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New optimized explicit modified RKN methods for the numerical solution of the Schrödinger equation

Yonglei Fang · Xiong You · Qinghe Ming

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Abstract This paper investigates a family of modified Runge-Kutta-Nyström (RKN) methods for the integration of second-order ordinary differential equations with oscillatory solutions. The order conditions for up to order five are presented. Two new optimized explicit four-stage modified RKN methods are derived by nullifying their dispersions and the dissipations in two different ways, respectively. These methods are checked to be of algebraic order five and both are dispersive of order six and dissipative of order five. The stability is examined and the error formulas are analyzed to show that advantages of the new methods compared with some highly efficient integrators from the recent literature. The high accuracy of the second new method is explained by its comparatively small dispersion and dissipation constants. In the integration of the resonance problem and the bound-states problem of the radial Schrödinger equation with the Woods-Saxon potential, the numerical results show the effectiveness and robustness of the new methods.

Y. Fang · Q. Ming
Department of Mathematics and Information Science, Zaozhuang University, Zaozhuang 277160, People's Republic of China

X. You (✉)
Department of Applied Mathematics, Nanjing Agricultural University, Nanjing 210095, People's Republic of China
e-mail: youx@njau.edu.cn

X. You
State Key Laboratory for Novel Software Technology at Nanjing University, Nanjing University, Nanjing 210093, People's Republic of China

Y. Fang
e-mail: ylfangmath@gmail.com

Q. Ming
e-mail: mqh@uzz.edu.cn

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1 Introduction

In the past two decades, there has been increasing interest in effective time-integration of the Schrödinger equation, which is of great importance in quantum physics, chemistry, biology etc. The radial or one dimensional Schrödinger equation we are concerned with in this paper has the form

$$y''(x) = \big(W(x) - E\big)y(x), \tag{1}$$

where the real number E is the *energy*, the function $W(x) = l(l+1)/x^2 + V(x)$ is the *effective potential* satisfying $W(x) \to 0$ as $x \to \infty$, the given integer l represents the *angular momentum* and the function $V(x)$ is the *potential*. Two boundary conditions are associated with this equation: one is $y(0) = 0$ and the other imposed at large x is determined by physical considerations. The form of this second boundary condition depends crucially on the sign of the energy E.

It has been universally acknowledged that when applied to the Schrödinger equation (1), general-purpose integrators cannot produce satisfactory numerical results. In the past decade, much attention has been concentrated on the design and analysis of effective and efficient integrators for the approximate solution of the radial Schrödinger equation (1) or for general second-order ordinary differential equations with oscillatory solutions ([1–71]). The vast literature in this direction can be broadly divided into four significant categories: (a) Runge-Kutta (RK) and Runge-Kutta Nyström (RKN) type methods that are phase-fitted and numerical methods with maximal dispersion order; (b) Exponentially/trigonometrically fitted RK and RKN or two-step methods; (c) Multistep phase-fitted methods and multistep methods with minimal phase-lag; (d) Symplectic and/or symmetric integrators for problems which can be regarded as Hamiltonian systems.

Compared with multistep methods whose implementation requires a series of starting values, Runge-Kutta (-Nyström) (RK(N)) type methods are more favorable because the initial values that are available in advance are sufficient for them to run. Regarding the oscillatory character of the solution to the Schrödinger equation (1), the task of this paper is to adapt modified RKN methods to the numerical integration of the radial Schrödinger equation (1). Section 2 presents order conditions and phase properties for modified RKN methods. In Sect. 3, we derive two new optimized modified RKN methods. In Sect. 4 we carry out the error analysis for the new methods and for five methods from the recent literature. In Sect. 5, we discuss the numerical stability of the new methods. Numerical results are reported in Sect. 6 to show the effectiveness and competence of our new methods. Section 7 is devoted to conclusions.

2 Modified RKN methods and phase properties

2.1 Order conditions for modified Runge-Kutta-Nyström methods

We start by considering the initial value problem of the second-order ODEs of the form

$$\begin{aligned} y'' &= f(x, y), \\ y(x_0) &= y_0,\ y'(x_0) = y'_0. \end{aligned} \tag{2}$$

Definition 1 An s-stage explicit modified Runge-Kutta-Nyström (RKN) method for the numerical solution of (2) reads

$$\begin{aligned} k_i &= f\Big(x_n + c_i h, \gamma_i y_n + c_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} k_j\Big),\ i = 1, \ldots, s, \\ y_{n+1} &= y_n + h y'_n + h^2 \sum_{i=1}^{s} \bar{b}_i k_i, \\ y'_{n+1} &= y'_n + h \sum_{i=1}^{s} b_i k_i, \end{aligned} \tag{3}$$

where $\gamma_i = \gamma_i(\nu)$ $(i = 1, \ldots, s)$ are even functions of $\nu = h\omega$. The scheme (3) can be expressed by the Butcher tableau

$$\begin{array}{c|c|c} c & \gamma & A \\ \hline & & \bar{b}^T \\ \hline & & b^T \end{array} = \begin{array}{c|c|cccc} 0 & \gamma_1 & & & & \\ c_2 & \gamma_2 & a_{21} & & & \\ \vdots & \vdots & \vdots & \vdots & & \\ c_s & \gamma_s & a_{s1} & \cdots & a_{ss-1} & \\ \hline & & \bar{b}_1 & \cdots & \bar{b}_{s-1} & \bar{b}_s \\ \hline & & b_1 & \cdots & b_{s-1} & b_s \end{array}$$

or can be simply denoted by $(c, \gamma, A, \bar{b}, b)$.

Here, following the approach of exponential-fitting and/or phase-fitting in [1,30,49], the frequency-depending parameters $\gamma_i = \gamma_i(\nu)$, $i = 1, \ldots, s$, are introduced to adapt the traditional RKN method to the oscillatory feature of the solution to the problem. It is assumed that $\lim_{\nu \to 0} \gamma_i(\nu) = 1$, $i = 1, \ldots, s$ so that as $\nu \to 0$, the modified RKN method (3) reduces to a traditional RKN method. In next section, we optimize the methods by nullifying the dispersion and dissipation.

