J Math Chem (2010) 48:925–958
DOI 10.1007/s10910-010-9718-y

ORIGINAL PAPER

High algebraic order methods with vanished phase-lag and its first derivative for the numerical solution of the Schrödinger equation

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Received: 21 June 2010 / Accepted: 2 July 2010 / Published online: 23 July 2010

Abstract In the present paper we develop a high algebraic order multistep method. The characteristic property of the new proposed method is the requirement of vanishing the phase-lag and its derivatives. The new method is applied for the approximate solution of the radial Schrödinger equation. The efficiency of the new methodology is proved via error analysis and numerical applications.

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

1 Introduction

The one-dimensional Schrödinger equation can be written as:

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

Many problems 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]).

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We give the definitions of some terms of (1):

- The function $W(x) = l(l+1)/x^2 + V(x)$ is called *the effective potential*. This satisfies $W(x) \to 0$ as $x \to \infty$
- 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:

$$y(0) = 0 \tag{2}$$

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

The last years an extended study on the development of numerical methods for the solution of the Schrödinger equation has been done. The aim of this research is the development of fast and reliable methods for the solution of the Schrödinger equation and related problems (see for example [5–37].

We can divide the numerical methods for the approximate 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]

The purpose of this paper is to describe a new methodology for the construction of numerical methods for the approximate solution periodic initial-value problems. The new methodology is based on the requirement of vanishing the phase-lag and its derivatives. We will apply the new proposed method in the numerical solution of the radial Schrödinger equation. The efficiency of the new methodology will be studied via the error analysis and the application to the specific potential.

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 derivative. We will investigate the stability and the error of the methods of the new family. Finally, we will apply both categories of methods the new obtained 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 a brief description of the literature on numerical methods with minimal phase-lag and on phase-fitted methods. In Sect. 3 we present the theory of the new methodology. In Sect. 4 we present the development of the new family of methods. The error analysis is presented in Sect. 5. In Sect. 6 we will investigate the stability properties of the new developed methods. In Sect. 7 the numerical results are presented. Finally, in Sect. 8 remarks and conclusions are discussed.

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

2 A brief description of the literature

2.1 Phase-fitted and minimal phase-lag Runge-Kutta and Runge-Kutta Nyström methods

In [9] the authors produced an embedded Runge-Kutta-Fehlberg. This method is based on the third algebraic order scheme with phase-lag of order six and dissipative order four and on the fourth algebraic order scheme with phase-lag of order four and dissipative order six. The authors used the scheme with phase-lag of order six in order to estimate the phase-lag error of the scheme with phase-lag of order four. The numerical results show the efficiency of the method.

In [10] a Runge-Kutta method is obtained for the numerical approximation of initial-value problems with oscillating solution. The new produced methods are based on the Runge-Kutta Fehlberg 2(3) method and Runge-Kutta methods with phase-lag of order infinity are finally constructed. Based on these methods the authors developed a new embedded Runge-Kutta Fehlberg 2(3) method with phase-lag of order infinity. The author called this method as Runge- Kutta Feldberg Phase Fitted method (RKFPF). The numerical results indicated the efficiency of the new proposed method.

In [11] the author developed the basic theory for the production of explicit Scaled Runge-Kutta methods (SRK) for the numerical approximation of first order differential equations having an oscillatory solution. In the same paper and based on the theory developed in the present paper and on the theory of Runge-Kutta methods with minimal phase-lag, the author obtained an embedded RungeKutta 10(12) method and an explicit scaled Runge-Kutta method. Numerical results indicate the efficiency of the new algorithms.

In [12] the author developed the theory of the phase-lag analysis for Runge-Kutta-Nyström methods and Runge-Kutta-Nyström interpolants. In the same paper the author developed a new Runge-Kutta-Nyström method with interpolation properties.

In [13] the author derives a Runge-Kutta type method which has an algebraic order eight, an interval of periodicity equal to (0, 30.7214582) and a phase-lag of order 12.

In [14] the authors have developed a new Runge-Kutta-Nyström fourth algebraic order method with phase-lag of order eight and interval of periodicity equal to [0, 9.1144751].

In [15] the author derives an Explicit Runge-Kutta type method which has an algebraic order six, an interval of periodicity equal to (0, 21.4812098756) and a phase-lag of order eight.

In [16] the authors have introduced Block Runge-Kutta methods with minimal phase-lag for first order periodic initial value problems. The new proposed methods are based on the Runge-Kutta methods of algebraic order three, and on a new error estimate introduced in this paper. The efficiency of the constructed scheme was presented via the numerical results.

In [17] the authors introduced new methods for the numerical numerical integration of the radial Schrödinger equation. They presented phase-lag analysis of the new methods. They called these methods embedded methods because of a simple natural error control mechanism. Numerical results for the radial Schrödinger equation show the validity of the developed theory.

In [18] the author derived a modified Runge-Kutta method with minimal phase-lag of order eight for the numerical approximation of the solution of ODEs with oscillating solutions. The produced method is based on the Runge-Kutta method of Sharp and Smart RK4SS(5) of order five. Numerical and theoretical results show the efficiency of the produced method.

In [19] the author produced: (1) A fourth algebraic order Runge-Kutta scheme with phase-lag of order six and (2) a block embedded Runge-Kutta scheme with phase lag of orders 8(2)12. These methods are based on Runge-Kutta 4(6) Fehlberg method.

In [20] an embedded Runge-Kutta method with phase-lag of order infinity is introduced. The algebraic order of the methods are four and five. The methods based on the well know Runge-Kutta Dormand-Prince pairs [26].

In [21] a modified Runge-Kutta-Nyström fourth-algebraic order phase-fitted method is derived.

In [22] the authors obtained a modified Runge-Kutta fourth-algebraic order phase-fitted method.

In [23] the author obtained a modified phase-fitted Runge-Kutta method (i.e. a method with phase-lag of order infinity) for the numerical integration of IVPs with periodical solutions. The new proposed method is based on the Runge-Kutta fifth algebraic order method of Dormand and Prince [26]. Numerical experiments show the efficiency of the new approach.

In [24] the authors has developed a Runge-Kutta-Nyström fourth algebraic order method with phase-lag of order infinity and almost P-stable (i.e. with interval of periodicity equal to: $(0, \infty) - S - (2.8, 3.2)$. The numerical results from the numerical solution of the Schrödinger equation show the efficiency of the new proposed method.

In [25] the authors have obtained three types of methods for the numerical solution of IVPs with periodical solution. The methods are: (i) phase-fitted, (ii) zero dissipative (iii) both zero dissipative and phase fitted. They presented some specific modifications of well-known explicit Runge-Kutta pairs of orders five and four. Numerical experiments show the efficiency of the new approaches.

In [29] the authors developed a Runge-Kutta method with minimal dispersion and dissipation error. The maximum order of dissipation is nine and maximum order of dispersion is eight. The authors used the Chebyshev pseudospectral method using spatial discretization and a new fourth-order six-stage Runge-Kutta scheme with optimal dispersion and dissipation properties is used for time advancing.

In [30] an Explicit Runge-Kutta method with algebraic order four, infinite order of phase-lag and eighth order of amplification error for the solution of well-known periodic orbital problems. Application of the new developed method to the well known orbital problems shows the efficiency of the method.

In [27] the authors constructed a family of explicit Rune-Kutta methods of fifth algebraic order. They presented the basic theory for the Runge-Kutta methods, the development of the method and the phase-lag analysis of the new proposed family. A study on the dependence of the obtained accuracy and of the product of the frequency of the problem and the integration stepsize is also presented.

In [28] the authors obtained a new explicit Rune-Kutta method of fifth algebraic order which is dispersive and dissipative fitted.

In [31] the authors produced new explicit Rune-Kutta methods of eight stages and of sixth algebraic order which have phase-lag of order ten or are phase-fitted.

In [32] the authors constructed a new Runge-Kutta-Nyström method, with phase-lag of order infinity, for the numerical solution of periodic IVPs. The proposed method is based on the Dormand, El-Mikkawy and Prince Runge-Kutta-Nyström method [8] of algebraic order four. Numerical results show the efficiency of the proposed method.

In [33] an optimized explicit Runge-Kutta fifth algebraic order with phase-lag of order eight is proposed.

