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New Trigonometrically Fitted Six-Step Symmetric Methods for the Efficient Solution of the Schrödinger Equation

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Abstract

In this paper we are developing a family of four trigonometrically fitted six-step symmetric methods with exponential order from one to four. The methods are constructed to solve numerically the radial one-dimensional time-independent Schrödinger equation during the resonance problem with use of the Woods-Saxon potential. The new four methods are being compared to the corresponding classical method as long as with other recently constructed optimized methods from the literature. With the use of various values of energy we come to the conclusion that the efficiency of the method increases while the exponential order increases and this is highly noticed for high values of energy. The new method of exponential order four is the most efficient among all the compared methods and also its efficiency increases slightly instead of decreasing while we use higher values of energy. Stability analysis of the new methods is made and some diagrams are presented that show their stability regions.

1 Introduction

Much research has been done on the numerical integration of the radial Schrödinger equation:

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

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where $\frac{l(l+1)}{x^2}$ is the *centrifugal potential*, $V(x)$ is the *potential*, E is the *energy* and $W(x) = \frac{l(l+1)}{x^2} + V(x)$ is the *effective potential*. It is valid that $\lim_{x\to\infty} V(x) = 0$ and therefore $\lim_{x\to\infty} W(x) = 0$.
Many problems in chemistry, physics, physical chemistry, chemical physics, electronics etc., are expressed by equation (1).

In this paper we will study the case of $E > 0$. We divide $[0, \infty)$ into subintervals $[a_i, b_i]$ so that $W(x)$ is a constant with value $\bar{W}_i$. After this the problem (1) can be expressed by the approximation

$$\begin{aligned} &y_i'' = (\bar{W} - E)\, y_i, \qquad \text{whose solution is} \\ &y_i(x) = A_i \exp\left(\sqrt{\bar{W} - E}\, x\right) + B_i \exp\left(-\sqrt{\bar{W} - E}\, x\right), \\ &A_i,\ B_i \in \mathbb{R}. \end{aligned} \tag{2}$$

This form of Schrödinger equation reveals the importance of exponential fitting when constructing new methods. This technique has been used in all types of numerical methods. Raptis and Allison have developed a two-step exponentially-fitted method of order four in [6] and Raptis has developed a four-step exponentially-fitted method of order six in [5]. More recently Simos has constructed a P-stable four-step exponentially-fitted method in [7] and a four-step exponentially-fitted method in [8] and Kalogiratou and Simos have constructed a two-step P-stable exponentially-fitted method of order four in [10]. Also Anastassi and Simos have constructed exponentially-fitted Runge-Kutta methods of various orders in [11], [12] and [13] and Van de Vyver has constructed some exponentially fitted Runge-Kutta-Nyström methods in [14] and [15].

Some other notable multistep methods for the numerical solution of oscillating IVPs have been developed by Chawla and Rao in [3], who produced a three-stage, two-Step P-stable method with minimal phase-lag and order six, by Henrici in [4], which is a four-step symmetric method of order six, and by Simos in [9], where a four-step P-stable method with minimal phase-lag is constructed.

Also some recent research work in numerical methods can be found in [19], [20], [21], [22], [23], [24], [25], [26], [27], [28], [29], [30], [31], [32], [33], [34], [35] and [36].

2 Basic theory

2.1 Exponential symmetric multistep methods

For the numerical solution of the initial value problem

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

multistep methods of the form

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \tag{4}$$

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

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

Method (4) is associated with the operator

$$L(x) = \sum_{i=0}^{m} a_i u(x + ih) - h^2 \sum_{i=0}^{m} b_i u''(x + ih) \tag{5}$$

where $u \in C^2$.

Definition 1 The multistep method (5) is called algebraic (or exponential) of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions 1, x, x^2, ..., x^{p+1} (or $\exp(\omega_0 x)$, $\exp(\omega_1 x), \ldots, \exp(\omega_{p+1} x)$, where $\omega_i | i = 0(1)p+1$ are real or complex numbers).

Remark 1 [1] If $\omega_i = \omega$ for $i = 0, 1, \ldots, n$, $n \leqslant p + 1$, then the operator L vanishes for any linear combination of $\exp(\omega x)$, $x \exp(\omega x)$, $x^2 \exp(\omega x)$, ..., $x^n \exp(\omega x)$, $\exp(\omega_{n+1} x)$, ..., $\exp(\omega_{p+1} x)$.

Remark 2 [1] Every exponential multistep method corresponds in a unique way to an algebraic method (by setting $\omega_i = 0$ for all i), which is called the *classical method*.

When we use an imaginary number for frequency, that is $I\omega$, then $\exp(I\omega x)$ can be expanded to $\cos(\omega x) + I \sin(\omega x)$, so we refer to a method that integrates exactly these functions as a trigonometrical multistep method.

2.2 Stability analysis of symmetric multistep methods

In this section we will present the definitions for the stability of symmetric linear multistep methods according to Lambert and Watson theory [17] as well as some definitions from the paper of Coleman and Ixaru for the stability of methods with variable coefficients [18].

We apply the symmetric linear m-step method (4) to the scalar test equation

$$y'' = -\theta^2 y \tag{6}$$

and then we solve the corresponding characteristic equation, which has m characteristic roots $\lambda_i, \ i = 0(1)m - 1$.