The algebraic order conditions presented in [72] are not fit for the modified RKN method (3). To overcome the difficulty, we write

$$\gamma_i = 1 + \gamma_i^{(2)} \nu^2 + \gamma_i^{(4)} \nu^4 + \gamma_i^{(6)} \nu^6 + \cdots,$$

where $\gamma_i^{(2j)} = \frac{1}{(2j)!}\frac{d^{2j}}{dv^{2j}}\gamma_i(0)$, $j = 1, 2, \ldots$, and obtain the following conditions for the explicit modified RKN method (3) to be of up to order five:

- Order 1 requires:

$$\sum_i b_i - 1 = 0. \tag{4}$$

- Order 2 requires in addition:

$$\sum_i b_i c_i - \frac{1}{2} = 0, \quad \sum_i \bar{b}_i - \frac{1}{2} = 0. \tag{5}$$

- Order 3 requires in addition:

$$\sum_i b_i c_i^2 - \frac{1}{3} = 0, \quad \sum_i \sum_k b_i a_{ik} - \frac{1}{6} = 0, \quad \sum_i b_i \gamma_i^{(2)} = 0, \quad \sum_i \bar{b}_i c_i - \frac{1}{6} = 0. \tag{6}$$

- Order 4 requires, in addition:

$$\begin{aligned} &\sum_i b_i c_i^3 - \frac{1}{4} = 0, \quad \sum_i \sum_k b_i c_i a_{ik} - \frac{1}{8} = 0, \quad \sum_i \sum_k b_i a_{ik} c_k - \frac{1}{24} = 0, \\ &\sum_i b_i c_i \gamma_i^{(2)} = 0, \quad \sum_i \bar{b}_i c_i^2 - \frac{1}{12} = 0, \quad \sum_i \sum_k \bar{b}_i a_{ik} - \frac{1}{24} = 0, \quad \sum_i \bar{b}_i \gamma_i^{(2)} = 0 \end{aligned} \tag{7}$$

- Order 5 requires, in addition:

$$\begin{aligned} &\sum_i b_i c_i^4 - \frac{1}{5} = 0, \quad \sum_i \sum_k b_i c_i^2 a_{ik} - \frac{1}{10} = 0, \quad \sum_i \sum_k \sum_l b_i c_i a_{ik} a_{il} - \frac{1}{20} = 0, \\ &\sum_i \sum_k b_i c_i a_{ik} c_k - \frac{1}{30} = 0, \quad \sum_i \sum_k b_i a_{ik} c_k^2 - \frac{1}{60} = 0, \\ &\sum_i \sum_k \sum_l b_i a_{ik} a_{kl} - \frac{1}{120} = 0, \\ &\sum_i b_i (\gamma_i^{(2)})^2 = 0, \quad \sum_i b_i c_i^2 \gamma_i^{(2)} = 0, \quad \sum_i \sum_k b_i a_{ik} \gamma_k^{(2)} = 0, \quad \sum_i b_i \gamma_i^{(4)} = 0, \\ &\sum_i \bar{b}_i c_i^3 - \frac{1}{20} = 0, \quad \sum_i \sum_k \bar{b}_i c_i a_{ik} - \frac{1}{40} = 0, \quad \sum_i \sum_k \bar{b}_i a_{ik} c_k - \frac{1}{120} = 0, \\ &\sum_i \bar{b}_i c_i \gamma_i^{(2)} = 0. \end{aligned} \tag{8}$$

2.2 Phase properties of modified RKN methods

For a traditional RKN method or the modified RKN method (3) solving oscillatory problems, apart from the local truncation error, the numerical solution may also have errors in phase and amplification factor. To specify, let us consider the test equation

$$y'' = -\omega^2 y,\ \omega \in \mathbb{R}^+, \tag{9}$$

whose exact solution at $x_n = x_0 + nh$ can be written in the form

$$y(x_n) = \alpha \cos(n\nu + \varphi_0), \quad \nu = h\omega,$$

where the constants α and φ_0 can be determined by the initial values of the problem. The solution to the test Eq. (9) and its derivative satisfy

$$\begin{pmatrix} y(x_n + h) \\ hy'(x_n + h) \end{pmatrix} = M_0(\nu) \begin{pmatrix} y(x_n) \\ hy'(x_n) \end{pmatrix},$$

where

$$M_0(\nu) = \begin{pmatrix} \cos(\nu) & \dfrac{\sin(\nu)}{\nu} \\ -\nu \sin(\nu) & \cos(\nu) \end{pmatrix}, \quad \nu = \omega h. \tag{10}$$

If we apply the modified RKN methods (3) to the test Eq. (9), we obtain the relation

$$\begin{pmatrix} y_{n+1} \\ hy'_{n+1} \end{pmatrix} = M(\nu) \begin{pmatrix} y_n \\ hy'_n \end{pmatrix},$$

where

$$M(\nu) = \begin{pmatrix} 1 - \nu^2 \bar{b}^T N^{-1} \gamma & 1 - \nu^2 \bar{b}^T N^{-1} c \\ -\nu^2 b^T N^{-1} \gamma & 1 - \nu^2 b^T N^{-1} c \end{pmatrix}, \tag{11}$$

with $N = I + \nu^2 A, e = (1, \ldots, 1)^T, \gamma = (\gamma_1, \ldots, \gamma_s)^T$, and the operation "$\cdot$" is understood as component-wise multiplication.

Definition 2 (see [73]) For a modified RKN method (3) with $M(\nu)$ given by (11), the two quantities

$$\phi(\nu) = \nu - \arccos\left(\frac{\mathrm{tr}\big(M(\nu)\big)}{2\sqrt{\det\big(M(\nu)\big)}} \right), \quad d(\nu) = 1 - \sqrt{\det\big(M(\nu)\big)},$$

are called the *dispersion* (or *phase lag*) and the *dissipation* (*error of amplification factor*) of the method, respectively. The method is said to be *dispersive of order q* and *dissipative of order r* if

$$\phi(v) = \mathcal{O}(v^{q+1}), \quad d(v) = \mathcal{O}(v^{r+1}).$$

If $\phi(v) = 0$, i.e., $q = \infty$, and $D(v) = 0$, i.e., $r = \infty$, then the method is said to be *zero-dispersive* (or *phase-fitted*) and *zero-dissipative* (or *amplification-fitted*), respectively.

It has been known that classical RKN methods with constant coefficients cannot give satisfactory results when applied to second-order oscillatory problems due to dispersion or dissipation. For example, for the fourth order RKN method

$$\begin{array}{c|cccc} 0 & & & & \\ 1/5 & 1/50 & & & \\ 2/3 & -1/27 & 7/27 & & \\ 1 & 3/10 & -2/35 & 9/35 & \\ \hline & 1/24 & 25/84 & 9/56 & 0 \\ & 1/24 & 125/336 & 27/56 & 5/48 \end{array} \tag{12}$$

the dispersion and dissipation are

$$\phi(v) = \frac{1}{6720}v^7 + (v^9), \quad d(v) = -\frac{1}{3600}v^6 + (v^8).$$

Therefore, the method (12) is dispersive of order six and dissipative of order five.

The idea of this paper is to choose appropriate coefficients $\gamma_i(v)$ $(i = 1, \ldots, s)$ such that the modified RKN method (3) can be zero-dispersive and zero-dissipative.

