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ORIGINAL PAPER

High order four-step hybrid method with vanished phase-lag and its derivatives for the approximate solution of the Schrödinger equation

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Abstract In this paper, we develop a new four-step hybrid method of sixth algebraic order with vanished phase-lag and its first and second derivatives. For the obtained method we study:

– its error and
– its stability

We apply the produced method to the Schrödinger equation in order to show its efficiency.

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

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1 Introduction

In this paper, we study the numerical solution of the one-dimensional time independent Schrödinger equation which can written as a boundary value problem with the following form:

$$q''(r) = \left[l(l+1)/r^2 + V(r) - k^2\right] q(r). \tag{1}$$

In applied sciences, there are many scientific areas for which the mathematical models of their problems can be written with the above mentioned boundary value problem. Some scientific areas are:

- astronomy,
- astrophysics,
- quantum mechanics,
- quantum chemistry,
- celestial mechanics,
- electronics
- physical chemistry
- chemical physics etc

(see for example [1–4])

For the above model (1), we give the following definitions:

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

The boundary conditions are:

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

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

In the last decades, much research has been done on the construction of efficient, fast and reliable algorithms for the approximate solution of the radial Schrödinger equation and related problems (see for example [5–105]). In the following, we mention some bibliography:

- Phase-fitted methods and numerical methods with minimal phase-lag of Runge-Kutta and Runge-Kutta Nyström type have been obtained in [5–11].
- In [12–17] exponentially and trigonometrically fitted Runge-Kutta and Runge-Kutta Nyström methods are constructed.
- Multistep phase-fitted methods and multistep methods with minimal phase-lag are obtained in [23–50].
- Symplectic integrators are investigated in [51–77].

– Exponentially and trigonometrically multistep methods have been produced in [78–98].
– Nonlinear methods have been studied in [99] and [100]
– Review papers have been presented in [101–105]
– Special issues and Symposia in International Conferences have been developed on this subject (see [106–112])

In this paper, we study a two-stage four-step hybrid sixth algebraic order method. More specifically, we study the effect of the vanishing of the phase-lag and its first and second derivatives on the efficiency of the obtained numerical scheme.

It is noted that the produced methods via the above procedure, are very effective on any problem with:

– periodic or
– oscillating solutions or
– solution which contains the functions cos and sin or
– solution that is a combination of the functions cos and sin.

More specifically, the aim of this paper is the calculation of the coefficients of the introduced hybrid two-stage four-step method in order to have:

– the the highest possible algebraic order
– the phase-lag vanished
– the first derivative of the phase-lag vanished as well
– the second derivative of the phase-lag vanished as well

The direct formula for the determination of the phase-lag for $2m$-method (see [29] and [26]) is used for the computation of the phase-lag and its first and second derivatives.

The investigation of the effectiveness of the new obtained scheme will be based on

– the investigation of the local truncation error of the new produced method and
– the study of the stability analysis of the new obtained method.
– the application of the new developed method to the resonance problem of the radial time independent Schrödinger equation. This is one of the most difficult problems arising from the radial Schrödinger equation.

The format of the paper is given below:

– The phase-lag analysis of symmetric $2k$-methods is developed in Sect. 2
– In Sect. 3, we obtain the new hybrid two-stage four-step method.
– The error analysis is presented in Sect. 4.
– In Sect. 5, the stability properties of the new produced method are studied.
– In Sect. 6, the numerical results are presented.
– Finally, in Sect. 7, remarks and conclusions are mentioned.

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

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

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

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

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

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

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

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

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

Theorem 1 [26] *and* [29] *The symmetric* $2k$*-step method with characteristic equation given by (6) has phase-lag order* q *and phase-lag constant* c *given by:*

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

The formula mentioned in the above theorem is a direct method for the computation of the phase-lag of any symmetric $2k$- step method.

3 Development of the new method

Let us consider the following family of hybrid (Runge-Kutta type) symmetric four-step methods for the numerical solution of problems of the form $q'' = f\,(x, q)$:

$$\begin{aligned} \hat{q}_{n+2} &= 2\, q_{n+1} - 2\, q_n + 2\, q_{n-1} - q_{n-2} + \frac{h^2}{6}\left(7\, f_{n+1} - 2\, f_n + 7\, y_{n-1}\right) \\ &q_{n+2} - 2\, q_{n+1} + 2\, q_n - 2\, q_{n-1} + q_{n-2} \\ &= h^2\left[b_0\, \left(\hat{f}_{n+2} + f_{n-2}\right) + b_1\, \left(f_{n+1} + f_{n-1}\right) + b_2\, f_n\right] \end{aligned} \tag{8}$$

In the above general form :

1. the coefficient b_0, b_1, b_2 are free parameters,
2. h is the step size of the integration ,

3. n is the number of steps,
4. q_n is the approximation of the solution on the point x_n
5. $f_n = f\,(x_n, q_n)$
6. $x_n = x_0 + n\,h$ and
7. x_0 is the initial value point.