2.2 Phase-fitted and minimal phase-lag hybrid and multistep methods

In [38] the authors have introduced, for the first time in the literature, the term of phase-fitted method. A method is called phase-fitted if its phase-lag order is equal to infinity. In the same paper the authors give, for the first time in the literature, a direct formula for the computation of the phase-lag for the symmetric four-step methods.

In [39] the conditions in order two-step hybrid fourth algebraic order methods with phase-lag of order six and eight to be P-stable are given. In the same paper two two-step fourth algebraic order methods with phase-lag of order eight and ten and internals of periodicity equal to (0, 8.27) and (0.8.89) are also obtained.

In [41] a explicit Numerov-type method with algebraic order four and phase-lag order eight and an extended interval of periodicity (equal to (, 21.48)) is developed.

In [40] a two-step phase-fitted hybrid sixth algebraic order method with interval of periodicity equals to (0, 9.59) is constructed.

In [43] two two-step almost P-stable methods with phase-lag of order infinite are developed. The first method is a hybrid Numerov-type method and the second one is a hybrid method. Both methods are almost P-stable, i.e. are P-stable except of some sets of points.

In [42] a family of explicit two-step hybrid sixth algebraic order methods is introduced. The family has free parameters which are determined in order phase-lag of order eight, ten and twelve to be achieved.

In [44] an explicit two-step phase-fitted hybrid fourth algebraic order method is produced. The method is almost P-stable i.e. its interval of periodicity is equal to $(0, \infty) - S$, where S is a set of distinct points.

In [45] the conditions in order two-step hybrid sixth algebraic order method with phase-lag of order eight to be P-stable are given. In the same paper a two-step sixth algebraic order method with phase-lag of order ten and internal of periodicity equals to (0, 8.16) is also determined.

In [46] two two-step hybrid methods are developed. The first method is of algebraic order four, has phase-lag of order ten and an interval of periodicity equals to (0, 31.70). The second one is of algebraic order four, has phase-lag of order eight and an interval of periodicity equals to (0, 21.48). Based on these methods a variable-step procedure is obtained.

In [47] the condition in order a two-step hybrid sixth algebraic order method to be phase-fitted is proved. The method for these values of parameters is also almost P-stable i.e. its interval of periodicity is equal to $(0, \infty) - S$, where S is a set if distinct points.

In [48] the condition in order a two-step hybrid fourth algebraic order method to be phase-fitted is given. The method for these values of parameters has interval of periodicity equals to $(0, \pi^2)$.

In [49] a tenth algebraic order Obrechkoff multoderivative P-stable phase-fitted method is derived.

In [50] an explicit four-step sixth algebraic order methods is obtained. The methods contains a free parameter which is determined in order the method to be phase-fitted (i.e. to have phase-lag equal to zero). The new produced method has interval of periodicity equals to $(0, 4.40831979^2)$.

In [51] two two-step hybrid sixth algebraic order methods with phase-lag of order eight and ten and intervals of periodicity equal to (0, 26) respectively are obtained. Based on these methods and a new error control procedure, a variable-step method is also proposed.

In [52] a family of P-stable two-step hybrid fourth algebraic order methods with phase-lag of order eight, ten and twelve is developed.

In [54] the author constructed a two-step second algebraic order P-stable phase-fitted method and a two-step fourth algebraic order P-stable phase-fitted method.

In [53] a two-step hybrid fourth algebraic order method with phase-lag of order ten and an interval of periodicity equal to $(0, \sqrt{720})$ is obtained.

In [55] two two-step methods of algebraic order $O(h^2)$ and $O(h^4)$ which are almost P-stable (i.e. its interval of periodicity is equal to $(0, \infty) - S$, where S is a set if distinct points) are obtained.

In [56] the author obtained a two-step fourth algebraic order method with phase-lag of order fourteen and interval of periodicity equal to (0, 29, 0974).

In [57] a four-step eighth algebraic order method with phase-lag of order eight is constructed.

In [58] the conditions in order a two-step hybrid sixth algebraic order method to have phase-lag of order ten and to be P-stable are given.

In [59] a hybrid two-step eighth algebraic order method with phase-lag of order ten and interval of periodicity equals to (0, 28.7979) is constructed.

In [60] two new hybrid two-step eighth algebraic order methods with phase?lag of order twelve and fourteen are produced. The first method has an interval of periodicity equal to (0, 32.58) while the second one has an interval of periodicity equal to (0, 62.75).

In [61] a hybrid four-step sixth algebraic order method with phase-lag of order eight is produced.

In [62] a family of hybrid P-stable two-step fourth algebraic order methods with phase-lag of order twelve, fourteen and sixteen is developed.

In [63] a family of hybrid P-stable two-step sixth algebraic order methods with phase-lag of order 10(2)20 is obtained.

In [64] a family of hybrid explicit two-step sixth algebraic order methods with phase-lag of order 12, 14 and intervals of periodicity equal to (0, 12.9394), (0, 12.6756) respectively is produced.

In [65] a hybrid explicit two-step sixth algebraic order method with phase-lag of order 12 and interval of periodicity equals to (0, 14.4576) is derived.

In [66] a hybrid explicit two-step sixth algebraic order method with phase-lag of order 10 and interval of periodicity equals to (0, 9.5301) is constructed.

In [67] the author developed a hybrid explicit two-step eighth algebraic order method with phase-lag of order 12 and interval of periodicity equals to (0, 16.886).

In [67] the author produced a family of hybrid explicit two-step fourth algebraic order methods with phase-lag of order 8(2)16 and intervals of periodicity equal to (0, 8.51), (0, 8.97), (0, 9.31), (0, 9.53), (0, 9.66) and (0, 9.75), respectively.

In [69] the author obtained high-algebraic, high-phase-lag methods for accurate computations for the elastic-scattering phase shift problem.

In [70] the author derived high-algebraic methods with minimal phase-lag.

In [71] a generator of hybrid two-step eighth algebraic order explicit methods is developed. The methods of this family have free parameters which determined in order methods with minimal phase-lag to be produced. In this paper a formula which determines the free parameters in order the method to have minimal phase-lag is proved.

In [72] the author produced a finite difference eighth algebraic order method with phase-lag of order ten.

In [73] the author obtained a family of four-step tenth algebraic order methods with phase-lag of order 18(2)26 and intervals of periodicity equal to (0, 9.81), (0, 9.33), (0, 9.86), (0, 9.69) and (0, 9.87). Based on these methods an new error estimation is introduced and a new variable-step method is proposed.

In [74] the author derived a family of two-step sixth algebraic order non-symmetric (dissipative) methods with phase-lag of order 10(2)26. Based on these methods an new error estimation is proposed and a new variable-step method is obtained.

In [75] the author obtained a family of explicit two-step eighth algebraic order methods with phase-lag of order 10(2)16.

In [76] the author developed a family of hybrid four-step tenth algebraic order methods with phase-lag of order 16(2)22 and intervals of periodicity equal to (0, 23.6551), (0, 17.9845), (0, 9.8214), (0, 9.8547).

In [77] a generator of hybrid two-step eighth algebraic order methods with minimal phase-lag is obtained in this paper. Based on this generator a new variable-step procedure is introduced and a variable-step method is derived.

In [78] a generator of dissipative hybrid explicit two-step sixth algebraic order methods with minimal phase-lag is derived in this paper. The dissipation of the family of methods is of order eighth. Based on this generator a new variable-step procedure is obtained and a variable-step method is produced.

In [79] a review for the development of variable-step methods is presented. Phase-lag and stability are studied.

In [80] two Numerov-type dissipative methods of algebraic order five and phase-lag order eight and ten are obtained in this paper. Based on these methods a new variable-step scheme is introduced and a variable-step method is developed.

In [81] a generator of explicit hybrid two-step methods of eighth algebraic order is introduced in this paper. In order the method to have minimal phase-lag the free parameters of the generator are determined using a theorem which is proved in this paper. The characteristic of this generator is the large intervals of periodicity which the members of the generator have. Based on this generator a new variable-step procedure is derived.

In [82] a four-step eighth algebraic order method with phase-lag of order eight and an interval of periodicity equals to (0, 0.65) is obtained.

In [83] a description of the methodologies for the development of efficient methods for the numerical integration of second order IVPs with oscillating solutions is presented.

In [84] and [85] a generator of hybrid two-step tenth algebraic order explicit methods is developed. In the papers a direct formula for the determination of the free parameters of the family in order in order the obtained methods to have minimal phase-lag is proved.