3 Construction of the new methods

In this paper, we consider the explicit four-stage modified RKN methods given by the tableau

$$\begin{array}{c|c|cccc} 0 & \gamma_1 & & & & \\ 1/5 & \gamma_2 & 1/50 & & & \\ 2/3 & \gamma_3 & -1/27 & 7/27 & & \\ 1 & \gamma_4 & 3/10 & -2/35 & 9/35 & \\ \hline & & 1/24 & 25/84 & 9/56 & 0 \\ & & 1/24 & 125/336 & 27/56 & 5/48 \end{array} \tag{13}$$

where $\gamma_i = 1,\ i = 1, \ldots, 4$, are generally even functions of $v = h\omega$. If we choose $\gamma_i = 1,\ i = 1, \ldots, 4$, the classical fifth order RKN method (12) is recovered in [72]. Following the lines in [18,19], for convenience of computation, we use the expression $\cos v - \dfrac{\mathrm{tr}\big(M(v)\big)}{2\sqrt{\det\big(M(v)\big)}}$ for the dispersion in place of $v - \arccos\left(\dfrac{\mathrm{tr}\big(M(v)\big)}{2\sqrt{\det\big(M(v)\big)}}\right)$ in Definition 2.

3.1 The first optimized modified RKN method

We first consider the case where $\gamma_1 = \gamma_4 = 1$ in (13) while γ_2 and γ_3 depend on ν. In this case, the dispersion and the dissipation can be given by

$$\phi(\nu) = \cos(\nu) - \frac{R}{2\sqrt{Q}}, \tag{14}$$

$$d(\nu) = 1 - \sqrt{Q}, \tag{15}$$

where

$$\begin{aligned} Q &= 20160 + 600(25\gamma_2 + 108\gamma_3 - 133)\nu^2 + 100(35 + 19\gamma_2 - 54\gamma_3)\nu^4 \\ &\quad +(427 - 675\gamma_2 + 360\gamma_3)\nu^6 - 14\nu^8, \\ R &= (25200 - 75(91 + 50\gamma_2 + 27\gamma_3)\nu^2 + 525(1 + \gamma_2)\nu^4 - 28\nu^6)/12600. \end{aligned}$$

Letting the expressions in (14) and (15) vanish yields

$$\begin{aligned} \gamma_2 &= \big(360\gamma_3(180-15\nu^2+\nu^4)+7(500\nu^2-11400+61\nu^4-2\nu^6)\big)/\big(25(27\nu^4-76\nu^2-600)\big), \\ \gamma_3 &= \big(432000 - 404280\nu^2 + 37620\nu^4 + 5655\nu^6 - 782\nu^8 + 30\nu^{10} - 432000\cos(\nu) \\ &\quad -54720\nu^2\cos(\nu) + 19440\nu^4\cos(\nu)\big)/\big(27\nu^2(2460\nu^2 - 9000 - 235\nu^4 + 8\nu^6)\big). \end{aligned}$$

For small ν, the above formulas are subject to heavy cancelations and in that case the following Taylor series expansions can be used

$$\begin{aligned} \gamma_2 &= 1 + \frac{2\nu^4}{625} + \frac{1469\nu^6}{3937500} + \frac{509\nu^8}{10546875} + \frac{3276761\nu^{10}}{649687500000} \\ &\quad + \frac{6162305399\nu^{12}}{1330235156250000} + \cdots, \\ \gamma_3 &= 1 - \frac{\nu^4}{405} - \frac{289\nu^6}{1701000} + \frac{131\nu^8}{12150000} + \frac{2648977\nu^{10}}{841995000000} \\ &\quad + \frac{5170488637\nu^{12}}{11493231750000000} + \cdots. \end{aligned}$$

The local truncation error formulas of this new method are given by

$$\begin{aligned} LTE &:= y(x_{n+1}) - y_{n+1} = \frac{\omega^4 y^{(2)}(x) - y^{(6)}(x)}{1800}h^6 + \mathcal{O}(h^7), \\ DLTE &:= y'(x_{n+1}) - y'_{n+1} = \left(\frac{43\omega^6 y^{(2)}(x)}{756000} + \frac{17\omega^4 y^{(4)}(x)}{54000} - \frac{y^{(8)}(x)}{16800}\right)h^7 + \mathcal{O}(h^8). \end{aligned}$$

Hence the method is of order five, and we denoted it as MODRKNA.

3.2 The second optimized modified RKN method

In order to construct another modified RKN method, we set $\gamma_i, i = 1, \ldots, 4$ free and nullify the phase-lag of the method for two different model equations of the form (9) with $\omega = \omega_1$ and $\omega = \omega_2$, respectively. Then substituting $v = v_1 = \omega_1 h$ and $v = v_2 = \omega_2 h$ in the Eqs. (14)–(15), we obtain a system of four linear equations in the four parameters $\gamma_i, i = 1, 2, 3, 4$. The solutions γ_i contain two parameters v_1 and v_2. By considering the limits $v_1 \to v$ and $v_2 \to v$, we get the γ-values as follow

$$
\begin{aligned}
\gamma_1 = {} & 2\big(207360 - 691200v^2 + 174240v^4 - 18720v^6 + 900v^8 - 40v^{10} + v^{12} \\
& -2073600\cos(v) + 691200v^2\cos(v) - 23040v^4\cos(v) - 2880v^6\cos(v) \\
& -1036800v\sin(v) + 86400v^3\sin(v) + 5760v^5\sin(v) - 720v^7\sin(v)\big)/3M, \\
\gamma_2 = {} & \big(51840000 - 21427200v^2 + 2606400v^4 - 60480v^6 - 30960v^8 + 4400v^{10} \\
& -195v^{12} + 3v^{14} - 51840000\cos(v) + 21427200v^2\cos(v) - 3686400v^4\cos(v) \\
& +190080v^6\cos(v) + 2160v^8\cos(v) - 25920000v\sin(v) + 10713600v^3\sin(v) \\
& -1324800v^5\sin(v) + 60480v^7\sin(v) - 360v^9\sin(v)\big)/75M, \\
\gamma_3 = {} & (-1244160000 + 1036800000v^2 - 277660800v^4 + 42537600v^6 - 3435120v^8 \\
& +76960v^{10} + 5800v^{12} - 380v^{14} + 7v^{16} + 1244160000\cos(v) + 321120v^9\sin(v) \\
& -1036800000v^2\cos(v) + 288460800v^4\cos(v) - 31737600v^6\cos(v) \\
& -20160v^{10}\cos(v) + 622080000v\sin(v) - 457920000v^3\sin(v) + 90662400v^5\sin(v) \\
& +1379520v^8\cos(v) - 7963200v^7\sin(v) - 5040v^{11}\sin(v))/1350M, \\
\gamma_4 = {} & (881280000 - 81260000v^2 + 234561600v^4 - 38203200v^6 + 3014640v^8 - 59120v^{10} \\
& -3875v^{12} + 235v^{14} - 4v^{16} - 881280000\cos(v) + 812160000v^2\cos(v) \\
& -214041600v^4\cos(v) + 19843200v^6\cos(v) - 631440v^8\cos(v) + 11520v^{10} \\
& +440640000v\sin(v) + 354240000v^3\sin(v) - 62956800v^5\sin(v) \\
& +4766400v^7\sin(v) - 161640v^9\sin(v) + 2880v^{11}\sin(v))/375M,
\end{aligned}
$$

