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A family of exponentially-fitted Runge–Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation

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We have constructed three Runge–Kutta methods based on a classical method of Fehlberg with eight stages and sixth algebraic order. These methods have exponential order one, two and three. We show through the error analysis of the methods that by increasing the exponential order, the maximum power of the energy in the error expression decreases. So the higher the exponential order the smaller the local truncation error of the method compared to the corresponding classical method. The difference is higher for higher values of energy. The results confirm this, when integrating the resonance problem of the one-dimensional time-independent Schrödinger equation.

KEY WORDS: Trigonometrical-fitting, Exponential-fitting, Schrödinger equation, Runge–Kutta, Explicit methods, Exponential order

Abbreviations: LTE – Local truncation error.

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1. Introduction

Much research has been done on the numerical integration of the radial Schrödinger equation (see for more details [1–36]):

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

where $\frac{l(l+1)}{x^2}$ is the *centrifugal potential*, $V(x)$ the *potential*, E 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 $\lim_{x\to\infty} W(x) = 0$.

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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 $\overline{W}_i$. After this the problem (1) can be expressed by the approximation

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

This form of Schrödinger equation reveals the importance of exponential fitting when constructing new methods. Related work can be found at [5–8]. In the next section, 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:

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

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 sets of equation (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:

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

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

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

Definition 1 [37]. 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: $y^{(n)}(x) = y^{(n)}_{\text{app.}}(x), \;\; n = 1, 2, \dots, p$.

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

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

where u is a continuously differentiable function.

Definition 2 [1]. 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 $\exp(\omega_0 x), \exp(\omega_1 x), \dots, \exp(\omega_p x)$, where $\omega_i | i = 0(1)p$ are real or complex numbers.

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

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

Definition 3 [1]. The corresponding algebraic method is called the classical method.

When we use an imaginary number for frequency, that is Iw, then $\exp(Iwx)$ can be expanded to $\cos(wx) + I\sin(wx)$, so we refer to a method that integrates exactly these functions as a trigonometrically fitted method.

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

We consider the explicit Runge–Kutta method Fehlberg II [3], which has eight stages and sixth algebraic order. The coefficients are shown in table (8).

$$
\begin{array}{c|cccccccc}
\frac{1}{6} & \frac{1}{6} & & & & & & & \\
\frac{4}{15} & \frac{4}{75} & \frac{16}{75} & & & & & & \\
\frac{2}{3} & \frac{5}{6} & \frac{-8}{3} & \frac{5}{2} & & & & & \\
\frac{4}{5} & \frac{-8}{5} & \frac{144}{25} & -4 & \frac{16}{25} & & & & \\
1 & \frac{361}{320} & \frac{-18}{5} & \frac{407}{128} & \frac{-11}{80} & \frac{55}{128} & & & \\
0 & \frac{-11}{640} & 0 & \frac{11}{256} & \frac{-11}{160} & \frac{11}{256} & 0 & & \\
1 & \frac{93}{640} & \frac{-18}{5} & \frac{803}{256} & \frac{-11}{160} & \frac{99}{256} & 0 & 1 & \\
\hline
 & \frac{7}{1408} & 0 & \frac{1125}{2816} & \frac{9}{32} & \frac{125}{768} & 0 & \frac{5}{66} & \frac{5}{66}
\end{array}
\qquad (8)
$$

We will construct three trigonometrically fitted methods.

3.1. *First-order trigonometrically fitted method*

We want the first method to integrate exactly the functions:

$\{1, x, x^2, x^3, x^4, x^5, x^6, \exp(Iwx)\}$ or equivalently
$\{1, x, x^2, x^3, x^4, x^5, x^6, \cos(wx), \sin(wx)\}$,

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

To achieve this we free the two coefficients b_7 and b_8 and leave the other coefficients the same as the classical method. Then we demand the approximate solution $y_{\text{app.}}$ to integrate exactly $\exp(Iwx)$ for the real and the imaginary part. From these two equations we derive b_7 and b_8.

The method has exponential order one and all the coefficients are the same as (8) except for:

$$b_7 = \frac{b_{7,\text{num}}}{b_{7,\text{den}}} \quad \text{and} \quad b_8 = \frac{b_{8,\text{num}}}{b_{8,\text{den}}},$$

where

$$\begin{aligned} b_{7,\text{num}} = & -229900\, v^{10} + 8551125\, v^8 \\ & + (-103504500 - 6534000 \cos(v))\, v^6 + 42471000 \sin(v)\, v^5 \\ & + (-16335000 \cos(v) + 225720000)\, v^4 - 588060000 \sin(v)\, v^3 \\ & + (202500000 - 1336500000 \cos(v))\, v^2 + 2673000000 \sin(v)\, v \\ & + 2673000000 \cos(v) - 2673000000, \end{aligned} \tag{9}$$

$$\begin{aligned} b_{8,\text{num}} = & \, 60500\, v^{10} - 1249875\, v^8 + 12474000\, v^6 \\ & - 6534000 \sin(v)\, v^5 + (50490000 + 16335000 \cos(v))\, v^4 \\ & - 1134000000\, v^2 + 2673000000 - 2673000000 \cos(v), \end{aligned}$$

$$\begin{aligned} b_{7,\text{den}} = b_{8,\text{den}} = & \, 15972\, v^{12} - 219615\, v^{10} + 6860700\, v^8 \\ & + 19602000\, v^6 - 588060000\, v^4 + 2673000000\, v^2, \end{aligned}$$

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

3.2. *Second-order trigonometrically fitted method*

The second method we construct will integrate exactly the functions:

$\{1, x, x^2, x^3, x^4, x^5, x^6, \exp(Iwx), x\exp(Iwx)\}$ or equivalently
$\{1, x, x^2, x^3, x^4, x^5, x^6, \cos(wx), \sin(wx), x\cos(wx), x\sin(wx)\}$.

To achieve this we free the four coefficients b_5, b_6, b_7 and b_8 and leave the other coefficients the same as the classical method. Then we demand the approximate solution $y_{\text{app.}}$ To integrate exactly $\exp(Iwx)$ and $x\exp(Iwx)$ for the real and the imaginary part. From these four equations we derive b_5, b_6, b_7 and b_8.

