 &+ 3456 v \cos(v) b_3 + 1152 v \cos(v) b_2 - 2304 \sin(v) v^2 b_4 \\
 &- 1728 \sin(v) v^2 b_3 - 576 \sin(v) v^2 b_2 - 4800 \sin(v) v^4 b_4 \\
 &- 3600 \sin(v) v^4 b_3 - 1200 \sin(v) v^4 b_2 + 3000 \sin(v) v^2 \\
 &+ 3125 \sin(v) v^4 + 576 \sin(v) \cos(v) v^2 b_2 \\
 &+ 1200 \sin(v) \cos(v) v^4 b_2 + 1680 v + 720 \sin(v) - 1152 \sin(v) \cos(v) \\
 &- 3456 \sin(v) \cos(v)^2 + 4608 \sin(v) \cos(v)^3 - 2400 \sin(v) \cos(v) v^2 \\
 &+ 4608 \sin(v) \cos(v)^3 v^2 b_4 + 9600 \sin(v) \cos(v)^3 v^4 b_4 \\
 &+ 1728 \sin(v) \cos(v)^2 v^2 b_3 + 3600 \sin(v) \cos(v)^2 v^4 b_3 \\
 &- 2304 \sin(v) \cos(v) v^2 b_4 - 4800 \sin(v) \cos(v) v^4 b_4 \\
 &+ 4800 \cos(v)^4 v - 4800 \cos(v)^3 v - 2400 \cos(v)^2 v - 576 \cos(v)^2 v b_2 \\
 &+ 2304 \cos(v)^2 v b_4 - 2304 \cos(v)^4 v b_4 - 1152 \cos(v)^3 v b_3 \\
 &+ 9600 \sin(v) \cos(v)^3 v^2 - 7200 \sin(v) \cos(v)^2 v^2 \Big] / \\
 &\left(12 + 25 v^2\right)^2 \tag{14}
 \end{aligned}$$

5. Computation of the corresponding second derivative of the phase-lag

The phase-lag’s first derivative is given by:

$$\begin{aligned}
 p\ddot{h}l = &\left[-\frac{1}{5} \left(33984 + 373248 v^2 b_4 + 172800 v^2 b_3 + 36288 v^2 b_2 \right. \right. \\
 &- 55296 b_4 - 27648 b_3 - 6912 b_2 + 91584 \cos(v) \\
 &- 68400 v^2 - 222336 \cos(v)^2 \\
 &+ 115200 v^4 b_4 - 28800 v^4 b_2 + 60000 v^4 - 93312 \cos(v) v^2 b_2 \\
 &- 28800 \cos(v) v^4 b_2 - 182016 \cos(v)^3 + 278784 \cos(v)^4 \\
 &+ 399600 \cos(v) v^2 - 158400 \cos(v)^3 v^2 - 626400 \cos(v)^2 v^2 \\
 &- 373248 \cos(v) v^2 b_4 - 115200 \cos(v) v^4 b_4 - 321408 \cos(v) v^2 b_3 \\
 &- 110592 v \sin(v) b_4 - 82944 v \sin(v) b_3 - 27648 v \sin(v) b_2 \\
 &- 120000 \cos(v) v^6 b_4 - 259200 \cos(v) v^4 b_3 - 270000 \cos(v) v^6 b_3 \\
 &- 30000 \cos(v) v^6 b_2 - 230400 v^3 \sin(v) b_4 - 172800 v^3 \sin(v) b_3 \\
 &- 57600 v^3 \sin(v) b_2 + 55296 \cos(v) b_4 + 41472 \cos(v) b_3 \\
 &+ 13824 \cos(v) b_2 + 472500 \cos(v) v^4 + 78125 \cos(v) v^6 \\
 &+ 27648 v b_2 \sin(v) \cos(v) + 57600 v^3 b_2 \sin(v) \cos(v) \\
 &+ 221184 \sin(v) \cos(v)^3 v b_4 + 460800 \sin(v) \cos(v)^3 v^3 b_4 \\
 &+ 172800 \sin(v) \cos(v)^2 v^3 b_3 + 82944 \sin(v) \cos(v)^2 v b_3 \\
 &- 110592 \sin(v) v \cos(v) b_4 - 230400 \sin(v) v^3 \cos(v) b_4 \\
 &+ 240000 \sin(v) \cos(v) v^3 + 115200 v \sin(v) \cos(v) + 120000 v^6 b_4 \\
 &\left. \left. - 30000 v^6 b_2 - 6912 \cos(v)^2 b_2 - 27648 \cos(v)^4 b_4 + 960000 \cos(v)^4 v^4 \right) \right]
 \end{aligned}$$

$$\begin{aligned}
& + 561600 \cos(v)^4 v^2 - 13824 \cos(v)^3 b_3 - 540000 \cos(v)^3 v^4 \\
& + 27648 \cos(v)^2 b_4 - 840000 \cos(v)^2 v^4 + 921600 \cos(v)^4 v^4 b_4 \\
& + 393984 \cos(v)^4 v^2 b_4 + 960000 \cos(v)^4 v^6 b_4 + 148608 \cos(v)^3 v^2 b_3 \\
& + 259200 \cos(v)^3 v^4 b_3 + 270000 \cos(v)^3 v^6 b_3 + 60000 \cos(v)^2 v^6 b_2 \\
& - 393984 \cos(v)^2 v^2 b_4 + 57024 \cos(v)^2 v^2 b_2 - 921600 \cos(v)^2 v^4 b_4 \\
& + 57600 \cos(v)^2 v^4 b_2 - 960000 \cos(v)^2 v^6 b_4 - 960000 \sin(v) \cos(v)^3 v^3 \\
& - 460800 \sin(v) \cos(v)^3 v + 720000 \sin(v) \cos(v)^2 v^3 \\
& + 345600 \sin(v) \cos(v)^2 v \Big] \Big/ \left(12 + 25 v^2\right)^3 \tag{15}
\end{aligned}$$

6. **Demand for the satisfaction of the relations (13), (14) and (15)**

We demand that the phase-lag and its first and second derivatives to be equal to zero, i.e. we demand the satisfaction of the relations (13), (14) and (15). We find out that:

$$\begin{aligned}
b_2 = & \frac{1}{24} \left(75 \cos(v) \sin(v)^6 + 336 \sin(v)^6 - 1605 \sin(v)^4 \right. \\
& - 841 \cos(v) \sin(v)^4 + 1780 \cos(v) \sin(v)^2 + 2284 \sin(v)^2 - 1008 \\
& - 1008 \cos(v) \left(243420 \cos(v) \sin(v)^8 v - 18144 \cos(v) \sin(v)^{10} v \right. \\
& + 73560 \cos(v) \sin(v)^5 v^2 - 524292 \cos(v) \sin(v)^6 v \\
& + 3600 \cos(v) \sin(v)^9 v^2 - 72288 \cos(v) \sin(v)^2 v \\
& + 387576 v \sin(v)^4 \cos(v) - 40824 \cos(v) \sin(v)^3 v^2 \\
& - 33888 \cos(v) \sin(v)^7 v^2 - 18144 v \cos(v) \\
& + 54432 \sin(v) \cos(v) + 63216 \sin(v)^2 v + 40824 \sin(v)^3 v^2 \\
& - 425988 \sin(v)^4 v - 318384 \cos(v) \sin(v)^3 - 42840 \sin(v)^3 v^4 \\
& + 725760 \sin(v)^6 v - 495132 \sin(v)^8 v + 41580 \sin(v)^7 v^2 \\
& - 79692 \sin(v)^5 v^2 - 2628 \sin(v)^9 v^2 + 109355 \sin(v)^5 v^4 \\
& - 94395 \sin(v)^7 v^4 + 28125 \sin(v)^9 v^4 + 105456 \sin(v)^{10} v \\
& + 603468 \cos(v) \sin(v)^5 - 420084 \cos(v) \sin(v)^7 \\
& + 21600 \sin(v)^{11} \cos(v) + 58032 \cos(v) \sin(v)^9 \\
& + 7200 \sin(v)^{12} v + 18144 v - 54432 \sin(v) + 345600 \sin(v)^3 \\
& \left. + 696132 \sin(v)^7 - 755856 \sin(v)^5 - 242172 \sin(v)^9 + 11232 \sin(v)^{11} \right) \Big/ \\
& \left(v^4 \left(5625 \sin(v)^6 - 18879 \sin(v)^4 + 21871 \sin(v)^2 - 8568 \right) \sin(v)^{11} \right) \tag{16}
\end{aligned}$$

$$b_3 = \frac{1}{48} \left(-880 \cos(v) \sin(v)^2 - 1168 \sin(v)^2 \right)$$

$$\begin{aligned}
 &+666 \sin(v)^4 + 576 + 298 \cos(v) \sin(v)^4 - 75 \sin(v)^6 + 576 \cos(v) \\
 &\left(- 28608 \cos(v) \sin(v)^5 v^2 + 71232 \cos(v) \sin(v)^6 v \right. \\
 &- 18144 \cos(v) \sin(v)^2 v - 83520 v \sin(v)^4 \cos(v) \\
 &+ 93120 \cos(v) \sin(v)^3 v^2 + 31104 v \cos(v) \\
 &- 31104 \sin(v) \cos(v) + 33696 \sin(v)^2 v - 134208 \sin(v)^3 v^2 \\
 &+ 66936 \sin(v)^4 v + 135648 \cos(v) \sin(v)^3 - 55480 \sin(v)^3 v^4 \\
 &- 98496 \sin(v)^6 v + 28800 \sin(v)^8 v - 7200 \sin(v)^7 v^2 \\
 &+ 77436 \sin(v)^5 v^2 + 28125 \sin(v)^5 v^4 - 148320 \cos(v) \sin(v)^5 \\
 &+ 43200 \cos(v) \sin(v)^7 - 31104 v + 31104 \sin(v) - 151200 \sin(v)^3 \\
 &- 85248 \sin(v)^7 + 205416 \sin(v)^5 + 63936 \sin(v) v^2 + 27360 \sin(v) v^4 \\
 &\left. - 63936 \sin(v) \cos(v) v^2 \right) / \\
 &\left(\sin(v)^9 \left(5472 - 11096 \sin(v)^2 + 5625 \sin(v)^4 \right) v^4 \right) \tag{17}
 \end{aligned}$$

$$\begin{aligned}
 b_4 = &-\frac{1}{96} \left(144 + 144 \cos(v) - 172 \cos(v) \sin(v)^2 \right. \\
 &\left. - 244 \sin(v)^2 + 93 \sin(v)^4 + 25 \cos(v) \sin(v)^4 \right) \\
 &\left(16512 \cos(v) \sin(v)^5 v^2 + 24384 \cos(v) \sin(v)^6 v \right. \\
 &+ 19584 \cos(v) \sin(v)^2 v - 47268 v \sin(v)^4 \cos(v) \\
 &- 12744 \cos(v) \sin(v)^3 v^2 - 2400 \cos(v) \sin(v)^7 v^2 \\
 &+ 2592 v \cos(v) - 7776 \sin(v) \cos(v) - 18288 \sin(v)^2 v \\
 &+ 12744 \sin(v)^3 v^2 + 57384 \sin(v)^4 v + 33264 \cos(v) \sin(v)^3 \\
 &- 2880 \sin(v)^3 v^4 - 44208 \sin(v)^6 v + 7200 \sin(v)^8 v \\
 &+ 8928 \sin(v)^7 v^2 - 21924 \sin(v)^5 v^2 + 3125 \sin(v)^5 v^4 \\
 &- 33552 \cos(v) \sin(v)^5 + 7200 \cos(v) \sin(v)^7 - 2592 v \\
 &+ 7776 \sin(v) - 37152 \sin(v)^3 - 19584 \sin(v)^7 \\
 &\left. + 49212 \sin(v)^5 \right) \left(\sin(v)^{11} \left(-576 + 625 \sin(v)^2 \right) v^4 \right) \tag{18}
 \end{aligned}$$

7. Taylor series expansions of the obtained coefficients

For small values of |v| the formulae given by (16)–(18) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$\begin{aligned}
 b_2 = &-\frac{33961}{181440} + \frac{58061}{380160} v^2 - \frac{114941161}{6227020800} v^4 + \frac{78851779}{78460462080} v^6 \\
 &- \frac{34785197}{494926848000} v^8 - \frac{13423756441}{24329020081766400} v^{10}
 \end{aligned}$$

$$\begin{aligned}
& - \frac{156136506251233}{562000363888803840000} v^{12} - \frac{8148804619499}{276985893630910464000} v^{14} \\
& - \frac{8745761934237617}{2419748766759633813504000} v^{16} + \dots \\
b_3 = & \frac{173531}{181440} - \frac{58061}{1330560} v^2 + \frac{60053897}{43589145600} v^4 - \frac{5734501}{156920924160} v^6 \\
& - \frac{651395527}{266765571072000} v^8 - \frac{11665883797}{42575785143091200} v^{10} \\
& - \frac{14989282592857}{562000363888803840000} v^{12} - \frac{5795535181309}{2215887149047283712000} v^{14} \\
& - \frac{231843167482133}{891486387753549299712000} v^{16} + \dots \\
b_4 = & \frac{45767}{725760} + \frac{58061}{10644480} v^2 + \frac{88852949}{174356582400} v^4 + \frac{81007601}{1569209241600} v^6 \\
& + \frac{857181503}{152437469184000} v^8 + \frac{2185407102427}{3406062811447296000} v^{10} \\
& + \frac{168261172258691}{224800145555215360000} v^{12} + \frac{170514753691237}{19389012554163732480000} v^{14} \\
& + \frac{69983291279922121}{67752965469269746778112000} v^{16} + \dots \quad (19)
\end{aligned}$$

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

8. Computation of the local truncation error

The local truncation error of the new proposed method is given by:

$$\text{LTE} = -\frac{58061 h^{12}}{31933440} \left(y_n^{(12)} + 3 \omega^2 y_n^{(10)} + 3 \omega^4 y_n^{(8)} + \omega^6 y_n^{(6)} \right) \quad (20)$$