Definition 2 [17] If the characteristic roots satisfy the conditions $|\lambda_0| = |\lambda_1| = 1$ and $|\lambda_i| \leqslant 1$, $i = 2(1)m-1$ for all $s < s_0$, where $s = \theta h$, then we say that the method has interval of periodicity $(0, s_0^2)$.

Definition 3 [17] Method (4) is called P-stable if its *interval of periodicity* is $(0, \infty)$.

We deliberately use frequency θ for the stability analysis that is different from frequency ω used for exponential-fitting. In this way we will be able to produce the $v - s$ plane, which gives the stability regions of the method.

Definition 4 [18] A *region of stability* for a multistep method is a region of the $v-s$ plane, throughout which the roots of the corresponding characteristic equation satisfy the conditions of Definition 2. If the conditions are valid for the equality only then that curve is called *stability boundary*.

If we set $r = \dfrac{v}{s} = \dfrac{\omega}{\theta}$, then we can say that the *principal interval of periodicity* is represented by the line segment from the beginning of the axes to the intersection of line $v = rs$ and the stability boundary. *Secondary intervals of periodicity* can be defined along the line $v = rs$ further from the beginning of the axes, but they are less important since the method must always be stable around the area where $h \to 0$.

3 Construction of the new trigonometrically fitted multistep methods

We consider the multistep symmetric method of Jenkins [2], with six steps and sixth algebraic order:

$$y_3 = -y_{-3} - a_2(y_2 + y_{-2}) + h^2 \left(b_2(f_2 + f_{-2}) + b_1(f_1 + f_{-1}) + b_0 f_0\right) \qquad (7)$$

where $a_2 = -1, \quad b_2 = \frac{67}{48}, \quad b_1 = -\frac{8}{48}, \quad b_0 = \frac{122}{48}$,
$y_i = y(x + ih)$ and $f_i = f(x + ih, y(x + ih))$

Based on this method we will construct four trigonometrically fitted methods.

3.1 First order trigonometrically fitted method

We want the first method to integrate exactly the functions:

$$\{1, x, \ldots, x^7, \exp(\pm I\omega x)\}$$

where ω is a real number and it is called frequency and $I = \sqrt{-1}$.

After satisfying the exact integration of the above functions, the method has exponential order one and all the coefficients are the same as (7) except for:

$$
\begin{aligned}
&b_i = \tfrac{b_{i,num}}{A}, \quad i = \{0,1,2\}, \quad \text{where} \\
&b_{0,num} = -144\,\cos(v)^3 + (72 - 70\,v^2)\cos(v)^2 + (-55\,v^2 + 108)\cos(v) \\
&-36 + 35\,v^2 \\
&b_{1,num} = 96\,\cos(v)^3 + (-48 + 65\,v^2)\cos(v)^2 - 72\,\cos(v) + 24 - 5\,v^2 \\
&b_{2,num} = \tfrac{1}{2}(-48\,\cos(v)^3 + 24\,\cos(v)^2 + (36 - 65\,v^2)\cos(v) - 12 + 35\,v^2) \\
&A = 12v^2(\cos(v) - 1)^2
\end{aligned}
\tag{8}
$$

where $v = \omega\,h$, ω is the frequency and h is the step length used.

3.2 Second order trigonometrically fitted method

The second method we construct integrates exactly the functions:

$$\{1,\, x,\, \ldots,\, x^7,\, \exp(\pm I\omega x),\, x\exp(\pm I\omega x)\}$$

After this the method has exponential order two and all the coefficients are the same as (7) except for:

$$b_i = \tfrac{b_{i,num}}{b_{i,den}}, \quad i = \{0,1,2\}, \quad \text{where} \tag{9}$$

$$
\begin{aligned}
&b_{0,num} = -16\,\cos(v)^5 v + 32\,\cos(v)^4\sin(v) + (24\,v + 10\,v^3)\cos(v)^3 \\
&+(8\,v + 10\,v^3 - 32\,\sin(v))\cos(v)^2 + (-4\,\sin(v) + 5\,v^3 - 8\,v)\cos(v) \\
&+5\,v^3 + 4\,\sin(v) - 8\,v \\
&b_{1,num} = 4\,\cos(v)^4 v - 8\,\cos(v)^3\sin(v) + (-9\,v + 4\,\sin(v))\cos(v)^2 \\
&+(-5\,v^3 + 2\,v + 6\,\sin(v))\cos(v) + 3\,v - 2\,\sin(v) \\
&b_{2,num} = -16\,\cos(v)^4 v + (16\,\sin(v) + 12\,v)\cos(v)^3 \\
&+(20\,v - 8\,\sin(v))\cos(v)^2 + (5\,v^3 - 12\,v - 12\,\sin(v))\cos(v) \\
&-4\,v + 5\,v^3 + 4\,\sin(v) \\
&b_{0,den} = 2\,(\cos(v) + 1)\,A, \qquad b_{1,den} = A, \qquad b_{2,den} = 4\,(\cos(v) + 1)\,A, \\
&A = v^3(\cos(v) - 1)^2
\end{aligned}
\tag{10}
$$

