Journal of Mathematical Chemistry Vol. 37, No. 3, April 2005 (© 2005)
DOI: 10.1007/s10910-004-1470-8

Trigonometrically fitted Runge–Kutta methods for the numerical solution of the Schrödinger equation

Z.A. Anastassi and T.E. Simos*,†

Department of Computer Science and Technology, Faculty of Sciences and Technology, University of Peloponnese, GR-22 100 Tripolis, Greece
E-mail: tsimos@mail.ariadne-t.gr

Received 20 February 2004; revised 25 April 2004

In this paper we construct two trigonometrically fitted methods based on a classical Runge–Kutta method of England with fifth algebraic order. The methods will be used for the integration of the radial Schrödinger equation and have high efficiency as the results show. The efficiency is higher when using higher energy and this can be explained by the error analysis of the methods. More specifically the new methods have lower powers of the energy in the local truncation error and that keeps the error at lower values.

KEY WORDS: Runge–Kutta, explicit methods, exponential fitting, trigonometrical fitting, radial Schrödinger equation, resonance problem, energy

Abbreviations: LTE – Local Truncation Error
PACS: 0.260, 95.10.E

1. Introduction

We consider the radial Schrödinger equation:

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

where $(l(l+1))/x^2$ is the *centrifugal potential*, $V(x)$ is the *potential*, E is the *energy* and $W(x) = (l(l+1)/x^2) + V(x)$ is the *effective potential*. It is valid that $\lim_{x\to\infty} V(x) = 0$ and therefore $\lim_{x\to\infty} W(x) = 0$. We will study the case of $E > 0$.

If we divide $[0, \infty]$ into small subintervals $[a_i, b_i]$ so that $W(x)$ is considered constant with value $\bar{W}_i$, then the problem (1) is reduced to the approximation

$$y_i'' = (\bar{W} - E)\, y_i,$$

* Active Member of the European Academy of Sciences and Arts.
† Corresponding author.

whose solution is

$$y_i(x) = A_i \exp\left(\sqrt{\bar{W} - E}\, x\right) + B_i \exp\left(-\sqrt{\bar{W} - E}\, x\right), \quad A_i,\ B_i \in \Re. \tag{2}$$

This form of Schrödinger equation shows why exponential fitting is so important when constructing new methods. In section 2 we will present the most important parts of the theory used.

2. Basic theory

2.1. Explicit Runge–Kutta methods

An s-stage explicit Runge–Kutta method used for the computation of the approximation of $y_{n+1}(x)$, when $y_n(x)$ is known, can be expressed by the following relations:

$$\begin{aligned} y_{n+1} &= y_n + \sum_{i=1}^{s} b_i k_i, \\ k_i &= hf\left(x_n + c_i h,\, y_n + h\sum_{j=1}^{i-1} a_{ij} k_j\right), \quad i = 1, \ldots, s, \end{aligned} \tag{3}$$

where in this case $f(x, y(x)) = (W(x) - E)\, y(x)$.

Actually to solve the second order ODE (1) using first order numerical method (3), (1) becomes:

$$\begin{aligned} z'(x) &= (W(x) - E)\, y(x), \\ y'(x) &= z(x). \end{aligned} \tag{4}$$

while we use two pairs of equations (3): one for y_{n+1} and one for z_{n+1}.

The method shown above can also be presented using the Butcher table below:

$$\begin{array}{c|ccccc} 0 & & & & & \\ c_2 & a_{21} & & & & \\ c_3 & a_{31} & a_{32} & & & \\ \vdots & \vdots & \vdots & & & \\ c_s & a_{s1} & a_{s2} & \ldots & a_{s,s-1} & \\ \hline & b_1 & b_2 & \ldots & b_{s-1} & b_s \end{array} \tag{5}$$

Coefficients $c_2, \ldots, c_s$ must satisfy the equations:

$$c_i = \sum_{j=1}^{i-1} a_{ij}, \quad i = 2, \ldots, s. \tag{6}$$

Definition 1 [1]. A Runge–Kutta method has algebraic order p when the method's series expansion agrees with the Taylor series expansion in the p first terms: $y^{(n)}(x) = y^{(n)}_{\text{app.}}(x), \quad n = 1, 2, \ldots, p$.

A convenient way to obtain a certain algebraic order is to satisfy a number of equations derived from Tree Theory. These equations will be shown during the construction of the new methods.