The method has exponential order two and all the coefficients are the same as (8) except for:

$$b_i = \frac{b_{i,\mathrm{num}}}{b_{i,\mathrm{den}}}, \quad i = \{5, 6, 7, 8\}, \tag{10}$$

where

$$\begin{aligned} b_{5,\mathrm{num}} = {} & 387200\, v^{14} - 6336000\, v^{12} - 7744000 \sin(v)\, v^{11} \\ & + (-181557750 - 81312000 \cos(v))\, v^{10} + 489456000 \sin(v)\, v^{9} \\ & + (1397880000 \cos(v) + 4933479375)\, v^{8} + 3247200000 \sin(v)\, v^{7} \\ & + (-40977112500 + 29818800000 \cos(v))\, v^{6} \\ & - 57024000000 \sin(v)\, v^{5} + 329184000000 \sin(v)\, v^{3} \\ & + (286713000000 - 147312000000 \cos(v))\, v^{4} \\ & + (900720000000 \cos(v) - 1354320000000)\, v^{2} \\ & + 129600000000 \sin(v)\, v - 648000000000 \cos(v) + 648000000000, \end{aligned}$$

$$\begin{aligned} b_{6,\mathrm{num}} = {} & -77440\, v^{16} + 2692800\, v^{14} + 1548800 \sin(v)\, v^{13} \\ & + (9292800 \cos(v) - 29315550)\, v^{12} - 17424000 \sin(v)\, v^{11} \\ & + (660441375 - 8712000 \cos(v))\, v^{10} - 452925000 \sin(v)\, v^{9} \\ & + (-14134387500 - 2035440000 \cos(v))\, v^{8} \\ & - 3984997500 \sin(v)\, v^{7} + 149910750000 \sin(v)\, v^{5} \\ & + (-58382775000 \cos(v) + 94984650000)\, v^{6} \\ & + (-682141500000 + 478021500000 \cos(v))\, v^{4} \\ & - 774562500000 \sin(v)\, v^{3} - 1166400000000 \sin(v)\, v \\ & + (2431215000000 - 1629315000000 \cos(v))\, v^{2} \\ & + 729000000000 - 729000000000 \cos(v), \end{aligned}$$

$$\begin{aligned} b_{7,\mathrm{num}} = {} & 387200\, v^{14} - 13464000\, v^{12} - 7744000 \sin(v)\, v^{11} \\ & + (136281750 - 46464000 \cos(v))\, v^{10} + 156816000 \sin(v)\, v^{9} \\ & + (-860569875 + 775368000 \cos(v))\, v^{8} - 1346895000 \sin(v)\, v^{7} \\ & + (6082666875 - 752400000 \cos(v))\, v^{6} - 5775907500 \sin(v)\, v^{5} \\ & + (6040237500 \cos(v) - 15862500)\, v^{4} - 29180250000 \sin(v)\, v^{3} \\ & + (-42211125000 \cos(v) + 50007375000)\, v^{2} \\ & - 2227500000 \sin(v)\, v - 11137500000 + 11137500000 \cos(v), \end{aligned}$$

$$
\begin{aligned}
b_{8,\text{num}} = {} & 3564000\,v^{12} + (-225027000 - 34848000\cos(v))\,v^{10} \\
& +209880000\sin(v)\,v^{9} + (508860000\cos(v) + 4504809375)\,v^{8} \\
& +2530440000\sin(v)\,v^{7} + (21758962500\cos(v) - 31628306250)\,v^{6} \\
& -47278687500\sin(v)\,v^{5} + 189185625000\sin(v)\,v^{3} \\
& +(-135988875000\cos(v) + 202611375000)\,v^{4} \\
& +(429603750000\cos(v) - 630078750000)\,v^{2} \\
& +291600000000\sin(v)\,v - 182250000000 + 182250000000\cos(v)\,,
\end{aligned}
$$

$$
b_{5,\text{den}} = 256\,A, \qquad b_{6,\text{den}} = 44\,v^2 A,
$$

$$
b_{7,\text{den}} = 22\,A, \qquad b_{8,den} = 11\,v^2 A,
$$

$$
\begin{aligned}
A = {} & 15488\,v^{14} - 218240\,v^{12} - 668250\,v^{10} - 14367375\,v^{8} \\
& -237127500\,v^{6} - 729000000\,v^{4},
\end{aligned} \tag{11}
$$

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

3.3. Third-order trigonometrically fitted method

The third method we construct will integrate exactly the functions:

$\{1,\ x,\ x^2,\ x^3,\ x^4,\ x^5,\ x^6,\ \exp(Iwx),\ x\exp(Iwx),\ x^2\exp(Iwx)\}$
or equivalently
$\{1,\ x,\ x^2,\ x^3,\ x^4,\ x^5,\ x^6,\ \cos(wx),\ \sin(wx),\ x\cos(wx),\ x\sin(wx)$
$x^2\cos(wx),\ x^2\sin(wx)\}$.

To achieve this we free all eight coefficients $b_i,\ i=1(1)8$ and leave the other coefficients the same as the classical method. Then we demand the approximate solution $y_{\text{app.}}$ to integrate exactly $\exp(Iwx)$, $x\exp(Iwx)$ and $x^2\exp(Iwx)$ for the real and the imaginary part and also we demand $b_2 = b_6$ and $b_7 = b_8$ as the coefficients of the classical method indicate. From these eight equations we derive the values of $b_i,\ i = 1(1)8$.

The new method has exponential order three and all of its coefficients are the same as (8) except for:

$$
\begin{aligned}
& b_i = \frac{b_{i,\text{num}}}{b_{i,\text{den}}}, \quad i = \{1, 2, 3, 4, 5, 7\}, \\
& b_6 = b_2 \quad \text{and} \quad b_8 = b_7,
\end{aligned}
$$

where

$$\begin{aligned}
b_{1,\text{num}} &= 30976\cos(v)\,v^{12} - 511104\sin(v)\,v^{11}\\
&\quad + (743424 - 5215584\cos(v))\,v^{10} + 28517280\sin(v)\,v^{9}\\
&\quad + (-54362880 + 107207760\cos(v))\,v^{8} - 293676900\sin(v)\,v^{7}\\
&\quad + (-442247190\cos(v) + 600483840)\,v^{6} - 176744700\sin(v)\,v^{5}\\
&\quad + (-323611200 - 691126425\cos(v))\,v^{4} + 2988191250\sin(v)\,v^{3}\\
&\quad + (-3090433500 + 4307104125\cos(v))\,v^{2} - 944510625\sin(v)\,v\\
&\quad -544320000 + 544320000\cos(v)\,,\\
b_{2,\text{num}} &= 1200\cos(v)\,v^{6} - 12600\sin(v)\,v^{5} - 65250\cos(v)\,v^{4}\\
&\quad +190125\sin(v)\,v^{3} + (246375\cos(v) - 216000)\,v^{2}\\
&\quad +50625\sin(v)\,v + 162000\cos(v) - 162000,
\end{aligned}\tag{12}$$