3.3 Third order trigonometrically fitted method

The third method we construct integrates exactly the functions:

$$\{1,\, x,\, \ldots,\, x^7,\, \exp(\pm I\omega x),\, x\exp(\pm I\omega x),\, x^2\exp(\pm I\omega x)\}$$

The new method has exponential order three and all of its coefficients are the same as (7) except for:

$$b_i = \tfrac{b_{i,num}}{A}, \quad i = \{0, 1, 2\}, \tag{11}$$

$$\begin{aligned}
&b_{0,num} = -24\,\cos(v)^5 v + (-8\,\sin(v)v^2 - 20\,v + 24\,\sin(v))\cos(v)^4 \\
&+(12\,\sin(v) - 8\,\sin(v)v^2 - 14\,v)\cos(v)^3 + (-12\,\sin(v)v^2 + 6\,\sin(v) \\
&-10\,v)\cos(v)^2 + (17\,v - 12\,\sin(v)v^2 + 6\,\sin(v))\cos(v) - 3\,\sin(v) + 6\,v
\end{aligned}$$

$$\begin{aligned}
&b_{1,num} = 32\,\cos(v)^4 v + (12\,\sin(v)v^2 + 24\,v - 24\,\sin(v))\cos(v)^3 \\
&+(12\,\sin(v)v^2 - 16\,v - 12\,\sin(v))\cos(v)^2 + (6\,\sin(v) - 8\,v \\
&+3\,\sin(v)v^2)\cos(v) + 3\,\sin(v)v^2 - 2\,v
\end{aligned}$$

$$\begin{aligned}
&b_{2,num} = -20\,\cos(v)^3 v + (-14\,v - 12\,\sin(v)v^2 + 12\,\sin(v))\cos(v)^2 \\
&+(13\,v - 10\,\sin(v)v^2 + 6\,\sin(v))\cos(v) - 3\,\sin(v) + 6\,v + 2\,\sin(v)v^2
\end{aligned}$$

$$\begin{aligned}
&b_{0,den} = A, \qquad b_{1,den} = A, \qquad b_{2,den} = 2\,A, \\
&A = v^4\sin(v)(\cos(v) + 1)
\end{aligned}$$

3.4 Fourth order trigonometrically fitted method

The fourth method we construct integrates exactly the functions:

$$\{1,\, x,\, \ldots,\, x^7,\, \exp(\pm I\omega x),\, x\exp(\pm I\omega x),\, x^2\exp(\pm I\omega x),\, x^3\exp(\pm I\omega x)\}$$

The new method has exponential order four and all of its coefficients are the same as (7) except for:

$$a_1 = \tfrac{a_{2,num}}{a_{2,den}}, \quad \textit{and} \quad b_i = \tfrac{b_{i,num}}{b_{i,den}}, \quad i = \{0, 1, 2\}, \tag{12}$$

$$a_{2,num} = 48\,\cos(v)^5 - 44\,\cos(v)^5 v^2 - 12\,v^3\sin(v)\cos(v)^4$$
$$+72\,\sin(v)\cos(v)^4 v - 84\,\cos(v)^3 + 101\,\cos(v)^3 v^2 - 108\,v\sin(v)\cos(v)^2$$
$$+24\,\cos(v)^2\sin(v)v^3 + 36\,\cos(v) - 60\,\cos(v)v^2 + 27\,v\sin(v) - 12\,\sin(v)v^3$$

$$b_{0,num} = 80\,\cos(v)^8 v^2 - 48\,\cos(v)^8 + 16\,v^3\sin(v)\cos(v)^7$$
$$-96\,v\sin(v)\cos(v)^7 + 20\,\cos(v)^6 v^2 + 60\,\cos(v)^6 + 48\,\sin(v)\cos(v)^5 v^3$$
$$-280\,\cos(v)^4 v^2 - 12\,\cos(v)^4 + 168\,\cos(v)^3\sin(v)v - 124\,\sin(v)\cos(v)^3 v^3$$
$$+105\,v^2\cos(v)^2 - 9\,\cos(v)^2 - 72\,\sin(v)\cos(v)v + 9 + 30\,v^2$$

$$b_{1,num} = 48\,\cos(v)^7 - 152\,\cos(v)^7 v^2 + 144\,v\sin(v)\cos(v)^6$$
$$-48\,v^3\sin(v)\cos(v)^6 + 266\,\cos(v)^5 v^2 - 84\,\cos(v)^5 - 180\,\sin(v)\cos(v)^4 v$$
$$+60\,v^3\sin(v)\cos(v)^4 + 54\,\cos(v)^3 - 51\,\cos(v)^3 v^2 + 18\,v\sin(v)\cos(v)^2$$
$$+24\,\cos(v)^2\sin(v)v^3 - 33\,\cos(v)v^2 - 18\,\cos(v) + 18\,v\sin(v) + 9\,\sin(v)v^3$$