2.2. *Exponentially fitted Runge–Kutta methods*

The method (3) is associated with the operator

$$\begin{aligned} L(x) &= u(x+h) - u(x) - h\sum_{i=1}^{s} b_i\, u'\left(x + c_i h, U_i\right), \\ U_i &= u(x) + h\sum_{j=1}^{i-1} a_{ij} u'\left(x + c_j h, U_j\right), \quad i = 1, \ldots, s, \end{aligned} \tag{7}$$

where u is a continuously differentiable function.

Definition 2 [2]. The method (7) is called exponential of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $\exp(v_0 x), \exp(v_1 x), \ldots, \exp(v_p x)$, where $v_i | i = 0(1)p$ are real or complex numbers.

Remark 1 [3]. If $v_i = v$ for $i = 0, 1, \ldots, n$, $n \leqslant p$, then the operator L vanishes for any linear combination of $\exp(vx)$, $x\exp(vx)$, $x^2\exp(vx)$, $\ldots$, $x^n\exp(vx)$, $\exp(v_{n+1}x)$, $\ldots$, $\exp(v_p x)$.

Remark 2 [3]. Every exponentially fitted method corresponds in a unique way to an algebraic method (by setting $v_i = 0$ for all i)

Definition 3 [2]. The corresponding algebraic method is called the classical method.

3. Construction of the new trigonometrically fitted Runge–Kutta methods

We consider the explicit Runge–Kutta method England-II [4] , which is of algebraic order five and has six stages. The coefficients are shown in (8).

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{1}{2} & \frac{1}{2} & & & & & \\
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} & & & & \\
1 & 0 & -1 & 2 & & & \\
\frac{2}{3} & \frac{7}{27} & \frac{10}{27} & 0 & \frac{1}{27} & & \\
\frac{1}{5} & \frac{28}{625} & -\frac{125}{625} & \frac{546}{625} & \frac{54}{625} & -\frac{378}{625} & \\
\hline
1 & \frac{1}{24} & 0 & 0 & \frac{5}{48} & \frac{27}{56} & \frac{125}{336}
\end{array}
\tag{8}
$$

We will construct two trigonometrically fitted methods.

3.1. *First trigonometrically fitted method*

The first method we construct will integrate exactly the functions:

$$
\{1,\, x,\, x^2,\, x^3,\, x^4,\, \exp(\mathrm{I}wx)\} \qquad \text{or equivalently}
$$
$$
\{1,\, x,\, x^2,\, x^3,\, x^4,\, \cos(wx),\, \sin(wx)\},
$$

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

To achieve this we consider all coefficients the same with the classical method except for b_5 and b_6. Then we demand the approximate solution $y_{\text{app.}}$ to integrate exactly $\exp(\mathrm{I}wx)$ for the real and the imaginary part. From these two equations we derive b_5 and b_6.

So the new method has all its coefficients the same as (8) except for:

$$
b_5 = \frac{9}{56}\frac{A}{C}, \quad b_6 = -\frac{625}{336}\frac{B}{C},
$$

where

$$
\begin{aligned}
A &= 135\, v^8 - 356\, v^6 + 1344\, v^5 \sin(v) - 2496\, v^4 \cos(v) + 6116\, v^4 \\
&\quad +4320\, \sin(v) v^3 - 22800\, v^2 + 4800\, v^2 \cos(v) - 48000\, \sin(v) v \\
&\quad +240000 - 240000\, \cos(v), \\
B &= 20736 - 120\, v^6 + 436\, v^4 - 4752\, v^2 - 192\, v^4 \cos(v) \\
&\quad +384\, \sin(v) v^3 + 5\, v^8 + 4608\, v^2 \cos(v) - 20736\, \cos(v) - 13824\, \sin(v)\, v, \\
C &= v^2 (272\, v^4 + 1180\, v^2 - 49\, v^6 + 2\, v^8 + 18000),
\end{aligned}
\tag{9}
$$

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

3.2. Second trigonometrically fitted method

The second method we construct will integrate exactly the functions:

$$\{1, x, x^2, \exp(\mathrm{I}wx),\ x\exp(\mathrm{I}wx)\} \qquad \text{or equivalently}$$
$$\{1,\ x,\ x^2,\ \cos(wx),\ \sin(wx),\ x\cos(wx),\ x\sin(wx)\}.$$

To achieve this we consider all coefficients the same with the classical method except for b_3, b_4, b_5 and b_6. Then we demand the approximate solution $y_{\text{app.}}$ to integrate exactly $\exp(\mathrm{I}wx)\ x\exp(\mathrm{I}wx)$ for the real and the imaginary part. From these four equations we derive b_3, b_4, b_5 and b_6.