In [86] an embedded Numerov-type method of algebraic order eight and phase-lag of orders 10(2)20 is introduced in this paper. The intervals of periodicity of the methods of the family are large.

In [87] a generator of hybrid dissipative two-step eighth algebraic order methods is derived.

In [88] a P-stable eighth eighth algebraic order method is produced. Based on this method and the method of Simos [63], a new variable-step method is proposed.

In [89] a hybrid eight-step eighth algebraic order family of explicit methods is developed. The methods of this family have free parameters which determined in order methods with minimal phase-lag be produced. More specifically the authors produced methods with phase-lag of order 10 (with interval of periodicity equal to (0, 0.64)), 12 (with interval of periodicity equal to (0, 0.64)), 14 (with interval of periodicity equal to (0, 0.64)).

In [91] a new explicit, zero dissipative, hybrid Numerov type method is constructed. The new method is of sixth algebraic order has a cost of seven stages per step while its phase lag order is fourteen.

In [90] a generator of hybrid four-step sixth algebraic order explicit methods is produced. The method contains free parameters. The authors determined these free parameters for phase-lag of order 8(2)16.

In [93] a hybrid two-step eighth algebraic order multiderivative family of methods is developed. The methods of this family have free parameters which determined in order methods with minimal phase-lag be produced. More specifically the authors produced methods with phase-lag of order 10 (with interval of periodicity equal to (0, 15.27)), 12 (with interval of periodicity equal to (0, 14.24)), 14 (with interval of periodicity equal to (0, 15.05)), 16 (with interval of periodicity equal to (0, 15.05)) and 18 (with interval of periodicity equal to (0, 13.57)).

In [92] a hybrid two-step eighth algebraic order multiderivative methods with phase-lag of order ten and interval of periodicity equal to (0, 15.84) is obtained.

In [94] an eight-step eighth algebraic order family of explicit methods is developed. The authors determined the free parameters of the proposed methods in order the phase-lag to be minimal or equal to zero.

In [95] a new methodology for the development of efficient methods for the approximate solution of second order periodic initial-value problems is presented. The new methodology is based on the requirement that the phase-lag and its derivatives to be vanished. More specifically in this paper a eighth algebraic order method with phase-lag and its first, second, third and fourth derivatives equal to zero is obtained.

In [96] an algorithm with phase-lag and its derivatives equal to zero is developed.

2.3 Review papers

In [97] the authors presented a review for the numerical methods used for the solution of the Schrödinger equation.

In [98] the authors present the recent development in the numerical solution of the Schrödinger equation and related systems of ordinary differential equations with periodical or oscillatory solutions, such as the *N*-body problem etc. In the present paper the authors investigated the multistep methods. Several types of multistep methods (explicit, implicit, predictor-corrector, hybrid) and several properties (P-stability, trigonometric fitting of various orders, phase fitting, high phase-lag order, algebraic order) are studied. The local truncation error and the stability of the methods is also investigated. An error analysis for the Schrödinger equation is also presented. With this analysis the relation of the error to the energy is revealed. The efficiency of the methods is studied through the integration of five problems. The authors presented and analyzed figures and some general conclusions are presented. Finally, code written in Maple is given for the development of all methods analyzed in this paper. Also the subroutines written in Matlab, for the usage of the methods, are presented.

In [99] the authors presented a review on multistep methods for the numerical solution of the Schrödinger equation. They produced some of the Bettis–Cowell methods, introducing a simple way that produces these methods for any algebraic and trigonometric order.

3 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$q'' = f(x, q) \tag{3}$$

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

$$q'' = -\omega^2 q \tag{4}$$

a difference equation of the form

$$\begin{aligned} A_k(\mathrm{v})\, q_{n+k} + \cdots + A_1(\mathrm{v})\, q_{n+1} + A_0(\mathrm{v})\, q_n + \\ + A_1(\mathrm{v})\, q_{n-1} + \cdots + A_k(\mathrm{v})\, q_{n-k} = 0 \end{aligned} \tag{5}$$

is obtained, where $\mathrm{v} = \omega h$, h is the step length and $A_0(\mathrm{v}), A_1(\mathrm{v}), \cdots, A_{\mathrm{k}}(v)$ are polynomials of v.

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

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

Theorem 1 *[104] The symmetric 2k-step method with characteristic equation given by (6) has phase-lag order r and phase-lag constant c given by*

$$\begin{aligned} &-c\,\mathrm{v}^{r+2} + O(\mathrm{v}^{r+4}) \\ &= \frac{2\,A_k(\mathrm{v})\,\cos(k\,\mathrm{v}) + \cdots + 2\,A_j(\mathrm{v})\,\cos(j\,\mathrm{v}) + \cdots + A_0(\mathrm{v})}{2\,k^2\,A_k(\mathrm{v}) + \cdots + 2\,j^2\,A_j(\mathrm{v}) + \cdots + 2\,A_1(\mathrm{v})} \end{aligned} \tag{7}$$

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

4 The new family of eight-step methods: construction of the new methods

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

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

where $a_4 = 1$.

Requiring the above method to have the maximum algebraic order, the following relations are obtained:

$$\begin{aligned} &a_0 = 0, \quad a_1 = -1, \quad a_2 = 2, \quad a_3 = -2, \quad a_4 = 1 \\ &b_0 = -\frac{601}{24} - 90\,b_4 - 20\,b_3, \quad b_1 = -\frac{101}{6} + 64\,b_4 + 15\,b_3 \\ &b_2 = \frac{109}{16} - 20\,b_4 - 6\,b_3 \end{aligned} \tag{9}$$

The application of the above method to the scalar test equation (4) gives the following difference equation:

$$\sum_{i=0}^{4} A_i(\mathrm{v})\,\left(q_{n+i} + q_{n-i}\right) = 0 \tag{10}$$

where $\mathrm{v} = \omega h$, h is the step length and $A_i(\mathrm{v}),\ i = 0(1)4$ are polynomials of v.

The characteristic equation associated with (10) is given by:

$$\sum_{i=0}^{4} A_i(\mathrm{v})\,\left(\lambda^i + \lambda^{-i}\right) = 0 \tag{11}$$

where

$$
\begin{aligned}
A_0(\mathrm{v}) &= \mathrm{v}^2 \left(-90\, b_4 - 20\, b_3 + \frac{601}{24}\right)\\
A_1(\mathrm{v}) &= -1 + \mathrm{v}^2 \left(64\, b_4 + 15\, b_3 - \frac{101}{6}\right)\\
A_2(\mathrm{v}) &= 2 + \mathrm{v}^2 \left(-20\, b_4 - 6\, b_3 + \frac{109}{16}\right)\\
A_3(\mathrm{v}) &= -2 + \mathrm{v}^2\, b_3\\
A_4(\mathrm{v}) &= 1 + \mathrm{v}^2\, b_4
\end{aligned}
$$

By applying $k = 4$ in the formula (7), we have that the phase-lag is equal to:

$$
\begin{aligned}
phl &= \frac{T_0}{T_1}\\
T_0 &= 2 \left(1 + \mathrm{v}^2\, b_4\right) \cos(4\,\mathrm{v}) + 2 \left(-2 + \mathrm{v}^2\, b_3\right) \cos(3\,\mathrm{v})\\
&\quad + 2 \left(2 + \mathrm{v}^2 \left(-20\, b_4 - 6\, b_3 + \frac{109}{16}\right)\right) \cos(2\,\mathrm{v})\\
&\quad + 2 \left(-1 + \mathrm{v}^2 \left(64\, b_4 + 15\, b_3 - \frac{101}{6}\right)\right) \cos(\mathrm{v})\\
&\quad + \mathrm{v}^2 \left(-90\, b_4 - 20\, b_3 + \frac{601}{24}\right)\\
T_1 &= 10 + 32\,\mathrm{v}^2\, b_4 + 18\,\mathrm{v}^2\, b_3 + 8\,\mathrm{v}^2 \left(-20\, b_4 - 6\, b_3 + \frac{109}{16}\right)\\
&\quad + 2\,\mathrm{v}^2 \left(64\, b_4 + 15\, b_3 - \frac{101}{6}\right)
\end{aligned}
\tag{12}
$$

