J Math Chem (2014) 52:1081–1098
DOI 10.1007/s10910-014-0328-y

ORIGINAL PAPER

A new embedded 5(3) pair of modified Runge–Kutta–Nyström methods for the numerical solution of the Schrödinger equation

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Received: 6 November 2013 / Accepted: 28 January 2014 / Published online: 14 February 2014

Abstract A new embedded 5(3) pair of modified Runge–Kutta–Nyström methods for the numerical solution of the Schrödinger equation is developed in this paper. The asymptotic expressions of the principal local truncation errors for large energies are obtained. We apply the new fifth-order method to the resonance problem, and apply the new embedded 5(3) pair to elastic scattering phase-shift problem. The numerical results show good numerical performance of the new embedded pair and the fifth-order method.

Keywords Embedded modified Runge–Kutta–Nyström methods · Exponential fitting · Schrödinger equation

1 Introduction

The radial Schrödinger equation has the form

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

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where the integer l representing the angular momentum, the term $l(l+1)/x^2$ is the *centrifugal potential*. The function $V(x)$ denotes the *potential* with $V(x) \to 0$ if $x \to \infty$, and $W(x) = l(l+1)/x^2 + V(x)$ is the *effective potential* satisfying $W(x) \to 0$ as $x \to \infty$. The real number E denotes the *energy*. The two boundary conditions associated with the equation are $y(0) = 0$ and the other imposed at large x, determined by physical considerations.

This type of equations appears often in scientific areas such as quantum chemistry, nuclear physics, molecular physics, celestial mechanics and so on. The past three decades, a lot of research has been performed on the numerical solution of the Schrödinger equation (1) or general ordinary differential equations with oscillatory character [1–38]. We remark that most of the techniques are multistep methods. Vigo–Aguiar and Simos gave an excellent review [20] on exponentially fitted multistep methods for the numerical solution of the Schrödinger equation. For variable stepsize multistep methods we refer the reader to [26]. A disadvantage of multistep methods is that they need many initial values. On the other hand, Runge–Kutta (–Nyström)[RK(N)] type methods have the simplicity of the initial start up. In addition, for variable-step algorithms, it is easy to change the steplength with RK(N) type methods than with multistep methods.

Very recently, Kalogiratou et al. [2] proposed a procedure for the numerical solution of the Schrödinger equation which is based on trigonometric fitting, the exponential order of the new methods is up to second. The numerical results show that the new methods have superior performance when solving the Schrödinger equation.

Based on the procedure of Kalogiratou et al. [2], we develop a new embedded 5(3) pair of modified Runge–Kutta–Nyström methods with four stages. In Sect. 2 we give the necessary conditions for constructing new methods. In Sect. 3 we derive the new 5(3) pair with modified Runge–Kutta–Nyström methods for second exponential order. In Sect. 4 we give the asymptotic expressions of the local truncation errors for large energies of the new pair and some related methods. In Sect. 5 the new fifth-order method is applied to the resonance problem, and the new embedded 5(3) pair of modified Runge–Kutta–Nyström methods is applied to elastic scattering phase-shift problem. Section 6 is devoted to conclusions.

2 Preliminaries

2.1 Embedded modified Runge–Kutta–Nyström methods

A modified RKN method is defined by

$$Y_i = y_n + c_i h y'_n + h \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, 2, \ldots, s,$$

$$y_{n+1} = g_1 y_n + g_2 h y'_n + h^2 \sum_{i=1}^{s} \bar{b}_i f(x_n + c_i h, Y_i),$$

$$y'_{n+1} = g_3 y'_n + h \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i). \tag{2}$$

The modified RKN method is associated with the following Butcher tableau:

$$\begin{array}{cc|cccc} & 0 & & & & \\ & c_2 & a_{21} & & & \\ & \vdots & \vdots & \ddots & & \\ & c_s & a_{s1} & \cdots & a_{s,s-1} & \\ \hline g_1 & g_2 & \bar{b}_1 & \cdots & \bar{b}_{s-1} & \bar{b}_s \\ \hline & g_3 & b_1 & \cdots & b_{s-1} & b_s \end{array}$$

or equivalently by the quintuple $(c, A, \bar{b}, b, g)$, where $A = (a_{i,j})_{s\times s} \in \mathbb{R}^{s\times s}$, $\bar{b}^T = (\bar{b}_1, \bar{b}_2, \ldots, \bar{b}_s)^T \in \mathbb{R}^s$, $b^T = (b_1, b_2, \ldots, b_s)^T \in \mathbb{R}^s$, $c = (c_1, c_2, \ldots, c_s)^T \in \mathbb{R}^s$, $g = (g_1, g_2, g_3) \in \mathbb{R}^3$, with $e = (1, 1, \ldots, 1)^T \in \mathbb{R}^s$. We note that for $g_1 = g_2 = g_3 = 1$ the modified RKN method is reduced to a standard RKN method.

An embedded $q(p)$ pair of modified RKN method is based on the modified RKN method $(c, A, \bar{b}, b, g)$ of order q and another modified RKN method $(c, A, \bar{b}^*, b^*, g^*)$ of order $p < q$. We obtain a local error estimation of the pth-order method at the integration point $x_{n+1} = x_n + h_n$ by means of the quantity

$$EST_{n+1} = max \left\{ \| y_{n+1} - y^*_{n+1} \|_\infty, \| y'_{n+1} - y'^*_{n+1} \|_\infty \right\}$$

There are many variable stepsize algorithms used in the literature. For the numerical integration of the Schrödinger equation (1) we use the stepsize algorithms proposed by Raptis and Cash [44]:

– if $EST_{n+1} < \frac{Tol}{100}$, $h_{n+1} = 2h_n$,
– if $\frac{Tol}{100} \le EST_{n+1} < Tol$, $h_{n+1} = h_n$,
– if $EST_{n+1} \ge Tol$, $h_{n+1} = \frac{h_n}{2}$ and repeat the step.

where Tol is the maximum allowable error.