$$b_{2,num} = -24\,\cos(v)^6 + 184\,\cos(v)^6 v^2 - 24\,\cos(v)^6 v^4 - 96\,\cos(v)^5\sin(v)v$$
$$+112\,\sin(v)\cos(v)^5 v^3 + 42\,\cos(v)^4 - 382\,\cos(v)^4 v^2 + 72\,\cos(v)^4 v^4$$
$$+132\,\cos(v)^3\sin(v)v - 214\,\sin(v)\cos(v)^3 v^3 - 27\,\cos(v)^2 + 207\,v^2\cos(v)^2$$
$$-72\,\cos(v)^2 v^4 + 72\,\sin(v)\cos(v)v^3 - 36\,\sin(v)\cos(v)v + 9 + 24\,v^4 - 24\,v^2$$

$$a_{2,den} = A, \qquad b_{0,den} = sin(v)\,v^3\,A,$$
$$b_{1,den} = sin(v)\,v^3\,A, \qquad b_{2,den} = 2\,sin(v)\,v^3\,A,$$

$$A = 4\,\cos(v)^4 v^2 + 11\,v^2 - 12\,\cos(v)^2 v^2 + 27\,\sin(v)\cos(v)v$$
$$-18\,\cos(v)^3\sin(v)v - 12 - 24\,\cos(v)^4 + 36\,\cos(v)^2$$

For small values of v the coefficients are subject to heavy cancelations, so we use the Taylor series expansions of the coefficients around zero. Of course the constant terms of the series are equal to the respective coefficients of the classical method.

4 Analysis of the new methods

4.1 Local truncation error analysis

In order to see the behavior of the error and which parameters it depends on, we will use the local truncation error (LTE), that is the Taylor series expansion of the difference between the theoretical and the approximate solution over the step length h. We see that indeed the order of the methods is six and we will present the principal term of the local truncation error for the methods below while integrating the Schrödinger equation:

a) The classical six-step symmetric method (7),
b) The first trigonometrically fitted method (8),
c) The second trigonometrically fitted method (9),
d) The third trigonometrically fitted method (11) and

e) The fourth trigonometrically fitted method (12)

In order to calculate the errors of methods b), c), d) and e) we need to determine the frequency ω. The formula for ω as it is used during calculations for the resonance problem is $\omega = \sqrt{E - \bar{W}}$ and this is also used during the error analysis.

$$\begin{aligned} LTE_a = \tfrac{h^8}{12096}\,[&787\,yE^4 - 3148\,yWE^3 + ((17314\,W'' + 4722\,W^2)y \\ &+9444\,W'y')E^2 + ((-12592\,W^{(4)} - 34628\,W''W - 3148\,W^3 \\ &-22036\,(W')^2)y - 18888\,W^{(3)}y' - 18888\,W'y'W)E \\ &+(787\,W^4 + 17314\,W''W^2 + (12592\,W^{(4)} + 22036\,(W')^2)W \\ &+11805\,(W'')^2 + 787\,W^{(6)} + 20462\,W^{(3)}W')y + 37776\,W'W''y' \\ &+4722\,(W^{(5)})y' + 9444\,W^2W'y' + 18888\,WW^{(3)}y'] \end{aligned} \tag{13}$$

$$\begin{aligned} LTE_b = \tfrac{h^8}{362880}\,[&(-23610\,yW + 23610\,y\,\bar{W})E^3 + (141660\,y'W' \\ &+70830\,yW^2 - 70830\,yW\,\bar{W} + 354150\,yW'')E^2 + (-70830\,yW^3 \\ &+70830\,yW^2\,\bar{W} + (-873570\,y(W'' - 424980\,y'W')W \\ &+(-354150\,W^{(4)} + 165270\,W''\,\bar{W} - 566640\,(W')^2)y - 472200\,y'W^{(3)} \\ &+141660\,y'W'\,\bar{W})E + 23610\,yW^4 - 23610\,yW^3\,\bar{W} + (283320\,y'W'(x) \\ &+519420\,yW'')W^2 + ((377760\,W^{(4)} + 661080\,(W')^2 \\ &-165270\,(W''\,\bar{W})y + 566640\,y'W^{(3)} - 141660\,y'W'\,\bar{W})W \\ &+(613860\,W'W^{(3)} + (-94440\,(W')^2 - 23610\,W^{(4)})\,\bar{W} + 23610\,W^{(6)} \\ &+354150\,((W'')^2)y + 1133280\,y'W'W'' + 141660\,y'W^{(5)} \\ &-94440\,y'W^{(3)}\,\bar{W}] \end{aligned} \tag{14}$$

$$\begin{aligned} LTE_c = \tfrac{h^8}{181440}\,[&((106245\,W'' + 11805\,W^2 + 11805\,\bar{W}^2 - 23610\,W\,\bar{W})y \\ &+23610\,y'W')E^2 + ((-23610\,W\,\bar{W}^2 + (141660\,W'' + 47220\,W^2)\,\bar{W} \\ &-354150\,WW'' - 236100\,(W')^2 - 165270\,W^{(4)} - 23610\,W^3)y \\ &-188880\,y'W^{(3)} - 141660\,y'WW' + 94440\,y'W'\,\bar{W})E \\ &+((11805\,W'' + 11805\,W^2)\,\bar{W}^2 + (-23610\,W^{(4)} - 23610\,W^3 \\ &-94440\,(W')^2 - 165270\,WW'')\,\bar{W} + 177075\,(W'')^2 + 330540\,W(W')^2 \\ &+188880\,WW^{(4)} + 306930\,W'W^{(3)} + 11805\,W^4 + 11805\,W^{(6)} \\ &+259710\,W^2W'')y + 23610\,y'W'\,\bar{W}^2 + (-141660\,y'WW' \\ &-94440\,y'W^{(3)})\,\bar{W} + 70830\,y'W^{(5)} + 141660\,y'W^2W' \\ &+283320\,y'WW^{(3)} + 566640\,y'W'(W'')] \end{aligned} \tag{15}$$

