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ORIGINAL PAPER

A new modified embedded 5(4) pair of explicit Runge–Kutta methods for the numerical solution of the Schrödinger equation

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Abstract In this work a new modified embedded 5(4) pair of explicit Runge–Kutta methods is developed for the numerical solution of the Schrödinger equation. We investigate the error of the new pair, based on the error analysis we apply the higher order method to the resonance problem, also we apply the new embedded pair to elastic scattering phase-shift problem. The applications show the efficiency of our new developed embedded pair and the higher order method.

Keywords Embedded Runge–Kutta methods · Error analysis · Schrödinger equation

1 Introduction

The radial time independent Schrödinger equation has the form

$$y''(r) = \big(\frac{l(l+1)}{r^2} + V(r) - E\big)y(r). \tag{1}$$

This type of problems appears often in many scientific areas such as astronomy, nuclear physics, quantum chemistry, molecular physics, celestial mechanics and so on.

For the above problem (1), we take the following notations: The quantity l is a given integer representing the angular momentum, the term $l(l+1)/r^2$ is called the *centrifugal potential*. $V(r)$ is a given function which denotes the *potential* with $V(r) \to 0$

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if $r \to \infty$. The function $W(r) = l(l+1)/r^2 + V(r)$ is called the *effective potential*. This satisfies $W(r) \to 0$ as $x \to \infty$. The quantity E is a real number denoting the *energy*.

In the past decade, many categories of numerical methods have been constructed for the approximate solution of the radial Schrödinger equation (1) or for general ordinary differential equations with oscillatory solutions ([1–50]), Most of these methods are: (a) Exponentially/trigonometrically fitted Runge–Kutta (RK) [1–4], Runge–Kutta Nyström (RKN), multistep methods and Exponential fitting BDF algorithms [46,47]; (b) Phase-fitted/amplification fitted RK, RKN, multistep methods; (c) Minimal phase lag RK, RKN, multistep methods; (d) Symplectic or symmetric methods for Hamiltonian systems.

For exponentially fitted multistep methods, there is an excellent review [39] by Vigo-Aguiar and Simos on multistep methods for the numerical solution of the Schrödinger equation, they present a simple procedure for the production of adapted Cowell methods of any algebraic, trigonometric and exponential order. It has been universally acknowledged that when applied to the Schrödinger equation general-purpose methods cannot produce satisfactory numerical results. Compared with multistep methods whose implements requires a series of starting values, Runge–Kutta type methods are favorable because the initial values that are available in advance are sufficient for them to run. In this paper we focus on modified RK methods and variable stepsize RK pair. For variable stepsize multistep methods one can refer to [45].

The Procedure of Kalogiratou and Simos [50] for the numerical ingegration of the Schrödinger equation is based on trigonometric fitting, the developed methods can integrate exactly the test equation $y'' = -\omega^2 y$ and the numerical results show the robustness of the new methods.

Here we develop a new trigonometrically fitted embedded 5(4) pair of explicit Runge–Kutta methods following the procedure of Kalogiratou and Simos [50], the new methods integrate exactly the test equation $y' = i\omega y$. In Sect. 2 we give the necessary conditions for such methods. In Sects. 3 we construct the new 5(4) pair of explicit Runge–Kutta methods and give an error analysis of the higher order method of the new pair and some related methods. In Sect. 4 we apply the higher order method to the resonance problem, also we apply the new embedded pair to elastic scattering phase-shift problem.

2 Preliminaries

2.1 Embedded Runge–Kutta methods

A Runge–Kutta (RK) method is defined by

$$\begin{aligned} Y_i &= y_n + h \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, 2, \ldots, s, \\ y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \end{aligned} \tag{2}$$

with the following associated Butcher tableau:

$$\begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ \vdots & \vdots & \ddots & & \\ c_s & a_{s1} & \cdots & a_{s,s-1} & \\ \hline & b_1 & \cdots & b_s & \end{array}$$

or in matrix form

$$\begin{array}{c|c} c & A \\ \hline & b \end{array}$$

where A is matrix $(a_{i,j})_{s\times s}$, $c = (c_1, c_2, \ldots, c_s)^T$, $b = (b_1, b_2, \ldots, b_s)$.