4 Comparative error analysis

We will study the following methods:

- The Numerov’s method which is indicated as **NUMEROV**
- The Exponentially-fitted two-step method developed by Raptis and Allison [38] which is indicated as **RAAL**
- The Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] which is indicated as **KALSIM**
- The Exponentially-fitted four-step method developed by Raptis [39] which is indicated as **RAP**
- The eight-step ninth algebraic order method developed by Quinlan and Tremaine [143] which is indicated as **QT9**
- The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143] which is indicated as **QT11**
- The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [143] which is indicated as **QT13**

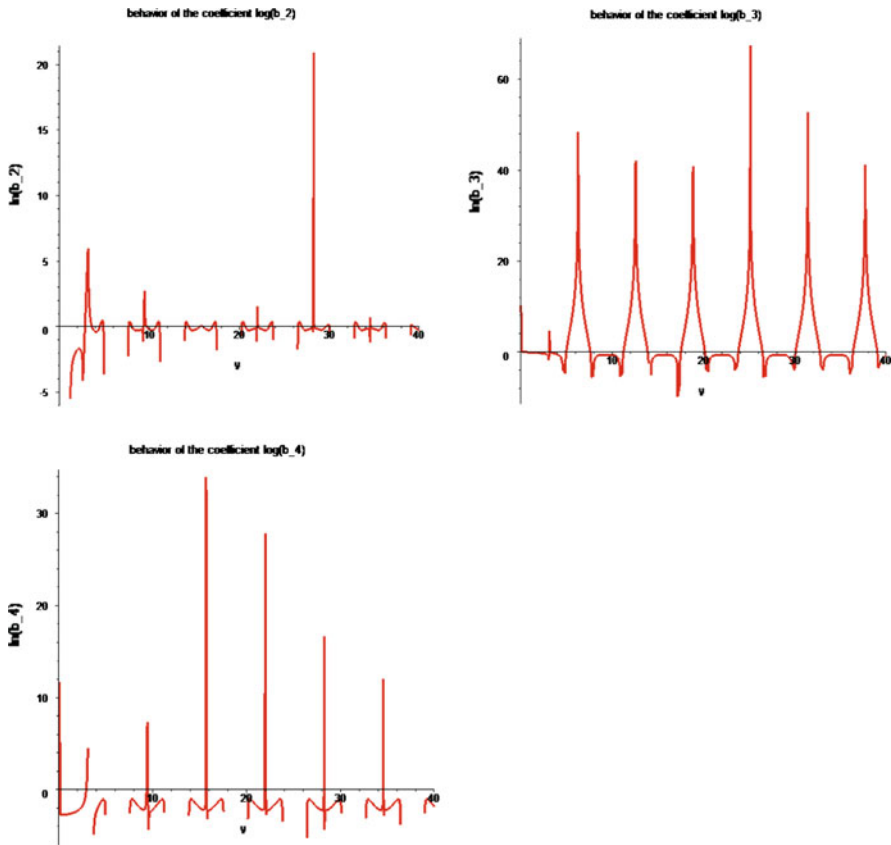


Fig. 1 Behavior of the coefficients of the new proposed method given by (16)–(18) for several values of v

- The classical eight-step method of the family of methods mentioned in paragraph 4 which is indicated as **CL**
- The method produced by Alolyan and Simos [144] which is indicated as **PLD1**
- The new developed eight-step method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 4 which is indicated as **PLD12**

The error analysis is based on the following steps:

1. The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x) y(x) \tag{21}$$

2. Based on the paper of Ixaru and Rizea [141], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \tag{22}$$

where $g(x) = V(x) - V_c = g$, where V_c is the constant approximation of the potential and $G = v^2 = V_c - E$.

3. We express the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \dots$, which are terms of the local truncation error formulae, in terms of the Eq. (21). The expressions are presented as polynomials of G .
4. Finally, we substitute the expressions of the derivatives, produced in the previous step, into the local truncation error formulae.

Based on the procedure mentioned above and on the formulae:

$$\begin{aligned}
 y_n^{(2)} &= (V(x) - V_c + G) y(x) \\
 y_n^{(4)} &= \left(\frac{d^2}{dx^2} V(x) \right) y(x) + 2 \left(\frac{d}{dx} V(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 &\quad + (V(x) - V_c + G) \left(\frac{d^2}{dx^2} y(x) \right) \\
 y_n^{(6)} &= \left(\frac{d^4}{dx^4} V(x) \right) y(x) + 4 \left(\frac{d^3}{dx^3} V(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 &\quad + 3 \left(\frac{d^2}{dx^2} V(x) \right) \left(\frac{d^2}{dx^2} y(x) \right) \\
 &\quad + 4 \left(\frac{d}{dx} V(x) \right)^2 y(x) \\
 &\quad + 6 (V(x) - V_c + G) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} V(x) \right) \\
 &\quad + 4 (U(x) - V_c + G) y(x) \left(\frac{d^2}{dx^2} V(x) \right) \\
 &\quad + (V(x) - V_c + G)^2 \left(\frac{d^2}{dx^2} y(x) \right) \dots
 \end{aligned}$$

we obtain the expressions mentioned in Appendix A for the above methods.

We consider two cases in terms of the value of E :

- The Energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in G are considered. Thus for these values of G , the methods are of comparable accuracy. This is because the free terms of the polynomials in G , are the same for the cases of the classical method and of the new developed methods.
- $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number. So, we have the following asymptotic expansions of the Eqs. (46)–(54).

The Numerov's method

$$\text{LTE}_{\text{NUMEROV}} = h^6 \left(-\frac{1}{240} y(x) G^3 + \dots \right) \quad (23)$$

The method of Raptis and Allison [38]

$$\text{LTE}_{\text{RAAL}} = h^6 \left(-\frac{1}{240} g(x) y(x) G^2 + \dots \right) \quad (24)$$

The exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40]

$$\text{LTE}_{\text{KALSIM}} = h^6 \left(-\frac{1}{144} y(x) G^3 + \dots \right) \quad (25)$$

The Exponentially-fitted four-step method developed by Raptis [39]

$$\text{LTE}_{\text{RAP}} = h^8 \left(-\frac{19}{6048} g(x) y(x) G^3 + \dots \right) \quad (26)$$

The eight-step ninth algebraic order method developed by Quinlan and Tremaine [143]

$$\text{LTE}_{\text{QT9}} = h^{10} \left(-\frac{45767}{725760} y(x) G^5 + \dots \right) \quad (27)$$

The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143]

$$\text{LTE}_{\text{QT11}} = h^{12} \left(-\frac{52559}{912384} y(x) G^6 + \dots \right) \quad (28)$$

The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [143]

$$\text{LTE}_{\text{QT13}} = h^{14} \left(-\frac{16301796103}{290594304000} y(x) G^7 + \dots \right) \quad (29)$$

The classical method of the family (see [144] for more details)²

$$\text{LTE}_{\text{CL}} = h^{12} \left(-\frac{58061}{31933440} y(x) G^6 + \dots \right) \quad (30)$$

² Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.

The method produced by Alolyan and Simos [144] (see [144] for more details)

$$\begin{aligned} \text{LTE}_{\text{PLD1}} = h^{12} & \left[\left(\frac{987037}{31933440} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \right. \right. \\ & + \frac{58061}{15966720} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\ & \left. \left. + \frac{58061}{31933440} g(x)^2 y(x) \right) G^4 + \dots \right] \end{aligned} \quad (31)$$

The new proposed method of the family

$$\text{LTE}_{\text{PLD12}} = h^{12} \left[\frac{58061}{7983360} G^4 \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \dots \right] \quad (32)$$

From the above equations and Table we have the following theorem: (Table 1)

Theorem 2 1. *Fourth Algebraic Order Methods:*

- For the Numerov's Method the error increases as the third power of G
- For the Method of Raptis and Allison [38] the error increases as the second power of G
- The Exponentially-fitted two-step P -stable method developed by Kalogitatu and Simos [40] the error increases as the third power of G

So, for the numerical solution of the time independent radial Schrödinger equation the Method of Raptis and Allison [38] is the most accurate Fourth Algebraic Order Method, especially for large values of $|G| = |V_c - E|$.

2. *Sixth and Eighth Algebraic Order Methods:*

- For the Exponentially-fitted four-step method developed by Raptis [39] the error increases as the third power of G
- For the eight-step ninth algebraic order method developed by Quinlan and Tremaine [143] the error increases as the fifth power of G

So, for the numerical solution of the time independent radial Schrödinger equation the Exponentially-fitted four-step method developed by Raptis [39] is the most accurate Method with Algebraic Order Six or Eight, especially for large values of $|G| = |V_c - E|$.

3. *High Algebraic Order Methods (Ten and Twelfth Algebraic Order Methods):*

- For the ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143] the error increases as the sixth power of G
- For the twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [143] the error increases as the seventh power of G
- For the Classical Method of the Family (see [144] for more details) the error increases as the sixth power of G
- For the method produced by Alolyan and Simos [144] the error increases as the fourth power of G
- For new proposed method produced in this paper the error increases as the fourth power of G but with smaller coefficient than the method of Alolyan and Simos [144]

Table 1 Comparative error analysis for the methods mentioned in Sect. 4

Method	Algebraic order	Order of G	$CFAE$
NUMEROV	4	3	$-\frac{1}{240}$
RAAL	4	2	$-\frac{1}{240}$
KALSIM	4	3	$-\frac{1}{144}$
RAP	6	3	$-\frac{19}{6048}$
QT9	8	5	$-\frac{45767}{725760}$
QT11	10	6	$-\frac{52559}{912384}$
QT13	12	7	$-\frac{16301796103}{290594304000}$
CL	10	6	$-\frac{58061}{31933440}$
PLD1	10	4	$\frac{987037}{31933440}$
PLD12	10	4	$\frac{58061}{7983360}$

We note that $CFAE$ is the coefficient of the maximum power of G in the asymptotic expansion and order of G is the order of the maximum power of G in the asymptotic expansion of the local truncation error

So, for the numerical solution of the time independent radial Schrödinger equation the new proposed method produced in this paper is the most accurate Method , especially for large values of $|G| = |V_c - E|$, since it is a tenth algebraic order methods for which the error increases as the fourth power of G but with smaller coefficient than the method of Alolyan and Simos [144].

5 Stability analysis

In order to define the interval of periodicity we follow the procedure:

1. **Application of the proposed method to the scalar test equation**

The method (8) with the coefficients (16)–(18) is applied to the scalar test equation:

$$\psi'' = -t^2\psi, \tag{33}$$

where $t \neq \omega$.

2. **Definition of the difference equation and the corresponding characteristic equation**

We obtain the following difference equation:

$$A_k(s) \psi_{n+k} + \cdots + A_1(s) \psi_{n+1} + A_0(s) \psi_n + A_1(s) \psi_{n-1} + \cdots + A_k(s) \psi_{n-k} = 0 \quad (34)$$

where $s = th$, h is the step length and $A_0(s), A_1(s), \dots, A_k(s)$ are polynomials of s .

The characteristic equation associated with (34) is given by:

$$A_k(s) \vartheta^k + \cdots + A_1(s) \vartheta + A_0(s) + A_1(s) \vartheta^{-1} + \cdots + A_k(s) \vartheta^{-k} = 0 \quad (35)$$

3. Development of the $s - v$ plane

Definition 1 (see [37]) A symmetric $2k$ -step method with the characteristic equation given by (35) is said to have an *interval of periodicity* $(0, s_0^2)$ if, for all $s \in (0, s_0^2)$, the roots z_i , $i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i \zeta(th)}, \quad |z_i| \leq 1, \quad i = 3, 4 \quad (36)$$

where $\zeta(th)$ is a real function of th and $s = th$.

Definition 2 (see [37]) A method is called P-stable if its interval of periodicity is equal to $(0, \infty)$.

Definition 3 A method is called singularly almost P-stable if its interval of periodicity is equal to $(0, \infty) - S^3$ only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $\mathit{mathrm}v = s$.

In Fig. 2 we present the $s - v$ plane for the method developed in this paper. A shadowed area denotes the $s - v$ region where the method is stable, while a white area denotes the region where the method is unstable.

4. Remarks and conclusions

In the case that the frequency of the scalar test equation is equal with the frequency of phase fitting, i.e. in the case that $v = s$, we have the following figure for the stability polynomials of the new developed methods. From the above diagram it is easy to see that the interval of periodicity of the new methods is equal to: $(0, 4.1)$.

Remark 2 For the solution of the Schrödinger equation the frequency of the exponential fitting is equal to the frequency of the scalar test equation. So, it is necessary to observe the surroundings of the first diagonal of the $s - v$ plane. The expression of the characteristic Eq. (35) in this case is shown in the Appendix B.

From the above analysis we have the following theorem:

Theorem 3 *The method (9) with the coefficients given by (9), (16), (17), (19) is of tenth algebraic order, has the phase-lag and its first derivative equal to zero and has an interval of periodicity equals to: $(0, 4.1)$.*

³ Where S is a set of distinct points.

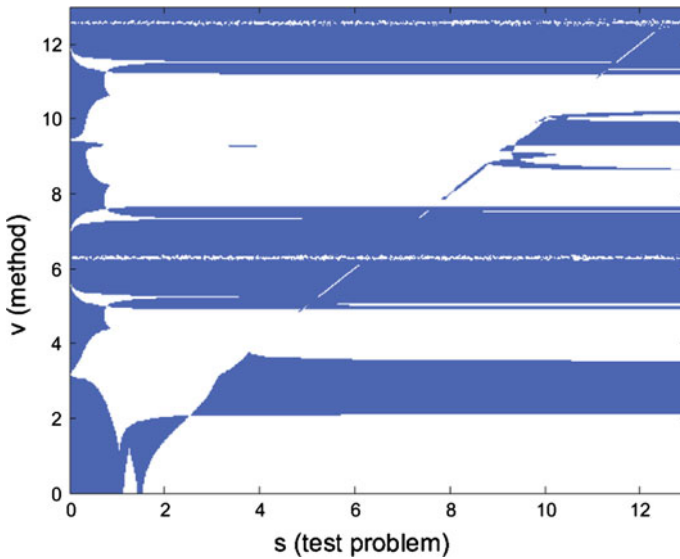


Fig. 2 $s - v$ plane of the New Method produced in Sect. 4

Table 2 Comparative stability analysis for the methods mentioned in the Sect. 5

Method	Interval of periodicity
NUMEROV	$(0, 6)$
RAAL	$(0, \infty) - S$
KALSIM	$(0, \infty) - S$
RAP	$(0, 9.87)$
QT9	$(0, 0.52)$
QT11	$(0, 0.17)$
QT13	$(0, 0.046)$
CL	$(0, 1.3)$
PLD1	$(0, 8.5264)$
PLD12	$(0, 4.1)$

Based on the analysis presented above, we studied the interval of periodicity of the ten methods mentioned in the previous paragraph. The results presented in the Table 2.