So the new method has all its coefficients the same as (8) except for:

$$\begin{aligned}
b_3 &= \frac{2}{3}\frac{D}{H}, \quad b_4 = \frac{1}{3}\frac{E}{H}, \quad b_5 = \frac{9}{14}\frac{F}{H}, \quad b_6 = -\frac{625}{21}\frac{G}{H},\\
D &= -672v^4\cos(v) + v^{10} + 38496\,v^3\sin(v) + 4776\sin(v)v^5\\
&\quad -57600 + 57600\cos(v) + 6v^{10}\cos(v) - 1224\,v^6\cos(v) + 54\,v^8\\
&\quad +43776\cos(v)v^2 - 93696\,v^2 + 408\,v^7\sin(v) - 42\,v^9\sin(v)\\
&\quad -240\,v^8\cos(v) - 5216\,v^4 + 528\,v^6 + 78720\sin(v)v,\\
E &= 6v^9\sin(v) - 29\,v^8 + 72v^8\cos(v) - 303v^7\sin(v) + 562\,v^6\\
&\quad -792v^6\cos(v) + 984\sin(v)v^5 - 24\,v^4\cos(v) - 2484\,v^4\\
&\quad -1044v^3\sin(v) - 10944\cos(v)v^2 + 3024\,v^2 + 18720\sin(v)v\\
&\quad -21600 + 21600\cos(v),\\
F &= 7\,v^8 + 84\,v^8\cos(v) - 96\,v^7\sin(v) + 1248\,v^6\cos(v) - 464\,v^6\\
&\quad -7344\sin(v)v^5 - 9216\,v^4\cos(v) + 15024\,v^4 - 22176\,v^3\sin(v)\\
&\quad -13056\cos(v)v^2 + 53376\,v^2 - 69120\sin(v)v + 57600\\
&\quad -57600\cos(v),\\
G &= 3\,v^7\sin(v) - 10\,v^6 + 24\,v^6\cos(v) - 96\sin(v)v^5 + 164\,v^4\\
&\quad -216\,v^4\cos(v) + 420\,v^3\sin(v) - 912\,v^2\\
&\quad +576\cos(v)v^2 + 480\sin(v)v + 288\cos(v) - 288,\\
H &= (v^8 - 8\,v^6 + 188\,v^4 + 1472\,v^2 - 960)v^4,
\end{aligned} \tag{10}$$

where again $v = w\,h$, w is the frequency and h is the step length used. For small values of v the coefficients are subject to heavy cancelations, thus we expand the coefficients over the Taylor series around zero.

4. Algebraic order of the new methods

The following equations must hold so that the new methods maintain the fifth algebraic order that the corresponding classical method (8) has. Number six met in these equations represents the number of stages.

1st Algebraic Order (1 equation)

$$\sum_{i=1}^{6} b_i = 1$$

2nd Algebraic Order (2 equations)

$$\sum_{i=1}^{6} b_i c_i = \frac{1}{2}$$

3rd Algebraic Order (4 equations)

$$\sum_{i=1}^{6} b_i c_i^2 = \frac{1}{3}$$

$$\sum_{i,j=1}^{6} b_i a_{ij} c_j = \frac{1}{6}$$

4th Algebraic Order (8 equations)

$$\sum_{i=1}^{6} b_i c_i^3 = \frac{1}{4}$$

$$\sum_{i,j=1}^{6} b_i c_i a_{ij} c_j = \frac{1}{8}$$

$$\sum_{i,j=1}^{6} b_i a_{ij} c_j^2 = \frac{1}{12}$$

$$\sum_{i,j,k=1}^{6} b_i a_{ij} a_{jk} c_k = \frac{1}{24}$$

5th Algebraic Order (17)