$$
\begin{aligned}
LTE_d = \tfrac{h^8}{362880}\,[&94440\,yW''E^2 + (-306930\,yW^{(4)} + ((354150\;\bar{W}\\
&-543030\,W)W'' + 23610\;\bar{W}^3 - 23610\,W^3 - 70830(\,W\,\bar{W}^2 + \,W^2\,\bar{W})\\
&-377760\,(W')^2)y - 283320\,y'W^{(3)} + (141660(\,y'\,\bar{W} - \,y'W)W')E\\
&+141660\,y'W^{(5)} + (-70830\;\bar{W} + 377760\,W)yW^{(4)} + (613860\,W'W^{(3)}\\
&+354150\,(W'')^2 + (519420\,W^2 - 495810\,W\,\bar{W} + 70830\;\bar{W}^2)W''\\
&+(661080\,W - 283320\;\bar{W})(W')^2 - 70830\,W^3\,\bar{W}\\
&+23610\,W^4 + 23610\,W^{(6)} - 23610\,W\,\bar{W}^3 + 70830\,W^2\,\bar{W}^2)y\\
&+(-283320\,y'\,\bar{W} + 566640\,y'W)W^{(3)}\\
&+1133280\,y'W'(W'' + (283320\,y'W^2\\
&-424980\,y'W\,\bar{W} + 141660\,y'\,\bar{W}^2)W']
\end{aligned}
\tag{16}
$$

$$
\begin{aligned}
LTE_e = \tfrac{h^8}{181440}\,[&((-141660\,W^{(4)} + (-188880\,W + 188880\;\bar{W})W''\\
&-141660\,(W')^2)y - 94440\,y'W^{(3)})E + (11805\,W^{(6)}\\
&+(188880\,W - 47220\;\bar{W})W^{(4)} + 306930\,W'W^{(3)} + 177075\,(W'')^2\\
&+(-330540\,W\,\bar{W} + 259710\,W^2 + 70830\;\bar{W}^2)(W'' + (-188880\;\bar{W}\\
&+330540\,W)(W')^2 + 11805\,W^4 - 47220\,W\,\bar{W}^3 + 11805\;\bar{W}^4\\
&-47220\;\bar{W}\,W^3 + 70830\,W^2\,\bar{W}^2)y + 70830\,y'W^{(5)} + (-188880\;\bar{W}\\
&+283320\,W)y'W^{(3)} + 566640\,y'W'W'' + (141660\;\bar{W}^2 + 141660\,W^2\\
&-283320\,W\,\bar{W})W'y']
\end{aligned}
\tag{17}
$$

where $y = y(x)$ and $W = W(x)$, while $\bar{W}$ is constant.

We notice the maximum power of energy E in these expressions. We see that for the classical method a) the maximum power of the energy is E^4. For the trigonometrically-fitted of first order method b) the maximum power becomes E^3, for the second order method c) E^2, for the third order method d) E^2 and for the fourth order method e) E.

The first conclusion that we come to is that when solving the equation using higher values of energy, all methods will be less efficient, because of the power of the energy in the local truncation error. Exception is the fourth exponential order method, which has a slight increase in accuracy while the energy increases. This can be shown in Figures 1 and 2 for the resonance problem while using the Woods-Saxon potential for 600 and 1200 function evaluations respectively. This indicates that we can use the fourth exponential order method to compute arbitrarily large eigenvalues for the Schrödinger equation with the same accuracy.

The second conclusion is that by increasing the exponential order of the method, the maximum power reduces and the method will gain efficiency as related to the other methods. It will always be more efficient than the methods of lower exponential order of the same family. The difference between them will be higher for higher values of energy.

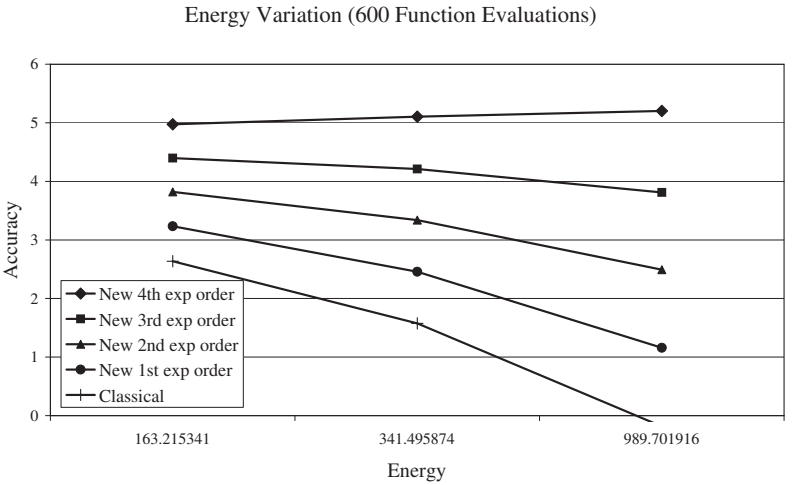

Figure 1: Accuracy of the new methods for various values of Energy (600 Function Evaluations)

