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A Six-Step P-stable Trigonometrically-Fitted Method for the Numerical Integration of the Radial Schrödinger Equation

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Abstract

In this paper we obtain a P–stable exponentially–fitted six–step method for the approximate solution of the one-dimensional Schrödinger equation. More specifically we present a method that is P-stable and also integrates exactly any linear combination of the functions $\{1,\, x,\, x^2,\, x^3,\, x^4,\, x^5,\, x^6,\, x^7,\, \exp(\pm I\, v\, x)\}$. The numerical experimentation showed that our new introduced method is considerably more efficient compared to well known methods used for the approximate solution of resonance problem of the radial Schrödinger equation.

1 Introduction

The one-dimensional Schrödinger equation can be written as:

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

The above boundary value problem occurs frequently in theoretical physics and chemistry, material sciences, quantum mechanics and quantum chemistry, electronics etc. (see for example [1] - [4]).
We give some definitions for (1):

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- 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 decades a lot of research has been done on the development of numerical methods for the solution of the Schrödinger equation. 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] - [42], [47] - [89]).
The methods for the numerical integration of the Schrödinger equation can be divided into two main categories:

- Methods with constant coefficients
- Methods with coefficients depending on the frequency of the problem [1].

In this paper we will investigate methods of the second category. More specifically we will study the exponentially-fitted methods. More specifically we will obtain an exponentially-fitted method of eighth algebraic order for the numerical solution of the radial Schrödinger equation. The developed method is also P-stable, that is it has an interval of periodicity equal to $(0, \infty)$. We apply the new obtained method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation. The above application shows the efficiency of the new obtained method. The paper is organized as follows. In Section 2 we present the development of the method. In the same section, the error analysis is presented. The stability of the new method is also studied. In Section 3 the numerical results are presented. Finally, in Section 4 remarks and conclusions are discussed.

[1]When using the trigonometrically-fitted method 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 The New Trigonometrically-Fitted Six-Step Method

2.1 Construction of the New Method

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

$$\begin{aligned} y_{n+3} + c_2\, y_{n+2} + c_1\, y_{n+1} - 2\, a_0\, y_n + c_1\, y_{n-1} + c_2\, y_{n-2} + y_{n-3} = \\ h^2 \left[b_0 \left(y''_{n+3} + y''_{n-3} \right) + b_1 \left(y''_{n+2} + y''_{n-2} \right) + b_2 \left(y''_{n+1} + y''_{n-1} \right) + b_3 y''_n \right] \end{aligned} \tag{3}$$

In order the above method (3) to be exact for any linear combination of the functions

$$\{1,\, x,\, x^2,\, x^3,\, x^4,\, x^5,\, x^6,\, x^7,\, \exp(\pm I\, v\, x)\} \tag{4}$$

where $I = \sqrt{-1}$, the following system of equations must hold:

$$\begin{aligned} & 2 \cos(3\, v\, h) + 2\, c_2 \cos(2\, v\, h) + 2\, c_1 \cos(v\, h) - 2\, a_0 \\ = \ & -2\, h^2\, v^2 \cos(3\, v\, h)\, b_0 - 2\, h^2\, v^2\, b_1 \cos(2\, v\, h) \\ - \ & 2\, h^2\, v^2\, b_2 \cos(v\, h) - h^2\, v^2\, b_3 \end{aligned} \tag{5}$$

$$2 + 2\, c_2 + 2\, c_1 - 2\, a_0 = 0 \tag{6}$$

$$18 + 8\, c_2 + 2\, c_1 = 4\, b_0 + 4\, b_1 + 4\, b_2 + 2\, b_3 \tag{7}$$

$$162 + 32\, c_2 + 2\, c_1 = 216\, b_0 + 96\, b_1 + 24\, b_2 \tag{8}$$

$$128\, c_2 + 1458 + 2\, c_1 = 4860\, b_0 + 960\, b_1 + 60\, b_2 \tag{9}$$

We apply the new method (3) to the scalar test equation:

$$y'' = -q^2\, y. \tag{10}$$

We obtain the following difference equation:

$$\begin{aligned} & A(q, h)\ (y_{n+3} + y_{n-3}) + B(q, h)\ (y_{n+2} + y_{n-2}) \\ & \quad + C(q, h)\ (y_{n+1} + y_{n-1}) + D(q, h)\, y_n = 0 \end{aligned} \tag{11}$$

where

$$\begin{aligned} A(q, h) = 1 + q^2\, h^2\, b_0,\ B(q, h) &= c_2 + q^2\, h^2\, b_1, \\ C(q, h) &= c_1 + q^2\, h^2\, b_2, \\ D(q, h) &= -2\, a_0 + q^2\, h^2\, b_3. \end{aligned} \tag{12}$$

The corresponding characteristic equation is given by:

$$A(v, h)\ \left(\lambda^6 + 1\right) + B(v, h)\ \left(\lambda^5 + \lambda\right) + C(v, h)\ \left(\lambda^4 + \lambda^2\right) + D(v, h)\, \lambda^3 = 0 \tag{13}$$

Definition 1 *(see [43]) A symmetric six-step method with the characteristic equation given by (13) is said to have an interval of periodicity* $(0, w_0^2)$ *if, for all* $w \in (0, w_0^2)$*, the roots* z_i*,* $i = 1, 2$ *satisfy*

$$z_{1,2} = e^{\pm i\,\theta(v\,h)},\ |z_i| \leq 1,\ i = 3(1)6 \tag{14}$$

where $\theta(v\,h)$ *is a real function of* $v\,h$ *and* $w = v\,h$ *.*

Definition 2 *(see [43]) A method is called P-stable if its interval of periodicity is equal to* $(0, \infty)$.