$$\sum_{i=1}^{6} b_i c_i^4 = \frac{1}{5}$$

$$\sum_{i,j=1}^{6} b_i c_i^2 a_{ij} c_j = \frac{1}{10}$$

$$\sum_{i,j=1}^{6} b_i c_i a_{ij} c_j^2 = \frac{1}{15}$$

$$\sum_{i,j,k=1}^{6} b_i c_i a_{ij} a_{jk} c_k = \frac{1}{30}$$

$$\sum_{i,j=1}^{6} b_i a_{ij} c_j^3 = \frac{1}{20}$$

$$\sum_{i,j,k=1}^{6} b_i a_{ij} c_j a_{jk} c_k = \frac{1}{40}$$

$$\sum_{i,j,k=1}^{6} b_i c_i a_{ij} a_{jk} c_k^2 = \frac{1}{60}$$

$$\sum_{i,j,k,l=1}^{6} b_i a_{ij} a_{jk} a_{kl} c_l = \frac{1}{120}$$

$$\sum_{i,j,k=1}^{6} b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20} \qquad (11)$$

4.1. Equations remainders for the first method

We present the remainders of the seventeen equations, that is the difference of the right part minus the left part, for the first method (9):

$$
\begin{aligned}
\mathrm{rem}_1 &= \frac{79}{60480}\,v^6 - \frac{2311}{27216000}\,v^8 + \cdots \\
\mathrm{rem}_2 &= \frac{1}{288}\,v^4 - \frac{19}{907200}\,v^6 - \frac{1061}{58320000}\,v^8 + \cdots \\
\mathrm{rem}_3 &= \frac{13}{4320}\,v^4 - \frac{2617}{13608000}\,v^6 - \frac{27221}{6123600000}\,v^8 + \cdots \\
\mathrm{rem}_4 &= \frac{13}{8640}\,v^4 - \frac{2617}{27216000}\,v^6 - \frac{27221}{12247200000}\,v^8 + \cdots \\
\mathrm{rem}_5 &= \frac{139}{64800}\,v^4 - \frac{33451}{204120000}\,v^6 - \frac{131063}{91854000000}\,v^8 + \cdots \\
\mathrm{rem}_6 &= \frac{139}{129600}\,v^4 - \frac{33451}{408240000}\,v^6 - \frac{131063}{183708000000}\,v^8 + \cdots \\
\mathrm{rem}_7 &= \frac{277}{259200}\,v^4 - \frac{85843}{816480000}\,v^6 + \frac{299941}{367416000000}\,v^8 + \cdots \\
\mathrm{rem}_8 &= \frac{1}{259200}\,v^4 + \frac{18941}{816480000}\,v^6 - \frac{562067}{367416000000}\,v^8 + \cdots \\
\mathrm{rem}_9 &= \frac{1417}{972000}\,v^4 - \frac{356353}{3061800000}\,v^6 - \frac{887189}{1377810000000}\,v^8 + \cdots \\
\mathrm{rem}_{10} &= \frac{1417}{1944000}\,v^4 - \frac{356353}{6123600000}\,v^6 - \frac{887189}{2755620000000}\,v^8 + \cdots \\
\mathrm{rem}_{11} &= \frac{2581}{3888000}\,v^4 - \frac{705529}{12247200000}\,v^6 + \frac{35323}{5511240000000}\,v^8 + \cdots \\
\mathrm{rem}_{12} &= \frac{253}{3888000}\,v^4 - \frac{7177}{12247200000}\,v^6 - \frac{1809701}{5511240000000}\,v^8 + \cdots \\
\mathrm{rem}_{13} &= \frac{197}{288000}\,v^4 - \frac{60623}{907200000}\,v^6 + \frac{200801}{408240000000}\,v^8 + \cdots \\
\mathrm{rem}_{14} &= \frac{199}{2592000}\,v^4 + \frac{36509}{8164800000}\,v^6 - \frac{2656583}{3674160000000}\,v^8 + \cdots \\
\mathrm{rem}_{15} &= \frac{221}{2592000}\,v^4 - \frac{80039}{8164800000}\,v^6 + \frac{577193}{3674160000000}\,v^8 + \cdots \\
\mathrm{rem}_{16} &= -\frac{11}{1296000}\,v^4 + \frac{29137}{2041200000}\,v^6 - \frac{28873}{32805000000}\,v^8 + \cdots \\
\mathrm{rem}_{17} &= \frac{1417}{3888000}\,v^4 - \frac{356353}{12247200000}\,v^6 - \frac{887189}{5511240000000}\,v^8 + \cdots
\end{aligned} \tag{12}
$$

We see that for $v = 0$ the 17 equations are held. That means that the new method maintains the algebraic order of the corresponding classical method.