An embedded $q(p)$ pair of RK method is based on the RK method (c, A, b) of order q and another RK method (c, A, b^*) of order $p < q$. An embedded pair is characterized by Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b \\ \hline & b^* \end{array}$$

Embedded pairs of explicit RK methods are widely used in variable stepsize algorithms because they provide a cheap error estimation. From embedded methods we obtain an estimate

$$EST_{n+1} = \| y_{n+1} - y^*_{n+1} \|$$

of the local trucation error of the p th-order method at the integration point $x_{n+1} = x_n + h_n$. For the numerical integration of the Schrödinger equation (1) we use the stepsize control precedure proposed by Raptis and Cash [59]:

- if $EST_{n+1} < \frac{Tol}{100}$, $h_{n+1} = 2h_n$,
- if $\frac{Tol}{100} \leq EST_{n+1} < Tol$, $h_{n+1} = h_n$,
- if $EST_{n+1} \geq Tol$, $h_{n+1} = \frac{h_n}{2}$ and repeat the step.

Where Tol is the requested local error. It should be noted that the q th-order approximation y_n is used as the initial value for the $(n+1)$th step, that is to say, the embedded pair is applied in local extrapolation mode or higher order mode.

2.2 Trigonometrically fitted Runge–Kutta methods

We define the operators $L(x)$ as follows:

$$\begin{aligned} Y_i(x) &= y(x) + h \sum_{j=1}^{i-1} a_{ij} Y_j'(x), \quad i = 1, 2, \ldots, s, \\ L(x) &= y(x+h) - y(x) - \sum_{i=1}^{s} b_i Y_i'(x), \end{aligned} \tag{3}$$

Definition 1 (see [2]) The method has exponential order p if the associated operator $L(x)$ vanishes for any linear combination of the functions

$$\exp(\omega_0 x), \exp(\omega_1 x), \ldots, \exp(\omega_p x),$$

where ω_i are real or complex numbers.

Remark 1 (see [51]) If $\omega_i = \omega$ for $i = 1, 2, \ldots, n, n \leq p$, then the operator $L(x)$ vanishes for any linear combination of

$$\exp(\omega x), x \exp(\omega x), x^2 \exp(\omega x), \ldots, x^n \exp(\omega x), \exp(\omega_{n+1} x), \ldots, \exp(\omega_p x).$$

Condition for the RK methods is given in the following theorem.

Theorem 1 *Method (2) is of exponential order p if the following conditions is satisfied:*

$$\cos(v) + i \sin(v) = 1 + \sum_{k=1}^{s} (iv)^k b A^{k-1} e, \tag{4}$$

where $v = \omega_i h$ for $i = 0, 1, \ldots, p$.

Remark 2 If $\omega_q = \omega_r = \omega$, for $q, r \in 0, 1, \ldots, p$ then the following additional condition is required:

$$-\sin(v) + i \cos(v) = \sum_{k=1}^{s} ik(iv)^{k-1} b A^{k-1} e, \tag{5}$$

On the basis of the above result we develop a new embedded 5(4) pair of explicit Runge–Kutta methods based on the embedded 5(4) pair of Runge–kutta formulas [52].

3 Construction of the new embedded 5(4) pair of explicit Runge–Kutta methods

We shall consider an embedded 5(4) pair of Explicit Runge–Kutta formulas which proposed by Dormand and Prince [52], it can be denoted by the Butcher tableau:

$$\begin{array}{c|c} c & A \\ \hline & b \\ \hline & b^* \end{array} = \begin{array}{c|cccccc} 0 & & & & & & \\ \frac{1}{5} & \frac{1}{5} & & & & & \\ \frac{3}{10} & \frac{3}{40} & \frac{9}{40} & & & & \\ \frac{3}{5} & \frac{3}{10} & \frac{-9}{10} & \frac{6}{5} & & & \\ \frac{2}{3} & \frac{226}{729} & \frac{-25}{27} & \frac{880}{729} & \frac{55}{729} & & \\ 1 & \frac{-181}{270} & \frac{5}{2} & \frac{-266}{297} & \frac{-91}{27} & \frac{189}{55} & \\ \hline & \frac{19}{216} & 0 & \frac{1000}{2079} & -\frac{125}{216} & \frac{81}{88} & \frac{5}{56} \\ \hline & \frac{31}{540} & 0 & \frac{190}{297} & -\frac{145}{108} & \frac{351}{220} & \frac{1}{20} \end{array} \tag{6}$$

We shall construct the new embedded 5(4) pair with second exponential order.