where $M = v^4(120 - 20v^2 + v^4)$. As $v \to 0$, γ_i $(i = 1, \ldots, 4)$ have the following Taylor series

$$
\begin{aligned}
\gamma_1 &= 1 + \frac{2v^2}{15} + \frac{v^4}{56} + \frac{v^6}{945} - \frac{v^8}{57024} - \frac{283v^{10}}{16816800} + \cdots, \\
\gamma_2 &= 1 - \frac{2v^2}{75} + \frac{187v^4}{2100} + \frac{v^6}{1512} + \frac{2137v^8}{49896000} - \frac{2v^{10}}{2837835} + \cdots, \\
\gamma_3 &= 1 + \frac{2v^2}{135} - \frac{929v^4}{37800} - \frac{v^6}{5250} + \frac{677v^8}{89812800} + \frac{230047v^{10}}{20432412000} + \cdots, \\
\gamma_4 &= 1 - \frac{2v^2}{75} + \frac{1571v^4}{21000} + \frac{2881v^6}{945000} + \frac{6817v^8}{49896000} - \frac{979v^{10}}{32248125} + \cdots.
\end{aligned}
$$

The local truncation error formulas of this method are given by

$$LTE := y(x_{n+1}) - y_{n+1} = -\frac{\omega^4 y^{(2)}(x_n) + 2\omega^2 y^{(4)}(x_n) + y^{(6)}(x_n)}{1800} h^6 + \mathcal{O}(h^7),$$

$$DLTE := y'(x_{n+1}) - y'_{n+1} = \left(\frac{13\omega^6 y^{(2)}(x_n)}{25200} + \frac{13\omega^4 y^{(4)}(x_n)}{16800} - \frac{y^{(8)}(x_n)}{16800} \right) h^7 + \mathcal{O}(h^8).$$

Therefore, the method is of order five, and we denoted it as MODRKNB.

4 Error analysis

In section, we follow the approach of by Simos for the numerical integration of Schrödinger equation in [5–7] and carry out the error analysis for the new methods derived in Sect. 3 as well as some other highly efficient methods we select from the literature. The methods we shall analyze are listed as follows:

- EFRKN5V: The fifth-order exponentially fitted RKN method given by Van de Vyver in [74].
- RKN5PL-AM-DAM: The optimized fifth-order RKN method derived by Kosti et al. in [18].
- RKN5PL-DPL-AM: The optimized fifth-order RKN method derived by Kosti et al. in [19].
- RKN5H: The fifth-order RKN method obtained by Van de Vyver in [75].
- EFRKN5S: The fifth-order exponentially fitted RKN method derived by Kalogiratou et al. in [44].
- MODRKNA: The new fifth-order RKN method derived in Sect. 3.1 of this paper.
- MODRKNB: The new fifth-order RKN method derived in Sect. 3.2 of this paper.

The following procedure of error analysis can also been found in Simos [41] and Alolyan et al. [42]:

i) Write the one-dimensional Schrödinger equation in the form

$$y''(x) = f(x)y(x). \tag{16}$$

ii) According Ixaru and Rizea [76], put the function $f(x)$ as

$$f(x) = g(x) + G, \tag{17}$$

where $g(x) = W(x) - V_c$, where V_c is a constant approximation of the potential E and $G = V_c - E$ is the error of the approximation.

iii) Give the derivative values of $y_n^{(i)}$, $i = 2, 3, 4 \ldots$, which are terms of the local truncation error formulas, associate with the Eq. (16), and can be expressed in the polynomials of G.

iv) Substitute the values of derivatives into the local truncation error.

Based on the previous discussions, the derivatives can be given by

$$\begin{aligned}
y_n^{(2)} &= (g(x_n)+G)y(x_n),\\
y_n^{(4)} &= g''(x_n)y(x_n)+2g'(x_n)y'(x_n)+\big(g(x_n)+G\big)^2y(x_n),\\
y_n^{(6)} &= g^{(4)}(x_n)y(x_n)+4g^{(3)}(x_n)y'(x_n)+7g''(x_n)\big(g(x_n)+G\big)y(x_n)\\
&\quad +4\big(g'(x_n)\big)^2y(x_n)+6g'(x_n)\big(g(x_n)+G\big)y'(x_n)+\big(g(x_n)+G\big)^3y(x_n),\\
&\quad \ldots
\end{aligned}$$

We consider two cases in terms of the value of E:

- The Energy is close to the potential, i.e. $G = V_c - E \approx 0$. In this case, only the free terms of the polynomials in G are considered. Thus for these values of G, the methods are of comparable accuracy. This is because the free terms of the polynomials in G, are the same for the cases of the classical methods and of the new developed methods.
- $G \gg 0$ or $G \ll 0$. Then $|G| = |V_c - E|$ is a large number.

Based on the above procedure, we obtain the following asymptotic expansions of the local truncation errors of the methods we have listed at the beginning of this section (see [5–7]):

For the method EFRKN5V,

$$\begin{aligned}
LTE_{\mathrm{EFRKN5V}} &= h^6\Big(g(x_n)y(x_n)G^2+\big(2g(x_n)^2y(x_n)+4g'(x_n)y'(x_n)+6g''(x_n)y(x_n)\big)G\\
&\quad +g(x_n)^3y(x_n)+g(x_n)(6g'(x_n)y'(x_n))+7g''(x_n)y(x_n)\\
&\quad +4g^{(3)}(x_n)y'(x_n)+y(x_n)\big(4g'(x_n)^2+g^{(4)}(x_n)\big)\Big)/1800.\\
DLTE_{\mathrm{EFRKN5V}} &= h^6\Big(1549((g(x_n)y'(x_n)+3y(x_n)g'(x_n))G^2+\big(4g(x_n)y(x_n)g'(x_n)\\
&\quad +g(x_n)^2y'(x_n)+3y'(x_n)g''(x_n)+y(x_n)g^{(3)}(x_n)\big)G\Big)/2520000.
\end{aligned}$$