6 Numerical results: conclusion

In order to illustrate the efficiency of the new methods obtained in paragraph 4, we apply them to the radial time independent Schrödinger equation.

In order to apply the new methods to the radial Schrödinger equation the value of parameter v is needed. For every problem of the one-dimensional Schrödinger equation given by (1) the parameter v is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \quad (37)$$

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

6.1 Woods–Saxon potential

We use the well known Woods–Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a(1+z)^2} \quad (38)$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

The behavior of Woods–Saxon potential is shown in the Fig. 3.

It is well known that for some potentials, such as the Woods–Saxon potential, the definition of parameter v is not given as a function of x but it is based on some critical points which have been defined from the investigation of the appropriate potential (see for details [142]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [142]):

$$v = \begin{cases} \sqrt{-50 + E}, & \text{for } x \in [0, 6.5 - 2h], \\ \sqrt{-37.5 + E}, & \text{for } x = 6.5 - h \\ \sqrt{-25 + E}, & \text{for } x = 6.5 \\ \sqrt{-12.5 + E}, & \text{for } x = 6.5 + h \\ \sqrt{E}, & \text{for } x \in [6.5 + 2h, 15] \end{cases} \quad (39)$$

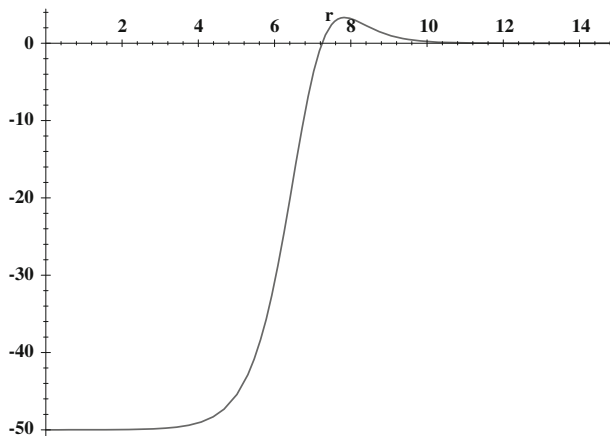


Fig. 3 The Woods–Saxon potential

6.2 Radial Schrödinger equation: the resonance problem

Consider the numerical solution of the radial time independent Schrödinger equation (1) in the well-known case of the Woods–Saxon potential (38). In order to solve this problem numerically we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $x \in [0, 15]$. We consider Eq. (1) in a rather large domain of energies, i.e. $E \in [1, 1000]$.

In the case of positive energies, $E = k^2$, the potential dies away faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{40}$$

for x greater than some value X .

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$ where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of Eq. (1) (when $x \rightarrow \infty$) has the asymptotic form

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC \left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan \delta_l \cos\left(kx - \frac{l\pi}{2}\right) \right] \end{aligned} \tag{41}$$

where δ_l is the phase shift, that is calculated from the formula

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{42}$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need $y_0, y_i, i = 1(1)8$ before starting an eight-step method. From the initial condition we obtain y_0 . The other values can be obtained using the Runge–Kutta–Nyström methods of Dormand et. al. (see [8]). With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l .

For positive energies we have the so-called resonance problem. This problem consists either of 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** when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

$$y(0) = 0, \quad y(x) = \cos\left(\sqrt{E}x\right) \text{ for large } x. \tag{43}$$

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

- The Numerov’s method which is indicated as **Method I**
- The Exponentially-fitted two-step method developed by Raptis and Allison [38] which is indicated as **Method II**
- The Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] which is indicated as **Method III**
- The Exponentially-fitted four-step method developed by Raptis [39] which is indicated as **Method IV**
- The eight-step ninth algebraic order method developed by Quinlan and Tremaine [143] which is indicated as **Method V**
- The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143] which is indicated as **Method VI**
- The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [143] which is indicated as **Method VII**
- The classical eight-step method of the family of methods mentioned in Sect. 3 which is indicated as **Method VIII**
- The method produced by Alolyan and Simos [144] which is indicated as **Method IX**
- The new developed eight-step method with phase-lag and its first and second derivatives equal to zero obtained in paragraph 4 which is indicated as **Method X**.

The computed eigenenergies are compared with exact ones. In Fig. 4 we present the maximum absolute error $\log_{10}(Err)$ where

$$Err = |E_{\text{calculated}} - E_{\text{accurate}}| \quad (44)$$

of the eigenenergy $E_2 = 341.495874$, for several values of NFE=Number of Function Evaluations. In Fig. 5 we present the maximum absolute error $\log_{10}(Err)$ where

$$Err = |E_{\text{calculated}} - E_{\text{accurate}}| \quad (45)$$

of the eigenenergy $E_3 = 989.701916$, for several values of NFE=Number of Function Evaluations.

7 Conclusions

In the present paper we have developed an eight-step method of tenth algebraic order with phase-lag and its first derivative equal to zero.

We have applied the new method to the resonance problem of the one-dimensional Schrödinger equation.

Based on the results presented above we have the following conclusions:

- The Exponentially-fitted two-step method developed by Raptis and Allison [38] (denoted as Method II) is more efficient than the Numerov’s Method (denoted Method I) and for low number of function evaluations is more efficient than the Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] (denoted as Method III).

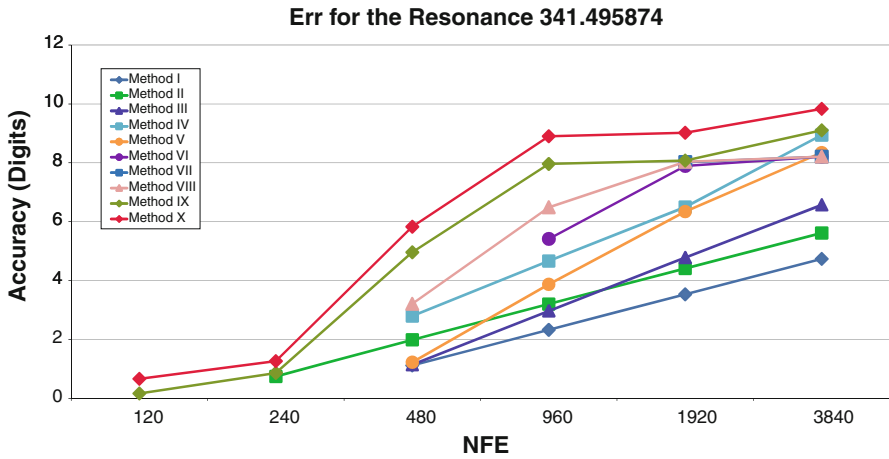


Fig. 4 Accuracy (*Digits*) for several values of *NFE* for the eigenvalue $E_2 = 341.495874$. The non-existence of a value of Accuracy (*Digits*) indicates that for this value of *NFE*, Accuracy (*Digits*) is less than 0

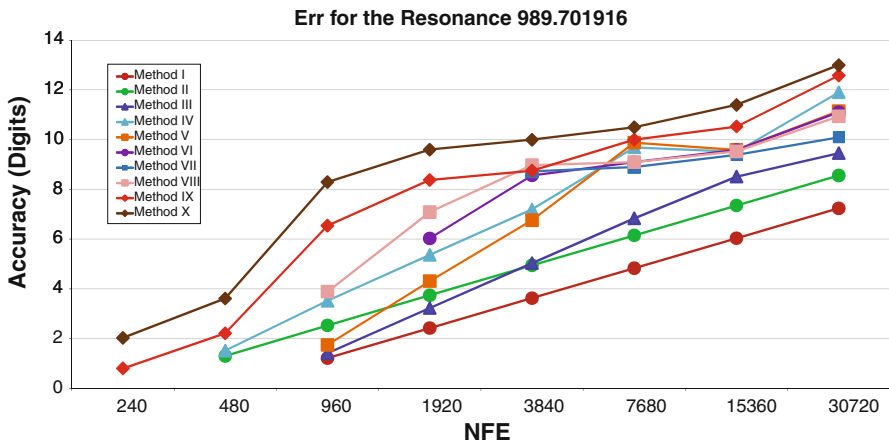


Fig. 5 Accuracy (*Digits*) for several values of *NFE* for the eigenvalue $E_3 = 989.701916$. The non-existence of a value of Accuracy (*Digits*) indicates that for this value of *NFE*, Accuracy (*Digits*) is less than 0

- The Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] (denoted as Method III) is more efficient than the Exponentially-fitted two-step method developed by Raptis and Allison [38] (denoted as Method II) for high number of function evaluations.
- The Exponentially-fitted four-step method developed by Raptis [39] (denoted as Method IV) is more efficient than the Numerov’ Method (denoted Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [38] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] (denoted as Method III)

- The eight-step ninth algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method V) is more efficient than the Numerov' Method (denoted Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [38] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] (denoted as Method III) and less efficient than the Exponentially-fitted four-step method developed by Raptis [39] (denoted as Method IV)
- The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method VI) is more efficient than the Numerov' Method (denoted Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [38] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] (denoted as Method III) and the Exponentially-fitted four-step method developed by Raptis [39] (denoted as Method IV) for small number of function evaluations
- The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method VII) is more efficient than the Numerov' Method (denoted Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [38] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [39] (denoted as Method IV) for small number of function evaluations, the eight-step ninth algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method V) for small number of function evaluations and the ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method VI) for small number of function evaluations
- The classical eight-step method of the family of methods mentioned in paragraph 4 (denoted as Method VIII) is more efficient than the Numerov' Method (denoted Method I), the Exponentially-fitted two-step method developed by Raptis and Allison [38] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [39] (denoted as Method IV) for small number of function evaluations, the eight-step ninth algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method V) for small number of function evaluations, the ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method VI) for small number of function evaluations and the twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [143] (denoted as Method VII) for small number of function evaluations
- The method produced by Alolyan and Simos [144] is more efficient than all the above mentioned methods
- The new developed eight-step method is more efficient than the method produced by Alolyan and Simos [144]

7.1 Summaries about the importance of properties for the numerical methods used for the solution of the radial Schrödinger equation

From the analysis presented above (comparative error analysis and comparative stability analysis) and from the numerical results presented above, the following summaries about the importance of the properties which have the numerical methods used for the approximate solution of the radial Schrödinger Equation are excluded:

- The Algebraic Order of the Numerical Method is a very important property for the numerical solution of this problem
- The Vanishing of the Phase-Lag and Its Derivatives is very important properties for the numerical solution of this problem since leads to the reduction of the power of $G = V_c - E$ (where V_c is the constant approximation of the potential) in the terms of the local truncation error
- The Large Interval of Periodicity doesn't play important role for the numerical solution of this problem although the existence of the non-vanishing interval of periodicity plays important role since in this problem we haven't abrupt changes of the function y (see (1) during the integration.

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

Appendix A

The Numerov's method

$$\begin{aligned}
 \text{LTE}_{\text{CL}} = h^6 & \left[-\frac{1}{240} y(x) G^3 - \frac{1}{80} g(x) y(x) G^2 \right. \\
 & + \left(-\frac{1}{40} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) - \frac{7}{240} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \right. \\
 & - \left. \frac{1}{80} g(x)^2 y(x) \right) G - \frac{1}{240} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \\
 & - \frac{1}{60} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) - \frac{7}{240} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & - \frac{1}{240} g(x)^3 y(x) - \frac{1}{60} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
 & \left. - \frac{1}{40} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \right] \tag{46}
 \end{aligned}$$

The Method of Raptis and Allison [38]

$$\text{LTE}_{\text{RAAL}} = h^6 \left[-\frac{1}{240} g(x) y(x) G^2 \right.$$

$$\begin{aligned}
& + \left(-\frac{1}{60} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) - \frac{1}{40} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \right. \\
& - \frac{1}{120} g(x)^2 y(x) \Big) G - \frac{1}{240} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \\
& - \frac{1}{60} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) - \frac{7}{240} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& - \frac{1}{240} g(x)^3 y(x) - \frac{1}{60} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
& \left. - \frac{1}{40} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \right] \quad (47)
\end{aligned}$$

The exponentially-fitted two-step P-stable method developed by Kalogitatu and Simos [40]

$$\begin{aligned}
\text{LTE}_{\text{KALSIM}} = h^6 & \left[-\frac{1}{144} y(x) G^3 + \left(-\frac{13}{720} g(x) y(x) \right. \right. \\
& - \frac{1}{144} y(x) \Big) G^2 + \left(-\frac{11}{720} g(x)^2 y(x) \right. \\
& - \frac{1}{72} g(x) y(x) - \frac{11}{360} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
& - \frac{23}{720} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \Big) G - \frac{1}{240} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \\
& - \frac{1}{60} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) - \frac{7}{240} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& - \frac{1}{144} g(x)^2 y(x) - \frac{1}{60} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
& - \frac{1}{40} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) - \frac{1}{144} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \\
& \left. - \frac{1}{240} g(x)^3 y(x) - \frac{1}{72} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right] \quad (48)
\end{aligned}$$