We note here that recently Wang [91] has proposed a methodology for constructing P-stable linear multistep methods for general periodic initial-value problems. In his methodology, the author assumes that all the roots of the characteristic equation must have a special form which leads to P-stable methods. We will follow his methodology in constructing our new trigonometrically-fitted P-stable method with a special arrangement mentioned below.
In order the new method to be P-stable[2] we require the characteristic equation (13) to have the following roots:

$$\exp(\pm I\,v\,h),\ -(-1)^{\left(\frac{1}{3}\right)}\exp(\pm I\,v\,h), (-1)^{\left(\frac{2}{3}\right)}\exp(\pm I\,v\,h) \tag{15}$$

In order (15) to be roots of the characteristic equation (13), the following system of equations must hold:

$$\begin{aligned}
8\,(1 + v^2\,h^2\,b_0)\cos(v\,h)^3 + 4\,(c_2 + v^2\,h^2\,b_1)\cos(v\,h)^2 & \\
+2\,(c_1 + v^2\,h^2\,b_2)\cos(v\,h) - 6\,(1 + v^2\,h^2\,b_0)\cos(v\,h) - 2\,c_2 & \\
-2\,v^2\,h^2\,b_1 - 2\,a_0 + h^2\,v^2\,b_3 &= 0 \qquad (16)\\
8\,(1 + v^2\,h^2\,b_0)\cos(v\,h)^3 + 4\,(c_2 + v^2\,h^2\,b_1)\cos(v\,h)^2 & \\
+2\,(c_1 + v^2\,h^2\,b_2)\cos(v\,h) - 6\,(1 + v^2\,h^2\,b_0)\cos(v\,h) & \\
-2\,c_2 - 2\,v^2\,h^2\,b_1 - 2\,a_0 + h^2\,v^2\,b_3 &= 0 \qquad (17)\\
-(c_1 + v^2\,h^2\,b_2)\cos(v\,h) + c_2 + v^2\,h^2\,b_1 - 2\,a_0 + h^2\,v^2\,b_3 & \\
-2\,(c_2 + v^2\,h^2\,b_1)\cos(v\,h)^2 - 6\,(1 + v^2\,h^2\,b_0)\cos(v\,h) & \\
+8\,(1 + v^2\,h^2\,b_0)\cos(v\,h)^3 + (c_1 + v^2\,h^2\,b_2)\sin(v\,h)\sqrt{3} & \\
-2\,(c_2 + v^2\,h^2\,b_1)\sin(v\,h)\cos(v\,h)\sqrt{3} &= 0 \qquad (18)
\end{aligned}$$

[2]in the case that the frequency of the exponential fitting is the same as the frequency of the scalar test equation (which in the case of (10) has been obtained), i.e. in the case that $q = v$. We will examine the case $q \neq v$ in another paper

$$\begin{aligned}
-(c_1+v^2\,h^2\,b_2)\sin(v\,h)\sqrt{3}+c_2+v^2\,h^2\,b_1-2\,a_0+h^2\,v^2\,b_3 & \\
-2\,(c_2+v^2\,h^2\,b_1)\cos(v\,h)^2-(c_1+v^2\,h^2\,b_2)\cos(v\,h) & \\
+8\,(1+v^2\,h^2\,b_0)\cos(v\,h)^3-6\,(1+v^2\,h^2\,b_0)\cos(v\,h) & \\
+2\,(c_2+v^2\,h^2\,b_1)\sin(v\,h)\cos(v\,h)\sqrt{3} &= 0 \qquad (19)
\end{aligned}$$

$$\begin{aligned}
-(c_1+v^2\,h^2\,b_2)\sin(v\,h)\sqrt{3}+c_2+v^2\,h^2\,b_1-2\,a_0+h^2\,v^2\,b_3 & \\
-2\,(c_2+v^2\,h^2\,b_1)\cos(v\,h)^2-(c_1+v^2\,h^2\,b_2)\cos(v\,h) & \\
+8\,(1+v^2\,h^2\,b_0)\cos(v\,h)^3-6\,(1+v^2\,h^2\,b_0)\cos(v\,h) & \\
+2\,(c_2+v^2\,h^2\,b_1)\sin(v\,h)\cos(v\,h)\sqrt{3} &= 0 \qquad (20)
\end{aligned}$$

$$\begin{aligned}
-(c_1+v^2\,h^2\,b_2)\cos(v\,h)+c_2+v^2\,h^2\,b_1-2\,a_0+h^2\,v^2\,b_3 & \\
-2\,(c_2+v^2\,h^2\,b_1)\cos(v\,h)^2-6\,(1+v^2\,h^2\,b_0)\cos(v\,h) & \\
+8\,(1+v^2\,h^2\,b_0)\cos(v\,h)^3+(c_1+v^2\,h^2\,b_2)\sin(v\,h)\sqrt{3} & \\
-2\,(c_2+v^2\,h^2\,b_1)\sin(v\,h)\cos(v\,h)\sqrt{3} &= 0 \qquad (21)
\end{aligned}$$

Solving the system of equations (5)–(9), (16)–(21) we obtain the following values of the coefficients of the methods:

$$\begin{aligned}
a_0 &= 10\Big(1440\cos(w)^3+196\cos(w)^3\,w^4+672\cos(w)^3\,w^2 \\
&- 1080\cos(w)-147\cos(w)\,w^4-504\cos(w)\,w^2 \\
&- 360-508\,w^4+1452\,w^2\Big)/T_0 \\
c_1 &= 45\Big(-183\,w^4-36\cos(w)\,w^4+48\cos(w)^3\,w^4 \\
&+ 488\,w^2-156\cos(w)\,w^2+208\cos(w)^3\,w^2-120 \\
&- 360\cos(w)+480\cos(w)^3\Big)/T_0 \\
c_2 &= -18\Big(-120-360\cos(w)+480\cos(w)^3+500\,w^2 \\
&- 9\cos(w)\,w^4+12\cos(w)^3\,w^4-120\cos(w)\,w^2 \\
&+ 160\cos(w)^3\,w^2-228\,w^4\Big)/T_0 \\
b_0 &= -(-360-12\cos(w)\,w^4+16\cos(w)^3\,w^4+1560\,w^2+180\,w^6 \\
&- 1080\cos(w)+1440\cos(w)^3-180\cos(w)\,w^2 \\
&+ 240\cos(w)^3\,w^2-949\,w^4)/T_1
\end{aligned}$$

$$
\begin{aligned}
b_1 &= 18(-120 - 360\cos(w) + 480\cos(w)^3 + 500\,w^2 - 9\cos(w)\,w^4 \\
&+ 12\cos(w)^3\,w^4 - 120\cos(w)\,w^2 \\
&+ 160\cos(w)^3\,w^2 - 228\,w^4)/T_1 \\
b_2 &= -45(-183\,w^4 - 36\cos(w)\,w^4 + 48\cos(w)^3\,w^4 + 488\,w^2 \\
&- 156\cos(w)\,w^2 + 208\cos(w)^3\,w^2 - 120 \\
&- 360\cos(w) + 480\cos(w)^3)/T_1 \\
b_3 &= 20(-54\,w^6\cos(w) + 72\,w^6\cos(w)^3 - 147\cos(w)\,w^4 \\
&+ 196\cos(w)^3\,w^4 - 508\,w^4 - 504\cos(w)\,w^2 \\
&+ 672\cos(w)^3\,w^2 + 1452\,w^2 - 1080\cos(w) - 360 + 1440\cos(w)^3)\,T_1
\end{aligned} \tag{22}
$$