2.2 Trigonometrically fitted modified Runge–Kutta–Nyström method

The operators $L(x)$ and $Lp(x)$ are defined as follows:

$$Y_i(x) = y(x) + c_i h y'(x) + h^2 \sum_{j=1}^{i-1} a_{ij} Y''_j(x), \quad i = 1, 2, \ldots, s,$$

$$L(x) = y(x+h) - g_1 y(x) - g_2 h y'(x) - h^2 \sum_{i=1}^{s} \bar{b}_i Y''_i(x),$$

$$Lp(x) = y'(x+h) - g_3 y'(x) - h \sum_{i=1}^{s} b_i Y''_i(x). \tag{3}$$

Definition 1 (See [39]) The method has exponential order p if the associated operator L 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 [39]) If $\omega_i = \omega$ for $i = 0, 1, \ldots, n, n \leq p$, then the operator L vanishes for any linear combination of

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

We give the conditions for modified RKN methods in the following theorem.

Theorem 1 *Modified RKN method (2) is of exponential order p if the following conditions are satisfied:*

$$\begin{aligned}
\cos v - g_1 &= -v^2 \sum_{k=0}^{s-1} (-1)^k (\bar{b}.A^k.e) v^{2k}, \\
\tfrac{\sin v}{v} - g_2 &= -v^2 \sum_{k=0}^{s-2} (-1)^k (\bar{b}.A^k.c) v^{2k}, \\
\tfrac{\sin v}{v} &= \sum_{k=0}^{s-1} (-1)^k (b.A^k.e) v^{2k}, \\
\cos v - g_3 &= -v^2 \sum_{k=0}^{s-2} (-1)^k (b.A^k.c) v^{2k}.
\end{aligned} \tag{4}$$

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:

$$\begin{aligned}
\sin v &= 2 \sum_{k=0}^{s-1} (-1)^k (k+1)(\bar{b}.A^k.e) v^{2k+1}, \\
\tfrac{\sin v - v \cos v}{v^3} &= 2 \sum_{k=0}^{s-2} (-1)^k (k+1)(\bar{b}.A^k.c) v^{2k}, \\
\cos v &= \sum_{k=0}^{s-1} (-1)^k (2k+1)(b.A^k.e) v^{2k}, \\
\sin v &= 2 \sum_{k=0}^{s-2} (-1)^k (k+1)(b.A^k.c) v^{2k+1}.
\end{aligned} \tag{5}$$

3 Derivation of the new embedded 5(3) pair

3.1 Trigonometrically fitted fifth order modified RKN method with second exponential order

We consider the four-stage modified RKN method formulas which can be denoted by the Butcher tableau:

$$\begin{array}{cc|cccc} & 0 & & & & \\ & \frac{1}{5} & \frac{1}{50} & & & \\ & \frac{2}{3} & -\frac{1}{27} & \frac{7}{27} & & \\ & 1 & \frac{3}{10} & -\frac{2}{35} & \frac{9}{35} & \\ \hline g_1 & g_2 & \bar{b}_1 & \bar{b}_2 & \bar{b}_3 & \bar{b}_4 \\ \hline & g_3 & b_1 & b_2 & b_3 & b_4 \end{array} \tag{6}$$

The c- and A-values are taken from the standard fifth-order RKN method [40]. Consider this modified RKN method, for second exponential order we require Eqs. (4, 5) to be satisfied:

$$\begin{aligned} &\cos v - g_1 = -(\bar{b}.e)v^2 + (\bar{b}.A.e)v^4 - (\bar{b}.A.A.e)v^6 + (\bar{b}.A.A.A.e)v^8, \\ &\tfrac{\sin v}{v} - g_2 = -(\bar{b}.c)v^2 + (\bar{b}.A.c)v^4 - (\bar{b}.A.A.c)v^6, \\ &\tfrac{\sin v}{v} = (b.e) - (b.A.e)v^2 + (b.A.A.e)v^4 - (b.A.A.A.e)v^6, \\ &\cos v - g_3 = -(b.c)v^2 + (b.A.c)v^4 - (b.A.A.c)v^6. \end{aligned} \tag{7}$$

and

$$\begin{aligned} &\sin v = 2(\bar{b}.e)v - 4(\bar{b}.A.e)v^3 + 6(\bar{b}.A.A.e)v^5 - 8(\bar{b}.A.A.A.e)v^7, \\ &\sin v - v\cos v = v^3(2(\bar{b}.c) - 4(\bar{b}.A.c)v^2 + 6(\bar{b}.A.A.c)v^4), \\ &\cos v = (b.e) - 3(b.A.e)v^2 + 5(b.A.A.e)v^4 - 7(b.A.A.A.e)v^6, \\ &\sin v = 2(b.c)v - 4(b.A.c)v^3 + 6(b.A.A.c)v^5. \end{aligned} \tag{8}$$