4.2. Equations remainders for the second method

Now we present the remainders of the equations for the second method (10):

$$
\begin{aligned}
\mathrm{rem}_1 &= \frac{71}{20160}\,v^6 + \frac{541}{86400}\,v^8 + \cdots \\
\mathrm{rem}_2 &= -\frac{1}{288}\,v^4 - \frac{1}{3360}\,v^6 - \frac{181}{172800}\,v^8 + \cdots \\
\mathrm{rem}_3 &= \frac{23}{1680}\,v^4 + \frac{5683}{226800}\,v^6 + \frac{6136723}{149688000}\,v^8 + \cdots \\
\mathrm{rem}_4 &= \frac{23}{3360}\,v^4 + \frac{5683}{453600}\,v^6 + \frac{6136723}{299376000}\,v^8 + \cdots \\
\mathrm{rem}_5 &= -\frac{1}{144}\,v^2 + \frac{281}{20160}\,v^4 + \frac{13933}{604800}\,v^6 + \frac{15156907}{399168000}\,v^8 + \cdots \\
\mathrm{rem}_6 &= -\frac{1}{288}\,v^2 + \frac{281}{40320}\,v^4 + \frac{13933}{1209600}\,v^6 + \frac{15156907}{798336000}\,v^8 + \cdots \\
\mathrm{rem}_7 &= \frac{1}{288}\,v^2 + \frac{17}{2240}\,v^4 + \frac{7057}{518400}\,v^6 + \frac{13336003}{598752000}\,v^8 + \cdots \\
\mathrm{rem}_8 &= -\frac{1}{144}\,v^2 - \frac{5}{8064}\,v^4 - \frac{19}{9072}\,v^6 - \frac{7873291}{2395008000}\,v^8 + \cdots \\
\mathrm{rem}_9 &= -\frac{71}{4320}\,v^2 + \frac{871}{201600}\,v^4 + \frac{307777}{54432000}\,v^6 + \frac{342152929}{35925120000}\,v^8 + \cdots \\
\mathrm{rem}_{10} &= -\frac{71}{8640}\,v^2 + \frac{871}{403200}\,v^4 + \frac{307777}{108864000}\,v^6 + \frac{342152929}{71850240000}\,v^8 + \cdots \\
\mathrm{rem}_{11} &= \frac{11}{8640}\,v^2 + \frac{1123}{134400}\,v^4 + \frac{1518203}{108864000}\,v^6 + \frac{1649683571}{71850240000}\,v^8 + \cdots \\
\mathrm{rem}_{12} &= -\frac{41}{4320}\,v^2 - \frac{1249}{201600}\,v^4 - \frac{86459}{7776000}\,v^6 - \frac{59433211}{3265920000}\,v^8 + \cdots \\
\mathrm{rem}_{13} &= \frac{19}{2880}\,v^2 + \frac{2449}{201600}\,v^4 + \frac{322393}{15552000}\,v^6 + \frac{611858623}{17962560000}\,v^8 + \cdots \\
\mathrm{rem}_{14} &= -\frac{1}{960}\,v^2 + \frac{1559}{403200}\,v^4 + \frac{643883}{108864000}\,v^6 + \frac{100791113}{10264320000}\,v^8 + \cdots \\
\mathrm{rem}_{15} &= -\frac{1}{240}\,v^2 - \frac{323}{134400}\,v^4 - \frac{235939}{54432000}\,v^6 - \frac{46343611}{6531840000}\,v^8 + \cdots \\
\mathrm{rem}_{16} &= \frac{1}{320}\,v^2 + \frac{79}{12600}\,v^4 + \frac{1115761}{108864000}\,v^6 + \frac{151914689}{8981280000}\,v^8 + \cdots \\
\mathrm{rem}_{17} &= -\frac{71}{17280}\,v^2 + \frac{871}{806400}\,v^4 + \frac{307777}{217728000}\,v^6 + \frac{342152929}{143700480000}\,v^8 + \cdots
\end{aligned}
\tag{13}
$$

We see that for $v = 0$ the 17 equations are held for this method too. Thus the new method has also fifth algebraic order.

5. Error analysis

The equations presented in Section 4 are useful when we need to see the order of the method. However if we want to see the behavior of the error and which parameters it depends on, we will have to use the local truncation error (LTE), that is the difference between the theoretical and the approximate solution. In fact we use the Taylor series expansion over the step length h and see that indeed the order of the methods is five, since the coefficients of the lowest powers $\{1, h, h^2, h^3, h^4, h^5\}$ vanish (see Definition 1). We will present the analytic form of the local truncation error for the three cases of:

(a) The classical England II method (8);

(b) The first trigonometrically fitted method (9);

(c) The second trigonometrically fitted method (10).