where $w = v\,h$ and:

$$
\begin{aligned}
T_0 &= 1560\,w^2 - 12\cos(w)\,w^4 + 16\cos(w)^3\,w^4 \\
&- 360 - 180\cos(w)\,w^2 - 1080\cos(w) \\
&+ 240\cos(w)^3\,w^2 + 1440\cos(w)^3 - 949\,w^4 \\
T_1 &= w^2(1560\,w^2 - 12\cos(w)\,w^4 + 16\cos(w)^3\,w^4 \\
&- 360 - 180\cos(w)\,w^2 - 1080\cos(w) + 240\cos(w)^3\,w^2 \\
&+ 1440\cos(w)^3 - 949\,w^4)
\end{aligned}
$$

For small values of $|w|$ the formulae given by (22) are subject to heavy cancelations. In this case the following Taylor series expansions should be used:

$$
\begin{aligned}
b_0 &= \frac{141}{2240} + \frac{15849}{5017600}\,w^2 + \frac{69131367}{123633664000}\,w^4 - \frac{154755991233}{3600212295680000}\,w^6 \\
&+ \frac{3604722515991}{1612895108464640000}\,w^8 + \frac{303074877872053197}{3378047515168342016000000}\,w^{10} \\
&- \frac{722325372352035227237}{1437697022455646362009600000000}\,w^{12} \\
&+ \frac{28079026902052066256650371}{4186573729390842206171955200000000}\,w^{14} + \cdots
\end{aligned}
$$

$$\begin{aligned}
b_1 &= \frac{243}{224} - \frac{209709}{2508800}\,w^2 - \frac{196254819}{61816832000}\,w^4 + \frac{2547621846117}{1800106147840000}\,w^6 \\
&- \frac{59213951695323}{310172136243200000}\,w^8 + \frac{1864820364102631323}{1299249044295516160000000}\,w^{10} \\
&- \frac{255394094069530455147}{14376970224556463620096000000}\,w^{12} \\
&- \frac{355344541025315275651177071}{2093286864695421103085977600000000}\,w^{14} + \cdots \\
b_2 &= \frac{4131}{2240} - \frac{6493689}{5017600}\,w^2 + \frac{28060843689}{123633664000}\,w^4 - \frac{71842643988399}{3600212295680000}\,w^6 \\
&+ \frac{4188870846789597}{8064475542323200000}\,w^8 + \frac{20678701847731525467}{135121900606733680640000}\,w^{10} \\
&- \frac{4509667346026274491744827}{143769702245564636200960000000}\,w^{12} \\
&+ \frac{13632665526031876066918751949}{41865737293908422061719552000000000}\,w^{14} + \cdots \\
b_3 &= \frac{1689}{560} - \frac{4307931}{1254400}\,w^2 + \frac{36466851051}{30908416000}\,w^4 - \frac{159401983253661}{900053073920000}\,w^6 \\
&+ \frac{27484868905253703}{20161188855808000000}\,w^8 - \frac{15328897621032309147}{168902375758417100800000}\,w^{10} \\
&- \frac{312020473132514612747889}{21142603271406564147200000000}\,w^{12} \\
&+ \frac{26429721303822676777504622871}{104664343234771055154298880000000000}\,w^{14} + \cdots \\
c_1 &= -\frac{4131}{2240}\,w^2 + \frac{6493689}{5017600}\,w^4 - \frac{28060843689}{123633664000}\,w^6 + \frac{71842643988399}{3600212295680000}\,w^8 \\
&- \frac{4188870846789597}{8064475542323200000}\,w^{10} - \frac{20678701847731525467}{135121900606733680640000}\,w^{12} \\
&+ \frac{4509667346026274491744827}{143769702245564636200960000000}\,w^{14} + \cdots \\
c_2 &= -\frac{243}{224}\,w^2 + \frac{209709}{2508800}\,w^4 + \frac{196254819}{61816832000}\,w^6 - \frac{2547621846117}{1800106147840000}\,w^8 \\
&+ \frac{59213951695323}{310172136243200000}\,w^{10} - \frac{1864820364102631323}{1299249044295516160000000}\,w^{12} \\
&+ \frac{255394094069530455147}{14376970224556463620096000000}\,w^{14} + \cdots
\end{aligned}$$

$$
\begin{aligned}
a_0 &= 1-\frac{6561}{2240}\,w^2+\frac{6913107}{5017600}\,w^4-\frac{27668334051}{123633664000}\,w^6+\frac{13349480059233}{720042459136000}\,w^8 \\
&- \frac{2649308102711199}{806447554232320000}\,w^{10}-\frac{565452875659956551073}{33780475151683420160000000}\,w^{12} \\
&+ \frac{3470939451513053689458 69}{1105920786504343355392000000 0}\,w^{14}+\cdots
\end{aligned}
\tag{23}
$$

The local truncation error of this method is given by:

$$
\mathrm{LTE}=-\frac{81\,h^10}{44800}\left(y_n^{(10)}+v^2\;y_n^{(8)}\right) \tag{24}
$$

2.2 Error Analysis

We will study the following methods:

Classical Method[3]

$$
\mathrm{LTE}_{\mathrm{CL}}=-\frac{81\,h^10}{44800}\,y_n^{(10)} \tag{25}
$$

Trigonometrically-fitted Method Produced in this paper

$$
\mathrm{LTE}=-\frac{81\,h^10}{44800}\left(y_n^{(10)}+v^2\;y_n^{(8)}\right) \tag{26}
$$

The algorithm we follow for the error analysis is:

- The radial time independent Schrödinger equation is of the form

$$
y''(x)=f(x)\,y(x) \tag{27}
$$

- Based on the paper of Ixaru and Rizea [48], the function f(x) can be written in the form:

$$
f(x)=g(x)+G \tag{28}
$$

  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 $y_n^{(i)}$, $i=2,3,4,\ldots,$ which are terms of the local truncation error formulae, in terms of the equation (27). 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

[3]i.e. the method with constant coefficients

Based on the procedure mentioned above and on the formulae:

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

we obtain the following expressions:

Classical Method

$$
\begin{aligned}
\mathrm{LTE}_{\mathrm{CL}} &= \frac{81}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\mathrm{V}(x))\;{V_c}^3 \\
&- \frac{81}{560}\,(\frac{d}{dx}\mathrm{y}(x))\,(\frac{d^3}{dx^3}\mathrm{V}(x))\;{V_c}^2 \\
&- \frac{17091}{44800}\,(\frac{d^2}{dx^2}\mathrm{V}(x))^2\,\mathrm{y}(x)\,\mathrm{V}(x) - \frac{2349}{44800}\,(\frac{d^6}{dx^6}\mathrm{V}(x))\,\mathrm{y}(x)\,\mathrm{V}(x) \\
&+ \frac{2349}{44800}\,(\frac{d^6}{dx^6}\mathrm{V}(x))\,\mathrm{y}(x)\;V_c \\
&- \frac{81}{8960}\,\mathrm{y}(x)\,\mathrm{V}(x)\;{V_c}^4 + \frac{81}{2240}\,(\frac{d}{dx}\mathrm{y}(x))\,(\frac{d}{dx}\mathrm{V}(x))\;{V_c}^3 \\
&- \frac{81}{560}\,(\frac{d}{dx}\mathrm{y}(x))\,(\frac{d^3}{dx^3}\mathrm{V}(x))\,\mathrm{V}(x)^2
\end{aligned}
$$

$$- \frac{81}{896} \mathrm{y}(x) \left(\frac{d^2}{dx^2} \mathrm{V}(x)\right) \mathrm{V}(x)^3 - \frac{81}{560} \left(\frac{d}{dx} \mathrm{V}(x)\right)^3 \left(\frac{d}{dx} \mathrm{y}(x)\right)$$
$$- \frac{2349}{5600} \left(\frac{d}{dx} \mathrm{V}(x)\right)^2 \mathrm{y}(x) \left(\frac{d^2}{dx^2} \mathrm{V}(x)\right)$$
$$- \frac{81}{4480} \mathrm{y}(x) \mathrm{V}(x)^3 \; {V_c}^2 + \frac{2511}{22400} \left(\frac{d^5}{dx^5} \mathrm{V}(x)\right) \left(\frac{d}{dx} \mathrm{y}(x)\right) \; V_c$$
$$- \frac{81}{700} \left(\frac{d}{dx} \mathrm{V}(x)\right) \mathrm{y}(x) \left(\frac{d^5}{dx^5} \mathrm{V}(x)\right)$$
$$- \frac{81}{160} \left(\frac{d^2}{dx^2} \mathrm{V}(x)\right) \left(\frac{d}{dx} \mathrm{y}(x)\right) \left(\frac{d^3}{dx^3} \mathrm{V}(x)\right)$$
$$- \frac{567}{3200} \left(\frac{d^2}{dx^2} \mathrm{V}(x)\right) \mathrm{y}(x) \left(\frac{d^4}{dx^4} \mathrm{V}(x)\right)$$
$$- \frac{729}{2240} \left(\frac{d}{dx} \mathrm{V}(x)\right) \left(\frac{d}{dx} \mathrm{y}(x)\right) \left(\frac{d^4}{dx^4} \mathrm{V}(x)\right) - \frac{81}{44800} \left(\frac{d^8}{dx^8} \mathrm{V}(x)\right) \mathrm{y}(x)$$
$$- \frac{81}{5600} \left(\frac{d^7}{dx^7} \mathrm{V}(x)\right) \left(\frac{d}{dx} \mathrm{y}(x)\right)$$
$$- \frac{81}{800} \left(\frac{d^3}{dx^3} \mathrm{V}(x)\right)^2 \mathrm{y}(x) - \frac{2511}{22400} \left(\frac{d^5}{dx^5} \mathrm{V}(x)\right) \left(\frac{d}{dx} \mathrm{y}(x)\right) \mathrm{V}(x)$$
$$- \frac{3483}{22400} \mathrm{y}(x) \left(\frac{d^4}{dx^4} \mathrm{V}(x)\right) \; {V_c}^2$$
$$- \frac{81}{2240} \left(\frac{d}{dx} \mathrm{y}(x)\right) \left(\frac{d}{dx} \mathrm{V}(x)\right) \mathrm{V}(x)^3 - \frac{81}{448} \mathrm{y}(x) \left(\frac{d}{dx} \mathrm{V}(x)\right)^2 \; {V_c}^2$$
$$- \frac{81}{448} \mathrm{y}(x) \left(\frac{d}{dx} \mathrm{V}(x)\right)^2 \mathrm{V}(x)^2$$
$$- \frac{3483}{22400} \mathrm{y}(x) \left(\frac{d^4}{dx^4} \mathrm{V}(x)\right) \mathrm{V}(x)^2 + \frac{17091}{44800} \left(\frac{d^2}{dx^2} \mathrm{V}(x)\right)^2 \mathrm{y}(x) \; V_c$$
$$+ \frac{81}{8960} \mathrm{y}(x) \mathrm{V}(x)^4 \; V_c$$
$$+ \frac{81}{4480} \mathrm{y}(x) \mathrm{V}(x)^2 \; {V_c}^3 + \frac{81}{224} \mathrm{y}(x) \left(\frac{d}{dx} \mathrm{V}(x)\right)^2 \mathrm{V}(x) \; V_c$$
$$- \frac{81}{44800} \mathrm{y}(x) \mathrm{V}(x)^5 + \frac{81}{44800} \mathrm{y}(x) \; {V_c}^5$$
$$+ \frac{243}{2240} \left(\frac{d}{dx} \mathrm{y}(x)\right) \left(\frac{d}{dx} \mathrm{V}(x)\right) \mathrm{V}(x)^2 \; V_c$$
$$- \frac{243}{2240} \left(\frac{d}{dx} \mathrm{y}(x)\right) \left(\frac{d}{dx} \mathrm{V}(x)\right) \mathrm{V}(x) \; {V_c}^2$$

