ICIC Express Letters
Part B: Applications
Volume **7**, Number **8**, August **2016**

ICIC International ©2016 ISSN 2185-2766
pp. 1835–1841

A TWO-DERIVATIVE RUNGE-KUTTA METHOD WITH INCREASED PHASE-LAG ORDER FOR THE SCHRÖDINGER EQUATION

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Received January 2016; accepted April 2016

Abstract. *An optimized explicit two-derivative Runge-Kutta (TDRK) method with increased phase-lag order for the numerical integration of the Schrödinger equation is constructed in this paper. The new method has algebraic order five and phase-lag order eight. Numerical results are reported to show the efficiency of the new method with the well-known Woods-Saxon potential.*
Keywords: TDRK method, Phase-lag, Schrödinger equation, Woods-Saxon potential

1. **Introduction.** In this paper, we are concerned with the numerical integration of the Schrödinger equation of the form

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

where the real number E is the *energy* and the function $W(x)$ is the *effective potential* satisfying $W(x) \to 0$ as $x \to \infty$. Two boundary conditions are associated with this equation: one is $y(0) = 0$ and the other imposed at large x is prescribed by physical considerations. This kind of problems arises frequently in a variety of applied fields such as mechanics, and astrophysics. For the numerical integration of Equation (1), a lot of numerical methods with frequency-dependent coefficients have been developed with special techniques like trigonometrical/exponential fitting (see [1-4]). An alternative way is to take into account the characteristic features of the problem. Two such features are the phase-lag and the amplification, which are actually two different types of truncation errors. To this end, a large number of papers have been published proposing methods with minimal phase-lag, see, for example, [5-8]. The methods of this category usually have constant coefficients. In this paper, we introduce the construction of optimized TDRK methods with constant coefficients for the Schrödinger equation based on the TDRK methods by Chan and Tasi [9]. The paper is arranged as follows. Firstly, we introduce the basic theory of the TDRK method and present the algebraic order conditions and the phase property of the TDRK methods. Secondly, we construct optimized TDRK methods with increased phase-lag order of eight. Thirdly, numerical results are reported to show the efficiency of new method with the Woods-Saxon potential. Finally, we give some conclusive remarks.

2. **Basic Theory.**

2.1. **Two-derivative Runge-Kutta methods.** We start by the numerical integration of the system of first order differential equations in the form

$$y' = f(x, y) \tag{2}$$

where $y \in \mathbb{R}^d$, $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a smooth function. A special s-stage explicit two-derivative Runge-Kutta (TDRK) method has the form (see Chan and Tasi [9])

$$\begin{cases} Y_1 = y_n, \\ Y_k = y_n + c_k h f(x_n, y_n) + h^2 \sum\limits_{j=1}^{k-1} a_{kj} g(x_n + c_j h, Y_j), \ k = 2, \ldots, s, \\ y_{n+1} = y_n + h f(x_n, y_n) + h^2 \sum\limits_{k=1}^{s} b_k g(x_n + c_k h, Y_k), \end{cases} \tag{3}$$

in which $g(x, y) := y''(x) = \frac{\partial}{\partial x} f(x, y) + \frac{\partial}{\partial y} f(x, y) \cdot f(x, y)$. The method (3) can be expressed briefly by the Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ \vdots & \vdots & \ddots & & \\ c_s & a_{s1} & \ldots & a_{ss-1} & \\ \hline & b_1 & \ldots & b_{s-1} & b_s \end{array}$$

or simply by (c, A, b). As the scheme (3) indicates, at each step, this special explicit TDRK method involves only one evaluation of the function f and s evaluations of the function g. Chan and Tasi [9] derived the order conditions for the TDRK methods through the rooted tree theory and B-series. The conditions for order two to order five are listed as follows.