Application of the method (8) to the scalar test equation (4) leads to the difference equation (5) with $k = 1$ and $A_j\,(v)\ ,\ \ j = 0, 1$ given by:

$$A_2\,(v) = 1,\ A_1\,(v) = -2 + v^2\left(b_0\left(2 - 7/6\,v^2\right) + b_1\right)$$
$$A_0\,(v) = 2 - 2\,b_0 v^2 + 1\Big/3\,v^4 b_0 + v^2 b_2 \tag{9}$$

We require the above mentioned method to have the phase-lag and its first and second derivatives vanished. Using the formulae (7) (for $k = 1$) and (9), the following equation is obtained:

$$\text{Phase} - \text{Lag} \ = \ -\frac{S_0}{D_0} = 0 \tag{10}$$

where

$$\begin{aligned} S_0 = {} & 12\ (\cos\,(v))^2 - 12\,\cos\,(v) + 12\,\cos\,(v)\,b_0 v^2 - 7\,\cos\,(v)\,v^4 b_0 \\ & +6\,\cos\,(v)\,v^2 b_1 - 6\,b_0 v^2 + v^4 b_0 + 3\,v^2 b_2 \\ \mathrm{D}_0 = {} & -12 - 12\,b_0 v^2 + 7\,v^4 b_0 - 6\,v^2 b_1 \end{aligned}$$

Requiring now the method to have the first derivative of the phase-lag vanished as well, the following equation is obtained:

$$\text{First Derivative of the Phase} - \text{Lag} \ = \ \frac{S_1}{D_0^2} = 0 \tag{11}$$

where

$$\begin{aligned} S_1 = {} & 84\,\sin\,(v)\,v^6 b_0 b_1 - 288\,\cos\,(v)\,\sin\,(v)\,b_0 v^2 + 168\,\cos\,(v)\,\sin\,(v)\,v^4 b_0 \\ & -144\,\cos\,(v)\,\sin\,(v)\,v^2 b_1 - 144\,\sin\,(v)\,b_0 v^4 b_1 - 144\,b_0 v + 48\,v^3 b_0 \\ & +72\,v\,b_2 - 288\,\sin\,(v)\,\cos\,(v) - 60\,{b_0}^2 v^5 + 576\,\cos\,(v)\,b_0 v - 672\,\cos\,(v)\,v^3 b_0 \\ & +288\,\cos\,(v)\,v\,b_1 - 144\,\sin\,(v)\,{b_0}^2 v^4 + 168\,\sin\,(v)\,{b_0}^2 v^6 - 49\,\sin\,(v)\,v^8 {b_0}^2 \\ & -36\,\sin\,(v)\,v^4 {b_1}^2 + 12\,v^5 b_0 b_1 + 42\,v^5 b_2 b_0 - 288\,v\,(\cos\,(v))^2\,b_0 \\ & +336\,(\cos\,(v))^2\,b_0 v^3 - 144\,v\,(\cos\,(v))^2\,b_1 + 144\,\sin\,(v) \end{aligned}$$

Finally, demanding for the new obtained method the second derivative of the phase-lag to be vanished as well, the following equation is obtained:

$$\text{Second Derivative of the Phase} - \text{Lag} \ = \ \frac{S_2}{D_0^3} = 0 \tag{12}$$

where

$$
\begin{aligned}
S_2 = {} & -3456 - 8064\,(\cos(v))^2\,v^4 b_0 - 252\,{b_0}^2 v^8 b_1 \\
& +216\,v^6 {b_0}^2 b_1 - 72\,b_0 v^6 {b_1}^2 - 504\,b_2 v^6 {b_0}^2 - 882\,b_2 v^8 {b_0}^2 \\
& +6912\,(\cos(v))^2\,v^2 b_1 + 25056\,(\cos(v))^2\,{b_0}^2 v^4 - 19824\,(\cos(v))^2\,v^6 {b_0}^2 \\
& +2352\,(\cos(v))^2\,v^8 {b_0}^2 + 1728\,(\cos(v))^2\,v^4 {b_1}^2 + 588\cos(v)\,v^8 {b_0}^2 \\
& -3024\cos(v)\,{b_0}^3 v^8 + 432\cos(v)\,v^4 {b_1}^2 + 1728\cos(v)\,{b_0}^3 v^6 + 13824\sin(v)\,{b_0}^2 v^3 \\
& +3456\,(\cos(v))^2\,b_0 - 8640\,b_0 v^2 + 4032\,v^4 b_0 - 3456\,v^2 b_1 - 6912\cos(v)\,b_0 \\
& +1728\,b_0 + 6912\,(\cos(v))^2 + 1764\cos(v)\,{b_0}^3 v^{10} - 24192\sin(v)\,{b_0}^2 v^5 \\
& -343\cos(v)\,v^{12} {b_0}^3 + 216\cos(v)\,v^6 {b_1}^3 + 9408\sin(v)\,v^7 {b_0}^2 + 3456\sin(v)\,v^3 {b_1}^2 \\
& -10368\,(\cos(v))^2\,{b_0}^2 v^2 + 1728\,(\cos(v))^2\,b_0 v^2 - 2592\,v^2\,(\cos(v))^2\,{b_1}^2 \\
& +20736\cos(v)\,{b_0}^2 v^2 + 24192\cos(v)\sin(v)\,{b_0}^2 v^5 - 9408\cos(v)\sin(v)\,{b_0}^2 v^7 \\
& -13824\cos(v)\sin(v)\,{b_0}^2 v^3 - 3456\cos(v)\sin(v)\,{b_1}^2 v^3 - 34560\cos(v)\,{b_0}^2 v^4 \\
& +21504\cos(v)\,v^6 {b_0}^2 + 5184\cos(v)\,v^2 {b_1}^2 + 16128\cos(v)\sin(v)\,b_0 v^3 \\
& -13824\,v\cos(v)\sin(v)\,b_0 - 6912\,v\cos(v)\sin(v)\,b_1 - 10368\,(\cos(v))^2\,b_0 v^2 b_1 \\
& -16416\cos(v)\,v^4 b_0 b_1 + 20736\cos(v)\,b_0 v^2 b_1 + 15984\,(\cos(v))^2\,v^4 b_0 b_1 \\
& -4032\,(\cos(v))^2\,v^6 b_0 b_1 + 1008\cos(v)\,v^4 b_0 + 22464\cos(v)\,b_0 v^2 \\
& -1008\cos(v)\,v^6 b_0 b_1 + 2592\cos(v)\,{b_0}^2 v^6 b_1 - 3024\cos(v)\,{b_0}^2 v^8 b_1 \\
& +1296\cos(v)\,b_0 v^6 {b_1}^2 + 13824\sin(v)\,b_0 v^3 b_1 + 882\cos(v)\,v^{10} {b_0}^2 b_1 \\
& -756\cos(v)\,v^8 b_0 {b_1}^2 - 16128\sin(v)\,b_0 v^3 - 5184\,{b_0}^2 v^2 + 7776\,{b_0}^2 v^4 \\
& -12096\sin(v)\,v^5 b_0 b_1 - 864\cos(v)\,v^2 b_1 - 2592\,b_0 v^2 b_1 + 12096\cos(v)\sin(v)\,b_0 v^5 b_1 \\
& -13824\cos(v)\sin(v)\,b_0 v^3 b_1 - 3888\,v^4 b_0 b_1 + 2592\,v^2 b_2 b_0 \\
& -6048\,v^4 b_2 b_0 + 1296\,v^2 b_2 b_1 - 3456\cos(v)\,b_1 - 864\,v^4 {b_1}^2 \\
& +13824\sin(v)\,b_0 v + 6912\sin(v)\,v b_1 - 252\,b_2 v^6 b_0 b_1 + 2016\,v^6 b_0 b_1 \\
& -864\,b_2 - 1728\cos(v) + 720\,v^6 {b_0}^3 + 1260\,v^8 {b_0}^3 + 1728\,(\cos(v))^2\,b_1 \\
& +2352\,v^6 {b_0}^2 - 1176\,{b_0}^2 v^8
\end{aligned}
$$