$$
\begin{aligned}
- & \quad \frac{81}{140}\,(\frac{d}{dx}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x) \\
+ & \quad \frac{81}{140}\,(\frac{d}{dx}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\;V_c \\
- & \quad \frac{13689}{22400}\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{y}(x)\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\,\mathrm{V}(x) \\
+ & \quad \frac{13689}{22400}\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{y}(x)\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\;V_c \\
+ & \quad \frac{3483}{11200}\,\mathrm{y}(x)\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\,\mathrm{V}(x)\;V_c \\
+ & \quad \frac{243}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x)^2\;V_c \\
+ & \quad \frac{81}{280}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\,\mathrm{V}(x)\;V_c - \frac{243}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x)\;{V_c}^2 \\
- & \quad \frac{81}{44800}\,\mathrm{y}(x)\,G^5 \\
+ & \quad \Big(\frac{81}{8960}\,\mathrm{y}(x)\;V_c - \frac{81}{8960}\,\mathrm{y}(x)\,\mathrm{V}(x)\Big)\,G^4 + \Big(-\frac{81}{896}\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{y}(x) \\
- & \quad \frac{81}{4480}\,\mathrm{y}(x)\;{V_c}^2 - \frac{81}{4480}\,\mathrm{y}(x)\,\mathrm{V}(x)^2 + \frac{81}{2240}\,\mathrm{y}(x)\,\mathrm{V}(x)\;V_c \\
- & \quad \frac{81}{2240}\,(\frac{d}{dx}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\Big)\,G^3 \\
- & \quad \Big(\frac{81}{560}\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x)) + \frac{243}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\;V_c \\
+ & \quad \frac{243}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\;V_c \\
- & \quad \frac{81}{4480}\,\mathrm{y}(x)\,\mathrm{V}(x)^3 \\
+ & \quad \frac{243}{4480}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\;V_c - \frac{243}{4480}\,\mathrm{y}(x)\,\mathrm{V}(x)\;{V_c}^2 + \frac{81}{4480}\,\mathrm{y}(x)\;{V_c}^3 \\
- & \quad \frac{243}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x) - \frac{3483}{22400}\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\,\mathrm{y}(x) \\
- & \quad \frac{81}{448}\,(\frac{d}{dx}\,\mathrm{V}(x))^2\,\mathrm{y}(x)
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{243}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x)\Big)G^2 + \Big(-\frac{2349}{44800}\,(\frac{d^6}{dx^6}\,\mathrm{V}(x))\,\mathrm{y}(x)\\
&- \frac{243}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x)^2\\
&+ \frac{81}{224}\,\mathrm{y}(x)\,(\frac{d}{dx}\,\mathrm{V}(x))^2\;V_c + \frac{3483}{11200}\,\mathrm{y}(x)\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\;V_c\\
&+ \frac{81}{2240}\,\mathrm{y}(x)\,\mathrm{V}(x)^3\;V_c\\
&- \frac{3483}{11200}\,\mathrm{y}(x)\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\,\mathrm{V}(x) - \frac{81}{224}\,\mathrm{y}(x)\,(\frac{d}{dx}\,\mathrm{V}(x))^2\,\mathrm{V}(x)\\
&- \frac{17091}{44800}\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))^2\,\mathrm{y}(x)\\
&- \frac{81}{140}\,(\frac{d}{dx}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^2}{dx^2}\,\mathrm{V}(x)) - \frac{81}{8960}\,\mathrm{y}(x)\;{V_c}^4\\
&+ \frac{81}{280}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\;V_c\\
&- \frac{2511}{22400}\,(\frac{d^5}{dx^5}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x)) - \frac{243}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\;{V_c}^2\\
&- \frac{243}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x)^2\\
&- \frac{243}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\;{V_c}^2 - \frac{81}{8960}\,\mathrm{y}(x)\,\mathrm{V}(x)^4\\
&- \frac{13689}{22400}\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{y}(x)\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\\
&+ \frac{243}{448}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x)\;V_c\\
&+ \frac{243}{1120}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x)\;V_c\\
&- \frac{81}{280}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\,\mathrm{V}(x)\\
&- \frac{243}{4480}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\;{V_c}^2 + \frac{81}{2240}\,\mathrm{y}(x)\,\mathrm{V}(x)\;{V_c}^3\Big)G \qquad (29)
\end{aligned}
$$

Trigonometrically-fitted Method produced in this paper

$$
\begin{aligned}
\mathrm{LTE_{NEW}} \;=\;& \frac{81}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\;{V_c}^3 - \frac{81}{560}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\;{V_c}^2 \\
&- \frac{17091}{44800}\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))^2\,\mathrm{y}(x)\,\mathrm{V}(x) \\
&- \frac{2349}{44800}\,(\frac{d^6}{dx^6}\,\mathrm{V}(x))\,\mathrm{y}(x)\,\mathrm{V}(x) + \frac{2349}{44800}\,(\frac{d^6}{dx^6}\,\mathrm{V}(x))\,\mathrm{y}(x)\;V_c \\
&- \frac{81}{8960}\,\mathrm{y}(x)\,\mathrm{V}(x)\;{V_c}^4 \\
&+ \frac{81}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\;{V_c}^3 - \frac{81}{560}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\,\mathrm{V}(x)^2 \\
&- \frac{81}{896}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x)^3 \\
&- \frac{81}{560}\,(\frac{d}{dx}\,\mathrm{V}(x))^3\,(\frac{d}{dx}\,\mathrm{y}(x)) - \frac{2349}{5600}\,(\frac{d}{dx}\,\mathrm{V}(x))^2\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x)) \\
&- \frac{81}{4480}\,\mathrm{y}(x)\,\mathrm{V}(x)^3\;{V_c}^2 \\
&+ \frac{2511}{22400}\,(\frac{d^5}{dx^5}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\;V_c - \frac{81}{700}\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{y}(x)\,(\frac{d^5}{dx^5}\,\mathrm{V}(x)) \\
&- \frac{81}{160}\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^3}{dx^3}\,\mathrm{V}(x)) \qquad (30) \\
&- \frac{567}{3200}\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{y}(x)\,(\frac{d^4}{dx^4}\,\mathrm{V}(x)) \\
&- \frac{729}{2240}\,(\frac{d}{dx}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d^4}{dx^4}\,\mathrm{V}(x)) - \frac{81}{44800}\,(\frac{d^8}{dx^8}\,\mathrm{V}(x))\,\mathrm{y}(x) \\
&- \frac{81}{5600}\,(\frac{d^7}{dx^7}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x)) - \frac{81}{800}\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))^2\,\mathrm{y}(x) \\
&- \frac{2511}{22400}\,(\frac{d^5}{dx^5}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\,\mathrm{V}(x) - \frac{3483}{22400}\,\mathrm{y}(x)\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\;{V_c}^2 \\
&- \frac{81}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x)^3 - \frac{81}{448}\,\mathrm{y}(x)\,(\frac{d}{dx}\,\mathrm{V}(x))^2\;{V_c}^2 \\
&- \frac{81}{448}\,\mathrm{y}(x)\,(\frac{d}{dx}\,\mathrm{V}(x))^2\,\mathrm{V}(x)^2 \\
&- \frac{3483}{22400}\,\mathrm{y}(x)\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\,\mathrm{V}(x)^2 + \frac{17091}{44800}\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))^2\,\mathrm{y}(x)\;V_c
\end{aligned}
$$

