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Two Optimized Runge-Kutta Methods for the Solution of the Schrödinger Equation

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Abstract

In this paper we are constructing two explicit Runge-Kutta methods, one with tenth order of phase-lag and constant coefficients and one with infinite order of phase-lag and variable coefficients. The new methods have eight stages and sixth algebraic order and will be used for the numerical integration of the radial time-independent Schrödinger equation. The efficiency of the new constructed methods is compared to that of a wide range of known methods from the literature. The numerical results are shown through the graphs of the accuracy versus the function evaluations when applied to the Resonance problem.

1 Introduction

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

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

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 $\lim\limits_{x\to\infty} V(x) = 0$ and therefore $\lim\limits_{x\to\infty} W(x) = 0$.

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

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

The classical methods that have been constructed in the previous decades are not efficient enough when integrating the Schrödinger equation. Some well known classical methods compared in this paper can be found in [1] and [6]. Many numerical methods have been constructed for the efficient solution of the Schrödinger equation. For example the explicit Runge-Kutta methods of Anastassi and Simos [9], [10] and Vande Berghe et al. [8]. Some recent research work in numerical methods can be found in [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22], [23], [24], [25], [26], [27] and [28].

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:

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

The methods mentioned previously can also be presented using the Butcher table below:

$$\begin{array}{c|ccccc} 0 & & & & & \\ c_2 & a_{21} & & & & \\ c_3 & a_{31} & a_{32} & & & \\ \vdots & \vdots & \vdots & & & \\ c_s & a_{s1} & a_{s2} & \ldots & a_{s,s-1} & \\ \hline & b_1 & b_2 & \ldots & b_{s-1} & b_s \end{array} \tag{4}$$

The following equations must always hold:

$$c_i = \sum_{j=1}^{s} a_{ij},\; i = 2, \ldots, s \tag{5}$$

Definition 1 [3] *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:*

$$y^{(n)}(x) = y_n^{(n)}(x), \quad n = 1, 2, \ldots, p.$$

Equivalently a Runge-Kutta method must satisfy a number of equations, in order to have a certain algebraic order. These equations will be shown later in this paper.

2.2 Phase-Lag Analysis of Runge-Kutta Methods

The phase-lag analysis of Runge-Kutta methods is based on the test equation

$$\boldsymbol{y' = i \;\; w \;\; y,\; w \; real} \tag{6}$$

Application of the Runge-Kutta method described in (3) to the scalar test equation (6) produces the numerical solution:

$$y_{n+1} = a_*^n y_n, \quad a_* = A_s(v^2) + ivB_s(v^2), \tag{7}$$

where $v = wh$ and A_s, B_s are polynomials in v^2 completely defined by Runge-Kutta parameters $a_{i,j}$, b_i and c_i, as shown in (4).

Definition 2 [4] In the explicit s-*stage Runge-Kutta method, presented in (4), the quantity*

$$t(v) = v - \arg[a_*(v)]$$

is called the phase-lag *or* dispersion error. *If $t(v) = O(v^{q+1})$ then the method is said to be of phase-lag order q.*

Although dispersion (or phase-lag) was introduced for cyclic orbit, Runge-Kutta methods with high phase-lag order are more efficient in many other problem types than methods with lower phase-lag order and higher algebraic order with the same number of stages. They are even more effective in problems with oscillating solutions.

3 Construction of the New Methods

We consider a 8-Stage explicit Runge-Kutta method as shown in (8):

$$\begin{array}{c|cccccccc}
0 & & & & & & & & \\
c_2 & a_{21} & & & & & & & \\
c_3 & a_{31} & a_{32} & & & & & & \\
c_4 & a_{41} & a_{42} & a_{43} & & & & & \\
c_5 & a_{51} & a_{52} & a_{53} & a_{54} & & & & \\
c_6 & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & & & \\
c_7 & a_{71} & a_{72} & a_{73} & a_{74} & a_{75} & a_{76} & & \\
c_8 & a_{81} & a_{82} & a_{83} & a_{84} & a_{85} & a_{86} & a_{87} & \\
\hline
1 & b_1 & b_2 & b_3 & b_4 & b_5 & b_6 & b_7 & b_8
\end{array} \tag{8}$$

There are 43 unknowns totally. The necessary equations that must hold so that the method has 6th algebraic order are the following 37:

1st Alg. Order (1 equation)

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

2nd Alg. Order (2 equations)

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

3rd Alg. Order (4 equations)

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

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

4th Alg. Order (8 equations)