The errors correspond to the ODE (4) and has two parts: one for $y(x)$ and one for $z(x)$. To calculate the errors of methods (b) and (c) we need to determine the frequency w. The formula for w as it is used during calculations for the resonance problem is $w = \sqrt{E - \bar{W}}$ and this is also used during the error analysis.

$$\begin{aligned} \mathrm{LTE}_{a,y} = {} & \frac{h^6}{4320}[15\,E^3\,y - 45\,E^2\,W\,y + E\,(45\,W^2\,y - 24\,W'\,y' - 9\,y\,W'') \\ & -15\,W^3\,y + 18\,y\,W'^2 + 24\,W\,W'\,y' + 9\,W\,y\,W'' \\ & +4\,y'\,W^{(3)} + y\,W^{(4)}] + O(h)^7, \end{aligned} \tag{14}$$

$$\begin{aligned} \mathrm{LTE}_{a,z} = {} & \frac{h^6}{108000}[375\,E^3\,y' + E^2\,(-945\,y\,W' - 1125\,W\,y') \\ & +E\,(1890\,W\,y\,W' + 1125\,W^2\,y' + 90\,y'\,W'' + 65\,y\,W^{(3)}) \\ & -945\,W^2\,y\,W' - 375\,W^3\,y' + 210\,W'^2\,y' + 240\,y\,W'\,W'' \\ & -90\,W\,y'\,W'' - 65\,W\,y\,W^{(3)} + 5\,y'\,W^{(4)} + y\,W^{(5)}] + O(h)^7, \end{aligned} \tag{15}$$

$$\begin{aligned} \mathrm{LTE}_{b,y} = {} & \frac{h^6}{4320}[E^2\,(30\,\bar{W}\,y - 30\,W\,y) + E\,(-15\,\bar{W}^2\,y - 30\,\bar{W}\,W\,y \\ & +45\,W^2\,y - 24\,W'\,y' - 9\,y\,W'') + 15\,\bar{W}^2\,W\,y - 15\,W^3\,y + 18\,y\,W'^2 \\ & +24\,W\,W'\,y' + 9\,W\,y\,W'' + 4\,y'\,W^{(3)} + y\,W^{(4)}] + O(h)^7, \end{aligned} \tag{16}$$

$$\begin{aligned} \mathrm{LTE}_{b,z} = {} & \frac{h^6}{108000}[E^2\,(-570\,y\,W' + 750\,\bar{W}\,y' - 750\,W\,y') \\ & +E\,(-750\,\bar{W}\,y\,W' + 1890\,W\,y\,W' - 375\,\bar{W}^2\,y' - 750\,\bar{W}\,W\,y' \\ & +1125\,W^2\,y' + 90\,y'\,W'' + 65\,y\,W^{(3)}) + 375\,\bar{W}^2\,y\,W' - 945\,W^2\,y\,W' \\ & +375\,\bar{W}^2\,W\,y' - 375\,W^3\,y' + 210\,W'^2\,y' + 240\,y\,W'\,W'' - 90\,W\,y'\,W'' \\ & -65\,W\,y\,W^{(3)} + 5\,y'\,W^{(4)} + y\,W^{(5)}] + O(h)^7, \end{aligned} \tag{17}$$

$$\begin{aligned}
\mathrm{LTE}_{c,y} = {} & \frac{h^6}{8640}\,[E\,(30\,\bar{W}^2\,y - 60\,\bar{W}\,W\,y + 30\,W^2\,y - 18\,W'\,y' \\
& -3\,y\,W'') - 30\,\bar{W}^2\,W\,y + 60\,\bar{W}\,W^2\,y - 30\,W^3\,y \\
& +36\,y\,W'^2 - 30\,\bar{W}\,W'\,y' + 48\,W\,W'\,y' \\
& -15\,\bar{W}\,y\,W'' + 18\,W\,y\,W'' + 8\,y'\,W^{(3)} + 2\,y\,W^{(4)}] + O(h)^7,
\end{aligned} \tag{18}$$