$$+ \quad \frac{81}{8960}\,\mathrm{y}(x)\,\mathrm{V}(x)^4\;V_c$$

$$+ \quad \frac{81}{4480}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\;{V_c}^3 + \frac{81}{224}\,\mathrm{y}(x)\,(\frac{d}{dx}\,\mathrm{V}(x))^2\,\mathrm{V}(x)\;V_c$$

$$- \quad \frac{81}{44800}\,\mathrm{y}(x)\,\mathrm{V}(x)^5 + \frac{81}{44800}\,\mathrm{y}(x)\;{V_c}^5$$

$$+ \quad \frac{243}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x)^2\;V_c$$

$$- \quad \frac{243}{2240}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x)\;{V_c}^2$$

$$+ \quad \Big(\frac{81}{44800}\,\mathrm{y}(x)\;V_c - \frac{81}{44800}\,\mathrm{y}(x)\,\mathrm{V}(x)\Big)\,G^4$$

$$+ \quad \Big(- \frac{81}{1600}\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{y}(x) - \frac{81}{11200}\,\mathrm{y}(x)\;{V_c}^2$$

$$- \quad \frac{81}{11200}\,\mathrm{y}(x)\,\mathrm{V}(x)^2 + \frac{81}{5600}\,\mathrm{y}(x)\,\mathrm{V}(x)\;V_c$$

$$- \quad \frac{81}{5600}\,(\frac{d}{dx}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x))\Big)\,G^3$$

$$- \quad \Big(\frac{81}{800}\,(\frac{d^3}{dx^3}\,\mathrm{V}(x))\,(\frac{d}{dx}\,\mathrm{y}(x)) + \frac{4293}{22400}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\;V_c$$

$$+ \quad \frac{729}{11200}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\;V_c$$

$$- \quad \frac{243}{22400}\,\mathrm{y}(x)\,\mathrm{V}(x)^3 + \frac{729}{22400}\,\mathrm{y}(x)\,\mathrm{V}(x)^2\;V_c$$

$$- \quad \frac{729}{22400}\,\mathrm{y}(x)\,\mathrm{V}(x)\;{V_c}^2 + \frac{243}{22400}\,\mathrm{y}(x)\;{V_c}^3$$

$$- \quad \frac{729}{11200}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x) - \frac{81}{640}\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\,\mathrm{y}(x)$$

$$- \quad \frac{729}{5600}\,(\frac{d}{dx}\,\mathrm{V}(x))^2\,\mathrm{y}(x)$$

$$- \quad \frac{4293}{22400}\,\mathrm{y}(x)\,(\frac{d^2}{dx^2}\,\mathrm{V}(x))\,\mathrm{V}(x)\Big)\,G^2 + \Big(- \frac{81}{1600}\,(\frac{d^6}{dx^6}\,\mathrm{V}(x))\,\mathrm{y}(x)$$

$$- \quad \frac{243}{2800}\,(\frac{d}{dx}\,\mathrm{y}(x))\,(\frac{d}{dx}\,\mathrm{V}(x))\,\mathrm{V}(x)^2$$

$$+ \quad \frac{3483}{11200}\,\mathrm{y}(x)\,(\frac{d}{dx}\,\mathrm{V}(x))^2\;V_c + \frac{3159}{11200}\,\mathrm{y}(x)\,(\frac{d^4}{dx^4}\,\mathrm{V}(x))\;V_c$$

$$
\begin{aligned}
&+ \quad \frac{81}{2800}\, \mathrm{y}(x)\, \mathrm{V}(x)^3\; V_c \\
&- \quad \frac{3159}{11200}\, \mathrm{y}(x)\, (\frac{d^4}{dx^4}\, \mathrm{V}(x))\, \mathrm{V}(x) - \frac{3483}{11200}\, \mathrm{y}(x)\, (\frac{d}{dx}\, \mathrm{V}(x))^2\, \mathrm{V}(x) \\
&- \quad \frac{567}{1600}\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))^2\, \mathrm{y}(x) \\
&- \quad \frac{1377}{2800}\, (\frac{d}{dx}\, \mathrm{V}(x))\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d^2}{dx^2}\, \mathrm{V}(x)) - \frac{81}{11200}\, \mathrm{y}(x)\; {V_c}^4 \\
&+ \quad \frac{1377}{5600}\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d^3}{dx^3}\, \mathrm{V}(x))\; V_c \\
&- \quad \frac{81}{800}\, (\frac{d^5}{dx^5}\, \mathrm{V}(x))\, (\frac{d}{dx}\, \mathrm{y}(x)) - \frac{243}{2800}\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d}{dx}\, \mathrm{V}(x))\; {V_c}^2 \\
&- \quad \frac{81}{350}\, \mathrm{y}(x)\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))\, \mathrm{V}(x)^2 \\
&- \quad \frac{81}{350}\, \mathrm{y}(x)\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))\; {V_c}^2 - \frac{81}{11200}\, \mathrm{y}(x)\, \mathrm{V}(x)^4 \\
&- \quad \frac{3159}{5600}\, (\frac{d}{dx}\, \mathrm{V}(x))\, \mathrm{y}(x)\, (\frac{d^3}{dx^3}\, \mathrm{V}(x)) \\
&+ \quad \frac{81}{175}\, \mathrm{y}(x)\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))\, \mathrm{V}(x)\; V_c + \frac{243}{1400}\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d}{dx}\, \mathrm{V}(x))\, \mathrm{V}(x)\; V_c \\
&- \quad \frac{1377}{5600}\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d^3}{dx^3}\, \mathrm{V}(x))\, \mathrm{V}(x) - \frac{243}{5600}\, \mathrm{y}(x)\, \mathrm{V}(x)^2\; {V_c}^2 \\
&+ \quad \frac{81}{2800}\, \mathrm{y}(x)\, \mathrm{V}(x)\; {V_c}^3 \Big) G \\
&- \quad \frac{81}{140}\, (\frac{d}{dx}\, \mathrm{V}(x))\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))\, \mathrm{V}(x) \\
&+ \quad \frac{81}{140}\, (\frac{d}{dx}\, \mathrm{V}(x))\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))\; V_c \\
&- \quad \frac{13689}{22400}\, (\frac{d}{dx}\, \mathrm{V}(x))\, \mathrm{y}(x)\, (\frac{d^3}{dx^3}\, \mathrm{V}(x))\, \mathrm{V}(x) \\
&+ \quad \frac{13689}{22400}\, (\frac{d}{dx}\, \mathrm{V}(x))\, \mathrm{y}(x)\, (\frac{d^3}{dx^3}\, \mathrm{V}(x))\; V_c \\
&+ \quad \frac{3483}{11200}\, \mathrm{y}(x)\, (\frac{d^4}{dx^4}\, \mathrm{V}(x))\, \mathrm{V}(x)\; V_c + \frac{243}{896}\, \mathrm{y}(x)\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))\, \mathrm{V}(x)^2\; V_c \\
&+ \quad \frac{81}{280}\, (\frac{d}{dx}\, \mathrm{y}(x))\, (\frac{d^3}{dx^3}\, \mathrm{V}(x))\, \mathrm{V}(x)\; V_c - \frac{243}{896}\, \mathrm{y}(x)\, (\frac{d^2}{dx^2}\, \mathrm{V}(x))\, \mathrm{V}(x)\; {V_c}^2
\end{aligned}
\tag{31}
$$