Then the modified RKN method integrates exactly the functions

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

We set $\bar{b}_1 = \frac{1}{24}, \bar{b}_2 = \frac{25}{84}, b_1 = \frac{1}{24}$. Solving the system of Eqs. (7) and (8), the coefficients $\bar{b}_3, \bar{b}_4, g_1, g_2, b_2, b_3, b_4, g_3$ of this method are:

$$\begin{aligned} \bar{b}_3 = \Big(&45\left(5v^3\left(2v^6 - 93v^4 + 768v^2 - 3525\right)\right. \\ &- 84v\left(2v^6 - 63v^4 + 375v^2 - 375\right)\cos(v) \\ &\left.+ 84\left(17v^6 - 183v^4 + 750v^2 - 375\right)\sin(v)\right)\Big)/(28Nv^3), \end{aligned}$$

$$\bar{b}_4 = 25\left(5v^3\left(v^4 - 54v^2 + 540\right) - 18v\left(7v^4 - 200v^2 + 450\right)\cos(v)\right.$$

$$+\ \left(966v^4-9000v^2+8100\right)\sin(v)\Big)/(4Nv^3),$$

$$g_1=\Big(\left(-7v^{10}+740v^8-17625v^6+66600v^4-269250v^2+675000\right)\cos(v)$$
$$+v\left(77v^8-4500v^6+41475v^4-209400v^2+618750\right)\sin(v)$$
$$+25v^4\left(25v^4-852v^2+1875\right)\Big)/(20N),$$

$$g_2=\Big(2v\left(7v^8-390v^6+6465v^4-11550v^2-33750\right)\cos(v)$$
$$-6\left(21v^8-610v^6+5215v^4-4250v^2-33750\right)\sin(v)$$
$$+5v^5\left(9v^4-320v^2+985\right)\Big)/(4Nv),$$

$$b_2=\Big(\left(-7v^{10}+670v^8-13725v^6+39150v^4-162750v^2+337500\right)\sin(v)$$
$$-10v\left(7v^8-390v^6+2745v^4-10650v^2+33750\right)\cos(v)$$
$$-25v^3\left(7v^4-152v^2+375\right)\Big)/(168Mv^3),$$

$$b_3=-9\Big(25\left(v^2-5\right)v^3+10\left(v^6-66v^4+450v^2-1500\right)v\cos(v)$$
$$+\left(v^8-106v^6+2160v^4-10500v^2+15000\right)\sin(v)\Big)/(28Mv^3),$$

$$b_4=-5\Big(25v^3+10\left(v^4-70v^2+450\right)v\cos(v)$$
$$+\left(v^6-110v^4+2050v^2-4500\right)\sin(v)\Big)/(8Mv^3),$$

$$g_3=\Big(\left(-20v^6+948v^4-6600v^2+9000\right)\cos(v)-5v^4$$
$$-2v\left(v^6-82v^4+1680v^2-3450\right)\sin(v)\Big)/(12M),$$

where $N=7v^8-180v^6-1815v^4+600v^2+33750$, $M=9v^4-350v^2+750$, $v=\omega h$.

For small values of $|v|$ the above formulae are subject to heavy cancelations. In that case the following Taylor series must be used:

$$\bar{b}_3=\frac{9}{56}+\frac{9v^4}{2800}-\frac{257v^6}{1890000}+\frac{5284049v^8}{37422000000}+\frac{2082554219v^{10}}{218918700000000}+\cdots,$$
$$\bar{b}_4=-\frac{13v^4}{8400}-\frac{311v^6}{3780000}-\frac{5428733v^8}{74844000000}-\frac{726787289v^{10}}{62548200000000}+\cdots,$$
$$g_1=1+\frac{v^6}{900}-\frac{3v^8}{22400}+\frac{1483v^{10}}{21262500}+\cdots,$$
$$g_2=1+\frac{v^6}{2520}-\frac{1349v^8}{15120000}+\frac{1187509v^{10}}{56133000000}+\cdots.$$
$$b_2=\frac{125}{336}+\frac{3v^4}{3136}+\frac{1787v^6}{4233600}+\frac{2723113v^8}{16765056000}+\frac{2452820737v^{10}}{32691859200000}+\cdots,$$

$$b_3 = \frac{27}{56} - \frac{9v^4}{3920} - \frac{41v^6}{44100} - \frac{443701v^8}{1164240000} - \frac{15295351v^{10}}{90810720000} + \cdots,$$
$$b_4 = \frac{5}{48} + \frac{3v^4}{2240} + \frac{379v^6}{604800} + \frac{3275269v^8}{11975040000} + \frac{561381377v^{10}}{4670265600000} + \cdots,$$
$$g_3 = 1 + \frac{v^8}{48000} + \frac{1187v^{10}}{68040000} + \frac{6537413v^{12}}{898128000000} + \cdots.$$

It is observed that when $v \to 0$, this method reduces to the classical fifth-order RKN method [40].

When apply this method to non-autonomous equation $Y'' = f(x, y)$ in the scalar case, the principal local truncation errors (PLTE) for y-component and its derivative are given as follows:

$$PLTE(y) = \frac{h^6}{21600}\left(-11 f_y y^{(4)} + 4y^{(3)}\left(f_{yy}y' + f_{xy}\right) - y^{(6)} + 36\omega^4 y^{(2)} + 24\omega^6 y\right),$$
$$PLTE(y') = \frac{h^6}{108000}(55 f_{xy} y^{(4)} + 9 f_y y^{(5)} - 10 f_y{}^2 y^{(3)} + y^{(7)} - 10 f_{yy} y^{(3)} y^{(2)}$$
$$+ 55 y' f_{yy} y^{(4)} - 10 f_{xxy} y^{(3)} - 10(y')^2 f_{yyy} y^{(3)} - 20 y' f_{xyy} y^{(3)}).$$

Hence this method is algebraically of fifth order, we denote this modified RKN method by RKN53NEWH.