3.1 Trigonometrically fitted higher order method with second exponential order

Consider the higher order Runge–kutta method, for second exponential order we requre Eqs. (4) and (5) to be satisfied, thus the following conditions should hold:

$$\cos(v) - 1 = -v^2 bAe + v^4 bA^3 e - v^6 bA^5 e,$$
$$\sin(v) = v(be - v^2 bA^2 e + v^4 bA^4 e),$$

and

$$-\sin(v) = -2vbAe + 4v^3 bA^3 e - 6v^5 bA^5 e,$$
$$\cos(v) = be - 3v^2 bA^2 e + 5v^4 bA^4 e.$$

Then the method integrates exactly the functions

$$\{1, x, \cos(\omega x), \sin(\omega x), x\cos(\omega x), x\sin(\omega x)\}.$$

We set $b_1 = \frac{19}{216}$, $b_2 = 0$ the coefficients b_3, b_4, b_5, b_6 of this method are:

$$\begin{aligned} b_3 = \Big(50\Big(&118503v^{10} + 4162410v^8 - 58835600v^6 + 41085600v^4 + 1572480000v^2 \\ &-450\left(6237v^8 - 99900v^6 - 23180v^4 + 2194800v^2 - 744000\right) v\sin(v) \\ &+18\Big(18711v^{10} - 771120v^8 + 3290100v^6 + 13290800v^4 \\ &-78960000v^2 + 54000000\Big)\cos(v) - 972000000\Big)\Big) / \left(2079v^4 N\right), \\ b_4 = 125(&-6183v^8 + 158900v^6 + 3286200v^4 - 59508000v^2 \\ &+18(v^2((9v^2 - 415)(9v^2 + 340)v^2 + 1924500) - 1200000)v\sin(v) \\ &+144(27v^8 + 2700v^6 - 76550v^4 + 394500v^2 - 337500)\cos(v) \\ &+48600000)/(27v^4 N), \\ b_5 = 675(&513v^8 + 29088v^6 - 653200v^4 + 8304000v^2 \\ &-240(81v^6 - 1755v^4 + 19850v^2 - 14000)v\sin(v) \end{aligned}$$

$$+36(81v^8 - 3168v^6 + 45200v^4 - 224000v^2 + 200000)\cos(v)$$
$$-7200000)/(22Nv^4),$$
$$b_6 = 250(-1206v^6 + 111500v^4 - 478800v^2 + 3(243v^6 - 16200v^4 + 80700v^2$$
$$-104000)v\sin(v) + 24(324v^6 - 5175v^4 + 21700v^2 - 22500)\cos(v)$$
$$+540000)/(7Nv^4),$$

where $N = 729v^8 - 16200v^6 + 404100v^4 - 112000v^2 - 600000$.

For small values of v the above formulae are subject to heavy cancelations and in that case the following series expansions must be used:

$$b_3 = \frac{1000}{2079} - \frac{5v^2}{462} + \frac{13423v^4}{582120} - \frac{12214v^6}{3274425} + \frac{570686189v^8}{34577928000} + \cdots,$$
$$b_4 = -\frac{125}{216} + \frac{5v^2}{48} - \frac{491v^4}{3024} + \frac{5203v^6}{77760} - \frac{195961v^8}{1603800} + \cdots,$$
$$b_5 = \frac{81}{88} - \frac{9v^2}{88} + \frac{1809v^4}{12320} - \frac{132443v^6}{1848000} + \frac{27538631v^8}{243936000} + \cdots,$$
$$b_6 = \frac{5}{56} + \frac{v^2}{112} - \frac{59v^4}{7840} + \frac{56683v^6}{6350400} - \frac{146864611v^8}{20956320000} + \cdots.$$

We shall refer to this method as RK54NEWH. We note that when $v \to 0$, this method reduces to the classical Runge–Kutta method of fifth algebraic order.

3.2 Trigonometrically fitted lower order method with second exponential order

Consider the lower order Runge–kutta method, for second exponential order we requre Eqs. (4) and (5) to be satisfied, thus the following conditions should hold:

$$\cos(v) - 1 = -v^2 b^* Ae + v^4 b^* A^3 e - v^6 b^* A^5 e,$$
$$\sin(v) = v(b^* e - v^2 b^* A^2 e + v^4 b^* A^4 e),$$

and

$$-\sin(v) = -2vb^* Ae + 4v^3 b^* A^3 e - 6v^5 b^* A^5 e,$$
$$\cos(v) = b^* e - 3v^2 b^* A^2 e + 5v^4 b^* A^4 e.$$