We consider two situations 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 three cases.
- $G \gg 0$ or $G \ll 0$. Then $\mid G \mid$ is a large number. So, we have the following asymptotic expansions of the equations (29) and (31).

Classical Method

$$\mathrm{LTE_{CL}} = -\frac{81}{44800}\,\mathrm{y}(x)\,G^5 + \cdots \tag{32}$$

Trigonometrically-fitted Method produced in this paper

$$\mathrm{LTE_{NEW}} = -\frac{81}{44800}\left(V_c - \mathrm{V}(x)\right)\mathrm{y}(x)\,G^4 + \cdots \tag{33}$$

¿From the above equations we have the following theorem:

Theorem 1 *For the Classical Six-Step Method the error increases as the fifth power of G. For the Trigonometrically-fitted Six-Step Method developed in this paper the error increases as the fourth power of G. So, for the numerical solution of the time independent radial Schrödinger equation the new obtained Trigonometrically-fitted six-step Method is the most accurate one, especially for large values of* $\mid G \mid = \mid V_c - E \mid$.

2.3 Stability Analysis

We apply the new method to the scalar test equation:

$$y'' = -q^2 y, \tag{34}$$

where $q \neq v$.
We obtain the difference equation (11) and the corresponding characteristic equation (12)
Substituting in the characteristic equation the values of the coefficients b_i, $i = 0(1)3$, c_i, $i = 0, 1$ and a_0, we obtain the following final form of the characteristic equation: (we note that $H = qh$)

$$
\begin{aligned}
& \Big(1-\Big(-360+180\,H^6+1560\,H^2 \\
- \;& 12\cos(H)\,H^4+16\cos(H)^3\,H^4-180\cos(H)\,H^2 \\
+ \;& 240\cos(H)^3\,H^2-1080\cos(H)+1440\cos(H)^3 \\
- \;& 949\,H^4\Big)/(\mathrm{S}_0)\Big)\Big(\lambda^3+\frac{1}{\lambda^3}\Big)-20\Big(1440\cos(H)^3 \\
+ \;& 196\cos(H)^3\,H^4+672\cos(H)^3\,H^2-1080\cos(H) \\
- \;& 147\cos(H)\,H^4-504\cos(H)\,H^2-360 \\
+ \;& 1452\,H^2-508\,H^4\Big)/\Big(\mathrm{S}_0\Big)+20\Big(-54\,H^6\cos(H) \\
+ \;& 72\,H^6\cos(H)^3-147\cos(H)\,H^4 \\
+ \;& 196\cos(H)^3\,H^4-508\,H^4-504\cos(H)\,H^2 \\
+ \;& 672\cos(H)^3\,H^2+1452\,H^2-360-1080\cos(H) \\
+ \;& 1440\cos(H)^3\Big)/\Big(\mathrm{S}_0\Big) \\
\mathrm{S}_0 = \;& -360-180\cos(H)\,H^2-1080\cos(H)+240\cos(H)^3\,H^2 \\
+ \;& 1440\cos(H)^3+1560\,H^2-12\cos(H)\,H^4 \\
+ \;& 16\cos(H)^3\,H^4-949\,H^4=0
\end{aligned}
\tag{35}
$$

where we have considered that $H = w$.
The roots of the above characteristic equation are give by:

$$
\begin{aligned}
&\Big\{\sqrt[3]{\cos(3\,v)-\sqrt{(\cos(3\,v))^2-1}} \;-\; \frac{1}{2}\sqrt[3]{\cos(3\,v)+\sqrt{(\cos(3\,v))^2-1}} \\
&-\frac{i\sqrt{3}}{2}\sqrt[3]{\cos(3\,v)+\sqrt{(\cos(3\,v))^2-1}} \;-\; \frac{1}{2}\sqrt[3]{\cos(3\,v)+\sqrt{(\cos(3\,v))^2-1}} \\
&+\frac{i\sqrt{3}}{2}\sqrt[3]{\cos(3\,v)+\sqrt{(\cos(3\,v))^2-1}} \;-\; \frac{1}{2}\sqrt[3]{\cos(3\,v)-\sqrt{(\cos(3\,v))^2-1}} \\
&-\frac{i\sqrt{3}}{2}\sqrt[3]{\cos(3\,v)-\sqrt{(\cos(3\,v))^2-1}} \;-\; \frac{1}{2}\sqrt[3]{\cos(3\,v)-\sqrt{(\cos(3\,v))^2-1}} \\
&+\frac{i\sqrt{3}}{2}\sqrt[3]{\cos(3\,v)-\sqrt{(\cos(3\,v))^2-1}} \;-\; \frac{1}{2}\sqrt[3]{\cos(3\,v)+\sqrt{(\cos(3\,v))^2-1}}\Big\}
\end{aligned}
$$

Based on the above roots of the characteristic equation and on the Definitions 1 and 2, it is easy for one to see that $\lambda_i \leq 1$, $i = 0(1)5$ for every $H^2 \in (0, \infty)$, i.e. the method is P-stable.

3 Numerical results - Conclusion

In order to illustrate the efficiency of the new obtained method given by coefficients (22) and (23) we apply it to the radial time independent Schrödinger equation.

In order to apply the new method 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

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|} \tag{36}$$

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

3.1 Woods-Saxon potential

We use as potential the well known Woods-Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a\,(1+z)^2} \tag{37}$$

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

The behavior of Woods-Saxon potential is shown in the Figure 1.