We demand now the coefficients of the new proposed method to satisfy the Eqs. (10–12). Therefore, the following coefficients of the new developed method are obtained:

$$b_0 = \frac{S_3}{D_1},\ b_1 = \frac{S_4}{D_1},\ b_2 = \frac{S_5}{D_1} \tag{13}$$

where:

$$
\begin{aligned}
S_3 = {} & -6\,v^2 \sin(3\,v) + 18\,\sin(v)\,v^2 + 42\cos(v)\,v - 18\,v\cos(3\,v) - 36\,v \\
& +12\,v\cos(2\,v) + 18\,\sin(3\,v) + 18\,\sin(v) - 36\,\sin(2\,v) \\
S_4 = {} & -36\,\sin(v) + 200\,v - 284\cos(v)\,v - 77\,\sin(v)\,v^2 - 84\,v^3 + 109\cos(v)\,v^3 \\
& -36\,\sin(3\,v) + 72\,\sin(2\,v) - 20\,v\cos(3\,v) + 104\,v\cos(2\,v) - 7\,v^4 \sin(3\,v) \\
& +21\,v^4 \sin(v) + 20\,v^3 \cos(2\,v) - 9\,v^2 \sin(3\,v) - 21\,v^3 \cos(3\,v) - 8\,v^2 \sin(2\,v)
\end{aligned}
$$

$$
\begin{aligned}
S_5 = {} & 128\,v + 36\,\sin(v) - 9\,v^3 - 300\,\cos(v)\,v + 12\,\sin(v)\,v^2 - 12\,\cos(v)\,v^3 \\
& -36\,v^2\sin(3\,v) - 164\,v\cos(3\,v) + 280\,v\cos(2\,v) + 36\,\sin(3\,v) - 6\,v^4\sin(v) \\
& +2\,v^4\sin(3\,v) - 32\,v^3\cos(2\,v) + 12\,v^3\cos(3\,v) + 98\,v^2\sin(2\,v) \\
& -7\,v^3\cos(4\,v) + 35\,v^2\sin(4\,v) + 56\,v\cos(4\,v) - 72\,\sin(2\,v) \\
D_1 = {} & -21\,v^5 + 7\,v^5\cos(2\,v) + 2\,v^5\cos(v) - 2\,v^4\sin(v) + 7\,v^4\sin(2\,v)
\end{aligned}
$$

For some values of $|\omega|$ the formulae given by (13) are subject to heavy cancellations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_0 = {} & \frac{3}{40} - \frac{751}{100800}\,v^2 + \frac{769}{4032000}\,v^4 - \frac{28543}{111767040000}\,v^6 \\
& + \frac{91697083}{174356582400000}\,v^8 + \frac{590544631}{11266117632000000}\,v^{10} \\
& + \frac{1243181826013}{298777439600640000000}\,v^{12} \\
& + \frac{4000700646135199}{1748445576542945280000000000}\,v^{14} \\
& + \frac{20035252700556811}{6294404075554603008000000000}\,v^{16} + \cdots \\
b_1 = {} & \frac{13}{15} + \frac{751}{25200}\,v^2 - \frac{8279}{1008000}\,v^4 + \frac{3086213}{27941760000}\,v^6 \\
& - \frac{322337753}{43589145600000}\,v^8 + \frac{7747502327}{36614882304000000}\,v^{10} \\
& + \frac{4147625909617}{74694359900160000000}\,v^{12} \\
& + \frac{10188357732421097}{14570379804524544000000000}\,v^{14} \\
& + \frac{987246637890099799}{15736010188886507520000000000}\,v^{16} + \cdots \\
b_2 = {} & \frac{7}{60} - \frac{751}{16800}\,v^2 + \frac{4621}{288000}\,v^4 - \frac{151101109}{55883520000}\,v^6 \\
& + \frac{12217462729}{87178291200000}\,v^8 - \frac{54378448079}{8136640512000000}\,v^{10} \\
& + \frac{25139050848319}{1493887198003200000000}\,v^{12} \\
& + \frac{40778649070486037}{87422278827147264000000000}\,v^{14} \\
& + \frac{195605063295660329}{18512953163395891200000000000}\,v^{16} + \cdots
\end{aligned}
\tag{14}
$$

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

The local truncation error of the new proposed method (mentioned as $NewMeth$) is given by:

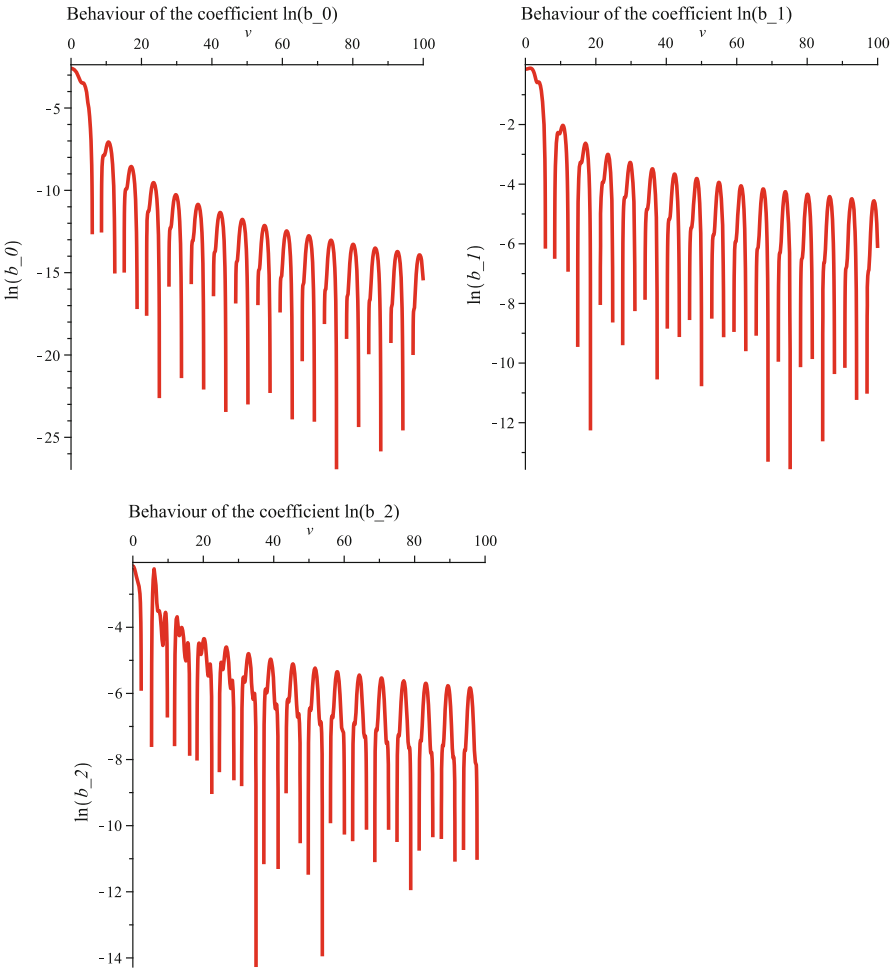

Fig. 1 Behavior of the coefficients of the new proposed method given by (13) for several values of $v = \omega h$

$$LTE_{NewMeth} = -\frac{751\,h^8}{302400}\left(q_n^{(8)} + 3\,\omega^2\,q_n^{(6)} + 3\,\omega^4\,q_n^{(4)} + \omega^6\,q_n^{(2)}\right) + O\left(h^{10}\right) \tag{15}$$

4 Comparative error analysis

We will study the following methods:

4.1 Classical method (i.e. the method (8) with constant coefficients)

$$LTE_{CL} = -\frac{751\,h^8}{302400}\,q_n^{(8)} + O\left(h^{10}\right) \tag{16}$$

4.2 The new proposed method with vanished phase-lag and its first and second derivatives

$$LTE_{NewMeth} = -\frac{751\,h^8}{302400}\left(q_n^{(8)} + 3\,\omega^2\,q_n^{(6)} + 3\,\omega^4\,q_n^{(4)} + \omega^6\,q_n^{(2)}\right) + O\left(h^{10}\right) \quad (17)$$

The following procedure is applied :

– The one-dimensional time independent Schrödinger equation can be written as:

$$q''(x) = f(x)\,q(x) \quad (18)$$

– Based on the paper of Ixaru and Rizea [78], the function $f(x)$ can be written in the form:

$$f(x) = g(x) + G \quad (19)$$

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

– We express the derivatives $q_n^{(i)}$, $i = 2, 3, 4, \ldots$, which are terms of the local truncation error formulae, in terms of the Eq. (19). 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

Using the procedure mentioned above and the formulae:

$$\begin{aligned}
q_n^{(2)} &= (V(x) - V_c + G)\,q(x)\\
q_n^{(4)} &= \left(\frac{d^2}{dx^2}V(x)\right)q(x) + 2\left(\frac{d}{dx}V(x)\right)\left(\frac{d}{dx}q(x)\right)\\
&\quad + (V(x) - V_c + G)\left(\frac{d^2}{dx^2}q(x)\right)\\
q_n^{(6)} &= \left(\frac{d^4}{dx^4}V(x)\right)q(x) + 4\left(\frac{d^3}{dx^3}V(x)\right)\left(\frac{d}{dx}q(x)\right)\\
&\quad + 3\left(\frac{d^2}{dx^2}V(x)\right)\left(\frac{d^2}{dx^2}q(x)\right) + 4\left(\frac{d}{dx}V(x)\right)^2 q(x)\\
&\quad + 6\,(V(x) - V_c + G)\left(\frac{d}{dx}V(x)\right)\left(\frac{d}{dx}q(x)\right)\\
&\quad + 4\,(V(x) - V_c + G)\,q(x)\left(\frac{d^2}{dx^2}V(x)\right)\\
&\quad + (V(x) - V_c + G)^2\left(\frac{d^2}{dx^2}q(x)\right)\ldots
\end{aligned} \quad (20)$$

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

we obtain the expressions of the Local Truncation Errors. For the methods mentioned above the expression can be found in the Appendix.