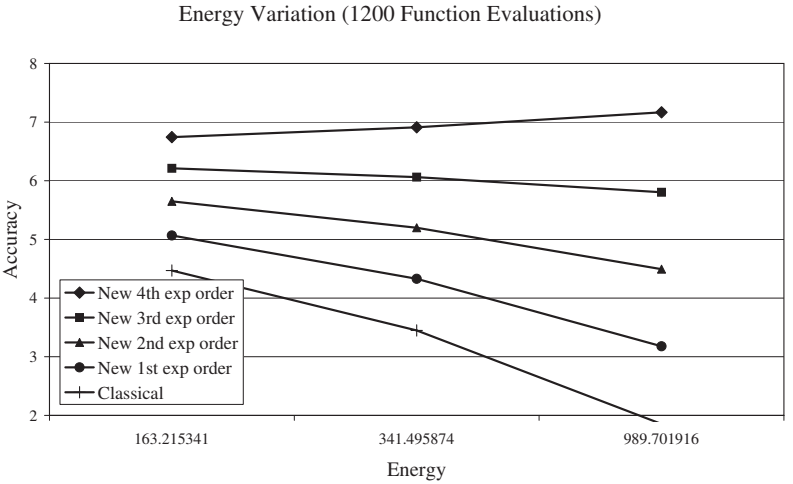

Figure 2: Accuracy of the new methods for various values of Energy (1200 Function Evaluations)

4.2 Stability analysis

We will use the stability theory to produce the $v - s$ plane of the four newly developed methods, where $v = \omega h$ and $s = \theta h$. The planes are presented in Figures 3-6, where the stability region of each method is represented by the shaded area. The critical part of the stability region is the one that includes the beginning of the axes, because we want the method to be stable as $h \to 0$.

A confirmation for the fact that all four exponentially-fitted methods are derived from the same classical method is that for line $r = 0$, that is the horizontal axis, the stability region ends at the same point $s_0 = 0.84$. We shall note that $r = 0 \Rightarrow v = 0 \Rightarrow \omega = 0$, which means that the exponentially-fitted method becomes the corresponding classical method.

In practice we are more interested for the principal interval of periodicity along line $r = 1$, that is when $\omega = \theta$. We are presenting the intervals for the four new methods and the corresponding classical one in Table 1.

Table 1: Interval of periodicity

Method	s_0	$(0, s_0^2)$
Corresponding classical method	0.84	$(0, 0.71)$
New TF method with exp. order 1	0.91	$(0, 0.83)$
New TF method with exp. order 2	1.02	$(0, 1.05)$
New TF method with exp. order 3	2.30	$(0, 5.29)$
New TF method with exp. order 4	1.61	$(0, 2.58)$

5 Numerical results

5.1 The resonance problem

The efficiency of the two newly constructed methods will be measured through the integration of problem (1) with $l = 0$ at the interval $[0, 15]$ using the well known Woods-Saxon potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\, q}{(1+q)^2}, \qquad q = \exp\left(\frac{x - x_0}{a}\right), \quad \text{where} \tag{18}$$
$$u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}$$

and with boundary condition $y(0) = 0$.

The potential $V(x)$ decays more quickly than $\frac{l\,(l+1)}{x^2}$, so for large x (asymptotic region) the Schrödinger equation (1) becomes