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

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

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

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

5th Algebraic Order (17)

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

6th Algebraic Order (37)

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

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

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

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

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

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

$$\sum_{i,j,k=1}^{s} b_i c_i a_{ij} c_j a_{jk} c_k = \frac{1}{48} \tag{9}$$

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

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

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

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

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

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

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

We select some coefficients giving them constant values in order to simplify the calculations afterwards: $a_{64} = -\frac{11}{80}$,$b_2 = 0$, $b_6 = 0$, $b_7 = \frac{5}{66}$, $c_2 = \frac{1}{6}$, $c_3 = \frac{4}{15}$, $c_4 = \frac{2}{3}$, $c_5 = \frac{4}{5}$, $c_6 = 1$, $c_7 = 0$ and $c_8 = 1$. After satisfying consistency conditions (5) and 6th algebraic order conditions (9), the coefficients depend now on a_{86} and a_{73}.

At this point we have two options: To create a method with constant coefficients, which has finite order of phase-lag, or to create a method with variable coefficients, which has infinite order of phase-lag.

In order to create a method with constant coefficients we expand the phase-lag (after satisfying the above equations) using Taylor series.

$$\begin{aligned}
phl = & \left(\frac{175}{1584}\,{a_{8,6}}^2 - \frac{8}{22275}\,a_{7,3} + \frac{2273}{95040}\,a_{8,6} + \frac{1}{453600} - \frac{28}{297}\,a_{8,6}a_{7,3}\right) v^7 \\
& + \left(-\frac{7}{396}\,{a_{8,6}}^2 - \frac{91}{10800}\,a_{8,6} - \frac{1}{45360} + \frac{112}{7425}\,a_{8,6}a_{7,3}\right) v^9 \\
& + \left(-\frac{7}{1188}\,{a_{8,6}}^2 - \frac{91}{32400}\,a_{8,6} + \frac{112}{22275}\,a_{8,6}a_{7,3} - \frac{1}{124740}\right) v^{11} + \ldots
\end{aligned}$$

By solving the coefficients of the lowest powers of the series for a_{86} and a_{73}, we achieve a higher order of phase-lag. So for

$$a_{7,3} = \frac{-20640763 + 338935\sqrt{1705}}{-29183616 + 1411200\sqrt{1705}} \quad \text{and} \quad a_{8,6} = -\frac{61}{10584} + \frac{1}{10584}\sqrt{1705}$$

phase-lag becomes

$$phl = -\frac{1}{1496880}v^{11} - \frac{1}{3603600}v^{13} - \frac{1151}{10216206000}v^{15} + \ldots$$

which means that the new method has 10th order of phase-lag. The coefficients of the new method are given below:

$$a_{21} = \frac{1}{6}, \quad a_{31} = \frac{4}{75}, \quad a_{32} = \frac{16}{75}, \quad a_{41} = 1/6\,\frac{3553 + 35\sqrt{1705}}{-517 + 25\sqrt{1705}}$$
$$a_{42} = -16/3\,\frac{253 + 5\sqrt{1705}}{-517 + 25\sqrt{1705}}, \quad a_{43} = \frac{75}{2}\,\frac{11 + \sqrt{1705}}{-517 + 25\sqrt{1705}}$$
$$a_{51} = -4\,\frac{407 + \sqrt{1705}}{-517 + 25\sqrt{1705}}, \quad a_{52} = \frac{48}{25}\,\frac{1859 + 25\sqrt{1705}}{-517 + 25\sqrt{1705}}$$
$$a_{53} = -8\,\frac{253 + 5\sqrt{1705}}{-517 + 25\sqrt{1705}}, \quad a_{54} = \frac{16}{25}$$
$$a_{61} = -\frac{1}{160}\,\frac{-251690417 + 3511589\sqrt{1705}}{\left(-517 + 25\sqrt{1705}\right)\left(-61 + \sqrt{1705}\right)}$$
$$a_{62} = \frac{12}{5}\,\frac{-1539527 + 18650\sqrt{1705}}{\left(-517 + 25\sqrt{1705}\right)\left(-61 + \sqrt{1705}\right)}$$
$$a_{63} = -\frac{11}{64}\,\frac{-12057133 + 124801\sqrt{1705}}{\left(-517 + 25\sqrt{1705}\right)\left(-61 + \sqrt{1705}\right)}, \quad a_{64} = -\frac{11}{80}, \quad a_{65} = \frac{231}{128}$$
$$a_{71} = \frac{11}{423360}\,\frac{-7871281 + 105085\sqrt{1705}}{-517 + 25\sqrt{1705}}, \quad a_{72} = -\frac{33}{20}\,\frac{-341 + 5\sqrt{1705}}{-517 + 25\sqrt{1705}}$$
$$a_{73} = \frac{1}{56448}\,\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}}, \quad a_{74} = -\frac{6347}{141120} - \frac{11}{28224}\sqrt{1705}$$
$$a_{75} = \frac{12331}{677376} + \frac{275}{677376}\sqrt{1705}, \quad a_{76} = \frac{61}{10584} - \frac{1}{10584}\sqrt{1705}$$
$$a_{81} = -\frac{1}{211680}\,\frac{-341912329 + 4484125\sqrt{1705}}{-517 + 25\sqrt{1705}}$$
$$a_{82} = -24\,\frac{110 + \sqrt{1705}}{-517 + 25\sqrt{1705}}, \quad a_{83} = \frac{1}{14112}\,\frac{16699507 + 527705\sqrt{1705}}{-517 + 25\sqrt{1705}}$$
$$a_{84} = -\frac{13057}{141120} + \frac{11}{28224}\sqrt{1705}, \quad a_{85} = \frac{278729}{677376} - \frac{275}{677376}\sqrt{1705}$$
$$a_{86} = -\frac{61}{10584} + \frac{1}{10584}\sqrt{1705}, \quad a87 = 1$$