- Order 2 requires:

$$\sum_{i=1}^{s} b_i = \frac{1}{2}. \tag{4}$$

- Order 3 requires, in addition:

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

- Order 4 requires, in addition:

$$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{12}. \tag{6}$$

- Order 5 requires, in addition:

$$\sum_{i=1}^{s} b_i c_i^3 = \frac{1}{20}. \quad \sum_{i=1}^{s} b_i a_{ij} c_j = \frac{1}{120}. \tag{7}$$

In order to apply the scheme (3) to the problem (1), one needs to transform the second-order ODE (1) into a form of first-order system

$$\begin{cases} y'(x) = z(x), \\ z'(x) = (W(x) - E) y(x). \end{cases} \tag{8}$$

For the practical computation of scheme (3), we have

$$\begin{cases} y''(x) = (W(x) - E) y(x), \\ z''(x) = (W(x) - E) z(x) + y(x) W'(x). \end{cases} \tag{9}$$

Therefore, we have two components of (3): one for y_{n+1} and the other for z_{n+1}.

2.2. **Phase-lag property of the TDRK methods.** For the purpose of phase analysis, we consider the following test equation

$$y' = \mathrm{i}\omega y, \quad \mathrm{i}^2 = -1, \tag{10}$$

in which $\omega > 0$ is the frequency of the solution. Applying the TDRK method (3) to (10) yields

$$y_{n+1} = M(\nu)y_n, \quad \nu = \omega h, \tag{11}$$

where $M(\nu)$ is called the *stability function*.

Definition 2.1. *(see* [8, 10]*) For the TDRK method (3) with stability function $M(\nu)$, the quantity*

$$PL(\nu) = \nu - \arg(M(\nu)) \tag{12}$$

is called phase-lag *or* dispersion. *If*

$$PL(\nu) = c_\phi \nu^{q+1} + \mathcal{O}\left(\nu^{q+3}\right),$$

the method is said to be of phase-lag order q*, where the* $c_\phi \neq 0$ *is called the* phase-lag constant*. If* $PL(\nu) = 0$*, then the method is called* phase-fitted.

Denoting $M(\nu) = U(\nu) + \mathrm{i}V(\nu)$ with $U(\nu)$, $V(\nu)$ the real and imaginary parts of $M(\nu)$, we have

$$U(\nu) = 1 - \nu^2 b^T (I + \nu^2 A)^{-1} e, \quad V(\nu) = \nu\big(1 - \nu^2 b^T (I + \nu^2 A)^{-1} c\big)$$

where the vector $e = (1, 1, \ldots, 1)^T$ and the phase-lag becomes

$$PL(\nu) = \nu - \arctan\left(\frac{V(\nu)}{U(\nu)}\right). \tag{13}$$

In particular, for an s-stage explicit TDRK method, that is, the coefficient matrix A is strictly lower-diagonal, $A^s = 0$ and

$$U(\nu) = 1 - \nu^2 b^T e + \nu^4 b^T A e - \ldots + (-1)^s \nu^{2s} A^{s-1} e,$$
$$V(\nu) = \nu - \nu^3 b^T c + \nu^5 b^T A c - \ldots + (-1)^s \nu^{2s+1} A^{s-1} c.$$

In the next section, we will derive an explicit fifth order TDRK method with increased phase-lag order.

3. **Construction of the New Method.** In this section, we shall construct a new fifth order TDRK method with increased phase-lag order. We consider the three stages explicit TDRK method which is given by the Butcher tableau

$$\begin{array}{c|ccc} 0 & & & \\ c_2 & a_{21} & & \\ c_3 & a_{31} & a_{32} & \\ \hline & b_1 & b_2 & b_3 \end{array} \tag{14}$$

Together with the simplifying assumptions $a_{21} = \dfrac{c_2^2}{2}$ and $a_{31} + a_{32} = \dfrac{c_3^2}{2}$, we solve Equations (4)-(7) and obtain the coefficients with a free parameter c_3 as follows:

$$c_2 = \frac{-3 + 5c_3}{-5 + 10c_3}, \quad a_{21} = \frac{c_2^2}{2}, \quad a_{31} = \frac{c_3(3 - 19c_3 + 35c_3^2 - 20c_3^3)}{10c_3 + 6},$$

$$a_{32} = \frac{c_3^2}{2} - a_{31}, \quad b_3 = -\frac{1 - 2c_2}{12c_3(c_2 - c_3)}, \quad b_2 = -\frac{-1 + 2c_3}{12c_2(c_2 - c_3)}, \quad b_1 = \frac{1}{2} - b_2 - b_3.$$