3.2 Trigonometrically fitted third order modified RKN method with second exponential order

For the purpose of developing an embedded 5(3) pair of modified RKN methods based on the above presented fifth-order modified RKN method $(A, c, \bar{b}, b, g)$, we consider the modified RKN method $(A, c, \bar{b}^*, b^*, g^*)$.

Following a similar approach as described above, for second exponential order, we require Eqs. (4, 5) to be satisfied, thus the following conditions should hold:

$$\begin{aligned}
&\cos v - g_1^* = -(\bar{b}^*.e)v^2 + (\bar{b}^*.A.e)v^4 - (\bar{b}^*.A.A.e)v^6 + (\bar{b}^*.A.A.A.e)v^8,\\
&\tfrac{\sin v}{v} - g_2^* = -(\bar{b}^*.c)v^2 + (\bar{b}^*.A.c)v^4 - (\bar{b}^*.A.A.c)v^6,\\
&\tfrac{\sin v}{v} = (b^*.e) - (b^*.A.e)v^2 + (b^*.A.A.e)v^4 - (b^*.A.A.A.e)v^6,\\
&\cos v - g_3^* = -(b^*.c)v^2 + (b^*.A.c)v^4 - (b^*.A.A.c)v^6.
\end{aligned} \tag{9}$$

and

$$\begin{aligned}
&\sin v = 2(\bar{b}^*.e)v - 4(\bar{b}^*.A.e)v^3 + 6(\bar{b}^*.A.A.e)v^5 - 8(\bar{b}^*.A.A.A.e)v^7,\\
&\sin v - v\cos v = v^3(2(\bar{b}^*.c) - 4(\bar{b}^*.A.c)v^2 + 6(\bar{b}^*.A.A.c)v^4),\\
&\cos v = (b^*.e) - 3(b^*.A.e)v^2 + 5(b^*.A.A.e)v^4 - 7(b^*.A.A.A.e)v^6,\\
&\sin v = 2(b^*.c)v - 4(b^*.A.c)v^3 + 6(b^*.A.A.c)v^5.
\end{aligned} \tag{10}$$

Then this modified RKN method integrates exactly the functions

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

We set $\bar{b}_1^* = -\frac{5}{24}$, $\bar{b}_2^* = \frac{125}{168}$, $b_1^* = -\frac{1}{12}$. Solving the system of Eqs. (9) and (10), the coefficients $\bar{b}_3^*, \bar{b}_4^*, g_1^*, g_2^*, b_2^*, b_3^*, b_4^*, g_3^*$ of this method are:

$$\begin{aligned}
\bar{b}_3^* &= \Big(45\Big(25v^3\Big(v^6-15v^4+132v^2-975\Big)-84v\Big(2v^6-63v^4+375v^2-375\Big)\cos(v)\\
&\quad+84\Big(17v^6-183v^4+750v^2-375\Big)\sin(v)\Big)\Big)/(28Nv^3),\\
\bar{b}_4^* &= 25\Big(25v^3\Big(v^4-12v^2+270\Big)-36v\Big(7v^4-200v^2+450\Big)\cos(v)\\
&\quad+12\Big(161v^4-1500v^2+1350\Big)\sin(v)\Big)/(8Nv^3),\\
g_1^* &= \Big(\Big(-7v^{10}+740v^8-17625v^6+66600v^4-269250v^2+675000\Big)\cos(v)\\
&\quad+v\Big(77v^8-4500v^6+41475v^4-209400v^2+618750\Big)\sin(v)\\
&\quad+125v^4\Big(2\Big(v^2-99\Big)v^2+375\Big)\Big)/(20N),\\
g_2^* &= \Big(25\Big(v^4-70v^2+215\Big)v^5+2\Big(7v^8-390v^6+6465v^4-11550v^2-33750\Big)v\cos(v)\\
&\quad-6\Big(21v^8-610v^6+5215v^4-4250v^2-33750\Big)\sin(v)\Big)/(4Nv),\\
b_2^* &= \Big(\Big(-7v^{10}+670v^8-13725v^6+39150v^4-162750v^2+337500\Big)\sin(v)\\
&\quad-10v\Big(7v^8-390v^6+2745v^4-10650v^2+33750\Big)\cos(v)\\
&\quad+50v^3\Big(7v^4-152v^2+375\Big)\Big)/(168Mv^3),\\
b_3^* &= -9\Big(10v\Big(v^6-66v^4+450v^2-1500\Big)\cos(v)-50v^3\Big(v^2-5\Big)\\
&\quad+\Big(v^8-106v^6+2160v^4-10500v^2+15000\Big)\sin(v)\Big)/(28Mv^3),\\
b_4^* &= -5\Big(10v\Big(v^4-70v^2+450\Big)\cos(v)-50v^3\\
&\quad+\Big(v^6-110v^4+2050v^2-4500\Big)\sin(v)\Big)/(8Mv^3),\\
g_3^* &= \Big(5v^4+\Big(-10v^6+474v^4-3300v^2+4500\Big)\cos(v)\\
&\quad-v\Big(v^6-82v^4+1680v^2-3450\Big)\sin(v)\Big)/(6M),
\end{aligned}$$

where $N = 7v^8-180v^6-1815v^4+600v^2+33750$, $M = 9v^4-350v^2+750$, $v = \omega h$.