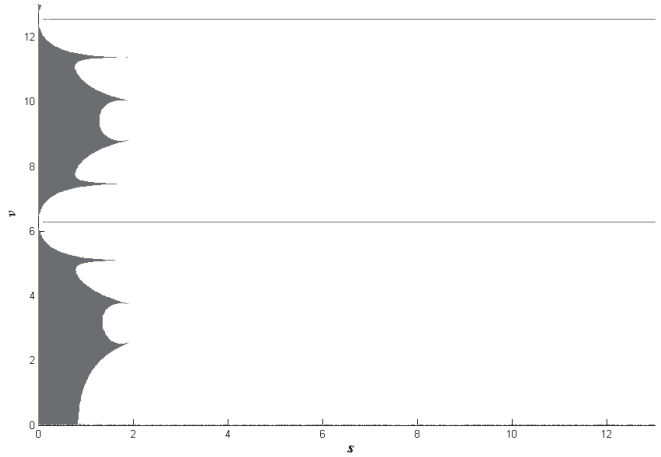

Figure 3: $v - s$ plane for the new method with 1st exponential order

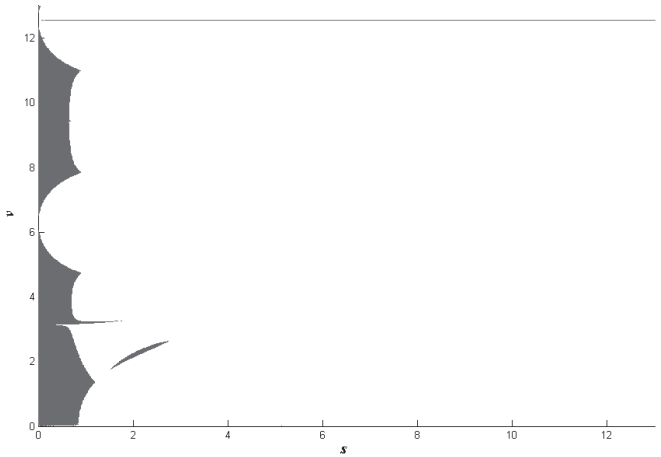

Figure 4: $v - s$ plane for the new method with 2nd exponential order

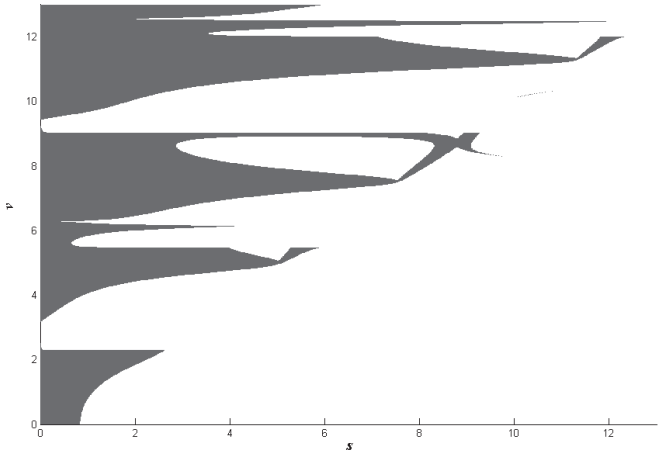

Figure 5: $v - s$ plane for the new method with 3rd exponential order

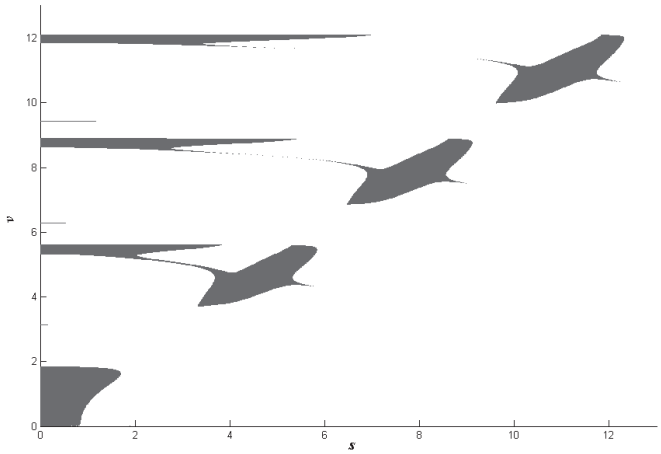

Figure 6: $v - s$ plane for the new method with 4th exponential order

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E \right) y(x) \tag{19}$$

The last equation has two linearly independent solutions $k\,x\,j_l(k\,x)$ and $k\,x\,n_l(k\,x)$, where j_l and n_l are the *spherical Bessel* and *Neumann* functions. When $x \to \infty$ the solution takes the asymptotic form

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{20}$$

where δ_l is called *scattering phase shift* and it is given by the following expression:

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{21}$$

where $S(x) = k\,x\,j_l(k\,x)$, $C(x) = k\,x\,n_l(k\,x)$ and $x_i < x_{i+1}$ and both belong to the asymptotic region. Given the energy we approximate the phase shift, the accurate value of which is $\pi/2$ for the above problem.

5.2 The methods

We have used several multistep methods for the integration of the Schrödinger equation. These are:

- The new method of exponential order four shown in (12)
- The new method of exponential order three shown in (11)
- The new method of exponential order two shown in (9)
- The new method of exponential order one shown in (8)
- The corresponding classical method of Jenkins of order six [2]
- The P-stable exponentially-fitted method of Simos of order six [7]
- The exponentially-fitted method of Raptis of order six [5]
- The P-stable method of Henrici with minimal phase-lag and order six [4]
- The exponentially-fitted method of Raptis and Allison of order four [6]
- The P-stable exponentially-fitted method of Kalogiratou and Simos of order four [10]
- The three-stage method of Chawla and Rao of order six [3]

5.3 Comparison

We will use three different values for the energy: i) 989.701916, ii) 341.495874 and iii) 163.215341. As for the frequency ω we will use the suggestion of Ixaru and Rizea [16]:

$$\omega = \begin{cases} \sqrt{E-50}, & x \in [0,\, 6.5] \\ \sqrt{E}, & x \in [6.5,\, 15] \end{cases} \tag{22}$$

We are presenting the **accuracy** of the tested methods expressed by the $-\log_{10}$(error at the end point) when comparing the phase shift to the actual value $\pi/2$ versus the $\log_{10}$(total function evaluations). The **function evaluations** per step are equal to the number of stages of the method multiplied by one, which is the dimension of the vector of the functions integrated for the resonance problem. In Figure 7 we see the results for $E = 989.701916$, in Figure 8 we have used $E = 341.495874$ and in Figure 9 we have used $E = 163.215341$.