As regarded to the new method with variable coefficients we want to produce the method that is corresponding to the previous method. This means that the constant coefficients of the previous method must be equal to the limit of the respective coefficients for $v \to 0$. In order to achieve this we set

$$a_{7,3} = \frac{-20640763 + 338935\sqrt{1705}}{-29183616 + 1411200\sqrt{1705}}$$

that is the same as before and then we satisfy $phl = 0$ obtaining the value of $a_{8,6}$ as shown below together with the other coefficients:

$$a_{21} = \frac{1}{6}, \quad a_{31} = \frac{4}{75}, \quad a_{32} = \frac{16}{75}$$

$$a_{41} = \frac{23}{24} - \frac{192}{5}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} + \frac{75}{22}a_{8,6}$$

$$a_{42} = -3\frac{512}{5}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} - \frac{100}{11}a_{8,6}$$

$$a_{43} = \frac{65}{24} + \frac{125}{22}a_{8,6} - 64\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}}$$

$$a_{51} = -\frac{19}{10} + \frac{2304}{25}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} - \frac{90}{11}a_{8,6}$$

$$a_{52} = \frac{164}{25} - \frac{6144}{25}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} + \frac{240}{11}a_{8,6}$$

$$a_{53} = -9/2 - \frac{150}{11}a_{8,6} + \frac{768}{5}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}}$$

$$a_{54} = \frac{16}{25}$$

$$a_{61} = \frac{1}{12800a_{8,6}}\Big(-158600\,a_{8,6} + 165 + 7096320\,a_{8,6}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} - 630000\,{a_{8,6}}^2 - 50688\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} + 3200\,a_{8,6}(-\frac{11}{80})\Big)$$

$$a_{62} = -\frac{1}{1600a_{8,6}}\Big(55 - 63800\,a_{8,6} + 2365440\,a_{8,6}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}}210000\,{a_{8,6}}^2 - 16896\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}}\Big)$$

$$a_{63} = -\frac{1}{2560a_{8,6}}\Big(72200\,a_{8,6} - 2365440\,a_{8,6}\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} + 210000\,{a_{8,6}}^2 - 55 + 16896\frac{5}{66}\frac{1}{56448}\frac{-20640763 + 338935\sqrt{1705}}{-517 + 25\sqrt{1705}} + 1600\,a_{8,6}(-\frac{11}{80})\Big)$$

$$a_{64} = -\frac{11}{80}, \quad a_{65} = \frac{55}{32} - \frac{5}{8}(-\frac{11}{80})$$

$$a_{71} = \frac{1}{84480}\,\frac{-6700\,a_{8,6} + 50688\,\frac{5}{66}\,\frac{1}{56448}\,\frac{-20640763+338935\,\sqrt{1705}}{-517+25\,\sqrt{1705}} - 275}{\frac{5}{66}}$$

$$a_{72} = -\frac{1}{10560}\,\frac{-1500\,a_{8,6} + 16896\,\frac{5}{66}\,\frac{1}{56448}\,\frac{-20640763+338935\,\sqrt{1705}}{-517+25\,\sqrt{1705}} - 55}{\frac{5}{66}}$$