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

$$
\begin{aligned}
\dot{phl} = \Big(&-2400 \sin(4\,\mathrm{v})\,\mathrm{v}^2 + 5448 \sin(v)\,\mathrm{v}^2\\
&- 6324 \sin(2\,\mathrm{v})\,\mathrm{v}^2 + 3600 \sin(3\,\mathrm{v})\,\mathrm{v}^2\\
&- 8175 \sin(2\,\mathrm{v})\,\mathrm{v}^4 + 10100 \sin(\mathrm{v})\,\mathrm{v}^4\\
&- 1200\,\mathrm{v} \cos(4\,\mathrm{v}) + 2400\,\mathrm{v} \cos(3\,\mathrm{v})\\
&+ 1524\,\mathrm{v} \cos(2\,\mathrm{v}) - 8496\,\mathrm{v} \cos(\mathrm{v})\\
&- 1152 \sin(4\,\mathrm{v}) + 1728 \sin(3\,\mathrm{v})\\
&- 1152 \sin(2\,\mathrm{v}) + 288 \sin(\mathrm{v}) + 7212\,\mathrm{v}\\
&+ 576\,\mathrm{v}\, b_3 \cos(3\,\mathrm{v}) + 576\,\mathrm{v}\, b_4 \cos(4\,\mathrm{v})\\
&- 1152 \sin(4\,\mathrm{v})\,\mathrm{v}^2\, b_4 - 864 \sin(3\,\mathrm{v})\,\mathrm{v}^2\, b_3\\
&- 11520\,\mathrm{v} \cos(2\,\mathrm{v})\, b_4 - 3456\,\mathrm{v} \cos(2\,\mathrm{v})\, b_3
\end{aligned}
$$

$$
\begin{aligned}
&+ 11520 \sin(2\,\mathrm{v})\,\mathrm{v}^2\, b_4 + 3456 \sin(2\,\mathrm{v})\,\mathrm{v}^2\, b_3\\
&+ 36864\,\mathrm{v} \cos(\mathrm{v})\, b_4 + 8640\,\mathrm{v} \cos(\mathrm{v})\, b_3\\
&- 18432 \sin(\mathrm{v})\,\mathrm{v}^2\, b_4 - 4320 \sin(\mathrm{v})\,\mathrm{v}^2\, b_3\\
&- 2400 \sin(4\,\mathrm{v})\,\mathrm{v}^4\, b_4 - 1800 \sin(3\,\mathrm{v})\,\mathrm{v}^4\, b_3\\
&+ 24000 \sin(2\,\mathrm{v})\,\mathrm{v}^4\, b_4 + 7200 \sin(2\,\mathrm{v})\,\mathrm{v}^4\, b_3\\
&- 38400 \sin(\mathrm{v})\,\mathrm{v}^4\, b_4 - 9000 \sin(\mathrm{v})\,\mathrm{v}^4\, b_3\\
&\left.-25920\,\mathrm{v}\, b_4 - 5760\,\mathrm{v}\, b_3\right) \Big/\\
&\left(1440 + 6000\,\mathrm{v}^2 + 6250\,\mathrm{v}^4\right) \qquad (13)
\end{aligned}
$$

We demand that the phase-lag and its first derivative to be equal to zero and we find out that:

$$
\begin{aligned}
b_3 = \frac{1}{48} &\Big(103680 - 319680\,\mathrm{v} \sin(\mathrm{v}) - 532800 \sin(\mathrm{v})^2\\
&- 136800\,\mathrm{v}^3 \sin(\mathrm{v}) - 103680 \cos(\mathrm{v})\\
&+ 319680\,\mathrm{v} \cos(\mathrm{v}) \sin(\mathrm{v}) + 970560 \sin(\mathrm{v})^3\,\mathrm{v}\\
&+ 379840 \sin(\mathrm{v})^3\,\mathrm{v}^3 + 480960 \cos(\mathrm{v}) \sin(\mathrm{v})^2\\
&+ 828888 \sin(\mathrm{v})^4 - 449160 \sin(\mathrm{v})^6\\
&- 942888 \sin(\mathrm{v})^5\,\mathrm{v} - 719520\,\mathrm{v} \cos(\mathrm{v}) \sin(\mathrm{v})^3\\
&+ 426228 \cos(\mathrm{v}) \sin(\mathrm{v})^5\,\mathrm{v} - 31392 \cos(\mathrm{v}) \sin(\mathrm{v})^7\,\mathrm{v}\\
&+ 53568 \sin(\mathrm{v})^8 - 346605 \sin(\mathrm{v})^5\,\mathrm{v}^3\\
&+ 287136 \sin(\mathrm{v})^7\,\mathrm{v} + 95136 \sin(\mathrm{v})^6 \cos(\mathrm{v})\\
&- 555768 \cos(\mathrm{v}) \sin(\mathrm{v})^4 + 62784 \sin(\mathrm{v})^8 \cos(\mathrm{v})\\
&+106929 \sin(\mathrm{v})^7\,\mathrm{v}^3\Big) \Big(-5778 \sin(\mathrm{v})^4\\
&- 2880 \cos(\mathrm{v}) - 2880 + 7360 \sin(\mathrm{v})^2\\
&- 3178 \cos(\mathrm{v}) \sin(\mathrm{v})^4 + 5920 \cos(\mathrm{v}) \sin(\mathrm{v})^2\\
&+327 \sin(\mathrm{v})^6 \cos(\mathrm{v}) + 1356 \sin(\mathrm{v})^6\Big) \Big/\\
&\Big(\sin(\mathrm{v})^9\,\mathrm{v}^3 \Big(-136800 + 379840 \sin(\mathrm{v})^2\\
&-346605 \sin(\mathrm{v})^4 + 106929 \sin(\mathrm{v})^6\Big)\Big) \qquad (14)
\end{aligned}
$$

$$
\begin{aligned}
b_4 = \frac{1}{192} &\Big(-327 \sin(\mathrm{v})^6 + 1154 \cos(\mathrm{v}) \sin(\mathrm{v})^4\\
&+ 2334 \sin(\mathrm{v})^4 - 3440 \sin(\mathrm{v})^2\\
&-2720 \cos(\mathrm{v}) \sin(\mathrm{v})^2 + 1440 + 1440 \cos(\mathrm{v})\Big)\\
&\Big(62784 \sin(\mathrm{v})^7\,\mathrm{v} - 192000 \sin(\mathrm{v})^6\\
&+ 125568 \sin(\mathrm{v})^6 \cos(\mathrm{v}) - 291168 \sin(\mathrm{v})^5\,\mathrm{v}
\end{aligned}
$$

$$
\begin{aligned}
&+221568\cos(\mathrm{v})\sin(\mathrm{v})^5\,\mathrm{v}+106929\sin(\mathrm{v})^5\,\mathrm{v}^3\\
&+410544\sin(\mathrm{v})^4-323904\cos(\mathrm{v})\sin(\mathrm{v})^4\\
&-360720\,\mathrm{v}\cos(\mathrm{v})\sin(\mathrm{v})^3+375600\sin(\mathrm{v})^3\,\mathrm{v}\\
&-194720\sin(\mathrm{v})^3\,\mathrm{v}^3-270720\sin(\mathrm{v})^2\\
&+244800\cos(\mathrm{v})\sin(\mathrm{v})^2-146880\,\mathrm{v}\sin(\mathrm{v})\\
&+87840\,\mathrm{v}^3\sin(\mathrm{v})+146880\,\mathrm{v}\cos(\mathrm{v})\sin(\mathrm{v})\\
&+51840-51840\cos(\mathrm{v})\Big)\Big/\Big(v^3(106929\sin(\mathrm{v})^4\\
&-194720\sin(\mathrm{v})^2+87840)\sin(\mathrm{v})^9\Big) \qquad (15)
\end{aligned}
$$