For the method RKN5PL-AM-DAM,

$$\begin{aligned}
LTE_{\mathrm{RKN5PL-AM-DAM}} &= h^6\Big(-2y(x_n)G^3-6g(x_n)y(x_n)G^2\\
&\quad +\big(g^2(x_n)y(x_n)+2g'(x_n)y'(x_n)\\
&\quad +21y(x_n)g''(x_n)\big)G+\big(5g^{(3)}(x_n)y(x_n)+20y(x_n)g'(x_n)^2\\
&\quad +30g(x_n)g'(x_n)y'(x_n)+35g(x_n)y(x_n)g''(x_n)\\
&\quad +20y'(x_n)g^{(3)}(x_n)+5y(x_n)g^{(4)}(x_n)\big)\Big)/14400.\\
DLTE_{\mathrm{RKN5PL-AM-DAM}} &= h^6\Big(y'(x_n)G^3+\big(9y(x_n)g'(x_n)+3g(x_n)y'(x_n)\big)G^2\\
&\quad +\big(18g(x_n)y(x_n)g'(x_n)+3g(x_n)^2y'(x_n)\\
&\quad +13y'(x_n)g''(x_n)+11y(x_n)g^{(3)}(x_n)\big)G\Big)/7200.
\end{aligned}$$

For the method RKN5PL-DPL-AM,

$$\begin{aligned}LTE_{\mathrm{RKN5PL-DPL-AM}} &= h^6\Big(-28y(x_n)G^3-53g(x_n)y(x_n)G^2\\ &\quad+\big(45g(x_n)^2y(x_n)+90g'(x_n)y'(x_n)\\ &\quad+325y(x_n)g''(x_n)\big)+70g(x_n)^3y(x_n)+280y(x_n)g'(x_n)^2\\ &\quad+420g(x_n)g'(x_n)y'(x_n)+490g(x_n)y(x_n)g''(x_n)\\ &\quad+280y'(x_n)g^{(3)}(x_n)+70y(x_n)g^{(4)}(x_n)\Big)/201600.\\ DLTE_{\mathrm{RKN5PL-DPL-AM}} &= h^6\Big(y'(x_n)G^3+\big(9y(x_n)g'(x_n)+3g(x_n)y'(x_n)\big)G^2\\ &\quad+\big(18g(x_n)y(x_n)g'(x_n)+3g(x_n)^2y'(x_n)+13y'(x_n)g''(x_n)\\ &\quad+11y(x_n)g^{(3)}(x_n)\big)G+\big(9g(x_n)^2y(x_n)g'(x_n)\\ &\quad+g(x_n)^3y'(x_n)+10g'(x_n)y'(x_n)\\ &\quad+15y(x_n)g'(x_n)g''(x_n)+13g(x_n)y'(x_n)g''(x_n)\\ &\quad+11g(x_n)y(x_n)g^{(3)}(x_n)+5y'(x_n)g^{(4)}(x_n)\\ &\quad+y(x_n)g^{(5)}(x_n)\big)\Big)/7200.\end{aligned}$$

For the method of RKN5H,

$$\begin{aligned}LTE_{\mathrm{RKN5H}} &= h^6\Big(g(x_n)y(x_n)G^2+\big(2g(x_n)^2y(x_n)+4g'(x_n)y'(x_n)\\ &\quad+6y(x_n)g''(x_n)\big)G+g(x_n)^3y(x_n)+4y(x_n)g'(x_n)^2+6g(x_n)g'(x_n)y'(x_n)\\ &\quad+7g(x_n)y(x_n)g''(x_n)+4y'(x_n)g^{(3)}(x_n)+y(x_n)g^{(4)}(x_n)\Big)/1800.\\ DLTE_{\mathrm{RKN5H}} &= h^7\Big(2g(x_n)y(x_n)G^3+\big(10y'(x_n)g'(x_n)+5g(x_n)^2y(x_n)\\ &\quad+21y(x_n)g''(x_n)\big)G^2+\big(4g(x_n)^3y(x_n)+28y(x_n)g'(x_n)^2\\ &\quad+24g(x_n)g'(x_n)y'(x_n)+44g(x_n)y(x_n)g''(x_n)+24y'(x_n)g^{(3)}(x_n)\\ &\quad+16y(x_n)g^{(4)}(x_n)\big)G+g(x_n)^4y(x_n)+28g(x_n)y(x_n)g'(x_n)^2\\ &\quad+12g(x_n)^2g'(x_n)y'(x_n)+22g(x_n)^2y(x_n)g''(x_n)+48g'(x_n)y'(x_n)g''\\ &\quad+15y(x_n)g''(x_n)^2+26y(x_n)g'(x_n)g^{(3)}(x_n)+24g(x_n)y'(x_n)g^{(3)}(x_n)\\ &\quad+16g(x_n)y(x_n)g^{(4)}(x_n)+y'(x_n)g^{(5)}(x_n)+y(x_n)g^{(6)}(x_n)\Big)/16800.\end{aligned}$$

For the method of EFRKN5S,

$$\begin{aligned}LTE_{\mathrm{EFRKN5S}} &= h^6\Big(g(x_n)y(x_n)G^2+\big(2g(x_n)^2y(x_n)+4g'(x_n)y'(x_n)+6g''(x_n)y(x_n)\big)G\\ &\quad+g(x_n)^3y(x_n)+g(x_n)(6g'(x_n)y'(x_n))+7g''(x_n)y(x_n)\\ &\quad+4g^{(3)}(x_n)y'(x_n)+y(x_n)\big(4g'(x_n)^2+g^{(4)}(x_n)\big)\Big)/1800.\end{aligned}$$

$$DLTE_{\mathrm{EFRKN5S}} = h^6\Big(1549((g(x_n)y'(x_n) + 3y(x_n)g'(x_n))G^2 + \big(4g(x_n)y(x_n)g'(x_n) + g(x_n)^2y'(x_n) + 3y'(x_n)g''(x_n) + y(x_n)g^{(3)}(x_n)\big)G\Big)/2520000.$$

For the method of MODRKNA,

$$\begin{aligned}LTE_{\mathrm{MODRKNA}} = h^6\Big(&2g(x_n)y(x_n)G^2 + \big(3g(x_n)^2y(x_n) + 6g'(x_n)y'(x_n)\\ &+7g''(x_n)y(x_n)\big)G + g(x_n)^3y(x_n) + g(x_n)(6g'(x_n)y'(x_n)\\ &+7y(x_n)g''(x_n)) + 4y'(x_n)g^{(3)}(x_n)\\ &+y(x_n)\big(4g'(x_n)^2 + g^{(4)}(x_n)\big)\Big)/1800.\end{aligned}$$

$$\begin{aligned}DLTE_{\mathrm{MODRKNA}} = h^7\Big(&-150y(x_n)G^4 - 253y(x_n)g(x_n)G^3 + \big(32g(x_n)^2y(x_n)\\ &+64g'(x_n)y'(x_n) + 752y(x_n)g''(x_n)\big)G^2 + \big(180g(x_n)^3y(x_n)\\ &+1260y(x_n)g'(x_n)^2 + 1080g(x_n)g'(x_n)y'(x_n)\\ &+1980g(x_n)y(x_n)g''(x_n) + 1080y'(x_n)g^{(3)}(x_n)\\ &+720y(x_n)g^{(4)}(x_n)\big)G + 45g(x_n)^4y(x_n) + 1260g(x_n)y(x_n)g'(x_n)^2\\ &+540g(x_n)^2g'(x_n)y'(x_n) + 990g(x_n)^2y(x_n)g''(x_n)\\ &+2160g'(x_n)y'(x_n)g''(x_n) + 675y(x_n)g''(x_n)^2\\ &+1170y(x_n)g'(x_n)g^{(3)}(x_n) + 1080g(x_n)y'(x_n)g^{(3)}(x_n)\\ &+720g(x_n)y(x_n)g^{(4)}(x_n) + 270y'(x_n)g^{(5)}(x_n)\\ &+45y(x_n)g^{(6)}(x_n)\Big)/756000.\end{aligned}$$