$$a_{73} = \frac{1}{56448}\,\frac{-20640763 + 338935\,\sqrt{1705}}{-517 + 25\,\sqrt{1705}}, \quad a_{74} = -\frac{1}{192}\,\frac{60\,a_{8,6} + 1}{\frac{5}{66}},$$

$$a_{75} = \frac{5}{1536}\,\frac{1 + 100\,a_{8,6}}{\frac{5}{66}}, \quad a_{76} = -\frac{5}{66}\,\frac{a_{8,6}}{\frac{5}{66}}$$

$$a_{81} = \frac{173}{128} - \frac{1584}{25}\,\frac{5}{66}\,\frac{1}{56448}\,\frac{-20640763 + 338935\,\sqrt{1705}}{-517 + 25\,\sqrt{1705}} + \frac{191}{32}\,a_{8,6} - \frac{66}{5}\,\frac{5}{66}$$

$$a_{82} = -\frac{83}{20} + \frac{4224}{25}\,\frac{5}{66}\,\frac{1}{56448}\,\frac{-20640763 + 338935\,\sqrt{1705}}{-517 + 25\,\sqrt{1705}} - 15\,a_{8,6}$$

$$a_{83} = \frac{891}{256} + \frac{525}{64}\,a_{8,6} - \frac{528}{5}\,\frac{5}{66}\,\frac{1}{56448}\,\frac{-20640763 + 338935\,\sqrt{1705}}{-517 + 25\,\sqrt{1705}}$$

$$a_{84} = -\frac{11}{160} + \frac{33}{8}\,a_{8,6}, \quad a_{85} = \frac{99}{256} - \frac{275}{64}\,a_{8,6}$$

$$\begin{aligned}
a_{86} = -\frac{1}{211680}\,\frac{1}{v^4\,(-25 + 4\,\tan(v)\,v)}\Big(&2732\,v^5\tan(v)\sqrt{1705} + \\
&+171532\,v^5\tan(v) - 383611\,v^4 - 17075\,v^4\sqrt{1705} + \\
\Big(&42149046944\,v^{10}(\tan(v))^2 + 937250848\,v^{10}(\tan(v))^2\sqrt{1705} - \\
&-7843714064\,v^9\tan(v)\sqrt{1705} - 283759702864\,v^9\tan(v) \\
&+601033675946\,v^8 + 12411851650\,v^8\sqrt{1705} + \\
&+40558023475200\,(\tan(v))^2 v^2 -, 20279011737600\,(\tan(v))^2 v^4 + \\
&+1689917644800\,(\tan(v))^2 v^6 - 56330588160\,(\tan(v))^2 v^8 \\
&+14082647040\,v^7\tan(v) - 3802314700800\,v^5\tan(v) \\
&+86185799884800\,\tan(v)\,v^3 - 253487646720000\,\tan(v)\,v \\
&+2112397056000\,v^6 - 42247941120000\,v^4 + 253487646720000\,v^2\Big)^{1/2}\Big)
\end{aligned}$$

$$a_{87} = 1$$

4 Numerical Results

4.1 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

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\,q}{(1+q)^2}, \qquad q = \exp\left(\frac{x-x_0}{a}\right), \quad \text{where} \tag{11}$$
$$u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}$$

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

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{12}$$

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

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{13}$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{14}$$

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.

4.2 The Methods

We will compare the new constructed method to a wide range of already known methods. These are explicit Runge-Kutta methods with algebraic order up to six, some of which are optimized for solving problems with oscillating solutions or Schrödinger equation specifically.

- Formulae Butcher (6th order), Fehlberg I (5th), Fehlberg II (6th), Fehlberg 4th, Fehlberg 5th, Kutta-Nyström (5th), England I (4th), England II (5th) and Gill (4th) from [1].
- Formulae 3.3 (5-2-2), 3.4 (4-2-6), 3.5 (6-2-10), 3.7 (4-4-6), 3.8 (5-4-8), 3.9 (6-4-10), 3.13 (3-2-2), 3.14 (4-1-2), 3.15 (5-1-2) and 3.17 (3-1-12) from [6]. In parentheses there are the number of stages, the algebraic order and the order of phase-lag respectively.
- The well known classical Runge-Kutta method with 4 stages and 4th algebraic order and the method of Zonneveld with 6 stages and 5th algebraic order.