Then the method integrates exactly the functions

$$\{1, x, \cos(\omega x), \sin(\omega x), x\cos(\omega x), x\sin(\omega x)\}.$$

We set $b_1^* = \frac{31}{540}$, $b_2^* = 0$, the coefficients $b_3^*, b_4^*, b_5^*, b_6^*$ of this method are:

$$\begin{aligned}
b_3^* = {} & (20(193347v^{10} + 12640950v^8 - 147372800v^6 + 92814000v^4 + 3931200000v^2 \\
& -1125(6237v^8 - 99900v^6 - 23180v^4 + 2194800v^2 - 744000)v\sin(v) \\
& +45(18711v^{10} - 771120v^8 + 3290100v^6 + 13290800v^4 - 78960000v^2 \\
& +54000000)\cos(v) - 2430000000))/(2079v^4 N), \\
b_4^* = {} & 250(-3537v^8 + 65920v^6 + 1692600v^4 - 29754000v^2 \\
& +9(v^2((9v^2 - 415)(9v^2 + 340)v^2 + 1924500) - 1200000)v\sin(v) \\
& +72(27v^8 + 2700v^6 - 76550v^4 + 394500v^2 - 337500)\cos(v) \\
& +24300000)/\left(24v^4 N\right), \\
b_5^* = {} & 135(837v^8 + 84600v^6 - 1666000v^4 + 20760000v^2 \\
& -600(81v^6 - 1755v^4 + 19850v^2 - 14000)v\sin(v) - 18000000 \\
& +90(81v^8 - 3168v^6 + 45200v^4 - 224000v^2 + 200000)\cos(v))/\left(11v^4 N\right), \\
b_6^* = {} & 250\left(-40\left(45v^6 - 2804v^4 + 11970v^2 - 13500\right)\right. \\
& +3v\left(243v^6 - 16200v^4 + 80700v^2 - 104000\right)\sin(v) \\
& \left.+24(324v^6 - 5175v^4 + 21700v^2 - 22500)\cos(v)\right)/\left(7v^4 N\right),
\end{aligned}$$

where $N = 729v^8 - 16200v^6 + 404100v^4 - 112000v^2 - 600000$.

For small values of v the above formulae are subject to heavy cancelations and in that case the following series expansions must be used:

$$\begin{aligned}
b_3^* &= \frac{190}{297} - \frac{622v^2}{17325} + \frac{4793357v^4}{48510000} - \frac{1224547537v^6}{32744250000} + \frac{32277838675363v^8}{432224100000000} + \cdots, \\
b_4^* &= -\frac{145}{108} + \frac{41v^2}{90} - \frac{741449v^4}{1008000} + \frac{83823949v^6}{194400000} - \frac{752693376863v^8}{1283040000000} + \cdots, \\
b_5^* &= \frac{351}{220} - \frac{648v^2}{1375} + \frac{10463367v^4}{15400000} - \frac{1011397441v^6}{2310000000} + \frac{8396527930067v^8}{15246000000000} + \cdots, \\
b_6^* &= \frac{1}{20} + \frac{271v^2}{5250} - \frac{7400567v^4}{176400000} + \frac{3585211223v^6}{79380000000} - \frac{19992488922001v^8}{523908000000000} + \cdots.
\end{aligned}$$

We shall refer to this method as RK54NEWL, and the new 5(4) pair as RK54NEW. We note that when $v \to 0$, this method reduces to the classical Runge–Kutta method of fourth algebraic order and the new pair RK54NEW reduces to the corresponding classical 5(4) pair.

3.3 Algebraic order of the new methods

The classical Butcher theory is described by Hairer et al. [53]. It is interesting to check the algebraic order conditions for the new methods. We expand the conditions using Taylor series over v and around zero:

First algebraic order:

$$be - 1 = \frac{221v^6}{504000} + \frac{3079v^8}{15120000} + \cdots,$$
$$b^*e - 1 = \frac{11v^4}{15000} + \frac{1109v^6}{984375} + \frac{7638311v^8}{12600000000} + \cdots.$$

Second algebraic order:

$$bc - \frac{1}{2} = -\frac{v^4}{7200} + \frac{11v^6}{63000} - \frac{3211v^8}{30240000} + \cdots,$$
$$b^*c - \frac{1}{2} = -\frac{31v^4}{45000} + \frac{48653v^6}{63000000} - \frac{22232951v^8}{37800000000} + \cdots.$$