For small values of |v| the formulae given by (15) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_3 =\ & \frac{173531}{181440}-\frac{58061}{1995840}\,\mathrm{v}^2\\
&+\frac{16818071}{43589145600}\,\mathrm{v}^4-\frac{155117}{3064861800}\,\mathrm{v}^6\\
&-\frac{673284671}{266765571072000}\,\mathrm{v}^8-\frac{4040637329}{21287892571545600}\,\mathrm{v}^{10}\\
&-\frac{53420333269}{3211430650793164800}\,\mathrm{v}^{12}-\frac{43018307527}{26166008845025280000}\,\mathrm{v}^{14}\\
&-\frac{14215306701522463}{84691206836587183472640000}\,\mathrm{v}^{16}\\
&-\frac{1147708651952909}{66861479081516197478400000}\,\mathrm{v}^{18}+\cdots\\
b_4 =\ & \frac{45767}{725760}+\frac{58061}{15966720}\,\mathrm{v}^2\\
&+\frac{31217597}{174356582400}\,\mathrm{v}^4+\frac{27054739}{3138418483200}\,\mathrm{v}^6\\
&+\frac{540777613}{1067062284288000}\,\mathrm{v}^8+\frac{34814241859}{851515702861824000}\,v^{10}\\
&+\frac{10243431577}{2569144520634531840}\,\mathrm{v}^{12}+\frac{42334355526431}{103408066955539906560000}\,\mathrm{v}^{14}\\
&+\frac{1296889165171339}{30796802486031703080960000}\,\mathrm{v}^{16}\\
&+\frac{8748478228936879}{2032588964078092403343360000}\,\mathrm{v}^{18}+\cdots \qquad (16)
\end{aligned}
$$

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

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

$$
\mathrm{LTE}=-\frac{58061\,h^{12}}{31933440}\left(y_n^{(12)}+2\,\omega^2\;y_n^{(10)}+\omega^4\;y_n^{(8)}\right) \qquad (17)
$$

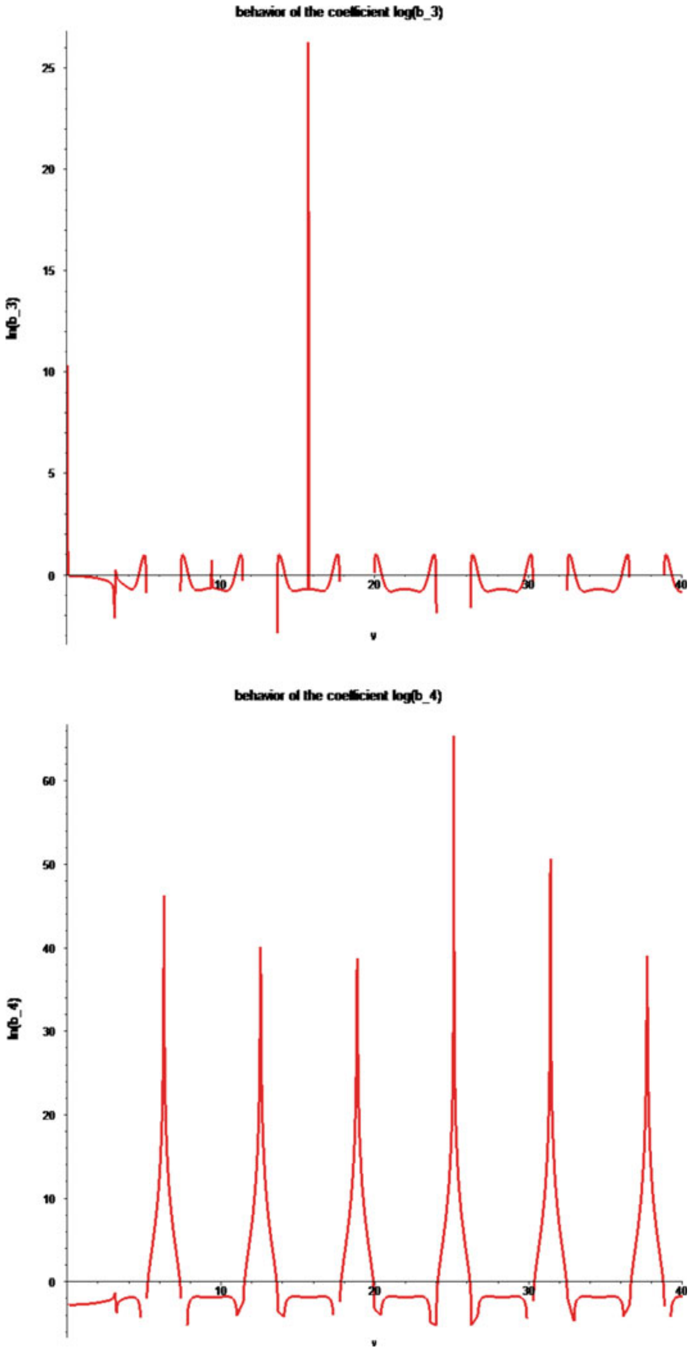

Fig. 1 Behavior of the coefficients of the new proposed method given by (15) for several values of H

5 Error analysis

We will study the following methods:

- The new proposed method of the family (mentioned as PL)
- The classical method of the family[2] (mentioned as CL)

The error analysis is based on the following steps:

- The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x)\, y(x) \tag{18}$$

- Based on the paper of Ixaru and Rizea [105], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \tag{19}$$

  where $g(x) = V(x) - V_c = g$, where V_c is the constant approximation of the potential and $G = v^2 = V_c - E$.
- We express the derivatives $y_n^{(i)}$, $i = 2, 3, 4, \cdots$, which are terms of the local truncation error formulae, in terms of the equation (18). The expressions are presented as polynomials of G.
- 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:

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

[2] Classical is called the method of the family with constant coefficients.

$$+ (V(x) - V_c + G)^2 \left(\frac{d^2}{dx^2} y(x) \right) \cdots$$

we obtain the expressions mentioned in Appendix.

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. 35 and 36.

The classical method of the family[3]

$$\text{LTE}_{\text{CL}} = h^{12} \left(-\frac{58061}{31933440} \, y(x) \, G^6 + \cdots \right) \tag{20}$$

The proposed method of the family

$$\begin{aligned} \text{LTE}_{\text{PL4}} = h^{12} \Bigg[\Bigg(& \frac{987037}{31933440} \left(\frac{d^2}{dx^2} g(x) \right) y(x) \\ & + \frac{58061}{15966720} \left(\frac{d}{dx} g(x) \right) \left(\frac{d}{dx} y(x) \right) \\ & + \frac{58061}{31933440} \, g(x)^2 \, y(x) \Bigg) G^4 + \cdots \Bigg] \end{aligned} \tag{21}$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Method of the New Family of Methods the error increases as the sixth power of G. For the Proposed Method of the New Family of Methods the error increases as the fourth power of G. So, for the numerical solution of the time independent radial Schrödinger equation the new Proposed Method of the New Family of Methods is the most accurate one, especially for large values of* $| G | = | V_c - E |$.

6 Stability analysis

We apply the new family of methods to the scalar test equation:

[3] Classical method of the family is the method of the family with constant coefficients which has the same algebraic order.

$$\phi'' = -t^2 \phi, \tag{22}$$

where $t \neq \omega$. We obtain the following difference equation:

$$\begin{aligned} A_k(s)\,\phi_{n+k} &+ \cdots + A_1(s)\,\phi_{n+1} + A_0(s)\,\phi_n + \\ &+ A_1(s)\,\phi_{n-1} + \cdots + A_k(s)\,\phi_{n-k} = 0 \end{aligned} \tag{23}$$

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

The characteristic equation associated with (23) is given by:

$$A_k(s)\,\theta^k + \cdots + A_1(s)\,\theta + A_0(s) + A_1(s)\,\theta^{-1} + \cdots + A_k(s)\,\theta^{-k} = 0 \tag{24}$$

Definition 1 (*see* [34]) A symmetric $2k$-step method with the characteristic equation given by is said to have an interval of periodicity $\left(0, s_0^2\right)$ if, for all $s \in \left(0, s_0^2\right)$, the roots z_i, $i = 1, 2$ satisfy

$$z_{1,2} = e^{\pm i\,\zeta(t\,h)},\ |z_i| \leq 1,\ i = 3, 4 \tag{25}$$

where $\zeta(t\,h)$ is a real function of $t\,h$ and $s = t\,h$.

Definition 2 (*see* [34]) 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 $(0, \infty) - S^4$ only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $H = s$.

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

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 $\mathrm{v} = s$, we have the following figure for the stability polynomials of the new developed methods. From the above diagram it is easy for one to see that the interval of periodicity of the new methods is equal to: $(0, 8.5264)$.

Remark 1 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.

From the above analysis we have the following theorem:

Theorem 3 *The method (8) with the coefficients given by (9), (14), (15), (16) is of tenth algebraic order, has the phase-lag and its first derivative equal to zero and has an interval of periodicity equals to:* $(0, 8.5264)$.

[4] Where S is a set of distinct points.