For small values of $|v|$ the above formulae are subject to heavy cancelations. In that case the following Taylor series should be used:

$$\bar{b}_3^* = -\frac{9}{56} - \frac{v^2}{50} - \frac{5941v^4}{630000} - \frac{281621v^6}{141750000} - \frac{1532110813v^8}{2806650000000} + \cdots,$$
$$\bar{b}_4^* = \frac{1}{8} + \frac{v^2}{50} + \frac{3911v^4}{630000} + \frac{431507v^6}{283500000} + \frac{2227141921v^8}{5613300000000} + \cdots,$$
$$g_1^* = 1 - \frac{v^6}{250} - \frac{135767v^8}{226800000} - \frac{627847v^{10}}{3189375000} + \cdots,$$
$$g_2^* = 1 + \frac{v^4}{300} - \frac{731v^6}{945000} - \frac{126901v^8}{3402000000} - \frac{104954033v^{10}}{4209975000000} + \cdots.$$
$$b_2^* = \frac{25}{42} + \frac{23v^2}{1680} + \frac{6233v^4}{705600} + \frac{416347v^6}{105840000} + \frac{715310257v^8}{419126400000} + \cdots,$$
$$b_3^* = \frac{9}{28} - \frac{3v^2}{70} - \frac{499v^4}{24500} - \frac{39023v^6}{4410000} - \frac{112343521v^8}{29106000000} + \cdots,$$
$$b_4^* = \frac{1}{6} + \frac{7v^2}{240} + \frac{7157v^4}{504000} + \frac{94931v^6}{15120000} + \frac{825291469v^8}{299376000000} + \cdots,$$
$$g_3^* = 1 + \frac{v^4}{600} + \frac{7v^6}{9000} + \frac{3929v^8}{10800000} + \frac{286043v^{10}}{1701000000} + \cdots.$$

It is observed that when $v \to 0$, this method reduces to the classical third-order RKN method [40].

When apply this method to non-autonomous equation $Y'' = f(x, y)$ in the scalar case, we present the PLTE for y-component and its derivative:

$$PLTE(y) = \frac{h^5}{900}(5y^{(5)} + 6\omega^2 y^{(3)} - 2f_y y^{(3)} + 3\omega^4 y'),$$
$$PLTE(y') = \frac{h^4}{1800}(5y^{(5)} + 6\omega^2 y^{(3)} - 2f_y y^{(3)} + 3\omega^4 y').$$

Therefore, this method is algebraically of third order, we denote this modified RKN method by RKN53NEWL, and we denote the new 5(3) pair of modified RKN methods by RKN53NEW.

4 Error analysis

In this paper we focus on solving the Schrödinger equation. In order to see the behavior of the error, we have to carry out the error analysis. We follow the approach of Ixaru and Rizea [42], one can find similar descriptions given by Anastassi and Simos [12], Van de Vyver [32]. We consider the following RKN-type methods and labeling:

– EFRKN5: The fifth-order exponentially fitted explicit RKN method derived by Van de Vyver [33].

- RKN5 PL-DPL-AF: The optimized fifth-order explicit RKN method given by Kosti et al. [34].
- RKN5 PL-AF-DAF: The optimized fifth-order explicit RKN method given by Kosti et al. [35].
- FRKN53H: The fifth-order explicit RKN method presented by Van de Vyver [36].
- RKN5S2: The second fifth-order explicit RKN method obtained by Kalogiratou et al. [2].
- RKN53NEWH: The fifth-order modified RKN method obtained in this paper.
- RKN53NEWL: The third-order modified RKN method obtained in this paper.

The fitted frequency ω determines the performance of the method. A reasonable strategy for frequencies approximations is: Divide $[a, b]$ in some subintervals and on each of them the function $W(x)$ is approximated by a constant $\bar{W}$, a choice for the fitted frequency ω in such a subinterval is given by $\omega = \sqrt{E - \bar{W}}$. Equation (1) is equivalent with $y'' = f(x, y)$, where $f(x, y) = (W(x) - E)y(x)$. We have found the following asymptotic expressions for large $|E|$:

$$
\begin{aligned}
PLTE(y)_{EFRKN5} &\approx -\frac{h^6}{1800}\mathrm{E}^2 y(x)\Delta W,\\
PLTE(y')_{EFRKN5} &\approx -\frac{h^6}{7560000}E^2\left(3107y(x)W'(x) + 4647\Delta W)y'(x)\right),\\
PLTE(y)_{RKN5PL-DPL-AF} &\approx -\frac{h^6}{7200}E^3 y(x),\\
PLTE(y')_{RKN5PL-DPL-AF} &\approx \frac{h^6}{7200}E^3 y'(x),\\
PLTE(y)_{RKN5PL-AF-DAF} &\approx -\frac{h^6}{7200}E^3 y(x),\\
PLTE(y')_{RKN5PL-AF-DAF} &\approx \frac{h^6}{7200}E^3 y'(x),\\
PLTE(y)_{FRKN53H} &\approx -\frac{h^6 y(x)}{1800}E^2\Delta W,\\
PLTE(y')_{FRKN53H} &\approx \frac{h^6}{1200}E^2 y(x)W'(x),\\
PLTE(y)_{RKN5S2} &\approx -\frac{h^6}{3600}E\left(y(x)W''(x) + 4W'(x)y'(x) - 2y(x)(\Delta W)^2\right),\\
PLTE(y')_{RKN5S2} &\approx \frac{h^6}{1200}E^2 y(x)W'(x),\\
PLTE(y)_{RKN53NEWH} &\approx \frac{h^6}{3600}E\left(3y(x)W''(x) + 4W'(x)y'(x) + 6y(x)(\Delta W)^2\right),\\
PLTE(y')_{RKN53NEWH} &\approx \frac{h^6}{1200}\mathrm{E}^2 y(x)W'(x),\\
PLTE(y)_{RKN53NEWL} &\approx -\frac{h^5}{75}Ey(x)W'(x),\\
PLTE(y')_{RKN53NEWL} &\approx -\frac{h^4}{150}\mathrm{E}y(x)W'(x),
\end{aligned}
$$

where $\Delta W = W(x) - \bar{W}$.