Third algebraic order:

$$bc^2 - \frac{1}{3} = \frac{19v^4}{14000} + \frac{4681v^6}{5670000} + \frac{4977923v^8}{7484400000} + \cdots,$$
$$bAc - \frac{1}{6} = \frac{19v^4}{28000} + \frac{4681v^6}{11340000} + \frac{4977923v^8}{14968800000} + \cdots,$$
$$b^*c^2 - \frac{1}{3} = \frac{11v^2}{3750} + \frac{32363v^4}{7875000} + \frac{69057299v^6}{28350000000} + \frac{100061121203v^8}{46777500000000} + \cdots,$$
$$b^*Ac - \frac{1}{6} = \frac{11v^2}{7500} + \frac{32363v^4}{15750000} + \frac{69057299v^6}{56700000000} + \frac{100061121203v^8}{93555000000000} + \cdots.$$

Fourth algebraic order:

$$bc^3 - \frac{1}{4} = \frac{v^2}{1200} + \frac{429v^4}{280000} + \frac{38611v^6}{18900000} + \frac{24706901v^8}{49896000000} + \cdots,$$
$$b(c * (Ac)) - \frac{1}{8} = \frac{v^2}{2400} + \frac{429v^4}{560000} + \frac{38611v^6}{37800000} + \frac{24706901v^8}{99792000000} + \cdots,$$
$$bAc^2 - \frac{1}{12} = \frac{v^2}{3600} + \frac{143v^4}{280000} + \frac{38611v^6}{56700000} + \frac{24706901v^8}{149688000000} + \cdots,$$
$$bA^2c - \frac{1}{24} = -\frac{v^2}{3600} + \frac{109v^4}{336000} - \frac{1201v^6}{5670000} + \frac{14964937v^8}{59875200000} + \cdots,$$
$$b^*c^3 - \frac{1}{4} = \frac{353v^2}{37500} + \frac{220363v^4}{70000000} + \frac{357420517v^6}{47250000000} + \frac{200287631617v^8}{623700000000000} + \cdots,$$

$$b^*(c*(Ac)) - \frac{1}{8} = \frac{353v^2}{75000} + \frac{220363v^4}{140000000} + \frac{357420517v^6}{94500000000} + \frac{200287631617v^8}{1247400000000000} + \cdots,$$

$$b^*Ac^2 - \frac{1}{12} = \frac{353v^2}{112500} + \frac{220363v^4}{210000000} + \frac{357420517v^6}{141750000000} + \frac{200287631617v^8}{1871100000000000} + \cdots,$$

$$b^*A^2c - \frac{1}{24} = -\frac{31v^2}{22500} + \frac{63829v^4}{42000000} - \frac{66667603v^6}{56700000000} + \frac{236625893843v^8}{187110000000000} + \cdots.$$

Fifth algebraic order:

$$bc^4 - \frac{1}{5} = \frac{77v^2}{36000} + \frac{5231v^4}{8400000} + \frac{725189v^6}{212625000} - \frac{167318833v^8}{408240000000} + \cdots,$$

$$b(c^2*(Ac)) - \frac{1}{10} = \frac{77v^2}{72000} + \frac{5231v^4}{16800000} + \frac{725189v^6}{425250000} - \frac{167318833v^8}{816480000000} + \cdots,$$

$$b(c*(Ac^2)) - \frac{1}{15} = \frac{77v^2}{108000} + \frac{5231v^4}{25200000} + \frac{725189v^6}{637875000} - \frac{167318833v^8}{1224720000000} + \cdots,$$

$$b(c*(A^2c)) - \frac{1}{30} = -\frac{23v^2}{108000} + \frac{2561v^4}{5040000} - \frac{5099v^6}{145800000} + \frac{899797183v^8}{2694384000000} + \cdots,$$

$$bAc^3 - \frac{1}{20} = \frac{11v^2}{12000} - \frac{937v^4}{8400000} + \frac{714047v^6}{567000000} - \frac{554934517v^8}{1496880000000} + \cdots,$$

$$bA(c*(Ac) - \frac{1}{40} = \frac{3v^2}{8000} - \frac{47v^4}{1120000} + \frac{117757v^6}{226800000} - \frac{454698949v^8}{2993760000000} + \cdots,$$

$$bA^2c^2 - \frac{1}{60} = \frac{v^2}{4000} - \frac{47v^4}{1680000} + \frac{117757v^6}{340200000} - \frac{454698949v^8}{4490640000000} + \cdots,$$

$$bA^3c - \frac{1}{120} = \frac{v^2}{24000} + \frac{89v^4}{420000} + \frac{4039v^6}{24300000} + \frac{112471651v^8}{1122660000000} + \cdots,$$

$$b(Ac)^2 - \frac{1}{20} = \frac{77v^2}{144000} + \frac{5231v^4}{33600000} + \frac{725189v^6}{850500000} - \frac{167318833v^8}{1632960000000} + \cdots.$$