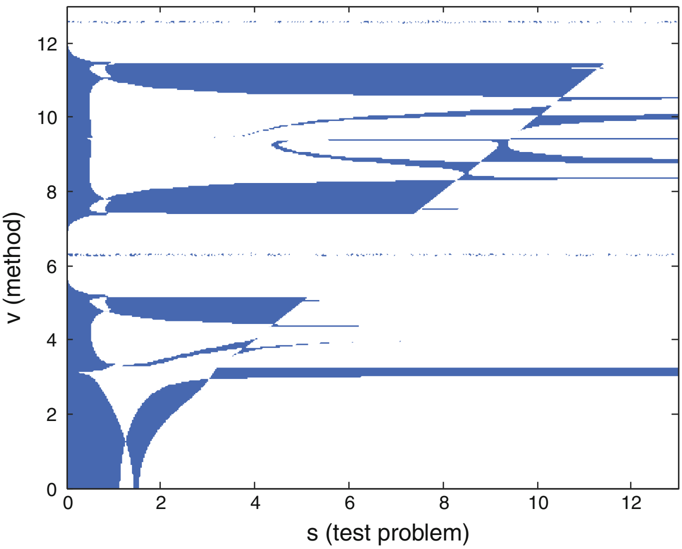

Fig. 2 $s-$v plane of the New Method produced in Sect. 4

7 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

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{26}$$

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

7.1 Woods-Saxon potential

We use the well known Woods-Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\,(1+z)^2} \tag{27}$$

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 [106]).

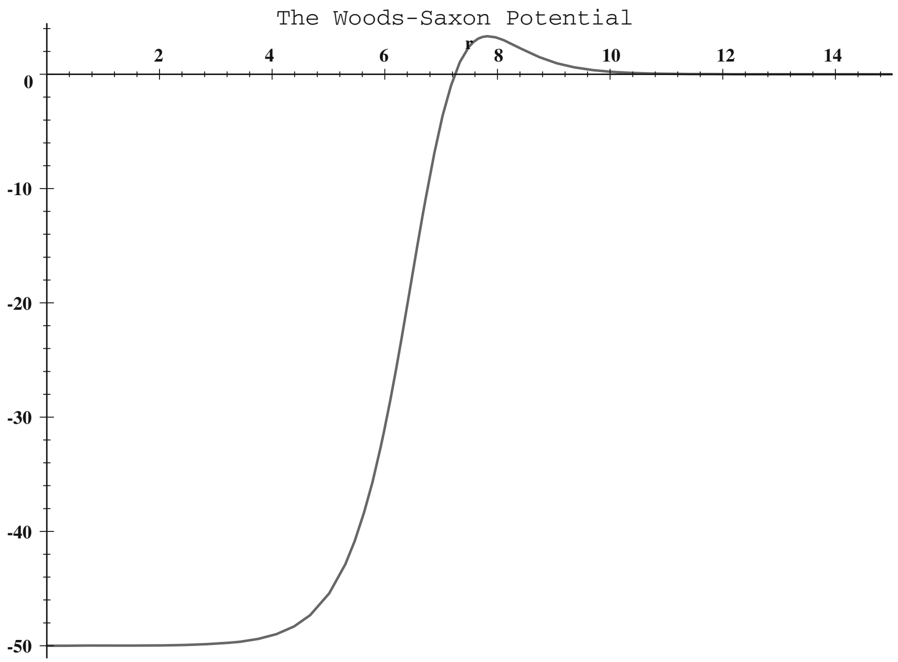

Fig. 3 The Woods-Saxon potential

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [106]):

$$v = \begin{cases} \sqrt{-50+E}, & \text{for x} \in [0, 6.5-2\text{h}], \\ \sqrt{-37.5+E}, & \text{for x} = 6.5-h \\ \sqrt{-25+E}, & \text{for x} = 6.5 \\ \sqrt{-12.5+E}, & \text{for x} = 6.5+h \\ \sqrt{E}, & \text{for x} \in [6.5+2\text{h}, 15] \end{cases} \tag{28}$$

7.2 Radial Schrödinger equation: the resonance problem

Consider the numerical solution of the radial time independent Schrödinger Eq. 1 in the well-known case of the Woods-Saxon potential (27). 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

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{29}$$

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 equation (1) (when $x \rightarrow \infty$) has the asymptotic form

$$
\begin{aligned}
y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\
&\simeq AC\left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan\delta_l \cos\left(kx - \frac{l\pi}{2}\right)\right]
\end{aligned}
\tag{30}
$$

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

$$
\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{31}
$$

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 a 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:

$$
y(0) = 0, \;\; y(x) = \cos\left(\sqrt{E}x\right) \;\text{ for large } x. \tag{32}
$$

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 [35] which is indicated as Method II.
- The Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] which is indicated as Method III.
- The Exponentially-fitted four-step method developed by Raptis [36] which is indicated as Method IV.
- The eight-step ninth algebraic order method developed by Quinlan and Tremaine [107] which is indicated as Method V.
- The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [107] which is indicated as Method VI.
- The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [107] which is indicated as Method VII.

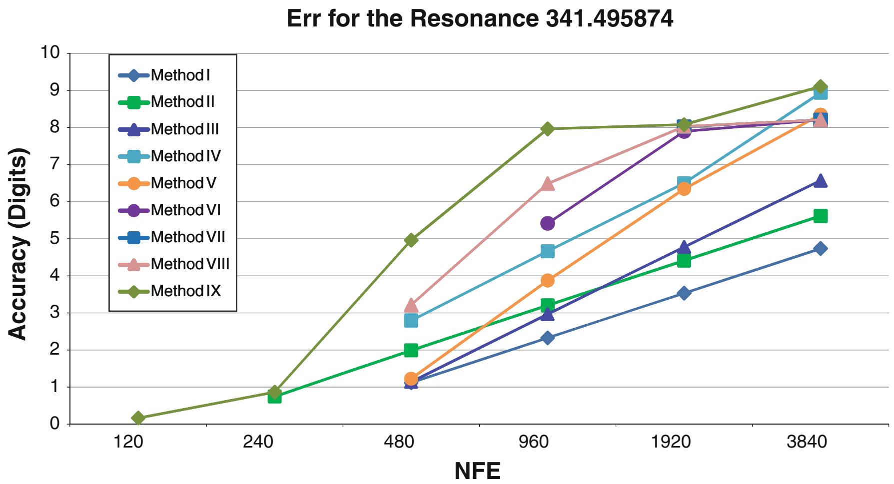

Fig. 4 Accuracy (Digits) for several values of NFE for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0

– The classical eight-step method of the family of methods mentioned in paragraph 4 which is indicated as Method VIII.
– The new developed eight-step method with phase-lag and its first derivative equal to zero obtained in paragraph 4 which is indicated as Method IX.

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

$$Err = |E_{\text{calculated}} - E_{\text{accurate}}| \tag{33}$$

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

$$\text{Err} = |E_{\text{calculated}} - E_{\text{accurate}}| \tag{34}$$

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

8 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 [35] (denoted as Method II) is more efficient than the Numerov's Method (denoted

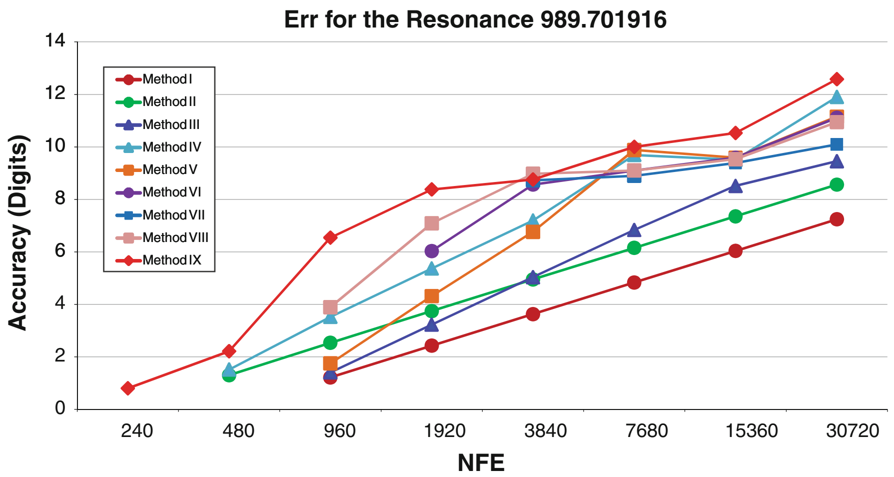

Fig. 5 Accuracy (Digits) for several values of NFE for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of NFE, Accuracy (Digits) is less than 0

Method I) and for low number of function evaluations is more efficient than the Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] (denoted as Method III).