$$\begin{aligned}
b_{3,\text{num}} &= 116160\cos(v)\,v^{10} - 1045440\sin(v)\,v^{9}\\
&\quad + (-5183640\cos(v) + 2787840)\,v^{8} + 16443900\sin(v)\,v^{7}\\
&\quad + (28195200\cos(v) - 36590400)\,v^{6} + 1014750\sin(v)\,v^{5}\\
&\quad + (19975725\cos(v) + 29660400)\,v^{4} - 157038750\sin(v)\,v^{3}\\
&\quad + (-235612125\cos(v) + 169141500)\,v^{2} + 58370625\sin(v)\,v\\
&\quad +16200000 - 16200000\cos(v),\\
b_{4,\text{num}} &= 7920\cos(v)\,v^{8} - 55440\sin(v)\,v^{7}\\
&\quad + (-164340\cos(v) + 95040)\,v^{6} + 362340\sin(v)\,v^{5}\\
&\quad + (443835\cos(v) - 736560)\,v^{4} + 645750\sin(v)\,v^{3}\\
&\quad + (-483300 + 925425\cos(v))\,v^{2} - 874125\sin(v)\,v\\
&\quad -864000\cos(v) + 864000,\\
b_{5,\text{num}} &= 6600\cos(v)\,v^{8} - 9900\sin(v)\,v^{7}\\
&\quad + (364100\cos(v) + 158400)\,v^{6} - 1493250\sin(v)\,v^{5}\\
&\quad + (-1748625\cos(v) + 2046000)\,v^{4} - 611250\sin(v)\,v^{3}\\
&\quad + (976500 - 528375\cos(v))\,v^{2} - 148125\sin(v)\,v\\
&\quad +600000\cos(v) - 600000,\\
b_{7,\text{num}} &= 4400\cos(v)\,v^{6} + 26400\sin(v)\,v^{5}\\
&\quad + (105600 + 323400\cos(v))\,v^{4} - 1146750\sin(v)\,v^{3}\\
&\quad + (1188000 - 1477875\cos(v))\,v^{2} - 35625\sin(v)\,v\\
&\quad +651000 - 651000\cos(v)\,,\\
b_{1,\text{den}} &= 31680\,A, \qquad b_{2,\text{den}} = 2\,A, \qquad b_{3,\text{den}} = 1408\,A,\\
b_{4,\text{den}} &= 16\,A, \qquad b_{5,\text{den}} = 128\,A, \qquad b_{7,\text{den}} = 11\,A,\\
A &= 176\,v^{10} - 660\,v^{8} - 895\,v^{6},
\end{aligned}\tag{13}$$

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, so we use the Taylor series expansions of the coefficients around zero.

4. Algebraic order of the new methods

The following 37 equations must be satisfied so that the new methods maintain the sixth algebraic order of the corresponding classical method (8). The number of stages is symbolized by s, where $s = 8$. Then we are presenting the Taylor series expansions of the remainders of these equations, that is the difference of the right part minus the left part.

First Algebraic Order (one equation)

$$\sum_{i=1}^{s} b_i = 1.$$

Second Algebraic Order (two equations)

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

Third Algebraic Order (four equations)

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

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

Fourth Algebraic Order (eight equations)

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

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

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

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

Fifth Algebraic Order (17)

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

Sixth Algebraic Order (37)

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

$$\sum_{i,j=1}^{s} b_i {c_i}^3 a_{ij} c_j = \frac{1}{12},$$

$$\sum_{i,j=1}^{s} b_i {c_i}^2 a_{ij} {c_j}^2 = \frac{1}{18},$$

$$\sum_{i,j,k=1}^{s} b_i c_i a_{ij} c_j a_{ik} c_k = \frac{1}{24},$$

$$\sum_{i,j,k=1}^{s} b_i {c_i}^2 a_{ij} a_{jk} c_k = \frac{1}{36},$$

$$\sum_{i,j=1}^{s} b_i c_i a_{ij} {c_j}^3 = \frac{1}{24},$$

$$\sum_{i,j,k=1}^{s} b_i c_i a_{ij} c_j a_{jk} c_k = \frac{1}{48}, \qquad (14)$$

$$\sum_{i,j,k=1}^{s} b_i a_{ij} c_j a_{ik} {c_k}^2 = \frac{1}{36},$$

$$\sum_{i,j,k,l=1}^{s} b_i c_i a_{ij} a_{jk} a_{kl} c_l = \frac{1}{144},$$

$$\sum_{i,j,k,l=1}^{s} b_i a_{ij} c_j a_{ik} a_{kl} c_l = \frac{1}{72},$$

$$\sum_{i,j,k=1}^{s} b_i c_i a_{ij} a_{jk} {c_k}^2 = \frac{1}{72},$$

$$\sum_{i,j=1}^{s} b_i a_{ij} {c_j}^4 = \frac{1}{30},$$

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

$$\sum_{i,j=1}^{s} b_i c_i^2 a_{ij} c_j = \tfrac{1}{10}, \qquad \sum_{i,j,k=1}^{s} b_i a_{ij} c_j a_{jk} {c_k}^2 = \tfrac{1}{90},$$
$$\sum_{i,j=1}^{s} b_i c_i a_{ij} c_j^2 = \tfrac{1}{15}, \qquad \sum_{i,j,k,l=1}^{s} b_i a_{ij} c_j a_{jk} a_{kl} c_l = \tfrac{1}{180},$$
$$\sum_{i,j,k=1}^{s} b_i c_i a_{ij} a_{jk} c_k = \tfrac{1}{30}, \qquad \sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} c_k a_{jl} c_l = \tfrac{1}{120},$$
$$\sum_{i,j=1}^{s} b_i a_{ij} c_j^3 = \tfrac{1}{20}, \qquad \sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} {c_k}^3 = \tfrac{1}{120},$$
$$\sum_{i,j,k=1}^{s} b_i a_{ij} c_j a_{jk} c_k = \tfrac{1}{40}, \qquad \sum_{i,j,k,l=1}^{s} b_i a_{ij} a_{jk} c_k a_{kl} c_l = \tfrac{1}{240},$$
$$\sum_{i,j,k=1}^{s} b_i c_i a_{ij} a_{jk} c_k^2 = \tfrac{1}{60}, \qquad \sum_{i,j,k,l=1}^{s} b_i a_{ij} a_{jk} a_{kl} {c_l}^2 = \tfrac{1}{360},$$
$$\sum_{i,j,k,l=1}^{s} b_i a_{ij} a_{jk} a_{kl} c_l = \tfrac{1}{120}, \qquad \sum_{i,j,k,l,m=1}^{s} b_i a_{ij} a_{jk} a_{kl} a_{lm} c_m = \tfrac{1}{720}.$$
$$\sum_{i,j,k=1}^{s} b_i a_{ij} c_j a_{ik} c_k = \tfrac{1}{20}.$$