Theorem 2 *(see [54]) The necessary and sufficient conditions for an adapted RK method to be of order p are given by*

$$b(v)\Phi(\tau) - \frac{1}{\gamma(\tau)} = O(v^{p+1-\rho(\tau)}), \quad \rho(\tau) = 1, 2, ..., p.$$

where τ is a rooted tree of order $\rho(\tau)$ and the function $\gamma(\tau)$ and $\Phi(\tau)$ are defined as in [53].

By **Theorem** 2 we conclude that the methods of the new pair RK54NEW have algebraic order five and four.

3.4 Error analysis

If we want to see the behavior of the error and which parameters it depends on, we have to use the local truncation error (LTE). We refer to the way given by Van de Vyver [55] and the approach given by Anastassi and Simos [56], we shall present the asymptotic expressions of the local truncation error for methods:

- PHRK54H: the higher order method of phase fitted RK pair from Simos [49],
- MODPHRK54H: the higher order method of phase fitted modified RK pair obtained by Van de Vyver [48],
- MODRK54H: the higher order method of modified RK pair presented by Van de Vyver [57],
- RK54NEWH: the higher order method of the new pair.

Eq.(1) is equivalent with $y'' = (W(x) - E)y(x)$, a nature choice for ω during calculations for resonance problem is $\omega = \sqrt{E - \overline{W}}$, where $\overline{W}$ is the constant approximation of the effective potential $w(x)$. We have found the following asymptotic expressions for large $|E|$:

$$LTE(PHRK54H) \approx \frac{h^6}{3600}\begin{pmatrix} E^3 y(x) \\ E^3 y'(x) \end{pmatrix},$$

$$LTE(MODPHRK54H) \approx \frac{37h^6}{914400}\begin{pmatrix} -E^3 y(x) \\ -E^3 y'(x) \end{pmatrix},$$

$$LTE(MODRK54H) \approx \frac{h^6}{124815600}\begin{pmatrix} 37111E^2 y(x)(\overline{W} - W(x)) \\ -E^2(180675y(x)W'(x) - 37111(\overline{W} - W(x))y'(x)) \end{pmatrix}.$$

$$LTE(RK54NEWH) \approx \frac{h^6}{7200}\begin{pmatrix} E(-2W'(x)y'(x) - y(x)((\overline{W} - W(x))^2 + 5W''(x))) \\ 2E^2 y(x)W'(x) \end{pmatrix},$$

It was explained in [58] (p.197) that the amplitude of the derivative y' is bigger by a factor $D^{1/2}$. Comparing D with E we can know that $D = \overline{W} - E$, so the amplitude of the derivative y' is bigger by a factor $E^{1/2}$ either. Finally, we conclude that the global error produced by PHRK54H increases with $E^{7/2}$, MODPHRK54H increases with $E^{7/2}$, MODPHRK54H increases with $E^{5/2}$, and RK54NEWH increases with E^2, Thus RK54NEWH is the method to choose for large energies and this will be confirmed by the numerical illustrations in the next section.

4 Numerical results

4.1 Comparison with fixed stepsize

In this section we consider the numerical integration of the Schrödinger equation(1) in the case of $l = 0$ and *Woods-Saxon* potential:

$$W(x) \;=\; \frac{u_0}{1+q} + \frac{u_1 q}{(1+q)^2}, \qquad q = \exp(\frac{x - x_0}{a}),$$

with

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

The domain of numerical integration is [0, 15]. For the test potential we shall consider *the resonance problem* which consists of finding those energies ($E > 0$), at which the phase-shift is equal to $\frac{\pi}{2}$. The boundary conditions for this eigenvalue problem are

$$y(0) = 0 \qquad and \qquad y(x) = \cos(\sqrt{E}x) \; for \; large \; x.$$

The choice of ω is given by

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

The numerical results obtained by the methods are compared with the analytical solution of the *Woods-Saxon* potential, rounded to six decimal places. We consider four resonances:53.588872, 163.215341, 341.495874, 989.701916. Figures 1, 2, 3 and 4 show the errors $-\log_{10}|E_{\text{analytical}} - E_{\text{calculated}}|$ as a function of $-\log_2(h)$.