In order to optimize the method, we calculate the phase-lag of the new method and expand it into a series in ν as follows

$$PL(\nu) = \frac{(11 - 15c_3)\nu^7}{8400(2c_3 - 1)} + \frac{(-17 + 25c_3)\nu^9}{64800(2c_3 - 1)} + \mathcal{O}(\nu^{11}). \tag{15}$$

By nullifying the leading term of the phase-lag (15), we obtain $c_3 = 11/15$. The new TDRK method thus obtained can be given by the Butcher tableau

$$\begin{array}{c|ccc} 0 & & & \\ \frac{2}{7} & \frac{2}{49} & & \\ \frac{11}{15} & \frac{11}{13500} & \frac{3619}{13500} & \\ \hline & \frac{23}{264} & \frac{343}{1128} & \frac{225}{2068} \end{array} \tag{16}$$

The phase-lag of this new method is now

$$PL(\nu) = \frac{\nu^9}{22680} + \mathcal{O}(\nu^{11}).$$

Therefore, this method has algebraic order five and phase-lag order eight and we denote it as TDRK5-8.

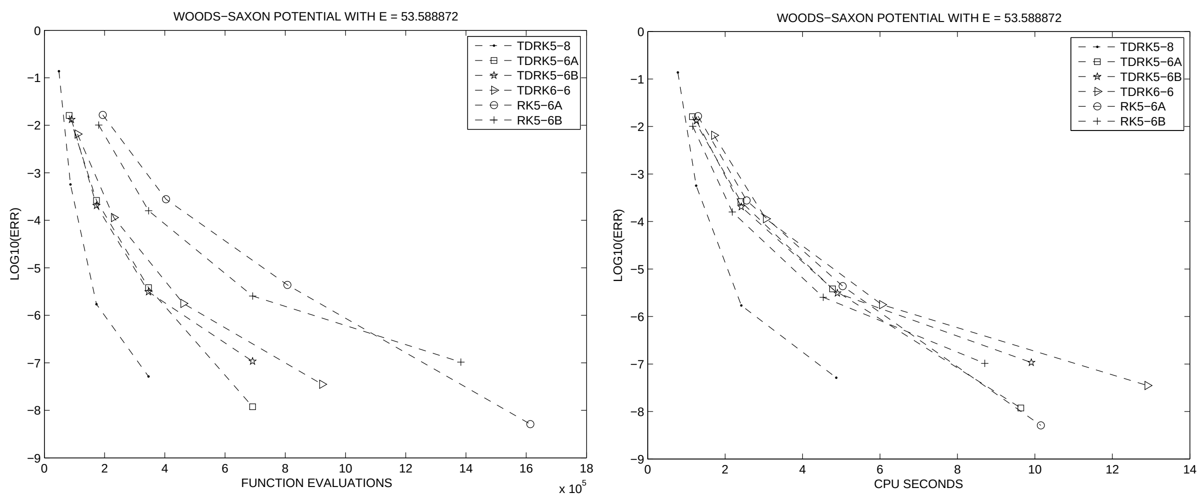

FIGURE 1. Efficiency curves for $E = 53.588872$

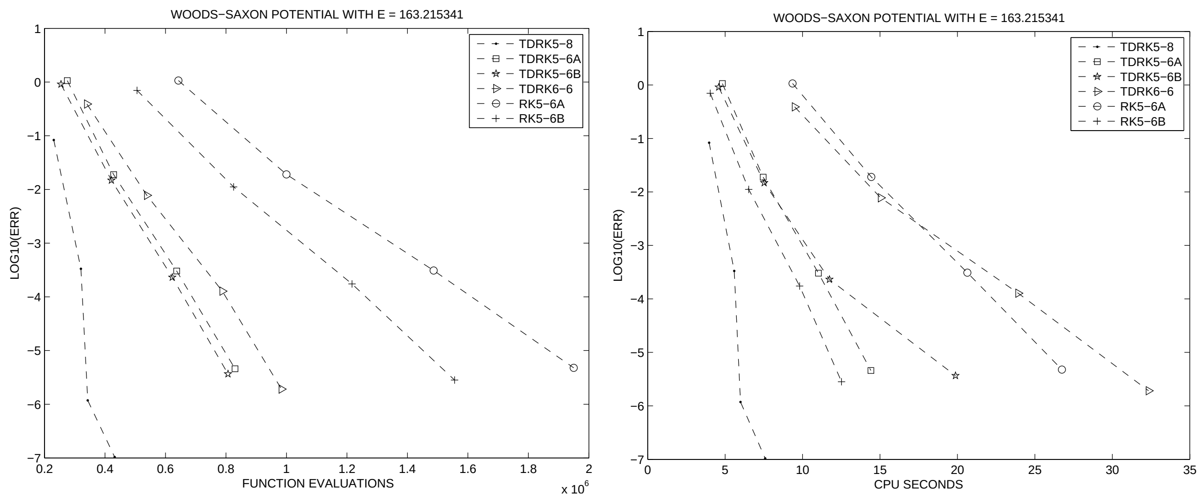

FIGURE 2. Efficiency curves for $E = 163.215341$

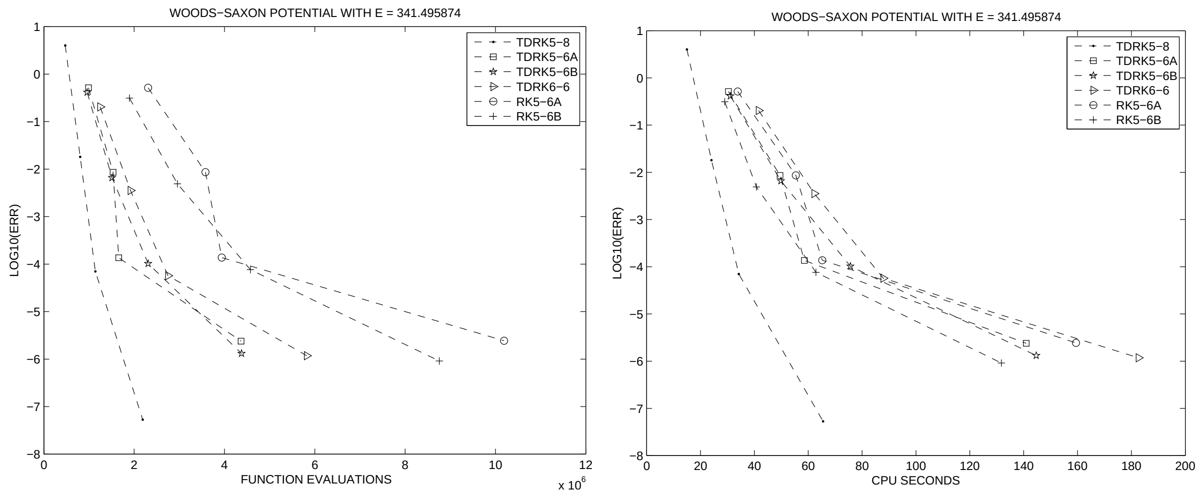

Figure 3. Efficiency curves for $E = 341.495874$

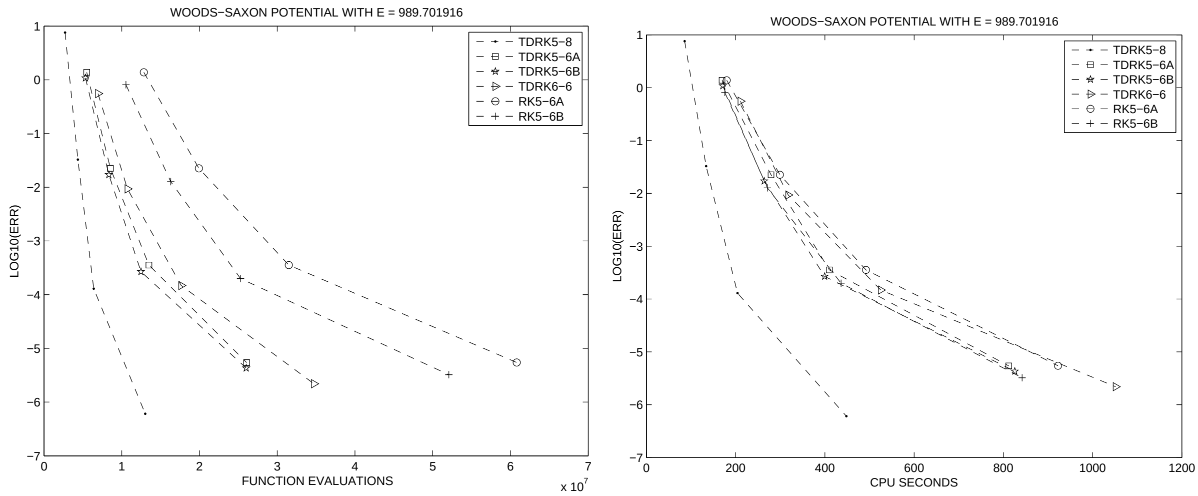

Figure 4. Efficiency curves for $E = 989.701916$

4. **Numerical Illustrations.** In this section, we shall examine the numerical performance of the new method in the integration of the radial Schrödinger equation with the Woods-Saxon potential. We compare the new method with some existing well-known methods in the literature. The methods we choose for comparison are:

- TDRK5-8: the optimized fifth order TDRK method derived in this paper.