- The trigonometrically fitted method of Vande Berghe et al. with 4 stages and 4th algebraic order from [8].
- The two trigonometrically fitted methods of Anastassi and Simos based on the classical method of England with 6 stages, 5th algebraic order and exponential orders one and two [9].
- The two trigonometrically fitted methods of Anastassi and Simos based on the classical method of Kutta-Nyström with 6 stages, 5th algebraic order and exponential orders one and two [10].
- The two trigonometrically fitted methods based on the classical method of Fehlberg I with 6 stages, 5th algebraic order and exponential orders one and two.
- The trigonometrically fitted method based on the classical method of Butcher with 8 stages, 6th algebraic order and first exponential order.
- The two new formulae 8-6-Inf and 8-6-10 constructed in this paper, where A-B-C means that the method has A stages, algebraic order B and phase-lag order C.

4.3 Comparison

We will use four values for the energy: 989.701916, 341.495874, 163.215341 and 53.588872. As for the frequency w we will use the suggestion of Ixaru and Rizea [7]:

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

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 Figures 1 - 3 we use $E = 989.701916$, in Figures 4 - 6 we use $E = 341.495874$, in Figures 7 - 9 we use 163.215341 and in Figures 10 - 12 we use 53.588872. The methods are divided into three groups depending on their efficiency with the first group including the most efficient ones.

As we see in the figures, the new method with constant coefficients is the most accurate among all the methods and for all values of energy. It also has the advantage of being independent from the frequency of the problem and the step-length. The second method developed in this paper that has variable coefficients is more accurate than all the other known methods when searching for high accuracy and this can be more clearly seen for the low values of energy (163.215341 and 53.588872).