It has been explained in [41] (p. 197) that the amplitude of the derivative y' is bigger by a factor $E^{1/2}$ than that of y. We conclude that the local errors produced by methods RKN5S2 and RKN53NEWH on y and y' are proportional with $E^{3/2}$ and E^2, respectively. Both of them will have good numerical performance than other fifth-order methods listed above when solving the Schrödinger equation especially for large Energies. Further more, we observe that the local errors produced by the new third-order method RKN53NEWL on y and y' are proportional with E and E, respectively. Thus the new 5(3) pair of modified RKN method RKN53NEW will have good numerical performance when solving the Schrödinger equation especially for large energies. This will be confirmed by the numerical results in the next section.

5 Numerical illustrations

5.1 Comparison with fixed step-size methods

In this subsection we will compare the numerical performance of the fifth-order method RKN53NEWH of the new 5(3) pair with other fifth-order RKN-type methods: EFRKN5, RKN5 PL-DPL-AF, RKN5 PL-AF-DAF, FRKN53H, RKN5S2 which have been listed in Sect. 4.

We consider the numerical integration of the Schrödinger equation (1) with the well-known *Woods-Saxon* potential and in the case of $l = 0$:

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

with

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

The domain of integration is taken as [0, 15].

For this test potential we consider the so-called *the resonance problem* which consists in finding those resonances(or energies) $E \in [0, 1000]$, at which the phase-shift is equal to $\frac{\pi}{2}$. The boundary conditions for this problem are

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

Following the suggestion by Ixaru and Rizea [42], the fitted frequency 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 RKN-type methods are compared with the analytical solution of the *Woods-Saxon* potential, which are rounded to six decimal places.

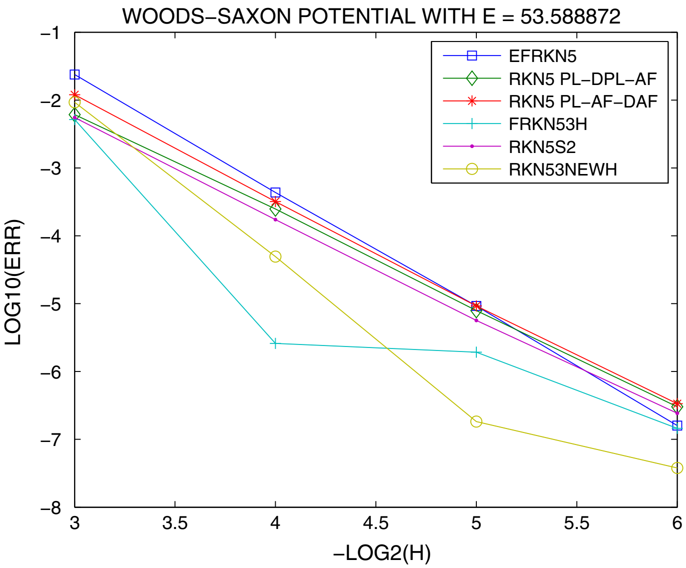

Fig. 1 Efficiency for the Schrödinger equation using $E = 53.588872$

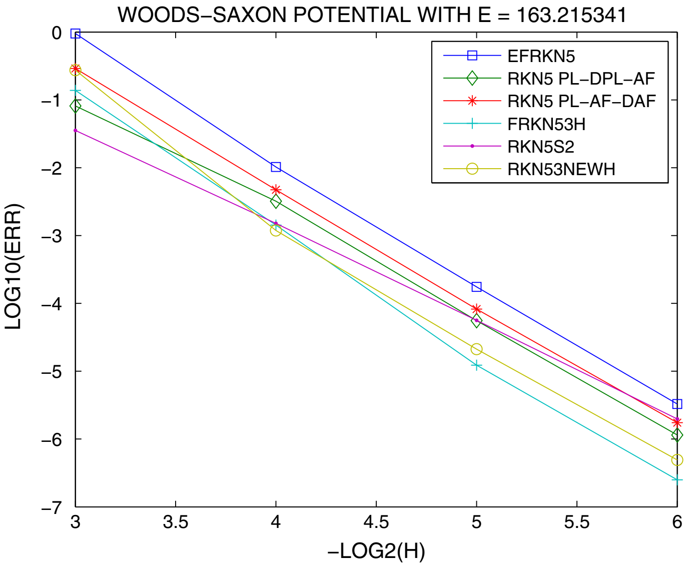

Fig. 2 Efficiency for the Schrödinger equation using $E = 163.215341$

Four resonances are considered:53.588872, 163.215341, 341.495874, 989.701916. Figures 1, 2, 3, and 4 show the errors $log_{10}|E_{\text{analytical}} - E_{\text{calculated}}|$ against $-log_2(h)$.