For the method of MODRKNB,

$$\begin{aligned}LTE_{\mathrm{MODRKNB}} = h^6\Big(&\big(g(x_n)^2y(x_n) + 2g'(x_n)y'(x_n) + 5g''(x_n)y(x_n)\big)G + g(x_n)^3y(x_n)\\ &+g(x_n)(6g'(x_n)y'(x_n) + 7y(x_n)g''(x_n)) + 4y'(x_n)g^{(3)}(x_n)\\ &+y(x_n)\big(4g'(x_n)^2 + g^{(4)}(x_n)\big)\Big)/1800.\end{aligned}$$

$$\begin{aligned}DLTE_{\mathrm{MODRKNB}} = h^7\Big(&-10y(x_n)G^4 - 40y(x_n)g(x_n)G^3\\ &+\big(-21g(x_n)^2y(x_n) - 42g'(x_n)y'(x_n)\\ &+27y(x_n)g''(x_n)\big)G^2 + \big(12g(x_n)^3y(x_n) + 84y(x_n)g'(x_n)^2\\ &+72g(x_n)g'(x_n)y'(x_n) + 132g(x_n)y(x_n)g''(x_n) + 72y'(x_n)g^{(3)}(x_n)\\ &+48y(x_n)g^{(4)}(x_n)\big)G + 3g(x_n)^4y(x_n) + 84g(x_n)y(x_n)g'(x_n)^2\\ &+36g(x_n)^2g'(x_n)y'(x_n) + 66g(x_n)^2y(x_n)g''(x_n)\\ &+144g'(x_n)y'(x_n)g''(x_n) + 45y(x_n)g''(x_n)^2\\ &+78y(x_n)g'(x_n)g^{(3)}(x_n) + 72g(x_n)y'(x_n)g^{(3)}(x_n)\\ &+48g(x_n)y(x_n)g^{(4)}(x_n) + 18y'(x_n)g^{(5)}(x_n) + 3y(x_n)g^{(6)}(x_n)\Big)/50400.\end{aligned}$$

In the above list, a lower power of G indicates a slower increase of the corresponding local truncation error for large values of $|G| = |V_c - E|$.

5 Stability and phase properties of the new method

Lambert and Watson's stability theory [77] was reformed by Coleman and Ixaru (see Ref. [78]) for the periodicity of exponentially-fitted symmetric methods for $y'' = f(x, y)$ which was further extended by Coleman and Duxbury [79] to ν-dependent RKN-type methods. Following their lines, we apply the modified RKN method (3) to the test equation

$$y'' = -\lambda^2 y,\ \lambda \in \mathbb{R}^+, \tag{18}$$

and obtain the difference equation

$$\begin{pmatrix} y_{n+1} \\ hy'_{n+1} \end{pmatrix} = M(\theta, \nu) \begin{pmatrix} y_n \\ hy'_n \end{pmatrix},\ \theta = h\lambda,$$

where

$$M(\theta, \nu) = \begin{pmatrix} 1 - \theta^2 \bar{b}^T N^{-1} e \cdot \gamma & 1 - \theta^2 \bar{b}^T N^{-1} c \\ -\theta^2 b^T N^{-1} e \cdot \gamma & 1 - \theta^2 b^T N^{-1} c \end{pmatrix}, \tag{19}$$

with $N = I + \theta^2 A$ and $e = (1, \ldots, 1)^T$.

The characteristic equation of the modified RKN method (3) is given by

$$\xi^2 - \mathrm{tr}\big(M(\theta, \nu)\big)\xi + \det\big(M(\theta, \nu)\big) = 0.$$

The stability, determined by the spectral radius $\rho\big(M(\theta, \nu)\big)$, imposes restriction to the step-size h which leads to the following definition:

Definition 3 For the modified RKN method (3) with the stability matrix $M(\theta, \nu)$ given by (19), a region in the θ-ν plane

$$R = \{(\theta, \nu) \big|\ \theta > 0, \nu > 0, \rho\big(M(\theta, \nu)\big) < 1\}$$

is called the *stability region* of the method. Any closed curve defined by $\rho\big(M(\theta, \nu)\big) = 1$ is called a *stability boundary*.

In determining the stability region of a method, it is convenient for us to use the following equivalent conditions

$$\det\big(M(\theta, \nu)\big) < 1 \quad \text{and} \quad |\mathrm{tr}\big(M(\theta, \nu)\big)| < \det\big(M(\theta, \nu)\big) + 1. \tag{20}$$

In Fig. 1, we depict the stability regions of the two new modified RKN methods MODRKNA and MODRKNB.

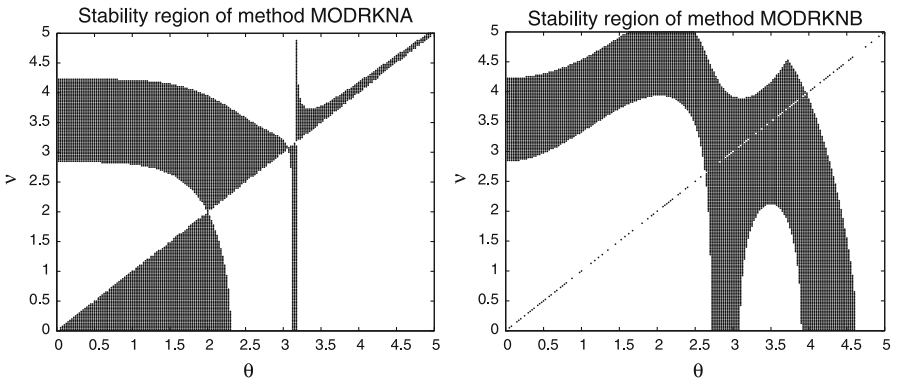


Fig. 1 Stability regions of MODRKNA and MODRKNB

In practice, the frequency of the problem to be solved is not exactly known. Mostly we can only have an estimate ω of the true frequency. Therefore, the errors in phase and in amplification factor will not vanish even if we have nullify the dispersion and dissipation in the derivation of the methods. This leads to the following definition of dispersion and dissipation.