4.1. Equations remainders for the first method

We are presenting the remainders of the 37 equations, for the first method (9):

$$\text{Rem}_1 = -\frac{1}{75600}v^6 - \frac{1}{103680}v^8 - \frac{1009}{374220000}v^{10} + \cdots,$$
$$\text{Rem}_2 = -\frac{1}{40320}v^6 - \frac{47}{9072000}v^8 - \frac{11617}{14968800000}v^{10} + \cdots,$$
$$\text{Rem}_3 = -\frac{1}{40320}v^6 - \frac{47}{9072000}v^8 - \frac{11617}{14968800000}v^{10} + \cdots,$$
$$\text{Rem}_4 = -\frac{1}{80640}v^6 - \frac{47}{18144000}v^8 - \frac{11617}{29937600000}v^{10} + \cdots,$$
$$\text{Rem}_5 = -\frac{1}{40320}v^6 - \frac{47}{9072000}v^8 - \frac{11617}{14968800000}v^{10} + \cdots,$$
$$\text{Rem}_6 = -\frac{1}{80640}v^6 - \frac{47}{18144000}v^8 - \frac{11617}{29937600000}v^{10} + \cdots,$$
$$\text{Rem}_7 = -\frac{17}{2016000}v^6 - \frac{799}{453600000}v^8 - \frac{197489}{748440000000}v^{10} + \cdots,$$
$$\text{Rem}_8 = -\frac{11}{2016000}v^6 - \frac{517}{453600000}v^8 - \frac{11617}{68040000000}v^{10} + \cdots,$$
$$\text{Rem}_9 = -\frac{1}{40320}v^6 - \frac{47}{9072000}v^8 - \frac{11617}{14968800000}v^{10} + \cdots,$$
$$\text{Rem}_{10} = -\frac{1}{80640}v^6 - \frac{47}{18144000}v^8 - \frac{11617}{29937600000}v^{10} + \cdots,$$

$$
\begin{aligned}
\mathrm{Rem}_{11} &= -\frac{17}{2016000}\, v^6 - \frac{799}{453600000}\, v^8 - \frac{197489}{748440000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{12} &= -\frac{11}{2016000}\, v^6 - \frac{517}{453600000}\, v^8 - \frac{11617}{68040000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{13} &= -\frac{14803}{2721600000}\, v^6 - \frac{94139}{81648000000}\, v^8 - \frac{11840237}{67359600000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{14} &= -\frac{1991}{680400000}\, v^6 - \frac{101189}{163296000000}\, v^8 - \frac{144449}{1530900000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{15} &= -\frac{11}{6048000}\, v^6 - \frac{517}{1360800000}\, v^8 - \frac{11617}{204120000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{16} &= \frac{11}{136080000}\, v^6 + \frac{11}{186624000}\, v^8 + \frac{1009}{61236000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{17} &= -\frac{1}{161280}\, v^6 - \frac{47}{36288000}\, v^8 - \frac{11617}{59875200000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{18} &= -\frac{1}{40320}\, v^6 - \frac{47}{9072000}\, v^8 - \frac{11617}{14968800000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{19} &= -\frac{1}{80640}\, v^6 - \frac{47}{18144000}\, v^8 - \frac{11617}{29937600000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{20} &= -\frac{17}{2016000}\, v^6 - \frac{799}{453600000}\, v^8 - \frac{197489}{748440000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{21} &= -\frac{1}{161280}\, v^6 - \frac{47}{36288000}\, v^8 - \frac{11617}{59875200000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{22} &= -\frac{11}{2016000}\, v^6 - \frac{517}{453600000}\, v^8 - \frac{11617}{68040000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{23} &= -\frac{31}{5670000}\, v^6 - \frac{1457}{1275750000}\, v^8 - \frac{360127}{2104987500000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{24} &= -\frac{1067}{362880000}\, v^6 - \frac{50149}{81648000000}\, v^8 - \frac{1126849}{12247200000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{25} &= -\frac{17}{4032000}\, v^6 - \frac{799}{907200000}\, v^8 - \frac{197489}{1496880000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{26} &= \frac{11}{72576000}\, v^6 + \frac{517}{16329600000}\, v^8 + \frac{11617}{2449440000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{27} &= -\frac{11}{4032000}\, v^6 - \frac{517}{907200000}\, v^8 - \frac{11617}{136080000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{28} &= -\frac{11}{6048000}\, v^6 - \frac{517}{1360800000}\, v^8 - \frac{11617}{204120000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{29} &= -\frac{315751}{81648000000}\, v^6 - \frac{205013}{244944000000}\, v^8 - \frac{52816117}{404157600000000}\, v^{10} + \cdots ,\\
\mathrm{Rem}_{30} &= -\frac{10043}{5103000000}\, v^6 - \frac{104269}{244944000000}\, v^8 - \frac{152521}{2296350000000}\, v^{10} + \cdots ,
\end{aligned} \tag{15}
$$

$$\text{Rem}_{31} = -\frac{2497}{2041200000}\,v^6 - \frac{12793}{48988800000}\,v^8 - \frac{5267}{131220000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{32} = \frac{11}{204120000}\,v^6 + \frac{11}{279936000}\,v^8 + \frac{1009}{91854000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{33} = -\frac{10043}{10206000000}\,v^6 - \frac{104269}{489888000000}\,v^8 - \frac{152521}{4592700000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{34} = -\frac{209}{151200000}\,v^6 - \frac{51271}{163296000000}\,v^8 - \frac{158057}{3061800000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{35} = -\frac{8591}{16329600000}\,v^6 - \frac{7073}{61236000000}\,v^8 - \frac{673187}{36741600000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{36} = -\frac{1529}{4082400000}\,v^6 - \frac{20537}{244944000000}\,v^8 - \frac{17819}{1312200000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{37} = -\frac{1991}{5443200000}\,v^6 - \frac{1903}{20412000000}\,v^8 - \frac{208507}{12247200000000}\,v^{10} + \cdots,$$