– The Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] (denoted as Method III) is more efficient than the Exponentially-fitted two-step method developed by Raptis and Allison [35] (denoted as Method II) for high number of function evaluations.
– The Exponentially-fitted four-step method developed by Raptis [36] (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 [35] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] (denoted as Method III).
– The eight-step ninth algebraic order method developed by Quinlan and Tremaine [107] (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 [35] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] (denoted as Method III) and less efficient than the Exponentially-fitted four-step method developed by Raptis [36] (denoted as Method IV).
– The ten-step eleventh algebraic order method developed by Quinlan and Tremaine [107] (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 [35] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] (denoted as Method III) and the Exponentially-fitted four-step method developed by Raptis [36] (denoted as Method IV) for small number of function evaluations.

- The twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [107] (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 [35] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [36] (denoted as Method IV) for small number of function evaluations, the eight-step ninth algebraic order method developed by Quinlan and Tremaine [107] (denoted as Method V) for small number of function evaluations and the ten-step eleventh algebraic order method developed by Quinlan and Tremaine [107] (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 [35] (denoted as Method II) and the Exponentially-fitted two-step P-stable method developed by Kalogitatou and Simos [37] (denoted as Method III), the Exponentially-fitted four-step method developed by Raptis [36] (denoted as Method IV) for small number of function evaluations, the eight-step ninth algebraic order method developed by Quinlan and Tremaine [107] (denoted as Method V) for small number of function evaluations, the ten-step eleventh algebraic order method developed by Quinlan and Tremaine [107] (denoted as Method VI) for small number of function evaluations and the twelve-step thirteenth algebraic order method developed by Quinlan and Tremaine [107] (denoted as Method VII) for small number of function evaluations.
- The new developed method is much more efficient than all the other methods.

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

Appendix

The classical case of the family

$$
\begin{aligned}
\mathrm{LTE}_{\mathrm{CL}} = h^{12}\Bigg[& -\frac{20495533}{3193344}\left(\frac{d}{\mathrm{d}x}g(x)\right)y(x)\left(\frac{d^3}{\mathrm{d}x^3}g(x)\right)\left(\frac{d^2}{\mathrm{d}x^2}g(x)\right) \\
& -\frac{58061}{31933440}\left(\frac{d^{10}}{\mathrm{d}x^{10}}g(x)\right)y(x) \\
& -\frac{58061}{3193344}\left(\frac{d^9}{\mathrm{d}x^9}g(x)\right)\left(\frac{d}{\mathrm{d}x}y(x)\right) \\
& -\frac{290305}{236544}\left(\frac{d^2}{\mathrm{d}x^2}g(x)\right)^3 y(x)-\frac{58061}{152064}\left(\frac{d^4}{\mathrm{d}x^4}g(x)\right)^2 y(x) \\
& -\frac{43139323}{7983360}g(x)\,y(x)\left(\frac{d}{\mathrm{d}x}g(x)\right)^2\left(\frac{d^2}{\mathrm{d}x^2}g(x)\right)
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{290305}{133056}\,g(x)^2\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)\\
&-\frac{18173093}{5322240}\,g(x)^2\,y(x)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)\\
&-\frac{1335403}{399168}\,g(x)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^4}{\mathrm{d}x^4}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\\
&-\frac{4238453}{798336}\,g(x)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)\\
&-\frac{18753703}{7983360}\,g(x)\,y(x)\left(\frac{d^5}{\mathrm{d}x^5}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\\
&-\frac{754793}{181440}\,g(x)\,y(x)\left(\frac{d^4}{\mathrm{d}x^4}\,g(x)\right)\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)\\
&-\frac{58061}{114048}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)^4 y(x)-\frac{987037}{2128896}\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)y(x)\left(\frac{d^6}{\mathrm{d}x^6}\,g(x)\right)\\
&-\frac{58061}{22176}\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^4}{\mathrm{d}x^4}\,g(x)\right)\\
&-\frac{754793}{3193344}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)y(x)\left(\frac{d^7}{\mathrm{d}x^7}\,g(x)\right)\\
&-\frac{6328649}{1596672}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)^2\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)\\
&-\frac{58061}{25344}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)^2 y(x)\left(\frac{d^4}{\mathrm{d}x^4}\,g(x)\right)\\
&-\frac{1799891}{2661120}\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)y(x)\left(\frac{d^5}{\mathrm{d}x^5}\,g(x)\right)\\
&-\frac{1103159}{591360}\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^5}{\mathrm{d}x^5}\,g(x)\right)\\
&-\frac{1799891}{354816}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\mathrm{Q}_0\\
&-\frac{406427}{456192}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^6}{\mathrm{d}x^6}\,g(x)\right)\\
&-\frac{290305}{266112}\,g(x)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)^3\\
&-\frac{58061}{1064448}\,g(x)^4\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\\
&-\frac{754793}{1596672}\,g(x)^3\,y(x)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)^2-\frac{58061}{5322240}\,g(x)\,y(x)\,G^5
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{290305}{798336}\, g(x)^3 \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^3}{dx^3}\, g(x)\right) \\
&- \frac{2496623}{997920}\, g(x)\, y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)^2 \\
&- \frac{1103159}{6386688}\, g(x)^4\, y(x) \left(\frac{d^2}{dx^2}\, g(x)\right) \\
&- \frac{1335403}{15966720}\, g(x)\, y(x) \left(\frac{d^8}{dx^8}\, g(x)\right) \\
&- \frac{2148257}{3991680}\, g(x)^3\, y(x) \left(\frac{d^4}{dx^4}\, g(x)\right) - \frac{69731261}{31933440}\, g(x)^2\, y(x)\, \mathrm{Q}_0 \\
&- \frac{13876579}{31933440}\, g(x)^2\, y(x) \left(\frac{d^6}{dx^6}\, g(x)\right) \\
&- \frac{9115577}{15966720}\, g(x)^2 \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^5}{dx^5}\, g(x)\right) \\
&- \frac{58061}{249480}\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^7}{dx^7}\, g(x)\right) \\
&- \frac{58061}{31933440}\, g(x)^6\, y(x) - \frac{58061}{31933440}\, y(x)\, G^6 \\
&+ \left(-\frac{58061}{1064448} \left(\frac{d}{dx}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right)\right. \\
&\left. - \frac{1103159}{6386688} \left(\frac{d^2}{dx^2}\, g(x)\right) y(x) - \frac{58061}{2128896}\, g(x)^2\, y(x)\right) G^4 \\
&+ \left(-\frac{1103159}{1596672}\, g(x)\, y(x) \left(\frac{d^2}{dx^2}\, g(x)\right) - \frac{2148257}{3991680} \left(\frac{d^4}{dx^4}\, g(x)\right) y(x)\right. \\
&- \frac{754793}{1596672} \left(\frac{d}{dx}\, g(x)\right)^2 y(x) - \frac{58061}{1596672}\, g(x)^3\, y(x) \\
&- \frac{58061}{266112}\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d}{dx}\, g(x)\right) \\
&\left. - \frac{290305}{798336} \left(\frac{d^3}{dx^3}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right)\right) G^3 \\
&+ \left(-\frac{9115577}{15966720} \left(\frac{d^5}{dx^5}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right)\right. \\
&- \frac{290305}{133056} \left(\frac{d}{dx}\, g(x)\right) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^2}{dx^2}\, g(x)\right) \\
&- \frac{18173093}{5322240} \left(\frac{d}{dx}\, g(x)\right) y(x) \left(\frac{d^3}{dx^3}\, g(x)\right)
\end{aligned}
$$

$$
\begin{aligned}
&-\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}\, \mathrm{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)\Bigg)\, G^2 \\
&+\Bigg(-\, \frac{9115577}{7983360}\, g(x) \left(\frac{d}{dx}\, y(x)\right) \left(\frac{d^5}{dx^5}\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) \\
&-\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) \\
&-\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)\, \mathrm{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)
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{13876579}{15966720}\,g(x)\,y(x)\,\left(\frac{d^6}{dx^6}\,g(x)\right)\\
&-\frac{58061}{266112}\,g(x)^3\,\left(\frac{d}{dx}\,y(x)\right)\left(\frac{d}{dx}\,g(x)\right)\\
&-\frac{1103159}{1596672}\,g(x)^3\,y(x)\,\left(\frac{d^2}{dx^2}\,g(x)\right)\\
&-\frac{2148257}{1330560}\,g(x)^2\,y(x)\,\left(\frac{d^4}{dx^4}\,g(x)\right)\Bigg)\,G\Bigg]
\end{aligned}
\tag{35}
$$