Definition 4 (see [73]) The quantities

$$\tilde{\phi}(\theta,\nu)=\theta-\arccos\left(\frac{\mathrm{tr}\big(M(\theta,\nu)\big)}{2\sqrt{\det\big(M(\theta,\nu)\big)}}\right),\quad \tilde{d}(\theta,\nu)=1-\sqrt{\det\big(M(\theta,\nu)\big)},$$

are called the *dispersion* and the *dissipation*, respectively. Hence the method is said to be *dispersive of order* q and *dissipative of order* p if

$$\tilde{\phi}(\theta,\nu)=c_\phi\theta^{q+1}+\mathcal{O}(\theta^{q+3}),\quad \tilde{d}(\theta,\nu)=c_d\theta^{p+1}\mathcal{O}(\theta^{p+3}),$$

where c_ϕ and c_d are called the *dispersion constant* and *dissipative constant*, respectively.

For convenience of phase property analysis, we denote the ratio $\frac{\omega}{\lambda}$ by r, thus $r=\frac{\nu}{\theta}$. Then the dispersion and the dissipation of the methods MODRKNA are

$$\tilde{\phi}(\theta)=-\frac{(r^2-1)(225+225r^2+43r^4)}{1512000}\theta^7+\mathcal{O}(\theta^9),\quad \tilde{d}(\theta)=\frac{(r^4-1)^2}{3600}\theta^6+\mathcal{O}(\theta^8),$$

respectively, and the dispersion and the dissipation of the method MODRKNB are

$$\tilde{\phi}(\theta)=\frac{(r^2-1)^2(26r^2-15)}{100800}\theta^7+\mathcal{O}(\theta^9),\quad \tilde{d}(\theta)=-\frac{(r^2-1)^2}{3600}\theta^6+\mathcal{O}(\theta^8),$$

respectively. Therefore both the two modified RKN methods are dispersive of order six and dissipative of order five, respectively.

6 Numerical results

In this section, we examine the numerical performance of the new methods. In order to show the competence of our new methods, we use seven fifth-order RKN type methods as listed in Sect. 4.

We consider the numerical integration of the Schrödinger equation (1) with the well-known Woods-Saxon potential

$$V(x) = c_0 z\big(1 - a(1 - z)\big),$$

where $z = \Big(\exp\big(a(x - b)\big) + 1\Big)^{-1}$, $c_0 = -50$, $a = 5/3$, $b = 7$. The problem is solved on the interval $[0, 15]$.

This potential was first put forward in the case of exponentially fitted algorithms by Ixaru and Rizea [80] and it has been widely adopted to examine the quality of a numerical method solving the Schrödinger equation. For this test potential, we study the resonant-state problem and the bound-state problem, respectively.

6.1 The resonance problem

The so-called resonance problem is to find the energies (or resonances) $E \in [0, 1000]$ for which the phase shift is equal to $\pi/2$. The boundary conditions for this problem are

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

In the case of the Woods-Saxon potential, we follow the lines of [49,80] and choose the fitting frequency

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

The numerical results $E_{\text{calculated}}$ are compared with the analytical solution $E_{\text{analytical}}$ of the Woods-Saxon potential, rounded to six decimal places. In Fig. 2 we plot the error $-\log_{10}|E_{\text{analytical}} - E_{\text{calculated}}|$ versus N (with the integration step-size $1/2^N$) for $E_{\text{analytical}} = 53.588872, 163.215341, 341.495874, 989.701916$, respectively.

6.2 The Bound-states problem

The second problem is to find the energies in the bound states, that is, we wish to find negative energies $E < 0$ which are such that the eigenfunctions vanish at both end points of the integration range. The boundary conditions for this problem are

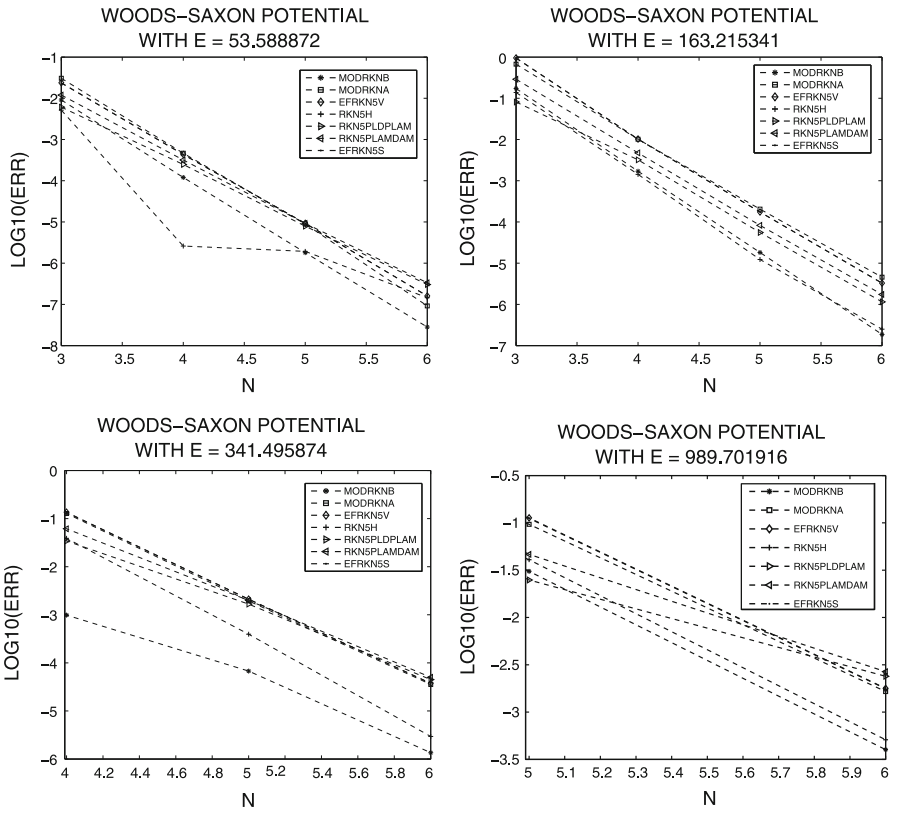


Fig. 2 $\log_{10}(E_{\text{analytical}} - E_{\text{calculated}})$ as a function of N for the resonant-state problem

$$y(0) = 0 \quad \text{and} \quad y(x) = \exp(-\sqrt{-E}x) \quad \text{for large } x.$$

The numerical results $E_{\text{calculated}}$ are compared with the analytical solution $E_{\text{analytical}}$ of the Woods-Saxon potential, rounded to nine decimal places. In Fig. 3, we plot the error $-\log_{10}|E_{\text{analytical}} - E_{\text{calculated}}|$ versus N (with the integration step-size $1/2^N$) for $E_{\text{analytical}} = -48.148430420$, -34.672313205, -13.436869040 and -3.908232481, respectively.