While comparing the four trigonometrically fitted methods (8), (9), (11) and (12) and the corresponding classical method of Jenkins (7), we can confirm all the conclusions of the error analysis that is the fourth method is the most efficient as it has the highest exponential order. We can see that every new method with higher exponential order is more efficient than another method from the same family, which guides us to use high exponential order methods for the integration of the Schrödinger equation.

We also see that the new method is more efficient than other exponential multistep methods, which have the same algebraic order, two or three stages or P-stability. However we conclude that higher exponential order crucial when integrating the Schrödinger equation.

6 Conclusions

In this paper we have constructed four trigonometrically-fitted methods of exponential order from one to four based on a symmetric six-step method of Jenkins. We have shown that the higher the exponential order is the more efficient the method is and also that for the maximum exponential order (four), the efficiency of the method actually increases while the energy used also increases. This is a very important conclusion in order to integrate problems with high values of energy. We have also shown that the new method of order four is much more efficient than the others methods compared of the same algebraic order.

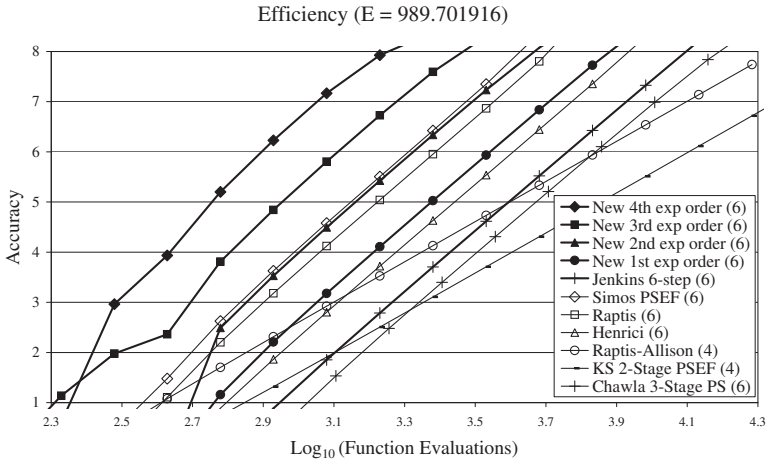

Figure 7: $-\log_{10}(\text{Error})$ versus $\log_{10}(\text{Function Evaluations})$ for the Resonance Problem using E = 989.701916

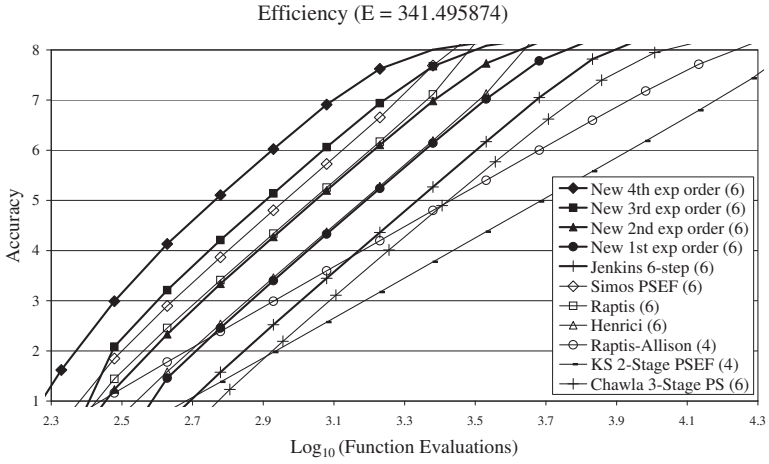

Figure 8: $-\log_{10}(\text{Error})$ versus $\log_{10}(\text{Function Evaluations})$ for the Resonance Problem using E = 341.495874

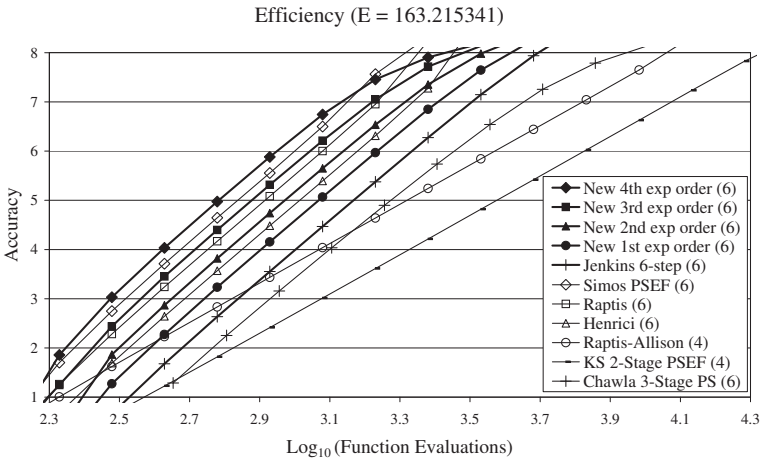

Figure 9: $-\log_{10}(\text{Error})$ versus $\log_{10}(\text{Function Evaluations})$ for the Resonance Problem using E = 163.215341

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