The exponentially-fitted four-step method developed by Raptis [39]

$$\begin{aligned}
\text{LTE}_{\text{RAP}} = h^8 & \left[-\frac{19}{6048} g(x) y(x) G^3 + \left(-\frac{95}{2016} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \right. \right. \\
& - \frac{19}{1008} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) - \frac{19}{2016} g(x)^2 y(x) \Big) G^2 \\
& + \left(-\frac{95}{2016} \left(\frac{d^4}{dx^4} g(x) \right) y(x) - \frac{95}{1512} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right.
\end{aligned}$$

$$\begin{aligned}
 & -\frac{19}{336} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right) - \frac{703}{6048} g(x) y(x) \left(\frac{d^2}{dx^2} g(x)\right) \\
 & -\frac{19}{252} \left(\frac{d}{dx} g(x)\right)^2 y(x) - \frac{19}{2016} g(x)^3 y(x) \Big) G \\
 & -\frac{19}{6048} \left(\frac{d^6}{dx^6} g(x)\right) y(x) - \frac{19}{1008} \left(\frac{d^5}{dx^5} g(x)\right) \left(\frac{d}{dx} y(x)\right) \\
 & -\frac{19}{378} g(x) y(x) \left(\frac{d^4}{dx^4} g(x)\right) - \frac{95}{2016} \left(\frac{d^2}{dx^2} g(x)\right)^2 y(x) \\
 & -\frac{247}{3024} \left(\frac{d}{dx} g(x)\right) y(x) \left(\frac{d^3}{dx^3} g(x)\right) \\
 & -\frac{19}{252} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^3}{dx^3} g(x)\right) \\
 & -\frac{19}{504} g(x)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right) \\
 & -\frac{19}{126} \left(\frac{d}{dx} g(x)\right) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^2}{dx^2} g(x)\right) \\
 & -\frac{209}{3024} g(x)^2 y(x) \left(\frac{d^2}{dx^2} g(x)\right) - \frac{19}{216} g(x) y(x) \left(\frac{d}{dx} g(x)\right)^2 \\
 & \left. -\frac{19}{6048} g(x)^4 y(x) \right] \tag{49}
 \end{aligned}$$

The eight-step ninth algebraic order method developed by Quinlan and Tremaine [143]

$$\begin{aligned}
 \text{LTE}_{\text{Q}9} = & -h^{10} \left[\frac{320369}{51840} \left(\frac{d^2}{dx^2} g(x)\right) y(x) \left(\frac{d^4}{dx^4} g(x)\right) \right. \\
 & + \left(\frac{45767}{12096} g(x)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right) \right. \\
 & + \frac{9656837}{725760} \left(\frac{d^2}{dx^2} g(x)\right)^2 y(x) + \frac{45767}{145152} g(x)^4 y(x) \\
 & + \frac{7734623}{362880} \left(\frac{d}{dx} g(x)\right) y(x) \left(\frac{d^3}{dx^3} g(x)\right) \\
 & + \frac{1418777}{362880} \left(\frac{d^5}{dx^5} g(x)\right) \left(\frac{d}{dx} y(x)\right) \\
 & + \frac{1327243}{725760} \left(\frac{d^6}{dx^6} g(x)\right) y(x) + \frac{45767}{4536} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^3}{dx^3} g(x)\right) \\
 & \left. + \frac{1967981}{181440} g(x) y(x) \left(\frac{d^4}{dx^4} g(x)\right) + \frac{228835}{24192} g(x)^2 y(x) \left(\frac{d^2}{dx^2} g(x)\right) \right]
 \end{aligned}$$

$$\begin{aligned}
& + \frac{45767}{2268} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{228835}{18144} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \Big) G \\
& + \frac{45767}{725760} y(x) G^5 + \left(\frac{45767}{36288} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right. \\
& + \left. \frac{228835}{72576} \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \frac{45767}{72576} g(x)^2 y(x) \right) G^3 \\
& + \left(\frac{45767}{12096} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) + \frac{228835}{24192} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \right. \\
& + \left. \frac{45767}{9072} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) + \frac{228835}{36288} \left(\frac{d}{dx} g(x) \right)^2 y(x) \right. \\
& + \left. \frac{45767}{72576} g(x)^3 y(x) + \frac{1967981}{362880} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \right) G^2 \\
& + \frac{45767}{9072} \left(\frac{d}{dx} g(x) \right)^3 \left(\frac{d}{dx} y(x) \right) + \frac{45767}{12960} \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) \\
& + \frac{45767}{725760} \left(\frac{d^8}{dx^8} g(x) \right) y(x) + \frac{45767}{90720} \left(\frac{d^7}{dx^7} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
& + \frac{45767}{725760} g(x)^5 y(x) + \frac{1327243}{90720} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{45767}{4032} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{45767}{11340} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{45767}{2592} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{45767}{2268} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{7734623}{362880} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{228835}{36288} g(x)^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{45767}{36288} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) + \frac{45767}{145152} g(x) y(x) G^4 \\
& + \frac{45767}{9072} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right)
\end{aligned}$$

$$\begin{aligned}
 & + \frac{228835}{72576} g(x)^3 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & + \frac{1418777}{362880} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & + \frac{1327243}{725760} g(x) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & + \frac{1967981}{362880} g(x)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & + \left. \frac{9656837}{725760} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^2 \right] \tag{50}
 \end{aligned}$$

The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [143]

$$\begin{aligned}
 LTE_{QT11} = & -h^{12} \left[\frac{1313975}{114048} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \right. \\
 & + \frac{52559}{912384} \left(\frac{d^{10}}{dx^{10}} g(x) \right) y(x) + \frac{262795}{456192} \left(\frac{d^9}{dx^9} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 & + \frac{1839565}{152064} \left(\frac{d^4}{dx^4} g(x) \right)^2 y(x) + \frac{1313975}{33792} \left(\frac{d^2}{dx^2} g(x) \right)^3 y(x) \\
 & + \frac{998621}{16896} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & + \frac{1839565}{114048} \left(\frac{d}{dx} g(x) \right)^4 y(x) + \frac{3416335}{456192} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^7}{dx^7} g(x) \right) \\
 & + \frac{28644655}{228096} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 & + \frac{12876955}{456192} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & + \frac{262795}{3168} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & + \frac{8146645}{50688} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) T_3 \\
 & + \frac{1839565}{25344} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & + \left. \frac{12561601}{912384} g(x)^2 y(x) \left(\frac{d^6}{dx^6} g(x) \right) \right]
 \end{aligned}$$

$$\begin{aligned}
& + \frac{1629329}{76032} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{4467515}{304128} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
& + \frac{92766635}{456192} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{39051337}{228096} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{6044285}{57024} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{16450967}{152064} g(x)^2 y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{1313975}{19008} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{16976557}{228096} g(x) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{19184035}{114048} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{683267}{5184} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{52559}{912384} g(x)^6 y(x) + \frac{52559}{912384} y(x) G^6 \\
& + \left(\frac{262795}{152064} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) + \frac{4993105}{912384} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \right) \\
& + \frac{262795}{304128} g(x)^2 y(x) G^4 + \left(\frac{262795}{38016} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \right) \\
& + \frac{1313975}{114048} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
& + \frac{1944683}{114048} \left(\frac{d^4}{dx^4} g(x) \right) y(x) + \frac{3416335}{228096} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
& + \frac{262795}{228096} g(x)^3 y(x) + \frac{4993105}{228096} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) G^3 \\
& + \left(\frac{12561601}{912384} \left(\frac{d^6}{dx^6} g(x) \right) y(x) + \frac{1944683}{38016} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \right) \\
& + \frac{262795}{304128} g(x)^4 y(x) + \frac{1313975}{19008} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right)
\end{aligned}$$

$$\begin{aligned}
& + \frac{1313975}{38016} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{8251763}{456192} \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
& + \frac{262795}{25344} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{3416335}{76032} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 + \frac{63123359}{912384} T_3 y(x) \\
& + \frac{4993105}{152064} g(x)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{16450967}{152064} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \Big) G^2 \\
& + \left(\frac{3416335}{76032} g(x)^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 \right. \\
& + \frac{8251763}{228096} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{16976557}{228096} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{262795}{38016} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{6044285}{57024} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{19184035}{114048} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{39051337}{228096} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{12561601}{456192} g(x) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
& + \frac{1313975}{9504} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{16450967}{76032} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{1313975}{38016} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{1944683}{38016} g(x)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right)
\end{aligned}$$

$$\begin{aligned}
& + \frac{683267}{5184} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{63123359}{456192} g(x) y(x) T_3 + \frac{4993105}{228096} g(x)^3 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{2260037}{28512} \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) + \frac{52559}{7128} \left(\frac{d^7}{dx^7} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
& + \frac{1208857}{456192} \left(\frac{d^8}{dx^8} g(x) \right) y(x) + \frac{52559}{152064} g(x)^5 y(x) \\
& + \frac{1313975}{38016} \left(\frac{d}{dx} g(x) \right)^3 \left(\frac{d}{dx} y(x) \right) \Big) G \\
& + \frac{3416335}{228096} g(x)^3 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{262795}{152064} g(x)^4 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{1313975}{38016} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 + \frac{52559}{152064} g(x) y(x) G^5 \\
& + \frac{4993105}{912384} g(x)^4 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{8251763}{456192} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{52559}{7128} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^7}{dx^7} g(x) \right) \\
& + \frac{1944683}{114048} g(x)^3 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{2260037}{28512} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 + \frac{63123359}{912384} g(x)^2 y(x) T_3 \\
& + \frac{1208857}{456192} g(x) y(x) \left(\frac{d^8}{dx^8} g(x) \right) \\
& T_3 = \left(\frac{d^2}{dx^2} g(x) \right)^2 \Big] \tag{51}
\end{aligned}$$

The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [143]

$$\text{LTE}_{\text{QT13}} = -h^{14} \left[\frac{277130533751}{943488000} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^6}{dx^6} g(x) \right) \right]$$

$$\begin{aligned}
 &+ \frac{505355679193}{384384000} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^3}{dx^3} g(x)\right) \left(\frac{d}{dx} g(x)\right)^2 \\
 &+ \frac{16301796103}{12418560} g(x) y(x) \left(\frac{d^4}{dx^4} g(x)\right) \left(\frac{d}{dx} g(x)\right)^2 \\
 &+ \frac{10253829748787}{10378368000} g(x)^2 y(x) \left(\frac{d^2}{dx^2} g(x)\right) \left(\frac{d}{dx} g(x)\right)^2 \\
 &+ \frac{1679084998609}{988416000} g(x) \left(\frac{d}{dx} y(x)\right) T_5 \left(\frac{d}{dx} g(x)\right) \\
 &+ \frac{5689326839947}{10378368000} g(x)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d^4}{dx^4} g(x)\right) \left(\frac{d}{dx} g(x)\right) \\
 &+ \frac{16301796103}{18532800} g(x)^2 \left(\frac{d}{dx} y(x)\right) \left(\frac{d^3}{dx^3} g(x)\right) \left(\frac{d^2}{dx^2} g(x)\right) \\
 &+ \frac{41553278266547}{72648576000} g(x)^2 y(x) \left(\frac{d^5}{dx^5} g(x)\right) \left(\frac{d}{dx} g(x)\right) \\
 &+ \frac{13970639260271}{13208832000} g(x)^2 y(x) \left(\frac{d^4}{dx^4} g(x)\right) \left(\frac{d^2}{dx^2} g(x)\right) \\
 &+ \frac{16301796103}{86486400} g(x)^3 \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right) \left(\frac{d^2}{dx^2} g(x)\right) \\
 &+ \frac{8297614216427}{20756736000} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^6}{dx^6} g(x)\right) \left(\frac{d}{dx} g(x)\right) \\
 &+ \frac{5982759169801}{6918912000} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^5}{dx^5} g(x)\right) \left(\frac{d^2}{dx^2} g(x)\right) \\
 &+ \frac{1157427523313}{2965248000} g(x)^3 y(x) \left(\frac{d^3}{dx^3} g(x)\right) \left(\frac{d}{dx} g(x)\right) \\
 &+ \frac{30500660508713}{145297152000} g(x) y(x) \left(\frac{d^7}{dx^7} g(x)\right) \left(\frac{d}{dx} g(x)\right) \\
 &+ \frac{46932870980537}{96864768000} g(x) y(x) \left(\frac{d^6}{dx^6} g(x)\right) \left(\frac{d^2}{dx^2} g(x)\right) \\
 &+ \frac{1287841892137}{1037836800} g(x) \left(\frac{d}{dx} y(x)\right) \left(\frac{d^4}{dx^4} g(x)\right) \left(\frac{d^3}{dx^3} g(x)\right) \\
 &+ \frac{56746552234543}{72648576000} g(x) y(x) \left(\frac{d^5}{dx^5} g(x)\right) \left(\frac{d^3}{dx^3} g(x)\right) \\
 &+ \frac{16301796103}{518918400} g(x)^4 y(x) \left(\frac{d}{dx} g(x)\right)^2 \\
 &+ \frac{16301796103}{6918912000} g(x)^5 \left(\frac{d}{dx} y(x)\right) \left(\frac{d}{dx} g(x)\right)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{16301796103}{79833600} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^4 \\
& + \frac{16301796103}{115315200} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 \\
& + \frac{16301796103}{41513472000} g(x) y(x) G^6 \\
& + \frac{374941310369}{7264857600} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^7}{dx^7} g(x) \right) \\
& + \frac{1842102959639}{41513472000} g(x)^4 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{1287841892137}{20756736000} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{10482054894229}{41513472000} g(x)^3 y(x) T_5 \\
& + \frac{7808560333337}{12108096000} g(x)^2 y(x) T_4 \\
& + \frac{4417786743913}{9686476800} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right)^2 \\
& + \frac{1092220338901}{290594304000} g(x) y(x) \left(\frac{d^{10}}{dx^{10}} g(x) \right) \\
& + \frac{374941310369}{29059430400} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^9}{dx^9} g(x) \right) \\
& + \frac{18958988867789}{290594304000} g(x)^3 y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
& + \frac{374941310369}{41513472000} g(x)^5 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{8819271691723}{290594304000} g(x)^2 y(x) \left(\frac{d^8}{dx^8} g(x) \right) \\
& + \frac{79340841633301}{96864768000} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right)^3 \\
& + \frac{16301796103}{691891200} g(x)^4 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{16301796103}{290594304000} g(x)^7 y(x) \\
& + \frac{16301796103}{290594304000} y(x) G^7 + \left(\frac{16301796103}{6918912000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right) \\
& + \frac{374941310369}{41513472000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \frac{16301796103}{13837824000} g(x)^2 y(x) \Big) G^5
\end{aligned}$$