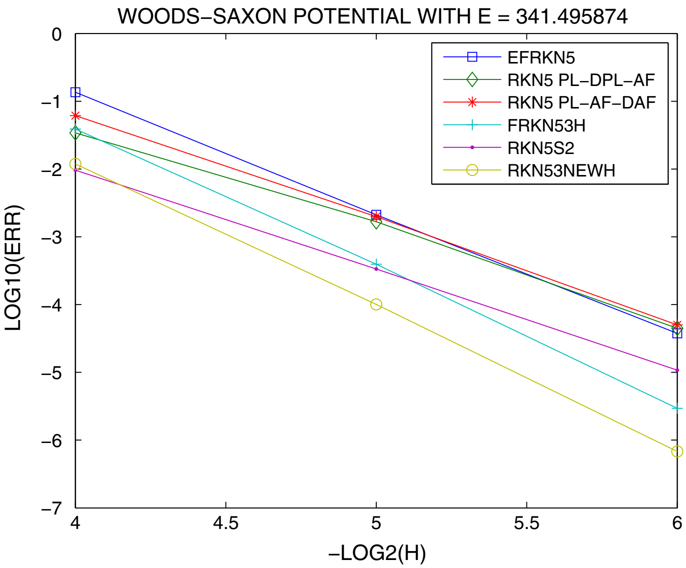

Fig. 3 Efficiency for the Schrödinger equation using $E = 341.495874$

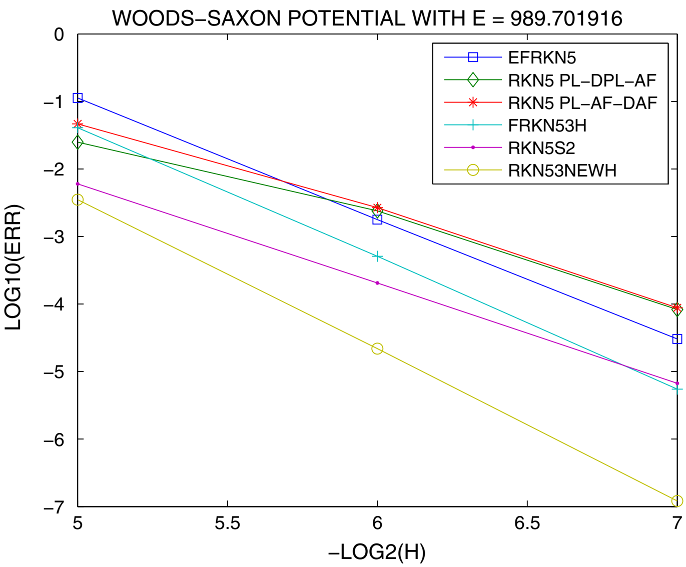

Fig. 4 Efficiency for the Schrödinger equation using $E = 989.701916$

5.2 Comparison with variable step-size methods

The methods used in the comparisons have been denoted by

– EFRKN43F: The exponentially fitted embedded 4(3) pair of explicit RKN methods with FSAL property derived by Franco [37],

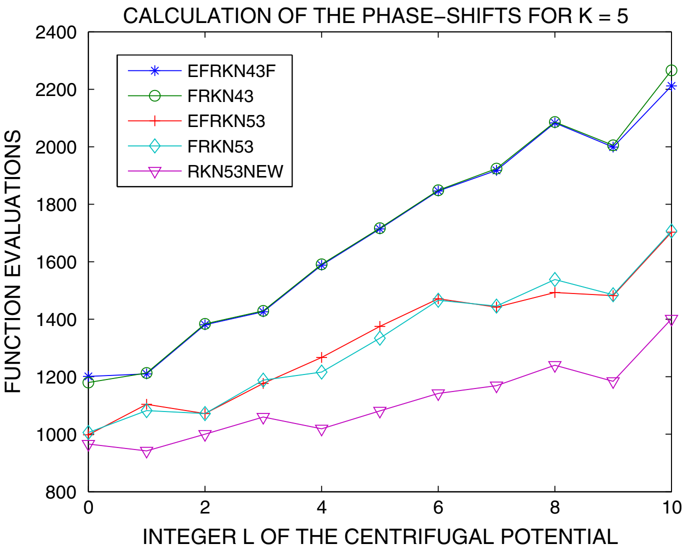

Fig. 5 The number of function evaluations used by the considered codes as a function of l from the centrifugal potential for energies $k^2 = 25$

- FRKN43: The embedded 4(3) pair of explicit RKN methods with FSAL property obtained by Van de Vyver [38],
- EFRKN53: The exponentially fitted embedded 5(3) pair of explicit RKN methods presented by Van de Vyver [33],
- FRKN53: The embedded 5(3) pair of explicit RKN methods given by Van de Vyver [36],
- RKN53NEW: the new embedded 5(3) pair of modified RKN methods derived in this paper.

We consider the numerical integration of the Schrödinger equation (1) with the widely discussed *Lennard–Jones potential* [29,43] which is given as follows

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

Following the work by Raptis and Allison [45], we start the numerical integration from $x_0 = 0.7$ with an initial stepsize $h = 0.01$. The first boundary condition can be transformed to $y(x_0) = 0$ [43], and we choose $y'(x_0) = 10^{-6}$ for the initial condition of the derivative. We use the variable stepsize algorithm in Sect. 2.1, and take $Tol = 10^{-8}$ for the computation of the phase-shifts correct to four decimal places that has been pointed out by Raptis and Cash [44].

We consider the energies $k^2 = 25$, $k^2 = 100$, $k^2 = 225$ and $k^2 = 900$ and choose the fitted frequency $\omega = k$. For the calculation of phase-shifts, Figs. 5, 6, 7, and 8 show the number of function evaluations as a function of $l = 0, \ldots, 10$.