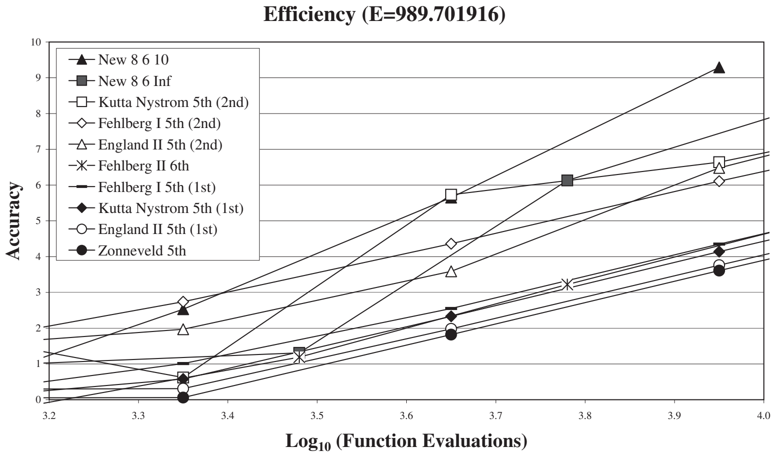

Figure 1: Efficiency for the first group of methods using E = 989.701916

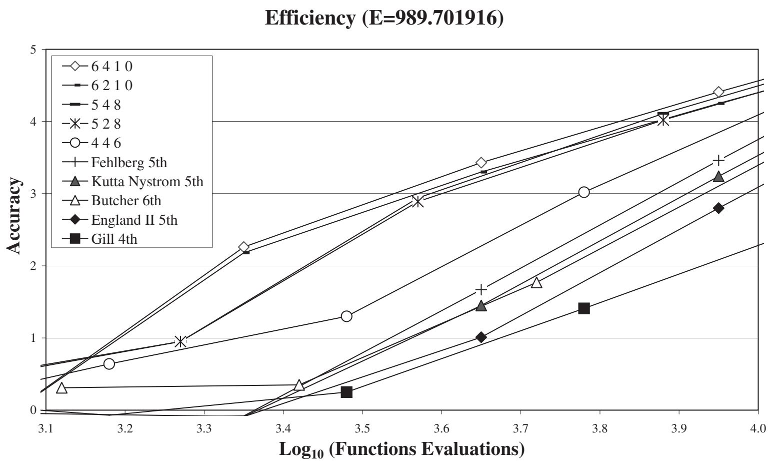

Figure 2: Efficiency for the second group of methods using E = 989.701916

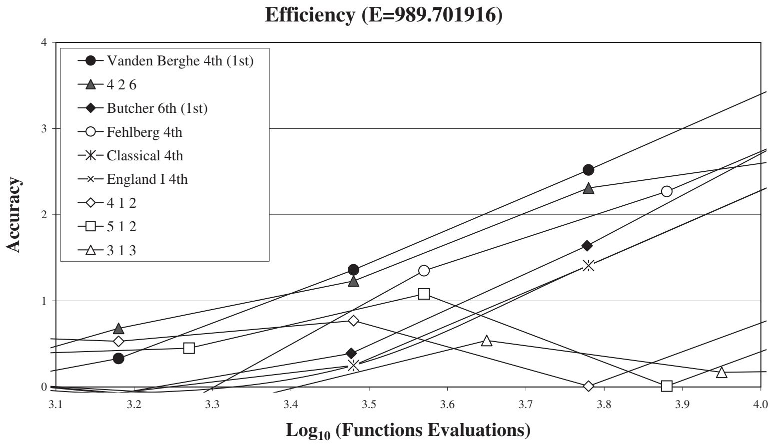

Figure 3: Efficiency for the third group of methods using E = 989.701916

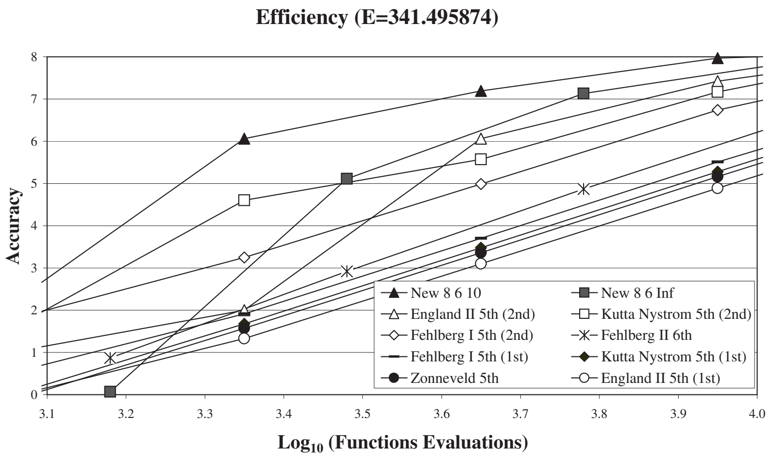

Figure 4: Efficiency for the first group of methods using E = 341.495874

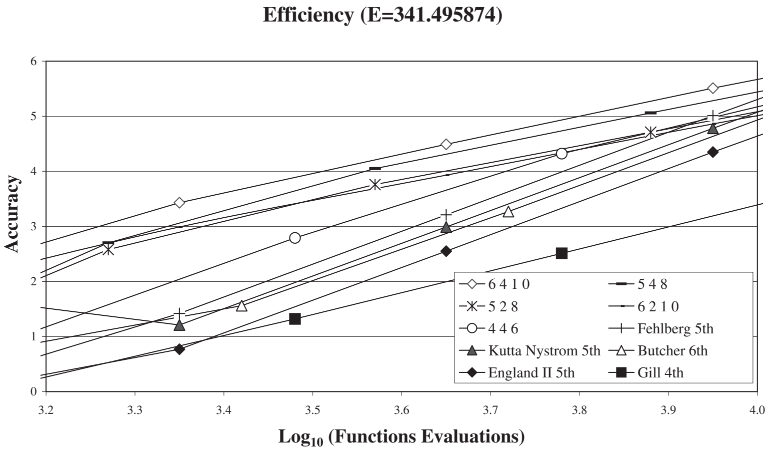

Figure 5: Efficiency for the second group of methods using E = 341.495874

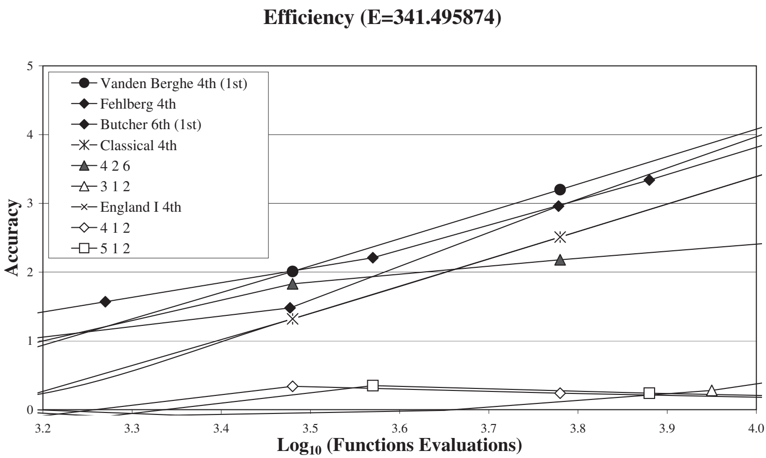

Figure 6: Efficiency for the third group of methods using E = 341.495874

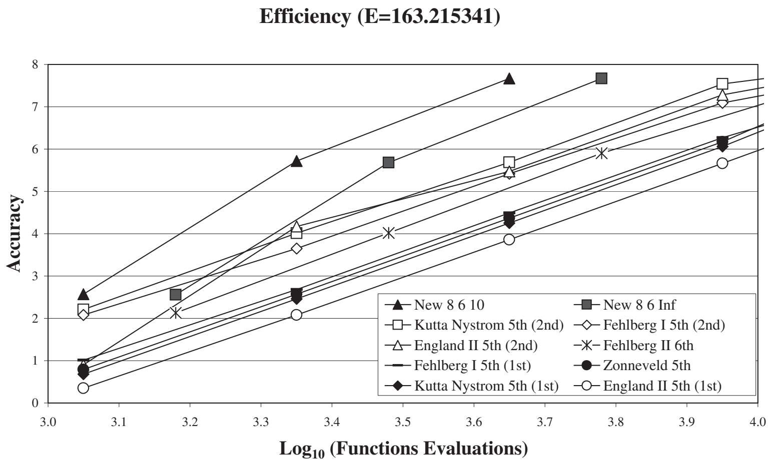

Figure 7: Efficiency for the first group of methods using E = 163.215341

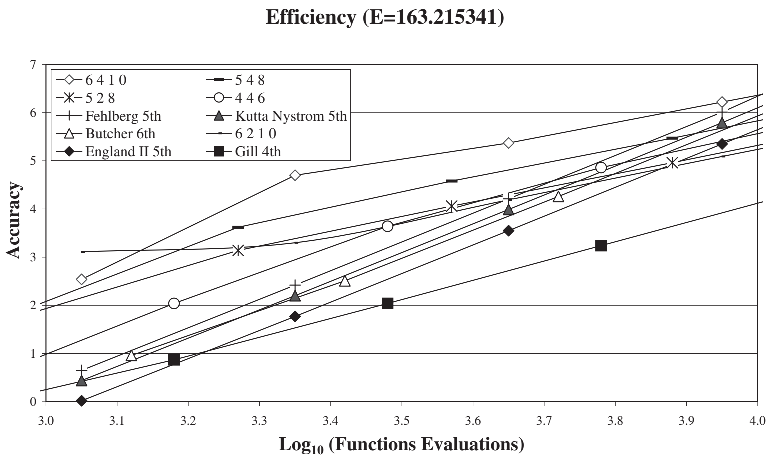