$$\begin{aligned}
 &+ \left(\frac{1842102959639}{41513472000} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \right. \\
 &+ \frac{374941310369}{8302694400} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 &+ \frac{16301796103}{1383782400} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) + \frac{16301796103}{8302694400} g(x)^3 y(x) \\
 &+ \frac{16301796103}{518918400} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
 &+ \left. \frac{16301796103}{691891200} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right) G^4 \\
 &+ \left(\frac{16301796103}{86486400} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \right. \\
 &+ \frac{16301796103}{172972800} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 &+ \frac{1287841892137}{20756736000} \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 &+ \frac{374941310369}{4151347200} g(x)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 &+ \frac{18958988867789}{290594304000} \left(\frac{d^6}{dx^6} g(x) \right) y(x) \\
 &+ \frac{1842102959639}{10378368000} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) + \frac{16301796103}{8302694400} g(x)^4 y(x) \\
 &+ \frac{1157427523313}{2965248000} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \\
 &+ \frac{10482054894229}{41513472000} T_5 y(x) \\
 &+ \frac{16301796103}{691891200} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
 &+ \frac{16301796103}{129729600} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \Big) G^3 \\
 &\left(\frac{1842102959639}{6918912000} g(x)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \right. \\
 &+ \frac{16301796103}{115315200} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 &+ \left. \frac{5689326839947}{10378368000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \right)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{16301796103}{115315200} \left(\frac{d}{dx} g(x) \right)^3 \left(\frac{d}{dx} y(x) \right) \\
& + \frac{1287841892137}{6918912000} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{10253829748787}{10378368000} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{10482054894229}{13837824000} g(x) y(x) T_5 \\
& + \frac{16301796103}{13837824000} g(x)^5 y(x) \\
& + \frac{16301796103}{28828800} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{374941310369}{7264857600} \left(\frac{d^7}{dx^7} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
& + \frac{41553278266547}{72648576000} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{7808560333337}{12108096000} T_4 y(x) \\
& + \frac{16301796103}{18532800} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{374941310369}{4151347200} g(x)^3 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{16301796103}{86486400} g(x)^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{1157427523313}{988416000} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{18958988867789}{96864768000} g(x) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
& + \frac{13970639260271}{13208832000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{8819271691723}{290594304000} \left(\frac{d^8}{dx^8} g(x) \right) y(x) \\
& + \frac{16301796103}{691891200} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) G^2 \\
& + \left(\frac{16301796103}{172972800} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \right) \\
& + \frac{1092220338901}{290594304000} \left(\frac{d^{10}}{dx^{10}} g(x) \right) y(x)
\end{aligned}$$

$$\begin{aligned}
 &+ \frac{374941310369}{29059430400} \left(\frac{d^9}{dx^9} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 &+ \frac{4417786743913}{9686476800} \left(\frac{d^4}{dx^4} g(x) \right)^2 y(x) \\
 &+ \frac{79340841633301}{96864768000} \left(\frac{d^2}{dx^2} g(x) \right)^3 y(x) \\
 &+ \frac{5982759169801}{6918912000} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 &+ \frac{16301796103}{79833600} \left(\frac{d}{dx} g(x) \right)^4 y(x) \\
 &+ \frac{30500660508713}{145297152000} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^7}{dx^7} g(x) \right) \\
 &+ \frac{505355679193}{384384000} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 &+ \frac{8297614216427}{20756736000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^6}{dx^6} g(x) \right) \\
 &+ \frac{1287841892137}{1037836800} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
 &+ \frac{1679084998609}{988416000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) T_5 \\
 &+ \frac{16301796103}{12418560} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 &+ \frac{18958988867789}{96864768000} g(x)^2 y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 &+ \frac{56746552234543}{72648576000} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
 &+ \frac{46932870980537}{96864768000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 &+ \frac{192573117364739}{48432384000} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
 &+ \frac{10253829748787}{5189184000} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right)^2 \\
 &+ \frac{5689326839947}{5189184000} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
 &+ \frac{1157427523313}{988416000} g(x)^2 y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} g(x) \right)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{16301796103}{28828800} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{41553278266547}{36324288000} g(x) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{16301796103}{9266400} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{13970639260271}{6604416000} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{16301796103}{41513472000} g(x)^6 y(x) \\
& + \frac{16301796103}{129729600} g(x)^3 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& + \frac{16301796103}{1383782400} g(x)^4 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{16301796103}{57657600} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 \\
& + \frac{374941310369}{8302694400} g(x)^4 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{1287841892137}{6918912000} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{374941310369}{3632428800} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^7}{dx^7} g(x) \right) \\
& + \frac{1842102959639}{10378368000} g(x)^3 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{7808560333337}{6054048000} g(x) y(x) T_4 + \frac{10482054894229}{13837824000} g(x)^2 y(x) T_5 \\
& + \frac{8819271691723}{145297152000} g(x) y(x) \left(\frac{d^8}{dx^8} g(x) \right) G \\
& + \frac{192573117364739}{48432384000} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{374941310369}{576576000} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{16301796103}{290594304000} \left(\frac{d^{12}}{dx^{12}} g(x) \right) y(x) \\
& + \frac{16301796103}{24216192000} \left(\frac{d^{11}}{dx^{11}} g(x) \right) \left(\frac{d}{dx} y(x) \right)
\end{aligned}$$

$$\begin{aligned}
 & + \frac{16301796103}{366912000} \left(\frac{d^5}{dx^5} g(x) \right)^2 y(x) \\
 & + \frac{374941310369}{6604416000} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \left(\frac{d^7}{dx^7} g(x) \right) \\
 & + \frac{16301796103}{41932800} \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & + \frac{277130533751}{8805888000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^8}{dx^8} g(x) \right) \\
 & + \frac{179319757133}{1100736000} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^7}{dx^7} g(x) \right) \\
 & + \frac{472752086987}{36324288000} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^9}{dx^9} g(x) \right) \\
 & + \frac{994409562283}{16144128000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^8}{dx^8} g(x) \right) \\
 & + \frac{700977232429}{8805888000} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & + \frac{31804804196953}{24216192000} \left(\frac{d}{dx} g(x) \right)^2 y(x) T_5 \\
 & + \frac{16301796103}{8985600} T_5 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 & + \frac{7449920819071}{5189184000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) T_4 \\
 & + \frac{6537020237303}{24216192000} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & + \frac{16301796103}{19656000} \left(\frac{d}{dx} g(x) \right)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & + \frac{16301796103}{22353408} \left(\frac{d}{dx} g(x) \right)^3 y(x) \left(\frac{d^3}{dx^3} g(x) \right) \\
 & + \frac{6863056159363}{8805888000} T_5 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & + \frac{16301796103}{18144000} \left(\frac{d^2}{dx^2} g(x) \right) y(x) T_4 \\
 & + \frac{16301796103}{6864000} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & + \frac{766184416841}{756756000} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{13383774600563}{9686476800} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
T_4 & = \left(\frac{d^3}{dx^3} g(x) \right)^2 \\
T_5 & = \left(\frac{d^2}{dx^2} g(x) \right)^2 \Big] \tag{52}
\end{aligned}$$

The Classical Method of the Family (see [144])

$$\begin{aligned}
\text{LTE}_{\text{CL}} & = h^{12} \left[-\frac{20495533}{3193344} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \right. \\
& - \frac{58061}{31933440} \left(\frac{d^{10}}{dx^{10}} g(x) \right) y(x) \\
& - \frac{58061}{3193344} \left(\frac{d^9}{dx^9} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
& - \frac{290305}{236544} \left(\frac{d^2}{dx^2} g(x) \right)^3 y(x) - \frac{58061}{152064} \left(\frac{d^4}{dx^4} g(x) \right)^2 y(x) \\
& - \frac{43139323}{7983360} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d^2}{dx^2} g(x) \right) \\
& - \frac{290305}{133056} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& - \frac{18173093}{5322240} g(x)^2 y(x) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& - \frac{1335403}{399168} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& - \frac{4238453}{798336} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& - \frac{18753703}{7983360} g(x) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& - \frac{754793}{181440} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& - \frac{58061}{114048} \left(\frac{d}{dx} g(x) \right)^4 y(x) - \frac{987037}{2128896} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
& - \frac{58061}{22176} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
& \left. - \frac{754793}{3193344} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^7}{dx^7} g(x) \right) \right]
\end{aligned}$$

$$\begin{aligned}
 & - \frac{6328649}{1596672} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 & - \frac{58061}{25344} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & - \frac{1799891}{2661120} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & - \frac{1103159}{591360} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & - \frac{1799891}{354816} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) Q_0 \\
 & - \frac{406427}{456192} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & - \frac{290305}{266112} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 \\
 & - \frac{58061}{1064448} g(x)^4 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
 & - \frac{754793}{1596672} g(x)^3 y(x) \left(\frac{d}{dx} g(x) \right)^2 - \frac{58061}{5322240} g(x) y(x) G^5 \\
 & - \frac{290305}{798336} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 & - \frac{2496623}{997920} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 \\
 & - \frac{1103159}{6386688} g(x)^4 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & - \frac{1335403}{15966720} g(x) y(x) \left(\frac{d^8}{dx^8} g(x) \right) \\
 & - \frac{2148257}{3991680} g(x)^3 y(x) \left(\frac{d^4}{dx^4} g(x) \right) - \frac{69731261}{31933440} g(x)^2 y(x) Q_0 \\
 & - \frac{13876579}{31933440} g(x)^2 y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & - \frac{9115577}{15966720} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & - \frac{58061}{249480} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^7}{dx^7} g(x) \right) \\
 & - \frac{58061}{31933440} g(x)^6 y(x) - \frac{58061}{31933440} y(x) G^6
 \end{aligned}$$

$$\begin{aligned}
& \left(-\frac{58061}{1064448} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right. \\
& - \frac{1103159}{6386688} \left(\frac{d^2}{dx^2} g(x) \right) y(x) - \frac{58061}{2128896} g(x)^2 y(x) \Big) G^4 \\
& + \left(-\frac{1103159}{1596672} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) - \frac{2148257}{3991680} \left(\frac{d^4}{dx^4} g(x) \right) y(x) \right. \\
& - \frac{754793}{1596672} \left(\frac{d}{dx} g(x) \right)^2 y(x) - \frac{58061}{1596672} g(x)^3 y(x) \\
& - \frac{58061}{266112} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& - \frac{290305}{798336} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \Big) G^3 \\
& + \left(-\frac{9115577}{15966720} \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right. \\
& - \frac{290305}{133056} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& - \frac{18173093}{5322240} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \\
& - \frac{58061}{2128896} g(x)^4 y(x) - \frac{2148257}{1330560} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& - \frac{290305}{266112} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) - \frac{69731261}{31933440} Q_0 y(x) \\
& - \frac{1103159}{1064448} g(x)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) - \frac{13876579}{31933440} \left(\frac{d^6}{dx^6} g(x) \right) y(x) \\
& - \frac{754793}{532224} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
& - \frac{58061}{177408} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \Big) G^2 + \\
& \left(-\frac{9115577}{7983360} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \right. \\
& - \frac{4238453}{798336} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& - \frac{290305}{266112} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) - \frac{58061}{5322240} g(x)^5 y(x) \\
& \left. - \frac{2496623}{997920} \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) - \frac{290305}{266112} \left(\frac{d}{dx} g(x) \right)^3 \left(\frac{d}{dx} y(x) \right) \right)
\end{aligned}$$

$$\begin{aligned}
 & - \frac{290305}{66528} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & - \frac{1335403}{15966720} \left(\frac{d^8}{dx^8} g(x) \right) y(x) \\
 & - \frac{43139323}{7983360} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & - \frac{18173093}{2661120} g(x) y(x) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 & - \frac{1335403}{399168} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & - \frac{58061}{249480} \left(\frac{d^7}{dx^7} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 & - \frac{69731261}{15966720} g(x) y(x) Q_0 - \frac{754793}{532224} g(x)^2 y(x) \left(\frac{d}{dx} g(x) \right)^2 \\
 & - \frac{18753703}{7983360} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & - \frac{754793}{181440} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & - \frac{13876579}{15966720} g(x) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & - \frac{58061}{266112} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
 & - \frac{1103159}{1596672} g(x)^3 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & - \frac{2148257}{1330560} g(x)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \Big] G \tag{53}
 \end{aligned}$$