4.2. Equations remainders for the second method

The remainders of the equations for the second method (10) are:

$$\text{Rem}_{1} = \frac{179}{7257600}\,v^6 - \frac{190937}{26127360000}\,v^8 - \frac{7933014923}{1034643456000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{2} = \frac{1891}{36288000}\,v^6 - \frac{4442611}{130636800000}\,v^8 + \frac{58386844871}{5173217280000000}\,v^{10} + \cdots,$$
$$\text{Rem}_{3} = \frac{131}{1814400}\,v^4 - \frac{128297}{6531840000}\,v^6 - \frac{1730673563}{258660864000000}\,v^8 + \cdots,$$
$$\text{Rem}_{4} = \frac{131}{3628800}\,v^4 - \frac{128297}{13063680000}\,v^6 - \frac{1730673563}{517321728000000}\,v^8 + \cdots,$$
$$\text{Rem}_{5} = \frac{131}{1008000}\,v^4 - \frac{279577}{3628800000}\,v^6 + \frac{2178824117}{143700480000000}\,v^8 + \cdots,$$
$$\text{Rem}_{6} = \frac{131}{2016000}\,v^4 - \frac{279577}{7257600000}\,v^6 + \frac{2178824117}{287400960000000}\,v^8 + \cdots,$$
$$\text{Rem}_{7} = \frac{131}{2592000}\,v^4 - \frac{2123447}{65318400000}\,v^6 + \frac{19552216267}{2586608640000000}\,v^8 + \cdots,$$
$$\text{Rem}_{8} = \frac{1441}{18144000}\,v^4 - \frac{4406611}{65318400000}\,v^6 + \frac{758060323}{33592320000000}\,v^8 + \cdots,$$
$$\text{Rem}_{9} = \frac{7991}{45360000}\,v^4 - \frac{20079797}{163296000000}\,v^6 + \frac{211098224737}{6466521600000000}\,v^8 + \cdots,$$
$$\text{Rem}_{10} = \frac{7991}{90720000}\,v^4 - \frac{20079797}{326592000000}\,v^6 + \frac{211098224737}{12933043200000000}\,v^8 + \cdots,$$
$$\text{Rem}_{11} = \frac{131}{2016000}\,v^4 - \frac{113363}{2419200000}\,v^6 + \frac{415847021}{31933440000000}\,v^8 + \cdots,$$

$$
\begin{aligned}
\mathrm{Rem}_{12} &= \frac{1441}{18144000}\,v^4 - \frac{4406611}{65318400000}\,v^6 + \frac{758060323}{33592320000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{13} &= \frac{13}{18144000}\,v^2 + \frac{342497}{65318400000}\,v^4 - \frac{535592317}{2586608640000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{14} &= \frac{13}{36288000}\,v^2 + \frac{1521497}{130636800000}\,v^4 - \frac{6384015331}{739031040000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{15} &= \frac{131}{18144000}\,v^4 - \frac{6259}{1866240000}\,v^6 + \frac{123005009}{517321728000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{16} &= -\frac{13}{7257600}\,v^2 - \frac{12377}{26127360000}\,v^4 + \frac{2418312931}{147806208000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{17} &= \frac{7991}{181440000}\,v^4 - \frac{20079797}{653184000000}\,v^6 + \frac{211098224737}{25866086400000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{18} &= \frac{5371}{25200000}\,v^4 - \frac{689917}{4320000000}\,v^6 + \frac{18613526933}{399168000000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{19} &= \frac{5371}{50400000}\,v^4 - \frac{689917}{8640000000}\,v^6 + \frac{18613526933}{798336000000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{20} &= \frac{6943}{90720000}\,v^4 - \frac{19053421}{326592000000}\,v^6 + \frac{224943613241}{12933043200000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{21} &= \frac{5371}{100800000}\,v^4 - \frac{689917}{17280000000}\,v^6 + \frac{18613526933}{1596672000000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{22} &= \frac{1441}{18144000}\,v^4 - \frac{4406611}{65318400000}\,v^6 + \frac{758060323}{33592320000000}\,v^8 + \cdots, \qquad (16)\\
\mathrm{Rem}_{23} &= \frac{13}{18144000}\,v^2 + \frac{1156007}{65318400000}\,v^4 - \frac{32377375147}{2586608640000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{24} &= \frac{13}{36288000}\,v^2 + \frac{2177807}{130636800000}\,v^4 - \frac{70343353747}{5173217280000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{25} &= \frac{6943}{181440000}\,v^4 - \frac{19053421}{653184000000}\,v^6 + \frac{224943613241}{25866086400000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{26} &= -\frac{13}{7257600}\,v^2 + \frac{136177}{26127360000}\,v^4 + \frac{10908370579}{1034643456000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{27} &= \frac{1441}{36288000}\,v^4 - \frac{4406611}{130636800000}\,v^6 + \frac{758060323}{67184640000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{28} &= \frac{3013}{272160000}\,v^4 - \frac{7035391}{979776000000}\,v^6 + \frac{65750945411}{38799129600000000}\,v^8 + \cdots,\\
\mathrm{Rem}_{29} &= \frac{169}{136080000}\,v^2 - \frac{5840209}{489888000000}\,v^4 + \frac{171450578549}{19399564800000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{30} &= \frac{169}{272160000}\,v^2 - \frac{4366459}{979776000000}\,v^4 + \frac{116259934799}{38799129600000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{31} &= \frac{13}{54432000}\,v^2 - \frac{553543}{195955200000}\,v^4 + \frac{25112610923}{7759825920000000}\,v^6 + \cdots,\\
\mathrm{Rem}_{32} &= -\frac{13}{10886400}\,v^2 - \frac{12377}{39191040000}\,v^4 + \frac{2418312931}{221709312000000}\,v^6 + \cdots,
\end{aligned}
$$

$$\mathrm{Rem}_{33} = \frac{169}{544320000}v^2 - \frac{4366459}{1959552000000}v^4 + \frac{116259934799}{7759825920000000}v^6 + \cdots,$$
$$\mathrm{Rem}_{34} = \frac{13}{36288000}v^2 + \frac{931997}{130636800000}v^4 - \frac{38310073897}{5173217280000000}v^6 + \cdots,$$
$$\mathrm{Rem}_{35} = -\frac{13}{108864000}v^2 + \frac{1131253}{391910400000}v^4 - \frac{10807147553}{15519651840000000}v^6 + \cdots,$$
$$\mathrm{Rem}_{36} = \frac{13}{54432000}v^2 - \frac{459223}{195955200000}v^4 + \frac{7562199803}{7759825920000000}v^6 + \cdots,$$
$$\mathrm{Rem}_{37} = \frac{13}{5184000}v^2 - \frac{4334611}{130636800000}v^4 + \frac{58343644871}{5173217280000000}v^6 + \cdots,$$