From Figs. 2 and 3, it is seen that the new method MODRKNB outperforms the other methods we select.

7 Conclusions and discussions

This paper proposes to consider the modified RKN methods with frequency-dependent coefficients. Based on a classical four-stage fifth order RKN method, the parameters of the corresponding modified RKN methods are obtained in two different ways: (1) For two-parameter case, using one test equation $y'' = -\omega^2 y$, simply nullify the dispersion and the dissipation and obtain the expressions of the two parameters γ_2 and γ_2;

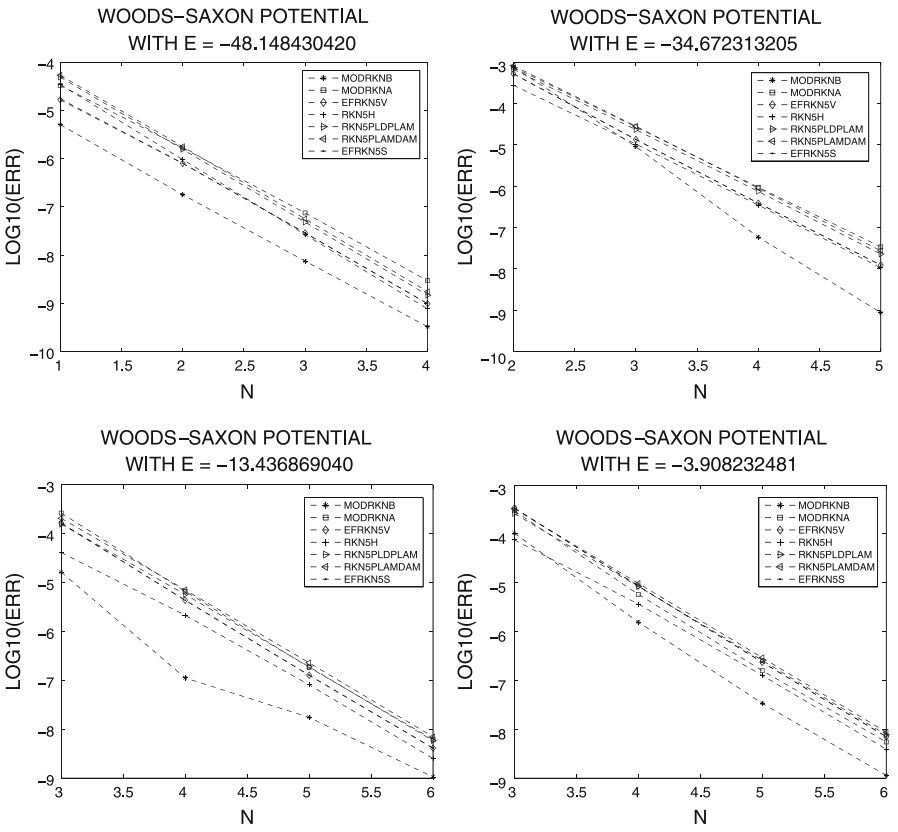


Fig. 3 $\log_{10}(E_{\text{analytical}} - E_{\text{calculated}})$ as a function of N for the bound-state problem

(2) For the four-parameter case, using two test equations $y'' = -\omega_1^2 y$ and $y'' = -\omega_1^2 y$, nullify the respect dispersion and the dissipation and obtain the expressions of the fours parameters γ_i, $(i = 1, \ldots, 4)$ as functions of $\nu_1 = h\omega_1$ and $\nu_2 = h\omega^2$. The final expressions of $\gamma_i(\nu)$, $(i = 1, \ldots, 4)$ are achieved by taking limits $\omega_1 \to \omega$ and $\omega_2 \to \omega$. The stability and phase properties of the two new methods MODRKNA and MODRKNB are examined and the error formulas are analyzed to show their theoretical advantages. Numerical experiments are carried out on the Schrödinger equation with the Woods-Saxon potential. Among all the methods we use in the experiments, the method MODRKNB is the most efficient.

To explain the high efficiency of the new method MODRKNB, we investigate the dispersion and dissipation from a novel point of view. Generally speaking, for numerical integrators of the same algebraic order, a higher dispersion order assumes a higher accuracy. For integrators of the same algebraic order and of the same dispersion order, a smaller dispersion constant assumes a higher accuracy. It is also true for dissipation. In Figs. 4 and 5, we depict the curves of the dispersion constant $|c_\phi|$ and dissipation constant $|c_d|$ as functions of $r = \omega/\lambda$, respectively, for each of the seven methods used in our first experiment. A method corresponding to a comparatively lower curve

Fig. 4 $|c_\phi(r)|$ as a function of r

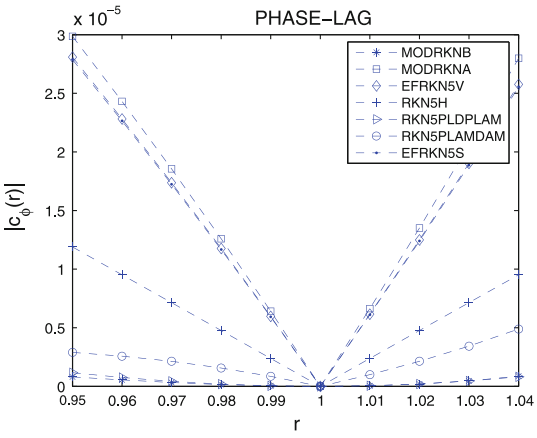
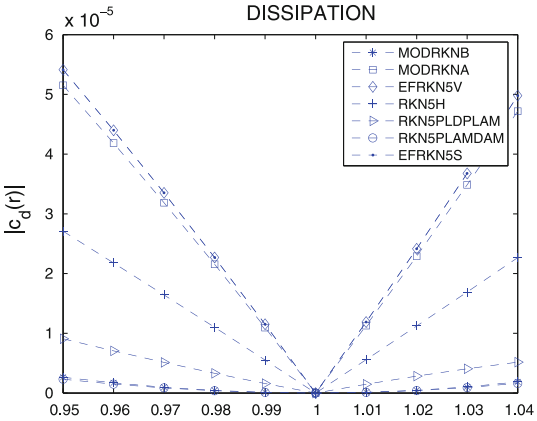


Fig. 5 $|c_d(r)|$ as a function of r



has a smaller dispersion/dissipation constant. As we can see in Figs. 4 and 5, the new method MODPHARK5 has the smallest dispersion constant and dissipation constant among all the methods considered.

Finally we note that, in practical computations of oscillatory problems, the true frequency is, in general, not available. The fitting frequency ω contained in the coefficients of the modified RKN methods is just an estimate of the true frequency. For techniques of estimating principal frequencies we refer to the papers [59,65,81].

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