The method produced by Alolyan and Simos [144]

$$\begin{aligned}
 LTE_{PL} = & h^{12} \left[\frac{20495533}{3193344} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \right. \\
 & + \frac{58061}{31933440} \left(\frac{d^{10}}{dx^{10}} g(x) \right) y(x) + \frac{58061}{3193344} \left(\frac{d^9}{dx^9} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 & + \frac{290305}{236544} \left(\frac{d^2}{dx^2} g(x) \right)^3 y(x) + \frac{58061}{152064} \left(\frac{d^4}{dx^4} g(x) \right)^2 y(x) \\
 & \left. + \frac{43139323}{7983360} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d^2}{dx^2} g(x) \right) \right]
 \end{aligned}$$

$$\begin{aligned}
& + \frac{290305}{133056} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{18173093}{5322240} g(x)^2 y(x) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{1335403}{399168} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{4238453}{798336} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{18753703}{7983360} g(x) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{754793}{181440} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{58061}{114048} \left(\frac{d}{dx} g(x) \right)^4 y(x) + \frac{987037}{2128896} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
& + \frac{58061}{22176} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{754793}{3193344} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^7}{dx^7} g(x) \right) \\
& + \frac{6328649}{1596672} \left(\frac{d}{dx} g(x) \right)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{58061}{25344} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{1799891}{2661120} \left(\frac{d^3}{dx^3} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{1103159}{591360} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{1799891}{354816} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) Q_0 \\
& + \frac{406427}{456192} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^6}{dx^6} g(x) \right) \\
& + \frac{290305}{266112} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right)^3 \\
& + \frac{58061}{1064448} g(x)^4 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{754793}{1596672} g(x)^3 y(x) \left(\frac{d}{dx} g(x) \right)^2
\end{aligned}$$

$$\begin{aligned}
 & + \frac{290305}{798336} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
 & + \frac{2496623}{997920} g(x) y(x) \left(\frac{d^3}{dx^3} g(x) \right)^2 \\
 & + \frac{1103159}{6386688} g(x)^4 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
 & + \frac{1335403}{15966720} g(x) y(x) \left(\frac{d^8}{dx^8} g(x) \right) \\
 & + \frac{2148257}{3991680} g(x)^3 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & + \frac{69731261}{31933440} g(x)^2 y(x) Q_0 \\
 & + \frac{13876579}{31933440} g(x)^2 y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & + \frac{9115577}{15966720} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & + \frac{58061}{249480} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^7}{dx^7} g(x) \right) \\
 & + \frac{58061}{31933440} g(x)^6 y(x) \\
 & \left(\frac{987037}{31933440} \left(\frac{d^2}{dx^2} g(x) \right) y(x) + \frac{58061}{15966720} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \right) \\
 & + \frac{58061}{31933440} g(x)^2 y(x) \Big) G^4 \\
 & + \left(\frac{1799891}{7983360} g(x) y(x) \left(\frac{d^2}{dx^2} g(x) \right) \right. \\
 & + \frac{58061}{228096} \left(\frac{d^4}{dx^4} g(x) \right) y(x) + \frac{58061}{7983360} g(x)^3 y(x) \\
 & + \frac{58061}{362880} \left(\frac{d}{dx} g(x) \right)^2 y(x) \\
 & + \frac{58061}{498960} \left(\frac{d^3}{dx^3} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\
 & + \left. \frac{58061}{1330560} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \right) G^3 \\
 & + \left(\frac{987037}{1330560} g(x) y(x) \left(\frac{d}{dx} g(x) \right)^2 \right. \\
 & + \left. \frac{58061}{443520} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \right)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{17824727}{7983360} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{1103159}{1995840} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{1103159}{997920} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{58061}{57024} g(x) y(x) \left(\frac{d^4}{dx^4} g(x) \right) + \frac{4238453}{7983360} g(x)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{58061}{5322240} g(x)^4 y(x) \\
& + \frac{23050217}{15966720} Q_0 y(x) + \frac{754793}{2280960} \left(\frac{d^6}{dx^6} g(x) \right) y(x) \\
& + \frac{406427}{1140480} \left(\frac{d^5}{dx^5} g(x) \right) \left(\frac{d}{dx} y(x) \right) \Big) G^2 \\
& + \left(\frac{3425599}{798336} \left(\frac{d^2}{dx^2} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \right. \\
& + \frac{58061}{18144} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{58061}{10368} g(x) y(x) \left(\frac{d}{dx} g(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{1103159}{241920} \left(\frac{d}{dx} g(x) \right)^2 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{2148257}{798336} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{5631917}{2661120} \left(\frac{d}{dx} g(x) \right) y(x) \left(\frac{d^5}{dx^5} g(x) \right) \\
& + \frac{30365903}{7983360} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
& + \frac{58061}{72576} g(x)^2 \left(\frac{d}{dx} y(x) \right) \left(\frac{d^3}{dx^3} g(x) \right) \\
& + \frac{58061}{399168} g(x)^3 \left(\frac{d}{dx} y(x) \right) \left(\frac{d}{dx} g(x) \right) \\
& + \frac{58061}{114048} g(x)^3 y(x) \left(\frac{d^2}{dx^2} g(x) \right) \\
& + \frac{1683769}{1596672} g(x)^2 y(x) \left(\frac{d}{dx} g(x) \right)^2
\end{aligned}$$

$$\begin{aligned}
 & + \frac{10392919}{7983360} g(x)^2 y(x) \left(\frac{d^4}{dx^4} g(x) \right) \\
 & + \frac{58061}{16128} g(x) y(x) Q_0 \\
 & + \frac{58061}{76032} g(x) y(x) \left(\frac{d^6}{dx^6} g(x) \right) \\
 & + \frac{58061}{63360} g(x) \left(\frac{d}{dx} y(x) \right) \left(\frac{d^5}{dx^5} g(x) \right) \\
 & + \frac{58061}{7983360} g(x)^5 y(x) \\
 & + \frac{4586819}{1995840} \left(\frac{d^3}{dx^3} g(x) \right)^2 y(x) + \frac{58061}{72576} \left(\frac{d}{dx} g(x) \right)^3 \left(\frac{d}{dx} y(x) \right) \\
 & + \frac{58061}{725760} \left(\frac{d^8}{dx^8} g(x) \right) y(x) \\
 & + \frac{58061}{285120} \left(\frac{d^7}{dx^7} g(x) \right) \left(\frac{d}{dx} y(x) \right) \Big] G \tag{54}
 \end{aligned}$$

where $Q_0 = \left(\frac{d^2}{dx^2} g(x) \right)^2$

Appendix B: The characteristic equation in the special case $s = v$

$$\begin{aligned}
 & \frac{1}{96} \left(36 - 72 \sin(v) v - 60 \cos(v)^3 v^2 - 125 \cos(v)^3 v^4 \right. \\
 & - 60 v^2 \cos(v)^2 - 215 \cos(v)^2 v^4 + 60 \cos(v) v^2 - 55 \cos(v) v^4 \\
 & + 60 v^2 + 35 v^4 + 288 \sin(v) v \cos(v)^5 - 480 \sin(v) v \cos(v)^4 \\
 & - 336 \sin(v) v \cos(v)^3 + 588 \sin(v) v \cos(v)^2 + 12 \sin(v) v \cos(v) \\
 & + 288 \cos(v)^6 - 288 \cos(v)^5 - 432 \cos(v)^4 + 468 \cos(v)^3 + 108 \cos(v)^2 \\
 & - 180 \cos(v) \Big) v^4 / (T_2 v^2) + \frac{1}{96} \left(-144 + 336 \sin(v) v + 360 v^2 \cos(v)^4 \right. \\
 & + 750 \cos(v)^4 v^4 + 480 \cos(v)^3 v^2 + 1480 \cos(v)^3 v^4 - 240 v^2 \cos(v)^2 \\
 & + 700 \cos(v)^2 v^4 - 480 \cos(v) v^2 - 40 \cos(v) v^4 - 120 v^2 - 10 v^4 \\
 & - 768 \sin(v) v \cos(v)^6 + 384 \sin(v) v \cos(v)^5 + 2688 \sin(v) v \cos(v)^4 \\
 & - 384 \sin(v) v \cos(v)^3 - 2256 \sin(v) v \cos(v)^2 - 1152 \cos(v)^7 \\
 & + 2880 \cos(v)^5 - 144 \cos(v)^4 - 2304 \cos(v)^3 \\
 & + 288 \cos(v)^2 + 576 \cos(v) \Big) v^3 / (T_2 v^2) \\
 & + \frac{1}{96} (288 + 240 v^2 - 864 \cos(v) + 140 v^4 + 384 \sin(v) v \cos(v)^7
 \end{aligned}$$

$$\begin{aligned}
& -4032 \sin(v) v \cos(v)^5 - 5808 \sin(v) v \cos(v)^4 + 3984 \sin(v) v \cos(v)^3 \\
& +4512 \sin(v) v \cos(v)^2 - 192 \sin(v) v \cos(v) \\
& +1920 \sin(v) v \cos(v)^6 - 1872 \cos(v)^2 \\
& -768 \sin(v) v - 720 \cos(v)^5 v^2 - 1500 \cos(v)^5 v^4 - 3720 \cos(v)^4 v^4 \\
& -240 \cos(v)^3 v^2 - 3380 \cos(v)^3 v^4 - 1460 \cos(v)^2 v^4 + 960 \cos(v) v^2 \\
& -160 \cos(v) v^4 - 1440 v^2 \cos(v)^4 + 1200 v^2 \cos(v)^2 \\
& -4032 \cos(v)^6 - 7344 \cos(v)^5 + 4752 \cos(v)^3 \\
& +1152 \cos(v)^8 + 4464 \cos(v)^4 + 3456 \cos(v)^7) \vartheta^2 / \\
& \left(T_2 v^2 \right) + \frac{1}{96} (-432 - 360 v^2 \\
& +1152 \cos(v) - 30 v^4 - 1536 \sin(v) v \cos(v)^7 + 8064 \sin(v) v \cos(v)^5 \\
& +6720 \sin(v) v \cos(v)^4 - 7104 \sin(v) v \cos(v)^3 - 7152 \sin(v) v \cos(v)^2 \\
& +576 \sin(v) v \cos(v) - 768 \sin(v) v \cos(v)^6 + 3168 \cos(v)^2 + 1200 \sin(v) v \\
& +1920 \cos(v)^5 v^2 + 4000 \cos(v)^5 v^4 + 7130 \cos(v)^4 v^4 - 480 \cos(v)^3 v^2 \\
& +6200 \cos(v)^3 v^4 + 1980 \cos(v)^2 v^4 - 1440 \cos(v) v^2 - 120 \cos(v) v^4 \\
& +480 v^2 \cos(v)^6 + 2040 v^2 \cos(v)^4 - 2160 v^2 \cos(v)^2 + 11520 \cos(v)^6 \\
& +8064 \cos(v)^5 - 5760 \cos(v)^3 - 4608 \cos(v)^8 \\
& -9648 \cos(v)^4 - 3456 \cos(v)^7 \\
& +1000 \cos(v)^6 v^4) \vartheta / \left(T_2 v^2 \right) + \frac{1}{96} (504 + 360 v^2 - 1368 \cos(v) + 210 v^4 \\
& +2304 \sin(v) v \cos(v)^7 - 9408 \sin(v) v \cos(v)^5 - 6240 \sin(v) v \cos(v)^4 \\
& +7680 \sin(v) v \cos(v)^3 + 8616 \sin(v) v \cos(v)^2 - 792 \sin(v) v \cos(v) \\
& -768 \sin(v) v \cos(v)^6 - 3384 \cos(v)^2 - 1392 \sin(v) v - 2400 \cos(v)^5 v^2 \\
& -5960 \cos(v)^5 v^4 - 8800 \cos(v)^4 v^4 + 600 \cos(v)^3 v^2 - 6430 \cos(v)^3 v^4 \\
& -2490 \cos(v)^2 v^4 + 1800 \cos(v) v^2 - 210 \cos(v) v^4 - 960 v^2 \cos(v)^6 \\
& -1920 v^2 \cos(v)^4 + 2520 v^2 \cos(v)^2 - 15552 \cos(v)^6 \\
& -6624 \cos(v)^5 + 5688 \cos(v)^3 \\
& +6912 \cos(v)^8 + 11520 \cos(v)^4 + 2304 \cos(v)^7 \\
& -1520 \cos(v)^6 v^4) / \left(T_2 v^2 \right) + \frac{1}{96} \\
& (-432 - 360 v^2 + 1152 \cos(v) - 30 v^4 - 1536 \sin(v) v \cos(v)^7 \\
& +8064 \sin(v) v \cos(v)^5 + 6720 \sin(v) v \cos(v)^4 - 7104 \sin(v) v \cos(v)^3 \\
& -7152 \sin(v) v \cos(v)^2 + 576 \sin(v) v \cos(v) \\
& -768 \sin(v) v \cos(v)^6 + 3168 \cos(v)^2 \\
& +1200 \sin(v) v + 1920 \cos(v)^5 v^2 + 4000 \cos(v)^5 v^4 + 7130 \cos(v)^4 v^4 \\
& -480 \cos(v)^3 v^2 + 6200 \cos(v)^3 v^4 + 1980 \cos(v)^2 v^4 - 1440 \cos(v) v^2 \\
& -120 \cos(v) v^4 + 480 v^2 \cos(v)^6 + 2040 v^2 \cos(v)^4 - 2160 v^2 \cos(v)^2 \\
& +11520 \cos(v)^6 + 8064 \cos(v)^5 - 5760 \cos(v)^3
\end{aligned}$$

$$\begin{aligned}
 & - 4608 \cos(v)^8 - 9648 \cos(v)^4 \\
 & - 3456 \cos(v)^7 + 1000 \cos(v)^6 v^4 \vartheta^{-1} / (T_2 v^2) \\
 & + \frac{1}{96} (288 + 240 v^2 - 864 \cos(v) \\
 & + 140 v^4 + 384 \sin(v) v \cos(v)^7 \\
 & - 4032 \sin(v) v \cos(v)^5 - 5808 \sin(v) v \cos(v)^4 \\
 & + 3984 \sin(v) v \cos(v)^3 + 4512 \sin(v) v \cos(v)^2 - 192 \sin(v) v \cos(v) \\
 & + 1920 \sin(v) v \cos(v)^6 - 1872 \cos(v)^2 - 768 \sin(v) v - 720 \cos(v)^5 v^2 \\
 & - 1500 \cos(v)^5 v^4 - 3720 \cos(v)^4 v^4 - 240 \cos(v)^3 v^2 - 3380 \cos(v)^3 v^4 \\
 & - 1460 \cos(v)^2 v^4 + 960 \cos(v) v^2 - 160 \cos(v) v^4 - 1440 v^2 \cos(v)^4 \\
 & + 1200 v^2 \cos(v)^2 - 4032 \cos(v)^6 - 7344 \cos(v)^5 \\
 & + 4752 \cos(v)^3 + 1152 \cos(v)^8 \\
 & + 4464 \cos(v)^4 + 3456 \cos(v)^7 \vartheta^{-2} / (T_2 v^2) + \frac{1}{96} (-144 + 336 \sin(v) v \\
 & + 360 v^2 \cos(v)^4 + 750 \cos(v)^4 v^4 + 480 \cos(v)^3 v^2 + 1480 \cos(v)^3 v^4 \\
 & - 240 v^2 \cos(v)^2 + 700 \cos(v)^2 v^4 - 480 \cos(v) v^2 \\
 & - 40 \cos(v) v^4 - 120 v^2 - 10 v^4 \\
 & - 768 \sin(v) v \cos(v)^6 + 384 \sin(v) v \cos(v)^5 + 2688 \sin(v) v \cos(v)^4 \\
 & - 384 \sin(v) v \cos(v)^3 - 2256 \sin(v) v \cos(v)^2 \\
 & - 1152 \cos(v)^7 + 2880 \cos(v)^5 \\
 & - 144 \cos(v)^4 - 2304 \cos(v)^3 + 288 \cos(v)^2 \\
 & + 576 \cos(v) \vartheta^{-3} / (T_2 v^2) + \frac{1}{96} (36 \\
 & - 72 \sin(v) v - 60 \cos(v)^3 v^2 - 125 \cos(v)^3 v^4 \\
 & - 60 v^2 \cos(v)^2 - 215 \cos(v)^2 v^4 \\
 & + 60 \cos(v) v^2 - 55 \cos(v) v^4 + 60 v^2 + 35 v^4 + 288 \sin(v) v \cos(v)^5 \\
 & - 480 \sin(v) v \cos(v)^4 - 336 \sin(v) v \cos(v)^3 + 588 \sin(v) v \cos(v)^2 \\
 & + 12 \sin(v) v \cos(v) + 288 \cos(v)^6 \\
 & - 288 \cos(v)^5 - 432 \cos(v)^4 + 468 \cos(v)^3 \\
 & + 108 \cos(v)^2 - 180 \cos(v) \vartheta^{-4} / (T_2 v^2) = 0 \\
 & T_2: = \cos(v)^6 - 2 \cos(v)^5 - \cos(v)^4 + 4 \cos(v)^3 - \cos(v)^2 - 2 \cos(v) + 1
 \end{aligned}$$