4.3. Equations remainders for the third method

The remainders of the equations for the third method (12) are:

$$\mathrm{Rem}_{1} = -\frac{1}{75600}v^6 + \frac{3253}{108259200}v^8 - \frac{50613137}{3197435472000}v^{10} + \cdots,$$
$$\mathrm{Rem}_{2} = -\frac{1}{40320}v^6 + \frac{1}{1209600}v^8 - \frac{1}{79833600}v^{10} + \cdots,$$
$$\mathrm{Rem}_{3} = -\frac{65}{240576}v^2 + \frac{90661}{1614866400}v^4 + \frac{186194591}{6937466054400}v^6 + \cdots,$$
$$\mathrm{Rem}_{4} = -\frac{1}{25200}v^4 + \frac{14191}{162388800}v^6 - \frac{101066069}{2131623648000}v^8 + \cdots,$$
$$\mathrm{Rem}_{5} = -\frac{21017}{36086400}v^2 - \frac{5311711}{24222996000}v^4 + \frac{2700188661011}{6868091393856000}v^6 + \cdots,$$
$$\mathrm{Rem}_{6} = -\frac{101}{375900}v^2 - \frac{3905849}{32297328000}v^4 + \frac{89672869973}{429255712116000}v^6 + \cdots,$$
$$\mathrm{Rem}_{7} = -\frac{101}{601440}v^2 - \frac{137077}{1614866400}v^4 + \frac{561638351}{4292557121160}v^6 + \cdots,$$
$$\mathrm{Rem}_{8} = -\frac{1}{13440}v^4 + \frac{1}{453600}v^6 - \frac{1}{31933440}v^8 + \cdots,$$
$$\mathrm{Rem}_{9} = -\frac{810109}{1082592000}v^2 - \frac{774398371}{1453379760000}v^4 + \frac{158233575147871}{206042741815680000}v^6 + \cdots,$$
$$\mathrm{Rem}_{10} = -\frac{4177}{11277000}v^2 - \frac{64989083}{242229960000}v^4 + \frac{4971259094953}{12877671363480000}v^6 + \cdots,$$
$$\mathrm{Rem}_{11} = -\frac{77}{322200}v^2 - \frac{9106091}{48445992000}v^4 + \frac{663766104521}{2575534272696000}v^6 + \cdots,$$
$$\mathrm{Rem}_{12} = -\frac{3}{50120}v^2 - \frac{1571929}{9689198400}v^4 + \frac{22591316081}{171702284846400}v^6 + \cdots,$$
$$\mathrm{Rem}_{13} = -\frac{4097}{18043200}v^2 - \frac{1754467}{19378396800}v^4 + \frac{483887337071}{2575534272696000}v^6 + \cdots,$$
$$\mathrm{Rem}_{14} = -\frac{449}{4510800}v^2 - \frac{61279}{1211149800}v^4 + \frac{143205387947}{1717022848464000}v^6 + \cdots,$$

$$\mathrm{Rem}_{15} = -\frac{101}{1503600}\,v^2 - \frac{207229}{9689198400}\,v^4 + \frac{39677081023}{858511424232000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{16} = -\frac{1}{25200}\,v^2 + \frac{277}{3383100}\,v^4 - \frac{151198591}{3197435472000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{17} = -\frac{4177}{22554000}\,v^2 - \frac{64989083}{484459920000}\,v^4 + \frac{4971259094953}{25755342726960000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{18} = -\frac{26905649}{32477760000}\,v^2 - \frac{34542927323}{43601392800000}\,v^4 + \frac{1314055254343807}{1236256450894080000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{19} = -\frac{69961}{169155000}\,v^2 - \frac{7502231}{18924215625}\,v^4 + \frac{20545343284913}{38633014090440000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{20} = -\frac{9167}{33831000}\,v^2 - \frac{200109169}{726689880000}\,v^4 + \frac{2778542002471}{7726602818088000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{21} = -\frac{69961}{338310000}\,v^2 - \frac{7502231}{37848431250}\,v^4 + \frac{20545343284913}{77266028180880000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{22} = -\frac{1}{10024}\,v^2 - \frac{32089}{145337976}\,v^4 + \frac{112199515657}{515106854539200}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{23} = -\frac{68419}{270648000}\,v^2 - \frac{39196631}{290675952000}\,v^4 + \frac{35200039930967}{154532056361760000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{24} = -\frac{21013}{180432000}\,v^2 - \frac{4580983}{58135190400}\,v^4 + \frac{11779924570019}{103021370907840000}\,v^6 + \cdots, \quad (17)$$
$$\mathrm{Rem}_{25} = -\frac{9167}{67662000}\,v^2 - \frac{200109169}{1453379760000}\,v^4 + \frac{2778542002471}{15453205636176000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{26} = \frac{4457}{180432000}\,v^2 + \frac{2912477}{96891984000}\,v^4 + \frac{41956293403}{34340456969280000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{27} = -\frac{1}{20048}\,v^2 - \frac{32089}{290675952}\,v^4 + \frac{112199515657}{1030213709078400}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{28} = -\frac{131}{1879500}\,v^2 - \frac{13223393}{290675952000}\,v^4 + \frac{41921514013}{585348698340000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{29} = -\frac{5321}{25776000}\,v^2 - \frac{55955023}{581351904000}\,v^4 + \frac{678214482439}{3512092190040000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{30} = -\frac{3413}{33831000}\,v^2 - \frac{296809}{6055749000}\,v^4 + \frac{1220780228959}{12877671363480000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{31} = -\frac{449}{6766200}\,v^2 - \frac{138419}{5813519040}\,v^4 + \frac{20349760457}{367933467528000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{32} = -\frac{1}{37800}\,v^2 + \frac{277}{5074650}\,v^4 - \frac{151198591}{4796153208000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{33} = -\frac{3413}{67662000}\,v^2 - \frac{296809}{12111498000}\,v^4 + \frac{1220780228959}{25755342726960000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{34} = -\frac{3361}{90216000}\,v^2 - \frac{3237137}{41525136000}\,v^4 + \frac{5271389780053}{51510685453920000}\,v^6 + \cdots,$$

$$\mathrm{Rem}_{35} = -\frac{1519}{77328000}\,v^2 - \frac{6845267}{290675952000}\,v^4 + \frac{1354227512051}{34340456969280000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{36} = -\frac{73}{3383100}\,v^2 - \frac{843643}{58135190400}\,v^4 + \frac{2350840501}{95390158248000}\,v^6 + \cdots,$$
$$\mathrm{Rem}_{37} = -\frac{1}{13440}\,v^2 + \frac{1}{604800}\,v^4 - \frac{1}{47900160}\,v^6.$$

We see that all three trigonometrically fitted methods retain the sixth algebraic order, since the constant term of all the remainders is missing. Despite the fact that it seems that the power of the principal term of h decreases, in the expression of the local truncation error these powers cancel each other leading to a power of h^7.

5. Error analysis

The equations presented in section 4 are useful when we need to verify 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 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 (the global error is one order less than the local error), since the coefficients of the lowest powers $\{1, h, h^2, h^3, h^4, h^5, h^6\}$ vanish (see definition 1). We will present the principal term of the local truncation error for the following methods:

(a) The classical Fehlberg II method (8),

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

(c) The second trigonometrically fitted method (10), and

(d) The third trigonometrically fitted method (12).