4.2 Comparison with variable stepsize

The variable stepsize embedded RK pairs used in the comparisions have been denoted by:

- PHRK54: the phase fitted RK pair from Simos [49],
- MODPHRK54: the phase fitted modified RK pair obtained by Van de Vyver [48],
- MODRK54: the modified RK pair presented by Van de Vyver [57],
- RK54NEW: the new pair presented this paper.

We consider the calculation of the phase-shifts with the *Lennard-Jones potential* [57] which is given by

$$V(x) = 500\Big(\frac{1}{x^{12}} - \frac{1}{x^6}\Big),$$

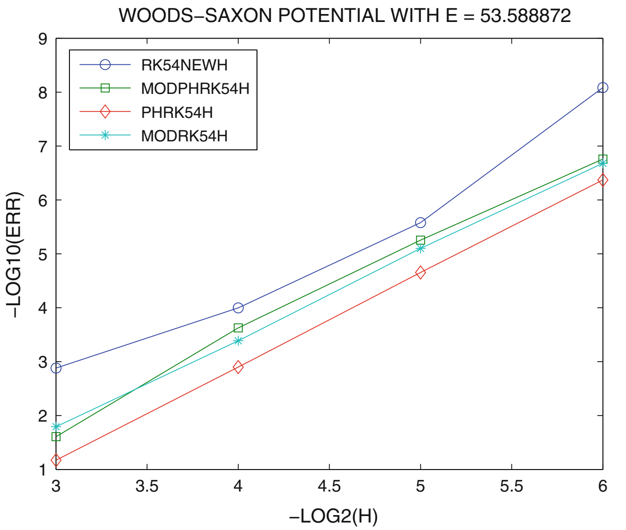

Fig. 1 Efficiency for the Schrödinger equation using $E = 53.588872$

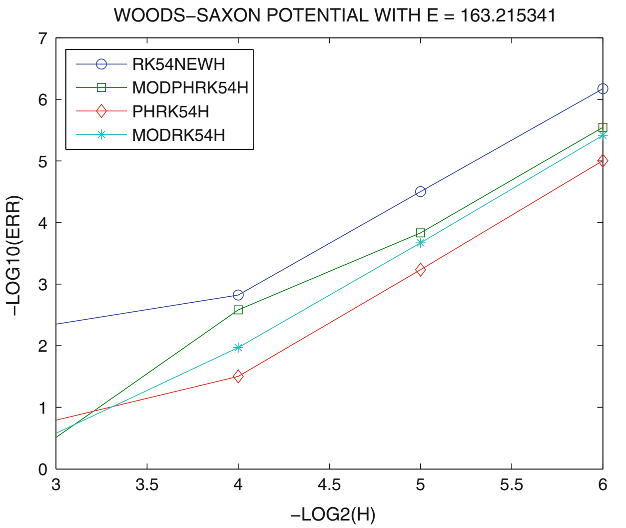

Fig. 2 Efficiency for the Schrödinger equation using $E = 163.215341$

Based on the work of Raptis and Cash [59], we start the integration from $x_0 = 0.7$ with an initial stepsize $h = 0.01$, for the initial condition of derivative we choose $y'(x_0) = 10^{-6}$, and take $Tol = 10^{-8}$ for the computation of the phase-shifts correct to four decimal places, we use the stepsize control procedure proposed by Raptis and Cash [59].

We consider the energies $k^2 = 25$ and $k^2 = 100$ and choose the $\omega = k$. For the calculation of phase-shifts, Figs. 5 and 6 show the number of function evaluations as a function of $l = 0, \ldots, 10$.