For some well known potentials, such as the Woods-Saxon potential, the definition of parameter v is not given as a function of x but based on some critical points which have been defined from the study of the appropriate potential (see for details [13]).

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (see for details [13]):

$$v = \begin{cases} \sqrt{-50 + E} & \text{for x} \in [0, 6.5 - 2\text{h}] \\ \sqrt{-37.5 + E} & \text{for x} = 6.5 - h \\ \sqrt{-25 + E} & \text{for x} = 6.5 \\ \sqrt{-12.5 + E} & \text{for x} = 6.5 + h \\ \sqrt{E} & \text{for x} \in [6.5 + 2\text{h}, 15] \end{cases} \tag{38}$$

3.2 Radial Schrödinger Equation - The Resonance Problem

Consider the numerical solution of the radial time independent Schrödinger equation (1) in the well-known case of the Woods-Saxon potential (37). In order to solve this problem numerically we need to approximate the true (infinite)

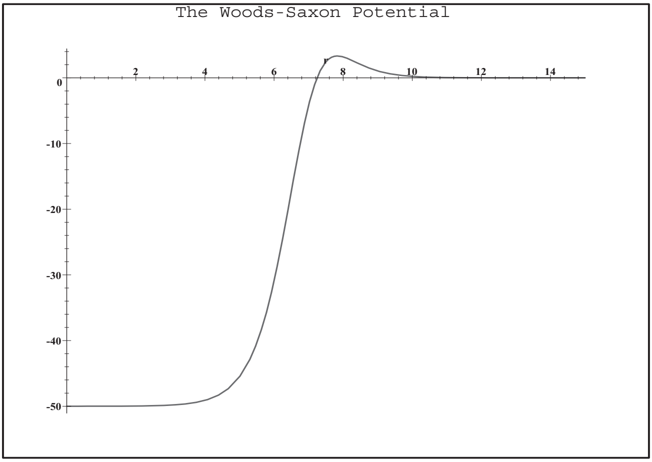

Figure 1: The Woods-Saxon potential.

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 equation (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 fades away faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0 \tag{39}$$

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) has (when $x \to \infty$) the asymptotic form

$$y(x) \simeq Akxj_l(kx) - Bkxn_l(kx)$$

$$\simeq AC \left[sin\left(kx - \frac{l\pi}{2}\right) + tan\delta_l \, cos\left(kx - \frac{l\pi}{2}\right)\right] \tag{40}$$

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

$$tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \tag{41}$$

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 before starting a one-step method. From the initial condition we obtain y_0. 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:

$$y(0) = 0, \;\; y(x) = \cos\left(\sqrt{E}x\right) \;\text{ for large } x. \tag{42}$$

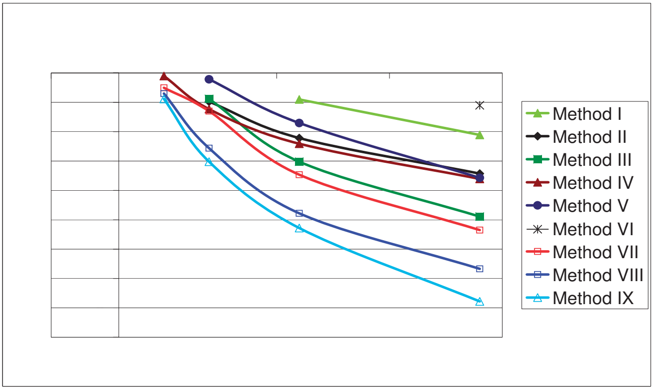

Figure 2: Comparison of the maximum errors Err in the computation of the resonance $E_3 = 989.701916$ using the Methods I-VIII. The values of Err have been obtained based on the $NFEx100$. The absence of values of Err for some methods indicates that for these values of NFEx100 = Number of Function Evaluations, the Err is positive.

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 method of Numerov type developed by Raptis and Allison [10] which is indicated as **Method II**
- the Exponentially-fitted four-step method developed by Raptis [16] which is indicated as **Method III**

- the Two-Step P-stable exponentially-fitted method developed by Kalogiratou and Simos [42] which is indicated as **Method IV**
- the Four-Step method mentioned in Henrici [45] which is indicated as **Method V**
- the Two-Step P-stable method obtained by Chawla [46] which is indicated as **Method VI**
- the P-stable trigonometrically-fitted four-step method obtained by Simos [90] which is indicated as **Method VII**
- the P-stable trigonometrically-fitted four-step method produced by Simos [92] which is indicated as **Method VIII**
- the New P-stable trigonometrically-fitted six-step method developed in this paper which is indicated as **Method IX**

The computed eigenenergies are compared with exact ones. In Figure 2 we present the maximum absolute error $log_{10}\,(Err)$ where

$$Err = |E_{calculated} - E_{accurate}| \tag{43}$$

of the eigenenergy E_3, for several values of NFEx100 = Number of Function Evaluations.

4 Conclusions

In the present paper we have obtained a new exponentially-fitted six-step method for the numerical solution of the radial Schrödinger equation. For this method we have examined the stability properties. We have also studied the error for the radial Schrödinger equation. The new method is almost P-stable only in the case that the frequency of the exponential fitting is the same as the frequency of the scalar test equation. The new method also integrates exactly every linear combination of the functions

$$\{1,\, x,\, x^2,\, x^3,\, x^4,\, x^5,\, x^6,\, x^7,\, \exp(\pm I\, v\, x)\}. \tag{44}$$

We have applied the new method to the resonance problem of the radial Schrödinger equation.
Based on the results presented above we have the following conclusions:

- The P-stable exponentially-fitted Numerov's type method of Kalogiratou and Simos (see [42]) is more efficient than the Numerov's method and the method of Raptis and Allison [10].
- The exponentially-fitted four-step method developed by Raptis [16] is more efficient than Numerov's method. For number of function evaluations equal to 400 the behavior is worse than the methods of Raptis and Allison [10] and Kalogiratou and Simos [42].

- The exponentially-fitted method Raptis and Allison [10] is more efficient than the Numerov's method.
- The P-stable trigonometrically-fitted four-step method obtained by Simos [90] is more efficient than all the other methods (except the new one).
- The method obtained by Simos [92] is much more efficient than all the above mentioned methods.
- The method developed in this paper is the most efficient one.

The reason of the better behavior of the new method is the combination of the P-stability, smallest LTE constant and the exponential fitting property.
All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

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