$$\begin{aligned}
\mathrm{LTE}_{c,z} = {} & \frac{h^6}{108000}\,[-1950\,E^2\,y\,W' + 10\,E\,(-375\,\bar{W}\,y\,W' + 765\,W\,y\,W' \\
& +375\,\bar{W}^2\,y' - 750\,\bar{W}\,W\,y' + 375\,W^2\,y' - 285\,y'\,W'' - 60\,y\,W^{(3)}) \\
& +10\,(-375\,\bar{W}^2\,y\,W' + 1125\,\bar{W}\,W\,y\,W' - 945\,W^2\,y\,W' - 375\,\bar{W}^2\,W\,y' \\
& +750\,\bar{W}\,W^2\,y' - 375\,W^3\,y' + 210\,W'^2\,y' + 240\,y\,W'\,W'' \\
& +375\,\bar{W}\,y'\,W'' - 90\,W\,y'\,W'' + 125\,\bar{W}\,y\,W^{(3)} - 65\,W\,y\,W^{(3)} \\
& +5\,y'\,W^{(4)} + y\,W^{(5)})] + O(h)^7,
\end{aligned} \tag{19}$$

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

By comparing the errors we come to some conclusions: The classical method a) includes at both $y(x)$ and $z(x)$ the third power of energy (E^3, E^3). In the error of method b) the maximum power of energy is decreased from three to two at both $y(x)$ and $z(x)$ (E^2, E^2). In the error of method (c) the maximum power is one for $y(x)$ and two for $z(x)$ (E, E^2).

These conclusions are very important for large energies, because the error will be significantly smaller and that can be shown in the actual testing later on. We note that it is not the maximum power of the two functions $y(x)$, $z(x)$ that plays critical role for the error propagation rather than each of the maximums separately. That happens because the new value of the derivative y'_{n+1} needs the value of z_{n+1} and the derivative z'_{n+1} needs y_{n+1} as seen in (4). This explains the higher efficiency of method (c) opposite to method (b).

6. Numerical results

6.1. The resonance problem

In order to measure the efficiency of the two new constructed methods in comparison with classical ones, we will integrate problem (1) with $l = 0$ at the interval [0, 15] using the Woods–Saxon potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\,q}{(1+q)^2}, \quad q = \exp\left(\frac{x - x_0}{a}\right), \tag{20}$$

$$\text{where} \quad u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}$$

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

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

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x). \tag{21}$$

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

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[\sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{22}$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{23}$$

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 will try to calculate the phase shift, the accurate value of which is $\pi/2$ for the above problem. We will use two values for the energy: 989.701916 and 341.495874. As for the frequency w we will use the suggestion of Ixaru and Rizea [5]:

$$w = \begin{cases} \sqrt{E-50} & x \in [0,\ 6.5], \\ \sqrt{E} & x \in [6.5,\ 15]. \end{cases} \tag{24}$$

We present 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 two that is the dimension of the vector of the functions $y(x)$ and $z(x)$ of the resonance problem. In figure 1 we use $E = 989.701916$ and in figure 2 we use $E = 341.495874$.

6.2. Comparison

We compare the two new trigonometrically fitted methods (9) and (10) to a variety of classical Runge–Kutta methods (followed by their algebraic order): Fehlberg II (6th), Butcher (6th), Fehlberg I (5th), Kutta–Nyström (5th), England II (5th), Fehlberg 5th, Fehlberg 4th, England I (4th), Gill (4th). The coefficients of the above methods have been taken from [4]. We also compare the new developed methods to the trigonometrically fitted method of Vanden Berghe et al. [6]. Among these we present the results of England II, which is the corresponding classical method to the two new methods, the two 6th order methods