The new proposed method of the family

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

$$+\frac{6328649}{1596672}\left(\frac{d}{\mathrm{d}x}g(x)\right)^2\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}g(x)\right)$$
$$+\frac{58061}{25344}\left(\frac{d}{\mathrm{d}x}g(x)\right)^2 y(x)\left(\frac{d^4}{\mathrm{d}x^4}g(x)\right)$$
$$+\frac{1799891}{2661120}\left(\frac{d^3}{\mathrm{d}x^3}g(x)\right)y(x)\left(\frac{d^5}{\mathrm{d}x^5}g(x)\right)$$
$$+\frac{1103159}{591360}\left(\frac{d^2}{\mathrm{d}x^2}g(x)\right)\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d^5}{\mathrm{d}x^5}g(x)\right)$$
$$+\frac{1799891}{354816}\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{\mathrm{d}x}y(x)\right)\mathrm{Q}_0$$
$$+\frac{406427}{456192}\left(\frac{d}{\mathrm{d}x}g(x)\right)\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d^6}{\mathrm{d}x^6}g(x)\right)$$
$$+\frac{290305}{266112}g(x)\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d}{\mathrm{d}x}g(x)\right)^3$$
$$+\frac{58061}{1064448}g(x)^4\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d}{\mathrm{d}x}g(x)\right)$$
$$+\frac{754793}{1596672}g(x)^3 y(x)\left(\frac{d}{\mathrm{d}x}g(x)\right)^2$$
$$+\frac{290305}{798336}g(x)^3\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}g(x)\right)$$
$$+\frac{2496623}{997920}g(x)\,y(x)\left(\frac{d^3}{\mathrm{d}x^3}g(x)\right)^2$$
$$+\frac{1103159}{6386688}g(x)^4 y(x)\left(\frac{d^2}{\mathrm{d}x^2}g(x)\right)$$
$$+\frac{1335403}{15966720}g(x)\,y(x)\left(\frac{d^8}{\mathrm{d}x^8}g(x)\right)$$
$$+\frac{2148257}{3991680}g(x)^3 y(x)\left(\frac{d^4}{\mathrm{d}x^4}g(x)\right)$$
$$+\frac{69731261}{31933440}g(x)^2 y(x)\,\mathrm{Q}_0$$
$$+\frac{13876579}{31933440}g(x)^2 y(x)\left(\frac{d^6}{\mathrm{d}x^6}g(x)\right)$$
$$+\frac{9115577}{15966720}g(x)^2\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d^5}{\mathrm{d}x^5}g(x)\right)$$
$$+\frac{58061}{249480}g(x)\left(\frac{d}{\mathrm{d}x}y(x)\right)\left(\frac{d^7}{\mathrm{d}x^7}g(x)\right)$$

$$
\begin{aligned}
&+\frac{58061}{31933440}\, g(x)^6\, y(x)\\
&+\left(\frac{987037}{31933440}\left(\frac{d^2}{\mathrm{d}x^2}\, g(x)\right) y(x)+\frac{58061}{15966720}\left(\frac{d}{\mathrm{d}x}\, g(x)\right)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\right.\\
&\left.+\frac{58061}{31933440}\, g(x)^2\, y(x)\right) G^4\\
&+\left(\frac{1799891}{7983360}\, g(x)\, y(x)\left(\frac{d^2}{\mathrm{d}x^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}{\mathrm{d}x}\, g(x)\right)^2 y(x)\\
&+\frac{58061}{498960}\left(\frac{d^3}{\mathrm{d}x^3}\, g(x)\right)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\\
&\left.+\frac{58061}{1330560}\, g(x)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\left(\frac{d}{\mathrm{d}x}\, g(x)\right)\right) G^3\\
&+\left(\frac{987037}{1330560}\, g(x)\, y(x)\left(\frac{d}{\mathrm{d}x}\, g(x)\right)^2\right.\\
&+\frac{58061}{443520}\, g(x)^2\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\left(\frac{d}{\mathrm{d}x}\, g(x)\right)\\
&+\frac{17824727}{7983360}\left(\frac{d}{dx}\, g(x)\right) y(x)\left(\frac{d^3}{\mathrm{d}x^3}\, g(x)\right)\\
&+\frac{1103159}{1995840}\, g(x)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}\, g(x)\right)\\
&+\frac{1103159}{997920}\left(\frac{d}{\mathrm{d}x}\, g(x)\right)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\left(\frac{d^2}{\mathrm{d}x^2}\, g(x)\right)\\
&+\frac{58061}{57024}\, g(x)\, y(x)\left(\frac{d^4}{\mathrm{d}x^4}\, g(x)\right)+\frac{4238453}{7983360}\, g(x)^2\, y(x)\left(\frac{d^2}{\mathrm{d}x^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}{\mathrm{d}x^6}\, g(x)\right) y(x)\\
&\left.+\frac{406427}{1140480}\left(\frac{d^5}{\mathrm{d}x^5}\, g(x)\right)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\right) G^2\\
&+\left(\frac{3425599}{798336}\left(\frac{d^2}{\mathrm{d}x^2}\, g(x)\right)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}\, g(x)\right)\right.\\
&+\frac{58061}{18144}\, g(x)\left(\frac{d}{\mathrm{d}x}\, y(x)\right)\left(\frac{d}{\mathrm{d}x}\, g(x)\right)\left(\frac{d^2}{\mathrm{d}x^2}\, g(x)\right)
\end{aligned}
$$

$$+\frac{58061}{10368}\,g(x)\,y(x)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)$$
$$+\frac{1103159}{241920}\left(\frac{d}{dx}\,g(x)\right)^2 y(x)\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)$$
$$+\frac{2148257}{798336}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^4}{\mathrm{d}x^4}\,g(x)\right)$$
$$+\frac{5631917}{2661120}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)y(x)\left(\frac{d^5}{\mathrm{d}x^5}\,g(x)\right)$$
$$+\frac{30365903}{7983360}\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)y(x)\left(\frac{d^4}{\mathrm{d}x^4}\,g(x)\right)$$
$$+\frac{58061}{72576}\,g(x)^2\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)$$
$$+\frac{58061}{399168}\,g(x)^3\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)$$
$$+\frac{58061}{114048}\,g(x)^3\,y(x)\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)$$
$$+\frac{1683769}{1596672}\,g(x)^2\,y(x)\left(\frac{d}{\mathrm{d}x}\,g(x)\right)^2$$
$$+\frac{10392919}{7983360}\,g(x)^2\,y(x)\left(\frac{d^4}{\mathrm{d}x^4}\,g(x)\right)$$
$$+\frac{58061}{16128}\,g(x)\,y(x)\,\mathrm{Q}_0$$
$$+\frac{58061}{76032}\,g(x)\,y(x)\left(\frac{d^6}{\mathrm{d}x^6}\,g(x)\right)$$
$$+\frac{58061}{63360}\,g(x)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\left(\frac{d^5}{\mathrm{d}x^5}\,g(x)\right)$$
$$+\frac{58061}{7983360}\,g(x)^5\,y(x)$$
$$+\frac{4586819}{1995840}\left(\frac{d^3}{\mathrm{d}x^3}\,g(x)\right)^2 y(x)+\frac{58061}{72576}\left(\frac{d}{\mathrm{d}x}\,g(x)\right)^3\left(\frac{d}{\mathrm{d}x}\,y(x)\right)$$
$$+\frac{58061}{725760}\left(\frac{d^8}{\mathrm{d}x^8}\,g(x)\right)y(x)$$
$$+\frac{58061}{285120}\left(\frac{d^7}{\mathrm{d}x^7}\,g(x)\right)\left(\frac{d}{\mathrm{d}x}\,y(x)\right)\Bigg)\,G\Bigg] \qquad (36)$$

where $\mathrm{Q}_0=\left(\frac{d^2}{\mathrm{d}x^2}\,g(x)\right)^2$

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