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 $w = \sqrt{E - \overline{W}}$ and this is also used during the error analysis.

$$\begin{aligned}\mathrm{LTE}_{a,y} = {}& \frac{1}{75600}\,h^7\,[y'E^3 + (-9\,W'y - 3\,y'W)E^2 \\ &+((18\,W'W + 11\,W^{(3)})y + 13\,y'W'' + 3\,y'W^2)E \\ &+(-W^{(5)} - 9\,W'W^2 - 11\,W^{(3)}W - 15\,W'W'')y - 5\,W^{(4)}y' \\ &-10\,y'(W')^2 - y'W^3 - 13\,y'W''W] + O(h)^8,\end{aligned} \tag{18}$$

$$\begin{aligned}
\mathrm{LTE}_{a,z} = {} & \frac{1}{75600}\, h^7\, [-yE^4 + 4\, yWE^3 \\
& +((-22\, W'' - 6\, W^2)y - 12\, W'y')E^2 + ((44\, W''W + 4\, W^3 \\
& +28\, (W')^2 + 16\, W^{(4)})y + 24\, W'y'W + 24\, y'W^{(3)})E \\
& +(-W^4 - 22\, W''W^2 + (-28\, (W')^2 - 16\, W^{(4)})W - 15\, (W'')^2 \\
& -26\, W'W^{(3)} - W^{(6)})y - 24\, WW^{(3)}y' - 6\, W^{(5)}y' - 12\, W^2W'y' \\
& -48\, W'W''y'] + O(h)^8, \\
\mathrm{LTE}_{b,y} = {} & \frac{1}{75600}\, h^7\, [(-3\, y'W + 3\, y'\overline{W} - 9\, W'y)E^2 \\
& +(13\, y'W'' + 18\, yW'W - 3\, y'\overline{W}^2 + 3\, y'W^2 + 11\, yW^{(3)})E \\
& +(-15\, W'y - 13\, y'W)W'' - y'W^3 - 10\, y'(W')^2 - yW^{(5)} \\
& -11\, yWW^{(3)} + y'\overline{W}^3 - 5\, y'W^{(4)} - 9\, yW^2W'] + O(h)^8,
\end{aligned}$$

$$\begin{aligned}
\mathrm{LTE}_{b,z} = {} & \frac{1}{75600}\, h^7\, [(-3\, y\overline{W} + 3\, Wy)E^3 \\
& +(3\, Wy\overline{W} - 12\, W'y' - 22\, yW'' + 3\, y\overline{W}^2 - 6\, yW^2)E^2 \\
& +(24\, y'W'W + 16\, yW^{(4)} - 3\, Wy\overline{W}^2 - y\overline{W}^3 + 44\, yWW'' \\
& +4\, yW^3 + 24\, y'W^{(3)} + 28\, y(W')^2)E \\
& -15\, y(W'')^2 + (-48\, W'y' - 22\, yW^2)W'' - 6\, y'W^{(5)} + y\overline{W}^3W \\
& -yW^4 - 12\, y'W^2W' + (-28\, y(W')^2 - 24\, y'W^{(3)} - 16\, yW^{(4)})W \\
& -yW^{(6)} - 26\, yW'W^{(3)}] + O(h)^8, \\
\mathrm{LTE}_{c,y} = {} & \frac{1}{7257600}\, h^7\, [-550\, W'yE^2 + (275\, y'W^2 + (1676\, W'y \\
& -550\, \overline{W}\, y')W + (1209\, W'' + 275\, \overline{W}^2)y' + 1043\, yW^{(3)} \\
& -576\, \overline{W}\, W'y)E - 96\, y'W^3 + (-864\, W'y + 13\, \overline{W}\, y')W^2 \\
& +((-1248\, W'' + 262\, \overline{W}^2)y' + 52\, \overline{W}\, W'y - 1056\, yW^{(3)})W \\
& +(-960\, (W')^2 + 39\, W''\overline{W} - 179\, \overline{W}^3 - 480\, W^{(4)})y' \\
& +262\, \overline{W}^2W'y + 13\, \overline{W}\, yW^{(3)} \\
& +(-96\, W^{(5)} - 1440\, W'W'')y] + O(h)^8,
\end{aligned} \tag{19}$$

$$\begin{aligned}
\mathrm{LTE}_{c,z} = {} & \frac{1}{7257600}\, h^7\, [(-275\, y\overline{W}^2 - 275\, yW^2 \\
& -1759\, yW'' - 550\, W'y' + 550\, Wy\overline{W})E^2 \\
& +(371\, yW^3 - 563\, \overline{W}\, yW^2 + (13\, y\overline{W}^2 + 2226\, W'y'
\end{aligned}$$

$$
\begin{aligned}
&+4133\, yW'')W + (-1126\, W'\overline{W} + 2252\, W^{(3)})y' + 179\, y\overline{W}^3 \\
&-615\, \overline{W}\, yW'' + (2636\,(W')^2 + 1523\, W^{(4)})y)E - 96\, yW^{(6)} \\
&-96\, yW^4 + 13\, \overline{W}\, yW^3 + (262\, y\overline{W}^2 - 1152\, W'y' \\
&-2112\, yW'')W^2 + ((78\, W'\overline{W} - 2304\, W^{(3)})y' - 179\, y\overline{W}^3 \\
&+91\, \overline{W}\, yW'' \\
&+(-1536\, W^{(4)} - 2688\,(W')^2)y)W + (-4608\, W'W'' \\
&+52\, W^{(3)}\overline{W} - 576\, W^{(5)} + 524\, W'\overline{W}^2)y' + 262\, \overline{W}^2 yW'' \\
&+(52\,(W')^2 + 13\, W^{(4)})y\overline{W} + (-1440\,(W'')^2 - 2496\, W'W^{(3)})y] \\
&+O(h)^8,
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{LTE}_{d,y} = \frac{1}{75600}\, h^7\, &[(6\, yW'W - 6\, yW'\overline{W} + 8\, yW^{(3)} + 4\, y'W'')E \\
&-y'W^3 + (-9\, yW' + 3\, y'\overline{W})W^2 + (-13\, y'W'' - 11\, yW^{(3)} \\
&+12\, yW'\overline{W} - 3\, \overline{W}^2 y')W - 10\, y'(W')^2 + (-3\, \overline{W}^2 - 15\, W'')yW' \\
&+9\, y'\overline{W}\, W'' - 5\, y'W^{(4)} + y'\overline{W}^3 + 3\, yW^{(3)}\overline{W} - yW^{(5)}] + O(h)^8,
\end{aligned} \tag{20}
$$