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

1. The Energy is close to the potential, i.e., $G = V_c - E \approx 0$. Consequently, the free terms of the polynomials in G are considered only. 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 methods with vanished the phase-lag and its derivatives.
2. $G >> 0$ or $G << 0$. Then $|G|$ is a large number.

Therefore, we have the following asymptotic expansions of the Local Truncation Errors:

4.3 Classical method

$$
LTE_{CL} = h^8\left(\frac{751}{302400}\,q\left(x\right)\,G^4 + \cdots\right) + O\left(h^{10}\right) \tag{21}
$$

4.4 The new proposed method with vanished phase-lag and its first and second derivatives

$$
LTE_{NewMeth} = h^8\left[\left(\frac{751}{75600}\,\left(\frac{d^2}{dx^2}g\left(x\right)\right)\,q\left(x\right)\right)G^2 + \cdots\right] + O\left(h^{10}\right) \tag{22}
$$

From the above equations we have the following theorem:

Theorem 2 *For the Classical Hybrid Four-Step Method the error increases as the fourth power of G. For the New Obtained Method with Vanished Phase-Lag and its First and Second Derivatives, the error increases as the second power of G. So, for the numerical solution of the time independent radial Schrödinger equation the New Proposed Method with Vanished Phase-Lag and its First and Second Derivatives is much more efficient, especially for large values of* $|G| = |V_c - E|$.

5 Stability analysis

Let us apply the new obtained method to the scalar test equation:

$$q'' = -z^2 q, \tag{23}$$

We note that $z \neq \omega$. Thus, we obtain the following difference equation:

$$A_2(s,v)\ (q_{n+2} + q_{n-2}) + A_1(s,v)\ (q_{n+1} + q_{n-1}) + A_0(s,v)\ q_n = 0 \tag{24}$$

where

$$A_2(s,v) = 1,\quad A_1(s,v) = 2\frac{S_6}{D_2},\quad A_0(s,v) = 2\frac{S_7}{D_2} \tag{25}$$

where

$$\begin{aligned}
S_6 = {} & -v^5\cos(v) + v^4\sin(v) - 4s^2v^2\sin(v)\cos(v) + 14v^5 + 14s^4v \\
& -26s^2v^3 - 5\sin(v)v^2s^2 - 8\cos(v)vs^2 + 7s^2v^4\sin(v) + 43s^2\cos(v)v^3 \\
& -7s^4\sin(v)v^2 - 28s^4\cos(v)v - 7v^4\sin(v)\cos(v) + 21s^4\sin(v)\cos(v) \\
& -7(\cos(v))^2v^5 - 21\sin(v)(\cos(v))^2v^2s^2 \\
& +7\sin(v)(\cos(v))^2s^4v^2 - 7\sin(v)(\cos(v))^2s^2v^4 \\
& -21(\cos(v))^3s^2v^3 + 21(\cos(v))^3s^4v - 56(\cos(v))^3vs^2 \\
& +64(\cos(v))^2vs^2 - 7(\cos(v))^2s^4v + 10(\cos(v))^2s^2v^3 \\
& -21\sin(v)(\cos(v))^2s^4 \\
S_7 = {} & v^5\cos(v) - v^4\sin(v) + 14s^2v^2\sin(v)\cos(v) - 14v^5 \\
& -14(\cos(v))^4s^2v^3 + 112(\cos(v))^4vs^2 \\
& +70\sin(v)(\cos(v))^3v^2s^2 - 4s^4v + 4s^2v^3 - 2s^2v^4\sin(v) \\
& -12s^2\cos(v)v^3 + 2s^4\sin(v)v^2 + 8s^4\cos(v)v + 7v^4\sin(v)\cos(v) \\
& -6s^4\sin(v)\cos(v) + 7(\cos(v))^2v^5 - 24\sin(v)(\cos(v))^2v^2s^2 \\
& -2\sin(v)(\cos(v))^2s^4v^2 + 2\sin(v)(\cos(v))^2s^2v^4 \\
& +12(\cos(v))^3s^2v^3 - 6(\cos(v))^3s^4v - 128(\cos(v))^3vs^2 \\
& +16(\cos(v))^2vs^2 + 2(\cos(v))^2s^4v \\
& -2(\cos(v))^2s^2v^3 + 6\sin(v)(\cos(v))^2s^4 \\
D_2 = {} & v^4\left(-\sin(v) + 7\sin(v)\cos(v) - 14v + 7v(\cos(v))^2 + \cos(v)v\right)
\end{aligned}$$

and $s = z\,h$.

The corresponding characteristic equation is given by:

$$A_2(s,v)\left(\lambda^4+1\right)+A_1(s,v)\left(\lambda^3+\lambda\right)+A_0(s,v)\,\lambda^2=0 \tag{26}$$

Definition 1 (see [18]) A symmetric $2k$-step method with the characteristic equation given by (6) is said to have an *interval of periodicity* $\left(0, v_0^2\right)$ if, for all $s \in \left(0, s_0^2\right)$, the roots λ_i, $i = 1(1)4$ satisfy

$$\lambda_{1,2} = e^{\pm i\,\zeta(s)},\ |\lambda_i| \leq 1,\ i = 3, 4, \ldots \tag{27}$$

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

Definition 2 (see [18]) 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 $(0, \infty) - S$[1] only when the frequency of the phase fitting is the same as the frequency of the scalar test equation, i.e. $s = v$.

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.

Remark 1 For the solution of the Schrödinger equation the frequency of the phase fitting is equal to the frequency of the scalar test equation. So, for this case of problems it is necessary to observe **the surroundings of the first diagonal of the $s - v$ plane**.