(55)

References

1. L.G. Ixaru, M. Micu, *Topics in Theoretical Physics* (Central Institute of Physics, Bucharest, 1978)
2. L.D. Landau, F.M. Lifshitz, *Quantum Mechanics* (Pergamon, New York, 1965)
3. I. Prigogine, S. Rice (eds.), *Advances in Chemical Physics vol. 93: New Methods in Computational Quantum Mechanics* (John Wiley & Sons, New York, 1997)

4. G. Herzberg, *Spectra of Diatomic Molecules* (Van Nostrand, Toronto, 1950)
5. T.E. Simos, Atomic structure computations in chemical modelling: applications and theory (Editor: A. Hinchliffe, UMIST). *R. Soc. Chem.* 38–142 (2000)
6. T.E. Simos, Numerical methods for 1D, 2D and 3D differential equations arising in chemical problems, chemical modelling: application and theory. *R. Soc. Chem.* **2**, 170–270 (2002)
7. T.E. Simos, Numerical Solution of Ordinary Differential Equations with Periodical Solution. Doctoral Dissertation, National Technical University of Athens, Greece, 1990 (in Greek)
8. J.R. Dormand, M.E.A. El-Mikkawy, P.J. Prince, Families of Runge-Kutta-Nyström formulae. *IMA J. Numer. Anal.* **7**, 235–250 (1987)
9. J.R. Dormand, P.J. Prince, A family of embedded Runge-Kutta formulae. *J. Comput. Appl. Math.* **6**, 1926 (1980)
10. A.B. Sideridis, T.E. Simos, A low-order embedded Runge-Kutta method for periodic initial-value problems. *J. Comput. Appl. Math.* **44**(2), 235–244 (1992)
11. T.E. Simos, A Runge-Kutta Fehlberg method with phase-lag of order infinity for initial value problems with oscillating solution. *Comput. Math. Appl.* **25**, 95–101 (1993)
12. T.E. Simos, Runge-Kutta interpolants with minimal phase-lag. *Comput. Math. Appl.* **26**, 43–49 (1993)
13. T.E. Simos, Runge-Kutta-Nyström interpolants for the numerical integration of special second-order periodic initial-value problems. *Comput. Math. Appl.* **26**, 7–15 (1993)
14. T.E. Simos, A high-order predictor-corrector method for periodic IVPs. *Appl. Math. Lett.* **6**(5), 9–12 (1993)
15. T.E. Simos, E. Dimas, A.B. Sideridis, A Runge-Kutta-Nyström method for the numerical-integration of special 2nd-order periodic initial-value problems. *J. Comput. Appl. Math.* **51**(3), 317–326 (1994)
16. T.E. Simos, An explicit high-order predictor-corrector method for periodic initial-value problems. *Math. Models Methods Appl. Sci.* **5**(2), 159–166 (1995)
17. G. Avdelas, T.E. Simos, Block Runge-Kutta methods for periodic initial-value problems. *Comput. Math. Appl.* **31**, 69–83 (1996)
18. G. Avdelas, T.E. Simos, Embedded methods for the numerical solution of the Schrödinger equation. *Comput. Math. Appl.* **31**, 85–102 (1996)
19. T.E. Simos, A modified Runge-Kutta method for the numerical solution of ODE's with oscillation solutions. *Appl. Math. Lett.* **9**(6), 61–66 (1996)
20. T.E. Simos, Some embedded modified Runge-Kutta methods for the numerical solution of some specific Schrödinger equations. *J. Math. Chem.* **24**(1–3), 23–37 (1998)
21. T.E. Simos, An embedded Runge-Kutta method with phase-lag of order infinity for the numerical solution of the Schrödinger equation. *Int. J. Mod. Phys. C* **11**, 1115–1133 (2000)
22. T.E. Simos, J. Vigo-Aguiar, A new modified Runge-Kutta-Nyström method with phase-lag of order infinity for the numerical solution of the Schrödinger equation and related problems. *Int. J. Mod. Phys. C* **11**, 1195–1208 (2000)
23. T.E. Simos, J. Vigo-Aguiar, A modified Runge-Kutta method with phase-lag of order infinity for the numerical solution of the of Schrödinger equation and related problems. *Comput. Chem.* **25**, 275–281 (2001)
24. T.E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **30**(1), 121–131 (2001)
25. T.E. Simos, P.S. Williams, A New Runge-Kutta-Nyström method with phase-lag of order infinity for the numerical solution of the Schrödinger equation. *MATCH Commun. Math. Comput. Chem.* **45**, 123–137 (2002)
26. C. Tsitouras, T.E. Simos, Optimized Runge-Kutta pairs for problems with oscillating solutions. *J. Comput. Appl. Math.* **147**(2), 397–409 (2002)
27. Z.A. Anastassi, T.E. Simos, Special optimized Runge-Kutta methods for IVPs with oscillating solutions. *Int. J. Mod. Phys. C* **15**, 1–15 (2004)
28. Z.A. Anastassi, T.E. Simos, A dispersive-fitted and dissipative-fitted explicit Runge-Kutta method for the numerical solution of orbital problems. *New Astron.* **10**, 31–37 (2004)
29. K. Tselios, T.E. Simos, Runge-Kutta methods with minimal dispersion and dissipation for problems arising from computational acoustics. *J. Comput. Appl. Math.* **175**(1), 173–181 (2005)
30. Z.A. Anastassi, T.E. Simos, An optimized Runge-Kutta method for the solution of orbital problems. *J. Comput. Appl. Math.* **175**(1), 1–9 (2005)
31. T.V. Triantafyllidis, Z.A. Anastassi, T.E. Simos, Two optimized Runge-Kutta methods for the solution of the Schrödinger equation. *MATCH Commun. Math. Comput. Chem.* **60**(3), 753–771 (2008)

32. D.F. Papadopoulos, Z.A. Anastassi, T.E. Simos, A phase-fitted Runge-Kutta-Nyström method for the numerical solution of initial value problems with oscillating solutions. *Comput. Phys. Commun.* **180**(10), 1839–1846 (2009)
33. A.A. Kosti, Z.A. Anastassi, T.E. Simos, An optimized explicit Runge-Kutta method with increased phase-lag order for the numerical solution of the Schrödinger equation and related problems. *J. Math. Chem.* **47**(1), 315–330 (2010)
34. Z. Kalogiratou, T.E. Simos, Construction of trigonometrically and exponentially fitted Runge-Kutta-Nyström methods for the numerical solution of the Schrödinger equation and related problems a method of 8th algebraic order. *J. Math. Chem.* **31**(2), 211–232 (2002)
35. Z.A. Anastassi, T.E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **37**(3), 281–293 (2005)
36. Z.A. Anastassi, T.E. Simos, A family of exponentially-fitted Runge-Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **41**(1), 79–100 (2007)
37. J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial values problems. *J. Inst. Math. Appl.* **18**, 189–202 (1976)
38. A.D. Raptis, A.C. Allison, Exponential—fitting methods for the numerical solution of the Schrödinger equation. *Comput. Phys. Commun.* **14**, 1–5 (1978)
39. A.D. Raptis, Exponentially-fitted solutions of the eigenvalue Schrödinger equation with automatic error control. *Comput. Phys. Commun.* **28**, 427–431 (1983)
40. Z. Kalogiratou, T.E. Simos, A P-stable exponentially-fitted method for the numerical integration of the Schrödinger equation. *Appl. Math. Comput.* **112**, 99–112 (2000)
41. A.D. Raptis, T.E. Simos, A four-step phase-fitted method for the numerical integration of second order initial-value problem. *BIT* **31**, 160–168 (1991)
42. T.E. Simos, A.D. Raptis, Numerov-type methods with minimal phase-lag for the numerical integration of the one-dimensional Schrödinger equation. *Computing* **45**, 175–181 (1990)
43. T.E. Simos, A two-step method with phase-lag of order infinity for the numerical integration of second order periodic initial-value problems. *Int. J. Comput. Math.* **39**, 135–140 (1991)
44. T.E. Simos, A Numerov-type method for the numerical-solution of the radial Schrödinger-equation. *Appl. Numer. Math.* **7**(2), 201–206 (1991)
45. T.E. Simos, Explicit two-step methods with minimal phase-lag for the numerical-integration of special second-order initial-value problems and their application to the one-dimensional Schrödinger-equation. *J. Comput. Appl. Math.* **39**(1), 89–94 (1992)
46. T.E. Simos, Two-step almost P-stable complete in phase methods for the numerical integration of second order periodic initial-value problems. *Inter. J. Comput. Math.* **46**, 77–85 (1992)
47. T.E. Simos, An explicit almost P-stable two-step method with phase-lag of order infinity for the numerical integration of second order periodic initial-value problems. *Appl. Math. Comput.* **49**, 261–268 (1992)
48. T.E. Simos, High—order methods with minimal phase-lag for the numerical integration of the special second order initial value problem and their application to the one-dimensional Schrödinger equation. *Comput. Phys. Commun.* **74**, 63–66 (1993)
49. T.E. Simos, A new variable-step method for the numerical-integration of special 2Nd-order initial-value problems and their application to the one-dimensional Schrödinger-equation. *Appl. Math. Lett.* **6**(3), 67–73 (1993)
50. T.E. Simos, A family of two-step almost P-stable methods with phase-lag of order infinity for the numerical integration of second order periodic initial-value problems. *Jpn. J. Ind. Appl. Math.* **10**, 289–297 (1993)
51. T.E. Simos, A predictor-corrector phase-fitted method for $y'' = f(x, y)$. *Math. Comput. Simul.* **35**, 153–159 (1993)
52. T.E. Simos, A P-stable complete in phase Obrechhoff trigonometric fitted method for periodic initial value problems. *Proc. R. Soc. Lond. A* **441**, 283–289 (1993)
53. T.E. Simos, An explicit 4-step phase-fitted method for the numerical-integration of 2nd-order initial-value problems. *J. Comput. Appl. Math.* **55**(2), 125–133 (1994)
54. T.E. Simos, Some new variable-step methods with minimal phase-lag for the numerical integration of special 2nd-order initial value problems. *Appl. Math. Comput.* **64**, 65–72 (1994)
55. T.E. Simos, G. Mousadis, Some new Numerov-type methods with minimal phase-lag for the numerical integration of the radial Schrödinger equation. *Mol. Phys.* **83**, 1145–1153 (1994)