$$
\begin{aligned}
\mathrm{LTE}_{d,z} = \frac{1}{75600}\, h^7\, &[-4\, W''yE^2 + (yW^3 - 3\, y\overline{W}\, W^2 \\
&+(6\, W'y' + (3\, \overline{W}^2 + 23\, W'')y)W + 16\, y(W')^2 - 6\, W'y'\overline{W} \\
&+(13\, W^{(4)} - 15\, W''\overline{W} - \overline{W}^3)y + 12\, y'W^{(3)})E \\
&-yW^4 + 3\, y\overline{W}\, W^3 + (-12\, W'y' + (-3\, \overline{W}^2 - 22\, W'')y)W^2 \\
&+(-28\, y(W')^2 + 18\, W'y'\overline{W} + (\overline{W}^3 - 16\, W^{(4)} + 21\, W''\overline{W})y \\
&-24\, y'W^{(3)})W + 12\, y\overline{W}\,(W')^2 + (-48\, y'W'' - 26\, yW^{(3)} \\
&-6\, \overline{W}^2 y')W' - 6\, y'W^{(5)} + (-3\, \overline{W}^2 W'' - W^{(6)} \\
&-15\,(W'')^2 + 3\, \overline{W}\, W^{(4)})y + 12\, y'\overline{W}\, W^{(3)}] + O(h)^8,
\end{aligned}
$$

where $y = y(x)$ and $W = W(x)$, while $\overline{W}$ 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 for the error of $y(x)$ and $z(x)$, respectively, are $(E^3,\ E^4)$. For the trigonometrically-fitted of first-order method (b) these powers become $(E^2,\ E^3)$, for the second-order method (c) $(E^2,\ E^2)$ and for the third-order method (d) $(E,\ E^2)$

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. The second and more important is that by increasing the exponential order of the method, this maximum power reduces and the method will gain efficiency. It will always be more efficient than the methods of lower exponential order. The difference between them will be higher for higher values of energy.

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 maximum powers 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 (1). This explains the higher efficiency of method (d) opposite to method (c).

6. Numerical results

6.1. *The resonance problem*

The efficiency of the two new 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

$$V(x) = \frac{u_0}{1+q} + \frac{u_1 q}{(1+q)^2}, \qquad q = \exp\left(\frac{x - x_0}{a}\right), \tag{21}$$

where

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

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

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x). \tag{22}$$

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

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[\sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{23}$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{24}$$

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.

6.2. Comparison

We will use three different values for the energy: (i) 989.701916, (ii) 341.495874, and (iii) 163.215341. As for the frequency w we will use the suggestion of Ixaru and Rizea [4]:

$$w = \begin{cases} \sqrt{E-50}, & x \in [0,\ 6.5], \\ \sqrt{E}, & x \in [6.5,\ 15]. \end{cases} \tag{25}$$

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 integrated for the resonance problem ($y(x)$ and $z(x)$). In figure 1 we use $E = 989.701916$, in figure 2 $E = 341.495874$, and in figure 3 $E = 163.215341$.

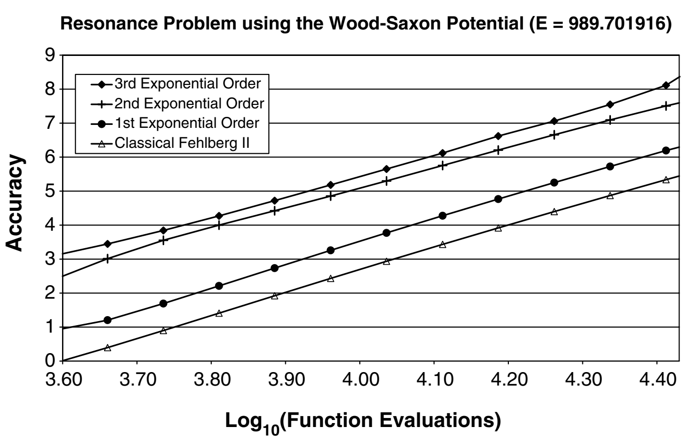

Figure 1. $-\log_{10}$(error) versus $\log_{10}$ (function evaluations) for the resonance problem using $E = 989.701916$.

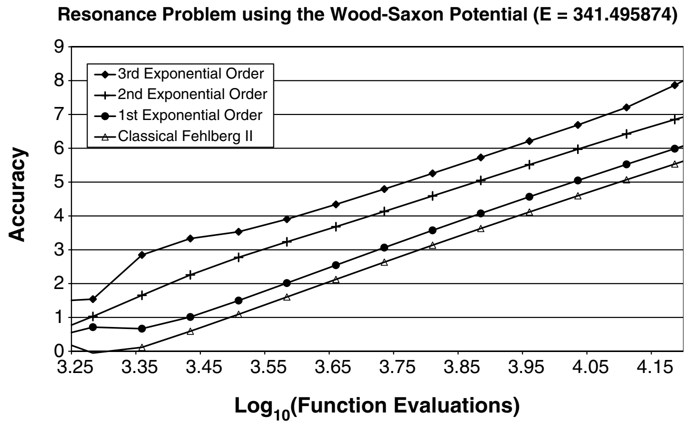

Figure 2. $-\log_{10}$(error) versus $\log_{10}$(function evaluations) for the resonance problem using $E = 341.495874$.

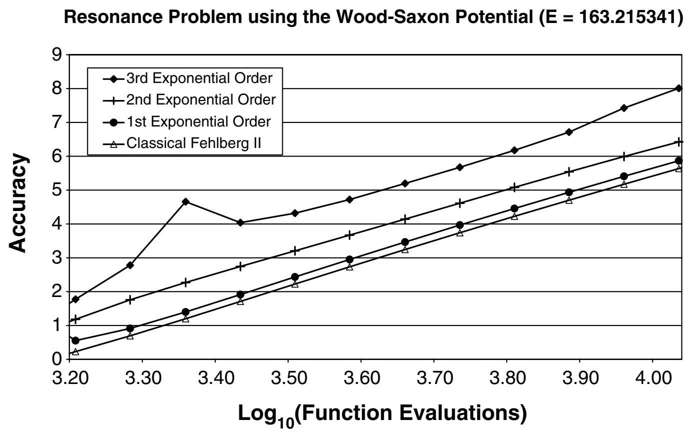

Figure 3. $-\log_{10}$(error) versus $\log_{10}$(function evaluations) for the resonance problem using $E = 163.215341$.

We compare the three trigonometrically fitted methods (9), (10), and (12) and the corresponding classical method Fehlberg II. The results confirm all the conclusions of the error analysis. We see that the third method is the most efficient, the second is the second most efficient, then comes the first and finally the classical method.

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