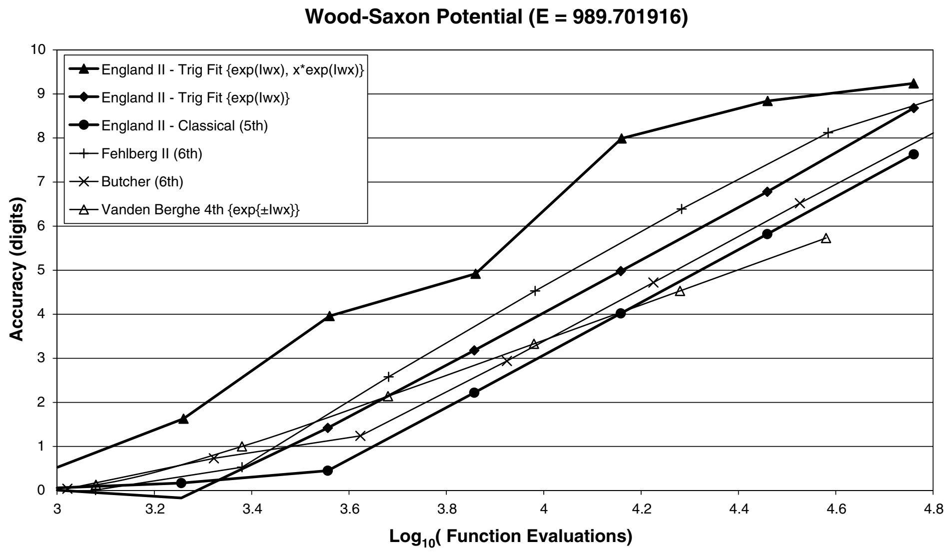

Figure 1. $-\log_{10}$(Error) for the resonance problem using $E = 989.701916$.

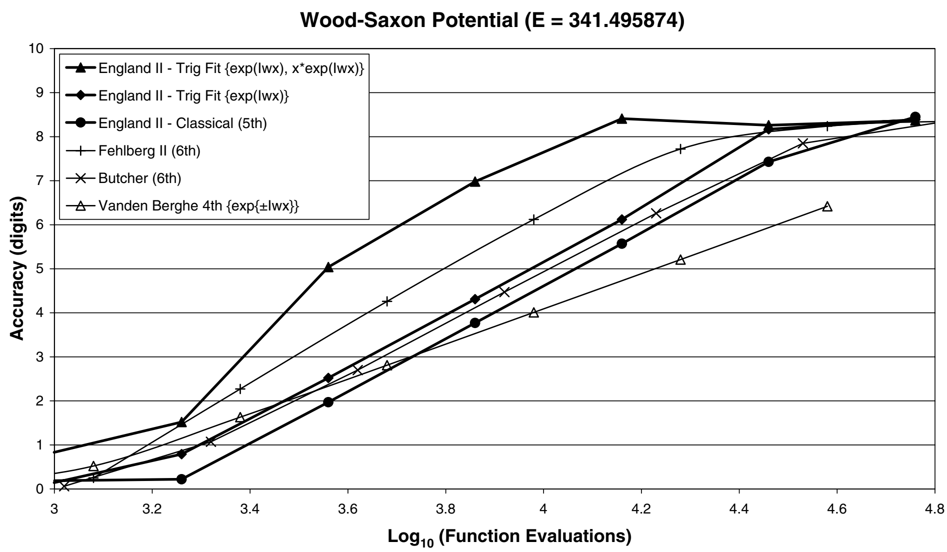

Figure 2. $-\log_{10}$(Error) for the resonance problem using $E = 341.495874$.

Fehlberg II and Butcher (despite that Fehlberg I, Kutta–Nyström (5th) and Fehlberg 5th were slightly better than the Butcher method using both energies) and the trigonometrically fitted method of Vanden Berghe et al. [6]. Method (9) was more efficient than all the methods of the same or lower algebraic order (5th) using high energy ($E = 989.701916$) and was also better than all the 5th and

4th order methods except for Fehlberg I and Fehlberg 5th using lower energy ($E = 341.495874$). The method was better than the 6th order method of Butcher using both energies. The second method constructed (10) was the most efficient of all with high difference from second best Fehlberg II. Again we mention that the main reason for this high efficiency is that we meet lower powers of energy E in the local truncation error of the new methods than in classical methods.

References

[1] E. Hairer, S.P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations I, Nonstiff Problems* (Springer-Verlag, Berlin, Heidelberg, 1993).
[2] T.E. Simos, An exponentially fiited Runge–Kutta method for the numerical integration of initial-value problems with periodic or oscillating solutions (1998).
[3] T. Lyche, Numer. Math. 19 (1972) 65.
[4] G. Engeln-Müllges, F. Uhlig, *Numerical Algorithms with Fortran* (Springer-Verlag, Berlin Heidelberg, 1996) p. 423.
[5] L.Gr. Ixaru and M. Rizea, Comp. Phys. Comm. 19 (1980) 23.
[6] G. Vanden Berghe, H. De Meyer, M. Van Daele and T. Van Hecke, Comp. Phys. Comm. 123 (1999) 7.