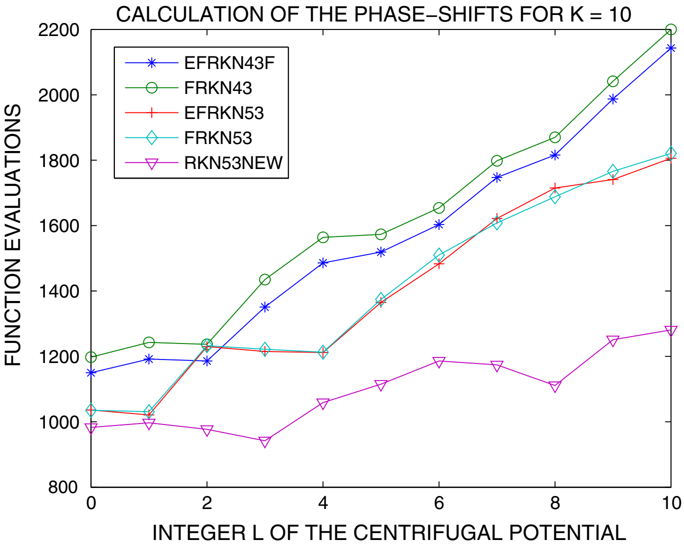

Fig. 6 The number of function evaluations used by the considered codes as a function of l from the centrifugal potential for energies $k^2 = 100$

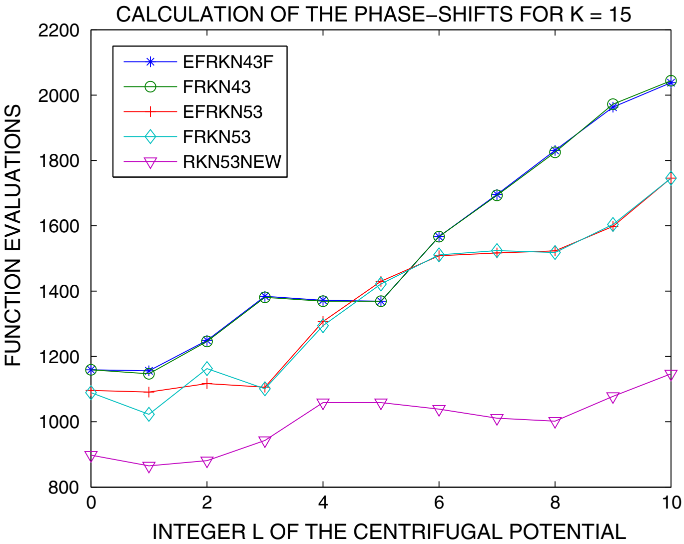

Fig. 7 The number of function evaluations used by the considered codes as a function of l from the centrifugal potential for energies $k^2 = 225$

6 Conclusions

On the basis of the procedure of Kalogiratou et al. [2], a new embedded 5(3) pair of modified Runge–Kutta–Nyström methods is developed in this paper. We carry out error analysis on the new 5(3) pair and some related methods, and obtain the asymp-

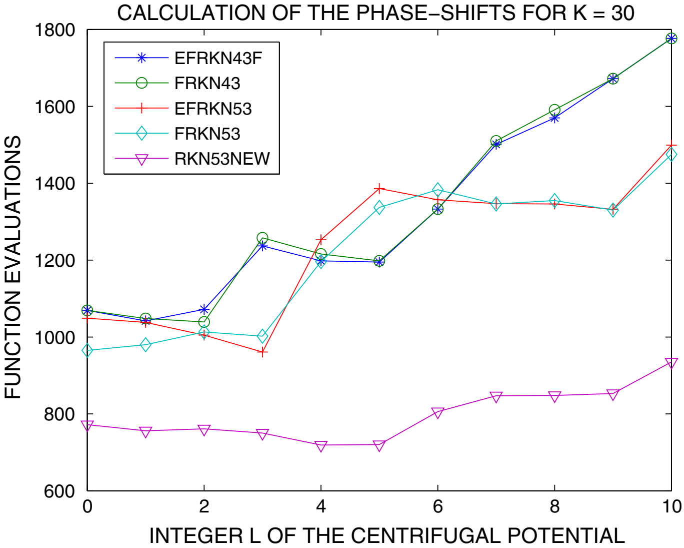

Fig. 8 The number of function evaluations used by the considered codes as a function of l from the centrifugal potential for energies $k^2 = 900$

totic expressions of the PLTEs for large energies. The analysis suggests theoretical advantages of the new 5(3) pair and the new fifth-order method when solving the Schrödinger equation. We apply the new fifth-order method to the Schrödinger equation with the Woods–Saxon potential (the resonance problem), and apply the new embedded 5(3) pair to elastic scattering phase-shift problem. The numerical results show good numerical performance of the new embedded 5(3) pair and the fifth-order method.

Finally, we note that the new developed 5(3) pair depend on the fitted frequency, we should keep in mind that the adapted methods can be applied only when a good estimate of the principal frequency is obtained in advance. For more techniques of estimating dominant frequency we refer the reader to the papers [46–49].

Acknowledgments This research was partially supported by NSFC (No. 11101357), the foundation of Shandong Outstanding Young Scientists Award Project (No. BS2010SF031), NSF of Shandong Province (No. ZR2011AL006) and the foundation of Scientific Research Project f Shangdong Universities (No. J11LG69).

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