Figure 8: Efficiency for the second group of methods using E = 163.215341

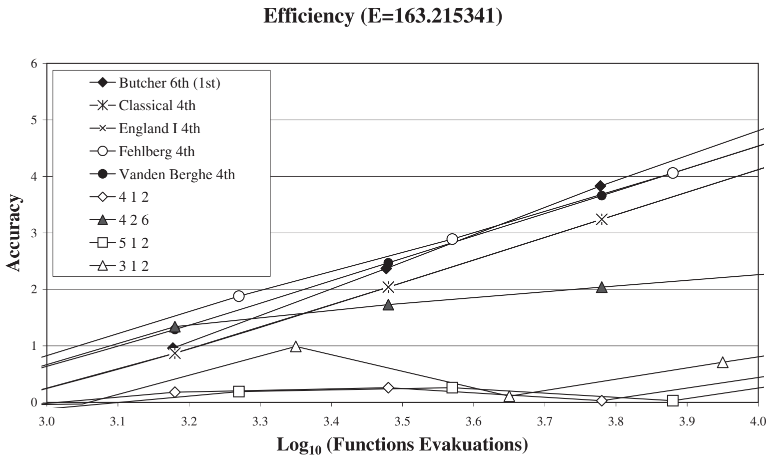

Figure 9: Efficiency for the third group of methods using E = 163.215341

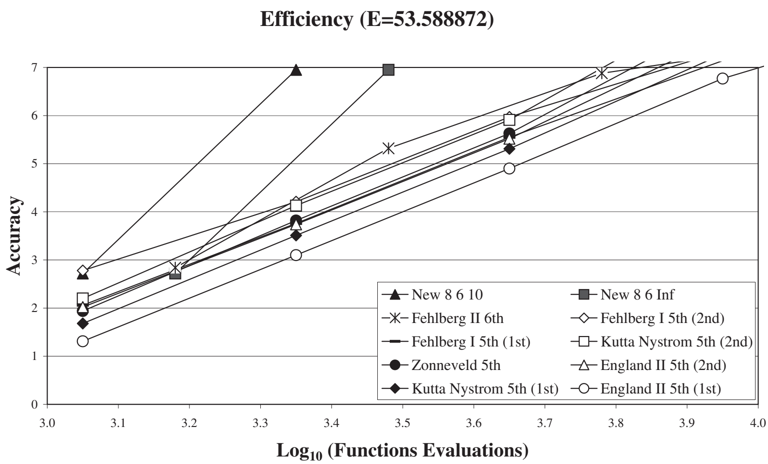

Figure 10: Efficiency for the first group of methods using E = 53.588872

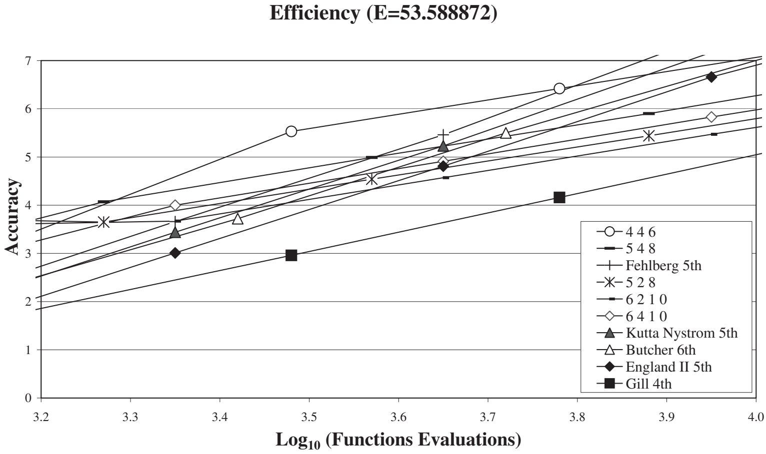

Figure 11: Efficiency for the second group of methods using E = 53.588872

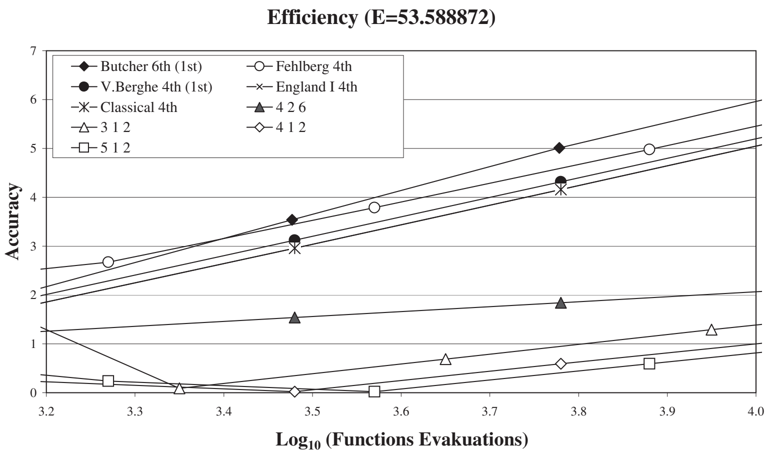

Figure 12: Efficiency for the third group of methods using E = 53.588872

Among the rest of the methods the ones that were competitive were the exponentially-fitted versions of Kutta-Nyström, Fehlberg I and England II. Especially the second exponential order methods were very efficient followed by the first exponential order methods of the families. The high efficiency of all optimized methods is more clear for high values of energy.

Method of Zonneveld and high phase-lag order methods from [6], like 6-4-10, 5-4-8 etc. were next in order of efficiency followed by the classical methods found in [1], i.e. Fehlberg 5th, Kutta-Nyström 5th etc., the optimized method of Vande Berghe, followed by the low algebraic and phase-lag order methods.

5 Conclusions

Two new explicit Runge-Kutta methods with eight stages, sixth algebraic order and order of phase-lag infinite and tenth are produced in this paper. After applying the new methods and a great variety of known methods we conclude that the newly developed methods are highly efficient when integrating the Resonance problem. This reveals the importance of phase-lag when solving ODEs with oscillating solutions, especially in the case of non-zero phase-lag, that is when we want to produce a method with constant coefficient.

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