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 $s = v$ (i.e. see the surroundings of the first diagonal of the $s - v$ plane), it is easy to see that the interval of periodicity of the new method developed in Sect. 3 is equal to: (0, 36.83054610).

From the above analysis we have the following theorem:

Theorem 3 *The method developed in Sect. 3 is of eighth algebraic order, has the phase-lag and its first and second derivatives equal to zero and has an interval of periodicity equals to:* (0, 36.83054610).

6 Numerical results

The efficiency of the application of the new obtained method to the radial time-independent Schrödinger equation (1) is studied in this section.

The new developed method belongs to the category of the frequency dependent methods. Therefore, the determination of the value of parameter ω is needed in order

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

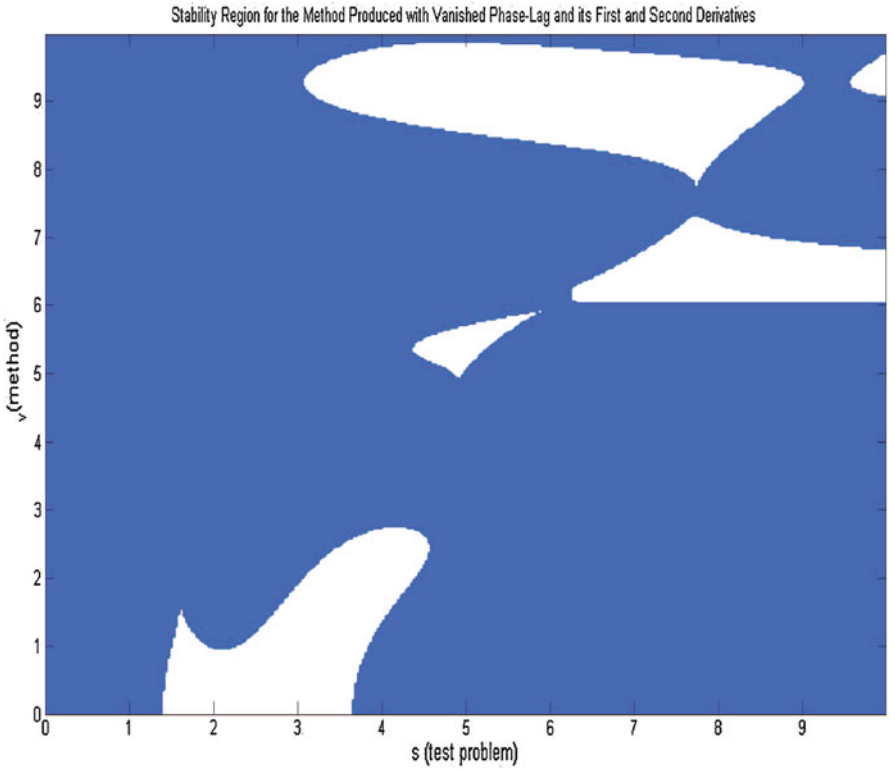

Fig. 2 $s - v$ plane of the the new developed method

to be possible the application of the new method to the radial Schrödinger equation. Based on (1), the parameter ω is given by (for the case $l = 0$):

$$\omega = \sqrt{|V(r) - k^2|} = \sqrt{|V(r) - E|} \tag{28}$$

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

6.1 Woods-Saxon potential

We use the well known Woods-Saxon potential which can be written as

$$V(r) = \frac{u_0}{1+y} - \frac{u_0\, y}{a\,(1+y)^2} \tag{29}$$

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

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

From the literature it is known that the definition of parameter ω for some potentials, such as the Woods-Saxon potential, is given not as a function of x but as based on

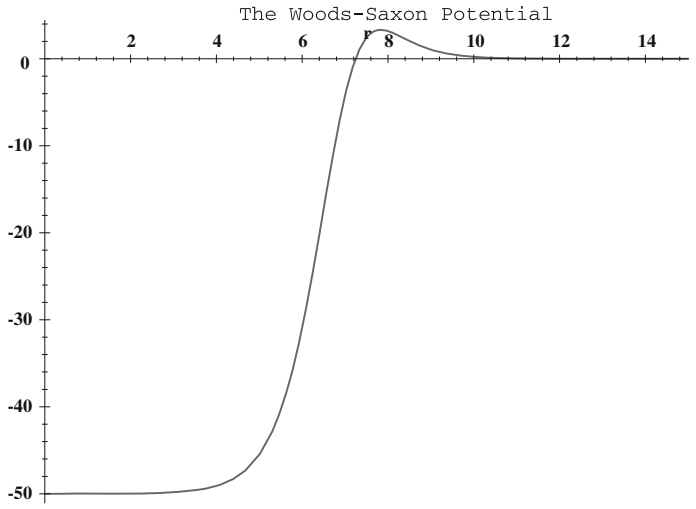

Fig. 3 The Woods-Saxon potential

some critical points which have been defined from the investigation of the appropriate potential (see for details [104]).

For the purpose of obtaining our numerical results, it is appropriate to choose v as follows (see for details [1] and [78]):

$$\omega = \begin{cases} \sqrt{-50+E}, & \text{for } r \in [0, 6.5-2h], \\ \sqrt{-37.5+E}, & \text{for } r = 6.5-h \\ \sqrt{-25+E}, & \text{for } r = 6.5 \\ \sqrt{-12.5+E}, & \text{for } r = 6.5+h \\ \sqrt{E}, & \text{for } r \in [6.5+2h, 15] \end{cases} \tag{30}$$

For example, in the point of the integration region $r = 6.5 + h$, the value of ω is equal to: $\sqrt{-12.5+E}$. So, $v = \omega\, h = \sqrt{-12.5+E}\, h$. In the point of the integration region $r = 6.5 + 3\,h$, the value of ω is equal to: $\sqrt{E}$, etc.