56. T.E. Simos, G. Mousadis, A two-step method for the numerical solution of the radial Schrödinger equation. *Comput. Math. Appl.* **29**, 31–37 (1995)
57. T.E. Simos, Predictor corrector phase-fitted methods for $Y''=F(X,Y)$ and an application to the Schrödinger-equation. *Int. J. Quantum Chem.* **53**(5), 473–483 (1995)
58. T.E. Simos, Some low-order two-step almost P-stable methods with phase-lag of order infinity for the numerical integration of the radial Schrödinger equation. *Int. J. Modern Phys. A* **10**, 2431–2438 (1995)
59. T.E. Simos, A new Numerov-type method for computing eigenvalues and resonances of the radial Schrödinger equation. *Int. J. Modern Phys. C-Phys. Comput.* **7**(1), 33–41 (1996)
60. G. Papakaliatakis, T.E. Simos, A new method for the numerical solution of fourth order BVPs with oscillating solutions. *Comput. Math. Appl.* **32**, 1–6 (1996)
61. T.E. Simos, Accurate computations for the elastic scattering phase-shift problem. *Comput. Chem.* **21**, 125–128 (1996)
62. T.E. Simos, An eighth order method with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. *Inter. J. Modern Phys. C* **7**, 825–835 (1996)
63. T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem. *J. Math. Chem.* **21**(4), 359–372 (1997)
64. T.E. Simos, An extended Numerov-type method for the numerical solution of the Schrödinger equation. *Comput. Math. Appl.* **33**, 67–78 (1997)
65. T.E. Simos, New Numerov-type methods for computing eigenvalues, resonances and phase shifts of the radial Schrödinger equation. *Int. J. Quantum Chem.* **62**, 467–475 (1997)
66. T.E. Simos, New P-stable high-order methods with minimal phase-lag for the numerical integration of the radial Schrödinger equation. *Phys. Scr.* **55**, 644–650 (1997)
67. T.E. Simos, Eighth order methods for elastic scattering phase-shifts. *Int. J. Theor. Phys.* **36**, 663–672 (1997)
68. T.E. Simos, G. Tougelidis, An explicit eighth order method with minimal phase-lag for the numerical solution of the Schrödinger equation. *Comput. Mater. Sci.* **8**, 317–326 (1997)
69. T.E. Simos, G. Tougelidis, An explicit eighth order method with minimal phase-lag for accurate computations of eigenvalues, resonances and phase shifts. *Comput. Chem.* **21**, 327–334 (1997)
70. T.E. Simos, Eighth order method for accurate computations for the elastic scattering phase-shift problem. *Int. J. Quantum Chem.* **68**, 191–200 (1998)
71. T.E. Simos, New embedded explicit methods with minimal phase-lag for the numerical integration of the Schrödinger equation. *Comput. Chem.* **22**, 433–440 (1998)
72. T.E. Simos, High-algebraic, high-phase-lag methods for accurate computations for the elastic-scattering phase shift problem. *Can. J. Phys.* **76**, 473–493 (1998)
73. T.E. Simos, High algebraic order methods with minimal phase-lag for accurate solution of the Schrödinger equation. *Int. J. Modern Phys. C* **9**, 1055–1071 (1998)
74. G. Avdelas, T.E. Simos, Embedded eighth order methods for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **26**(4), 327–341 (1999)
75. T.E. Simos, A new finite difference scheme with minimal phase-lag for the numerical solution of the Schrödinger equation. *Appl. Math. Comput.* **106**, 245–264 (1999)
76. T.E. Simos, High algebraic order explicit methods with reduced phase-lag for an efficient solution of the Schrödinger equation. *Int. J. Quantum Chem.* **73**, 479–496 (1999)
77. T.E. Simos, Dissipative high phase-lag order Numerov-type methods for the numerical solution of the Schrödinger equation. *Comput. Chem.* **23**, 439–446 (1999)
78. T.E. Simos, Explicit eighth order methods for the numerical integration of initial-value problems with periodic or oscillating solutions. *Comput. Phys. Commun.* **119**, 32–44 (1999)
79. T.E. Simos, High algebraic order methods for the numerical solution of the Schrödinger equation. *Mol. Simul.* **22**, 303–349 (1999)
80. G. Avdelas, A. Konguetsof, T.E. Simos, A family of hybrid eighth order methods with minimal phase-lag for the numerical solution of the Schrödinger equation and related problems. *Int. J. Modern Phys. C* **11**, 415–437 (2000)
81. G. Avdelas, T.E. Simos, Dissipative high phase-lag order Numerov-type methods for the numerical solution of the Schrödinger equation. *Phys. Rev. E* **62**, 1375–1381 (2000)
82. G. Avdelas, T.E. Simos, On variable-step methods for the numerical solution of Schrödinger equation and related problems. *Comput. Chem.* **25**, 3–13 (2001)
83. T.E. Simos, P.S. Williams, New insights in the development of Numerov-type methods with minimal phase-lag for the numerical solution of the Schrödinger equation. *Comput. Chem.* **25**, 77–82 (2001)

84. G. Avdelas, A. Konguetsof, T.E. Simos, A generator of hybrid explicit methods for the numerical solution of the Schrödinger equation and related problems. *Comput. Phys. Commun.* **136**, 14–28 (2001)
85. T.E. Simos, J. Vigo-Aguiar, A symmetric high-order method with minimal phase-lag for the numerical solution of the Schrödinger equation. *Int. J. Modern Phys. C* **12**, 1035–1042 (2001)
86. T.E. Simos, J. Vigo-Aguiar, On the construction of efficient methods for second order IVPs with oscillating solution. *Int. J. Modern Phys. C* **12**, 1453–1476 (2001)
87. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 1. Development of the basic method. *J. Math. Chem.* **29**(4), 281–291 (2001)
88. G. Avdelas, A. Konguetsof, T.E. Simos, A generator and an optimized generator of high-order hybrid explicit methods for the numerical solution of the Schrödinger equation. Part 2. Development of the generator; optimization of the generator and numerical results. *J. Math. Chem.* **29**(4), 293–305 (2001)
89. Ch. Tsitouras, T.E. Simos, High algebraic, high phase-lag order embedded Numerov-type methods for oscillatory problems. *Appl. Math. Comput.* **131**, 201–211 (2002)
90. G. Avdelas, A. Konguetsof, T.E. Simos, A generator of dissipative methods for the numerical solution of the Schrödinger equation. *Comput. Phys. Commun.* **148**, 59–73 (2002)
91. A. Konguetsof, T.E. Simos, P-stable eighth algebraic order methods for the numerical solution of the Schrödinger equation. *Comput. Chem.* **26**, 105–111 (2002)
92. T.E. Simos, J. Vigo-Aguiar, Symmetric eighth algebraic order methods with minimal phase-lag for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **31**(2), 135–144 (2002)
93. A. Konguetsof, T.E. Simos, A generator of hybrid symmetric four-step methods for the numerical solution of the Schrödinger equation. *J. Comput. Appl. Math.* **158**(1), 93–106 (2003)
94. T.E. Simos, I.T. Famelis, Ch. Tsitouras, Zero dissipative, explicit Numerov-type methods for second order IVPs with oscillating solutions. *Numer. Algorithms* **34**(1), 27–40 (2003)
95. D.P. Sakas, T.E. Simos, Multiderivative methods of eighth algebraic order with minimal phase-lag for the numerical solution of the radial Schrödinger equation. *J. Comput. Appl. Math.* **175**(1), 161–172 (2005)
96. D.P. Sakas, T.E. Simos, A family of multiderivative methods for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **37**(3), 317–331 (2005)
97. G.A. Panopoulos, Z.A. Anastassi, T.E. Simos, Two new optimized eight-step symmetric methods for the efficient solution of the Schrödinger equation and related problems. *MATCH Commun. Math. Comput. Chem.* **60**(3), 773–785 (2008)
98. T.E. Simos, A new Numerov-type method for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **46**(3), 981–1007 (2009)
99. T.E. Simos, A family of 4-step exponentially fitted predictor-corrector methods for the numerical integration of the Schrödinger equation. *J. Comput. Appl. Math.* **58**(3), 337–344 (1995)
100. R.M. Thomas, T.E. Simos, G.V. Mitsou, A family of Numerov-type exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. *J. Comput. Appl. Math.* **67**(2), 255–270 (1996)
101. R.M. Thomas, T.E. Simos, A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. *J. Comput. Appl. Math.* **87**(2), 215–226 (1997)
102. G. Psihoyios, T.E. Simos, Trigonometrically fitted predictor-corrector methods for IVPs with oscillating solutions. *J. Comput. Appl. Math.* **158**(1), 135–144 (2003)
103. A. Konguetsof, A new two-step hybrid method for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **47**(2), 871–890 (2010)
104. K. Tselios, T.E. Simos, Symplectic methods for the numerical solution of the radial Schrödinger equation. *J. Math. Chem.* **34**(1–2), 83–94 (2003)
105. K. Tselios, T.E. Simos, Symplectic methods of fifth order for the numerical solution of the radial Schrödinger equation. *J. Math. Chem.* **35**(1), 55–63 (2004)
106. T. Monovasilis, T.E. Simos, New second-order exponentially and trigonometrically fitted symplectic integrators for the numerical solution of the time-independent Schrödinger equation. *J. Math. Chem.* **42**(3), 535–545 (2007)
107. T. Monovasilis, Z. Kalogiratou, T.E. Simos, Exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. *J. Math. Chem.* **37**(3), 263–270 (2005)

108. T. Monovasilis, Z. Kalogiratu, T.E. Simos, Trigonometrically fitted and exponentially fitted symplectic methods for the numerical integration of the Schrödinger equation. *J. Math. Chem.* **40**(3), 257–267 (2006)
109. Z. Kalogiratu, T.E. Simos, Newton-Cotes formulae for long-time integration. *J. Comput. Appl. Math.* **158**(1), 75–82 (2003)
110. T.E. Simos, High order closed Newton-Cotes trigonometrically-fitted formulae for the numerical solution of the Schrödinger equation. *Appl. Math. Comput.* **209**(1), 137–151 (2009)
111. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for the solution of the Schrödinger equation. *MATCH Commun. Math. Comput. Chem.* **60**(3), 787–801 (2008)
112. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high order for the numerical integration of the Schrödinger equation. *J. Math. Chem.* **44**(2), 483–499 (2008)
113. T.E. Simos, High-order closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. *Comput. Phys. Commun.* **178**(3), 199–207 (2008)
114. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for numerical integration of the Schrödinger equation. *Comput. Lett.* **3**(1), 45–57 (2007)
115. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration of orbital problems. *Revista Mexicana de Astronomia y Astrofisica* **42**(2), 167–177 (2006)
116. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae for long-time integration. *Int. J. Modern Phys. C* **14**(8), 1061–1074 (2003)
117. Z. Kalogiratu, T. Monovasilis, T.E. Simos, Symplectic integrators for the numerical solution of the Schrödinger equation. *J. Comput. Appl. Math.* **158**(1), 83–92 (2003)
118. T.E. Simos, Closed Newton-Cotes trigonometrically-fitted formulae of high-order for long-time integration of orbital problems. *Appl. Math. Lett.* **22**(10), 1616–1621 (2009)
119. T.E. Simos, A family of P-stable exponentially-fitted methods for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **25**(1), 65–84 (1999)
120. J. Vigo-Aguiar, T.E. Simos, Family of twelve steps exponential fitting symmetric multistep methods for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **32**(3), 257–270 (2002)
121. G. Avdelas, E. Kefalidis, T.E. Simos, New P-stable eighth algebraic order exponentially-fitted methods for the numerical integration of the Schrödinger equation. *J. Math. Chem.* **31**(4), 371–404 (2002)
122. T.E. Simos, A family of trigonometrically-fitted symmetric methods for the efficient solution of the Schrödinger equation and related problems. *J. Math. Chem.* **34**(1–2), 39–58 (2003)
123. T.E. Simos, Exponentially—fitted multiderivative methods for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **36**(1), 13–27 (2004)
124. T.E. Simos, A four-step exponentially fitted method for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **40**(3), 305–318 (2006)
125. T.E. Simos, A family of four-step trigonometrically-fitted methods and its application to the Schrödinger equation. *J. Math. Chem.* **44**(2), 447–466 (2009)
126. T.E. Simos, Exponentially and trigonometrically fitted methods for the solution of the Schrödinger equation. *Acta Appl. Math.* **110**(3), 1331–1352 (2010)
127. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. *J. Math. Chem.* **45**(4), 1102–1129 (2009)
128. G. Psihoyios, T.E. Simos, Sixth algebraic order trigonometrically fitted predictor-corrector methods for the numerical solution of the radial Schrödinger equation. *J. Math. Chem.* **37**(3), 295–316 (2005)
129. G. Psihoyios, T.E. Simos, The numerical solution of the radial Schrödinger equation via a trigonometrically fitted family of seventh algebraic order Predictor-Corrector methods. *J. Math. Chem.* **40**(3), 269–293 (2006)
130. T.E. Simos, A new explicit Bessel and Neumann fitted eighth algebraic order method for the numerical solution of the Schrödinger equation. *J. Math. Chem.* **27**(4), 343–356 (2000)
131. Z.A. Anastassi, T.E. Simos, A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution. *J. Math. Chem.* **45**(4), 1102–1129 (2009)
132. T.E. Simos, Dissipative trigonometrically-fitted methods for linear second-order IVPs with oscillating solution. *Appl. Math. Lett.* **17**(5), 601–607 (2004)
133. T.E. Simos, P.S. Williams, On finite difference methods for the solution of the Schrödinger equation. *Comput. Chem.* **23**, 513–554 (1999)

134. Z.A. Anastassi, T.E. Simos, Numerical multistep methods for the efficient solution of quantum mechanics and related problems. *Phys. Rep. Rev. Sect. Phys. Lett.* **482**, 1–240 (2009)
135. J. Vigo-Aguiar, T.E. Simos, Review of multistep methods for the numerical solution of the radial Schrödinger equation. *Int. J. Quantum Chem.* **103**(3), 278–290 (2005)
136. T.E. Simos, A.D. Zdzetsis, G. Psihoyios, Z.A. Anastassi, Special issue on mathematical chemistry based on papers presented within ICCMSE 2005 preface. *J. Math. Chem.* **46**(3), 727–728 (2009)
137. T.E. Simos, G. Psihoyios, Special issue: the international conference on computational methods in sciences and engineering 2004—preface. *J. Comput. Appl. Math.* **191**(2), 165–165 (2004)
138. T.E. Simos, G. Psihoyios, Special issue—selected papers of the international conference on computational methods in sciences and engineering (ICCMSE 2003) Kastoria, Greece, 12–16 September 2003—preface. *J. Comput. Appl. Math.* **175**(1), IX–IX (2005)
139. T.E. Simos, J. Vigo-Aguiar, Special issue—selected papers from the conference on computational and mathematical methods for science and engineering (CMMSE-2002)—Alicante University, Spain, 20–25 September 2002—preface. *J. Comput. Appl. Math.* **158**(1), IX–IX (2003)
140. T.E. Simos, P.S. Williams, A finite-difference method for the numerical solution of the Schrödinger equation. *J. Comput. Appl. Math.* **79**(2), 189–205 (1997)
141. L.G. Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation. *Comput. Phys. Commun.* **38**(3), 329–337 (1985)
142. L.G. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies. *Comput. Phys. Commun.* **19**, 23–27 (1980)
143. G.D. Quinlan, S. Tremaine, Symmetric multistep methods for the numerical integration of planetary orbits. *Astron. J.* **100**(5), 1694–1700 (1990)
144. I. Alolyan, T.E. Simos, High algebraic order methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation. *J. Math. Chem.* (2010). doi:[10.1007/s10910-010-9718-y](https://doi.org/10.1007/s10910-010-9718-y)