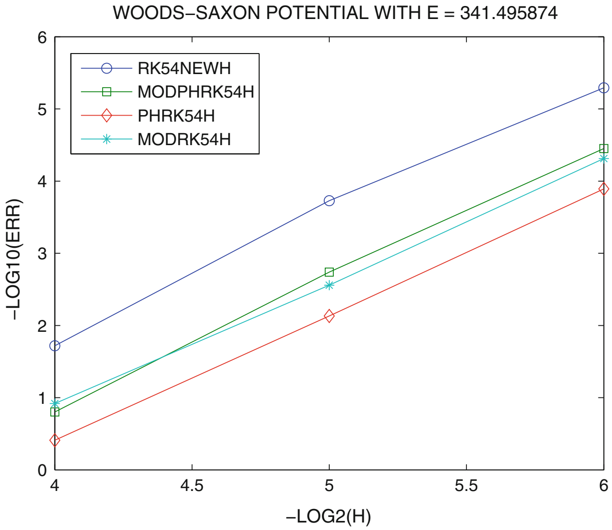

Fig. 3 Efficiency for the Schrödinger equation using $E = 341.495874$

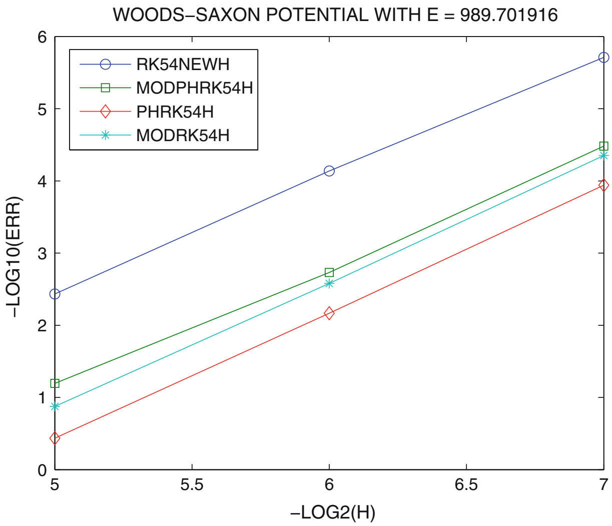

Fig. 4 Efficiency for the Schrödinger equation using $E = 989.701916$

5 Conclusions

Based on the approach introduced by Kalogiratou and Simos [50], we develop a new modified embedded 5(4) pair of explicit Runge–Kutta methods and give the asymptotic expression of the local errors for large energies, this can explain the numerical result in case of resonance problem. We apply the higher order method to the resonance problem and apply the new embedded pair to elastic scattering phase-shift problem.

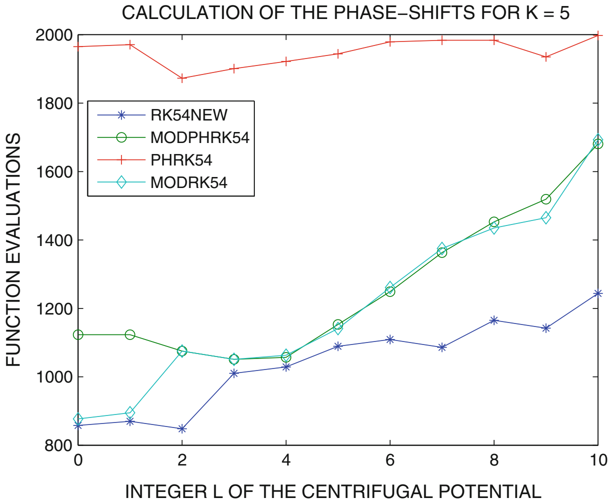

Fig. 5 The number of function evaluations used by the considered codes as a function of l from the centrifugal potential for energies $k^2 = 25$

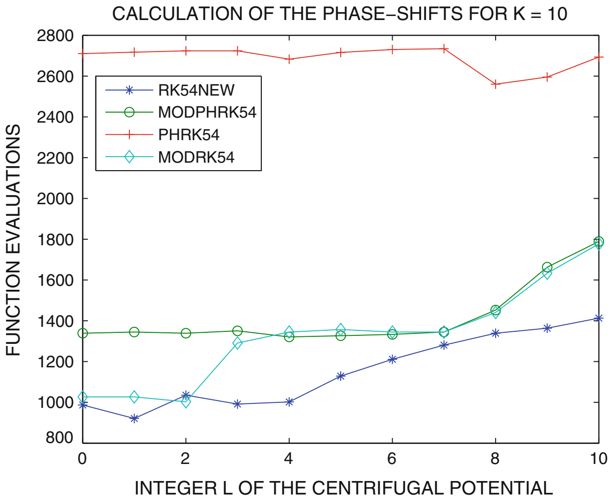

Fig. 6 The number of function evaluations used by the considered codes as a function of l from the centrifugal potential for energies $k^2 = 100$

The applications show the efficiency of our new developed embedded pair and the higher order method.

It is noted that in practical computations our new methods can be applied only when a good estimate of the dominant frequency of the solution is known in advance. For the techniques of estimating principal frequency we refer to the papers [60,61].

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