6.2 Radial Schrödinger equation: the resonance problem

For the purpose of this application, we consider the numerical solution of the radial time independent Schrödinger equation (1) in the known case of the Woods-Saxon potential (29). The numerical solution of this problem requires the approximation of the true (infinite) interval of integration by a finite interval. For our numerical purposes, we take the domain of integration as $r \in [0, 15]$. 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 decays faster than the term $\frac{l(l+1)}{r^2}$ and the Schrödinger equation effectively reduces to

$$q''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right) q(r) = 0 \tag{31}$$

for r greater than some value R.

The above equation has linearly independent solutions $krj_l(kr)$ and $krn_l(kr)$, where $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions respectively. Thus, the solution of Eq. (1) (when $r \to \infty$), has the asymptotic form

$$\begin{aligned} q(r) &\approx Akrj_l(kr) - Bkrn_l(kr) \\ &\approx AC\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan d_l \cos\left(kr - \frac{l\pi}{2}\right)\right] \end{aligned} \tag{32}$$

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

$$\tan\delta_l = \frac{q(r_2)S(r_1) - q(r_1)S(r_2)}{q(r_1)C(r_1) - q(r_2)C(r_2)} \tag{33}$$

for r_1 and r_2 distinct points in the asymptotic region (we choose r_1 as the right hand end point of the interval of integration and $r_2 = r_1 - h$) with $S(r) = krj_l(kr)$ and $C(r) = -krn_l(kr)$. Since the problem is treated as an initial-value problem, we need $q_j,\ j = 0, (1)3$ before starting a four-step method. From the initial condition, we obtain q_0. The values $q_i,\ i = 1(1)3$ are obtained by using high order Runge-Kutta-Nyström methods (see [113] and [114]). With these starting values, we evaluate at r_2 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**.

The boundary conditions for this problem are:

$$q(0) = 0,\ q(r) = \cos\left(\sqrt{E}r\right) \text{ for large } r. \tag{34}$$

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

- The eighth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT8**.
- The tenth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10**.
- The twelfth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT12**.
- The fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as **Method MCR4**
- The exponentially-fitted method of Raptis and Allison [79], which is indicated as **Method MRA**
- The hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [24], which is indicated as **Method MCR6**

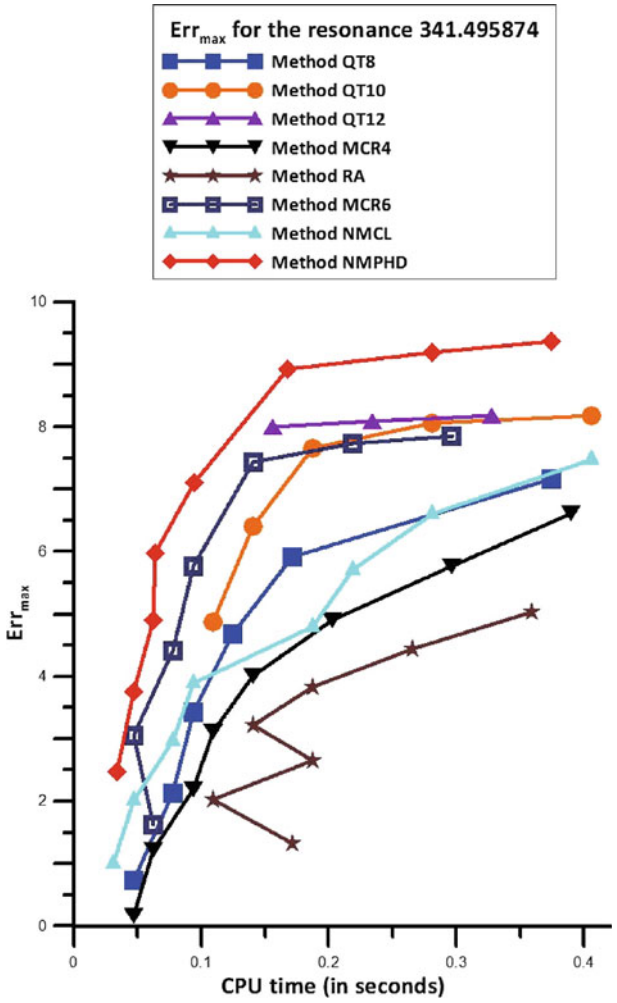

Fig. 4 Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_2 = 341.495874$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is <0

– The classical form of the sixth algebraic order four-step method developed in Sect. 3, which is indicated as **Method NMCL**.[2]
– The hybrid four-step method of sixth algebraic order with vanished phase-lag and its first and second derivatives (obtained in Sect. 3), which is indicated as **Method NMPHD**

The computed eigenenergies are compared with reference values.[3] In Figs. 4 and 5, we present the maximum absolute error $Err_{max} = |log_{10}(Err)|$ where

[2] With the term classical we mean the method of Sect. 3 with constant coefficients.

[3] The reference values are computed using the well known two-step method of Chawla and Rao [24] with small step size for the integration.