- TDRK5-6A: the fifth order TDRK method with $c_3 = \frac{3}{4}$ obtained in [9].
- TDRK5-6B: the fifth order TDRK method with $c_3 = \frac{2}{3}$ presented in [9].
- TDRK6-6: the sixth order TDRK method with $c_4 = \frac{2}{3}$ given in [9].
- RK5-6A: the optimized fifth order RK method given in [11].
- RK5-6B: the optimized fifth order RK method derived by Anastassi in [12].

We consider the numerical integration of the Schrödinger Equation (1) with the well-known Woods-Saxon potential of the form in [2, 4]

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

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

In the numerical experiments, we consider the so-called resonant-state problem $E > 0$; that is to find the energies (or resonances) $E \in [0, 1000]$ for which the phase shift is equal to $\frac{\pi}{2}$. 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 Figures 1-4, we plot the logarithm of error $|E_{\text{analytical}} - E_{\text{calculated}}|$ (LOG(ERR)) versus the computational effort by the number of function evaluations (FUNCTION EVALUATIONS) and the CPU times (CPU SECONDS) required by each method for $E_{\text{analytical}} = 53.588872$, 163.215341, 341.495874, and 989.701916, respectively. The calculations are carried out on a Thinkpad with i5-2400 CPU, 4.0GB memory.

In view of Figures 1-4, we observe that the new method TDRK5-8 shows more advantages over the other methods we select. This can be explained by the fact that the new method is associated with optimized phase property which is very essential to the numerical integration of oscillatory problems.

5. **Conclusions.** In this paper, we have constructed an explicit two-derivative Runge-Kutta (TDRK) method of algebraic order five and maximal phase-lag order eight. Numerical results of the experiment on the Schrödinger equation show the high efficiency of the new method.

For the numerical methods with frequency-dependent coefficients, one has to evaluate the principal frequency. However, in practical problems such as the Schrödinger equation, the principal frequency is not available or not easy to estimate in advance. This is why we pursue the methods with constant coefficients but having a maximal phase-lag order.

To explain the superiority of the new TDRK method, we observe that, due to the employment of the second derivative in the scheme, TDRK methods have the possibility of gaining one algebraic order higher than RK methods of the same number of internal stages. On the other hand, increased phase-lag order has tuned TDRK methods to the oscillatory feature of the Schrödinger equation.

We note that, following the approach of this work, higher order TDRK methods with increased phase-lag order can be derived by taking more stages. Also, embedded TDRK pairs with step control might achieve higher efficiency. Finally, dissipation of the method is another quantity which we can consider to get optimized.

Acknowledgment. This research is partially supported by NSFC (No. 11571302) and the foundation of Scientific Research Project of Shandong Universities (No. J14LI04).

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