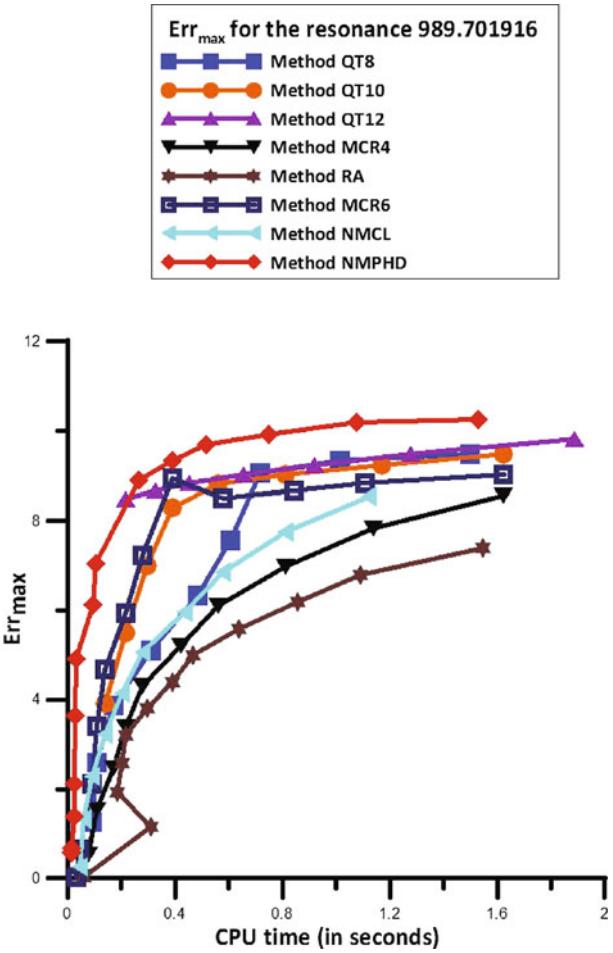

Fig. 5 Accuracy (Digits) for several values of CPU Time (in Seconds) for the eigenvalue $E_3 = 989.701916$. The nonexistence of a value of Accuracy (Digits) indicates that for this value of CPU, Accuracy (Digits) is <0

$$Err = |E_{calculated} - E_{accurate}| \tag{35}$$

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

7 Conclusions

In this paper we have investigated a family of two-stage four-step sixth algebraic order methods and the influencing of the procedure of vanishing phase-lag and its derivatives on the efficiency of the above mentioned methods for the numerical solution of

the radial Schrödinger equation and related problems. As a result of the above, a two-stage four-step sixth algebraic order methods with vanished phase-lag and its first and second derivatives was produced. This new method is very efficient on any problem with oscillating solutions or problems with solutions contain the functions cos and sin or any combination of them.

From the results presented above, we can make the following remarks:

1. The classical form of the sixth algebraic order four-step method developed in Sect. 3, which is indicated as **Method NMCL** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as **Method MCR4**. Both the above mentioned methods are more efficient than the exponentially-fitted method of Raptis and Allison [79], which is indicated as **Method MRA**.
2. The tenth algebraic order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10** is more efficient than the fourth algebraic order method of Chawla and Rao with minimal phase-lag [25], which is indicated as **Method MCR4**. The **Method QT10** is also more efficient than the eighth order multi-step method developed by Quinlan and Tremaine [19], which is indicated as **Method QT8**. Finally, the **Method QT10** is more efficient than the hybrid sixth algebraic order method developed by Chawla and Rao with minimal phase-lag [24], which is indicated as **Method MCR6** for large CPU time and less efficient than the **Method MCR6** for small CPU time.
3. The twelfth algebraic order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT12** is more efficient than the tenth order multistep method developed by Quinlan and Tremaine [19], which is indicated as **Method QT10**
4. Finally, the new developed hybrid four-step two-stage sixth algebraic order method with vanished phase-lag and its first and second derivatives (obtained in Sect. 3), which is indicated as **Method NMPHD** is the most efficient one.

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

Appendix

New method with vanished phase-lag and its first, second and third derivative (developed in Sect. 3)

$$\begin{aligned} \mathrm{LTE}_{\mathrm{NM}} = h^8 \Bigg[& \left(\frac{751}{75600} \left(\frac{d^2}{dx^2} g(x) \right) q(x) \right) G^2 \\ & + \left(\frac{9763}{302400} \left(\frac{d^4}{dx^4} g(x) \right) q(x) + \frac{751}{25200} \left(\frac{d^3}{dx^3} g(x) \right) \right. \\ & \left. \frac{d}{dx} q(x) + \frac{751}{50400} g(x) \left(\frac{d}{dx} q(x) \right) \frac{d}{dx} g(x) \right) \end{aligned}$$

$$+\frac{17273}{302400}\,g\,(x)\,q\,(x)\,\frac{d^2}{dx^2}g\,(x)+\frac{751}{18900}$$
$$\left(\frac{d}{dx}g\,(x)\right)^2 q\,(x)+\frac{751}{302400}\,(g\,(x))^3\,q\,(x)\Bigg)\,G$$
$$+\frac{751}{302400}\left(\frac{d^6}{dx^6}g\,(x)\right)q\,(x)+\frac{751}{50400}\left(\frac{d^5}{dx^5}g\,(x)\right)$$
$$\frac{d}{dx}q\,(x)+\frac{751}{18900}\,g\,(x)\,q\,(x)\,\frac{d^4}{dx^4}g\,(x)$$
$$+\frac{751}{20160}\left(\frac{d^2}{dx^2}g\,(x)\right)^2 q\,(x)+\frac{9763}{151200}\left(\frac{d}{dx}g\,(x)\right)$$
$$q\,(x)\,\frac{d^3}{dx^3}g\,(x)+\frac{751}{12600}\,g\,(x)\left(\frac{d}{dx}q\,(x)\right)$$
$$\frac{d^3}{dx^3}g\,(x)+\frac{751}{25200}\,(g\,(x))^2\left(\frac{d}{dx}q\,(x)\right)$$
$$\frac{d}{dx}g\,(x)+\frac{751}{6300}\left(\frac{d}{dx}g\,(x)\right)\left(\frac{d}{dx}q\,(x)\right)$$
$$\frac{d^2}{dx^2}g\,(x)+\frac{8261}{151200}\,(g\,(x))^2\,q\,(x)\,\frac{d^2}{dx^2}g\,(x)$$
$$+\frac{751}{10800}\,g\,(x)\,q\,(x)\left(\frac{d}{dx}g\,(x)\right)^2+\frac{751}{302400}\,(g\,(x))^4\,q\,(x)\Bigg] \quad (36)$$

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