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ORIGINAL PAPER

New optimized two-derivative Runge-Kutta type methods for solving the radial Schrödinger equation

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Abstract This paper focuses on adapted two-derivative Runge-Kutta (TDRK) type methods for solving the Schrödinger equation. Two new TDRK methods are derived by nullifying their phase-lags and the first derivatives of the phase-lags. Error analysis is carried out by means of asymptotic expressions of the local errors. Numerical results are reported to show the efficiency and robustness of the new methods in comparison with some RK type methods specially tuned to the integration of the radial time-independent Schrödinger equation with the Woods–Saxon potential.

Keywords Two-derivative Runge-Kutta methods · Phase fitting · Schrödinger equation · Error analysis

1 Introduction

In molecular dynamics, quantum physics and chemistry, no other equation has been studied more profoundly than the Schrödinger equation [1]–[7]. The radial time-independent Schrödinger equation has the form

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

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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 determined by physical considerations. The form of this second boundary condition depends crucially on the sign of the energy E. Compared with multistep methods whose implementation requires a series of starting values, Runge-Kutta (–Nyström) (RK(N)) type methods are favorable because the initial values that are available are sufficient for them to run. Regarding the oscillatory character of the solution to the Schrödinger Eq. (1), there have appeared a lot of adapted-type integrators, one step or multistep, of , a pronounced class of which is based on important properties such as exponentially/trigometrically-fitted or phase optimized (see [1]–[44]). Very recently, Anastassi et al. [32] constructed optimized Runge-Kutta methods with zero phase-lag and its derivatives, which were tested to be very effective for the radial Schrödinger equation.

The purpose of this paper is to investigate modified two-derivative Runge-Kutta (TDRK) methods adapted to the oscillatory character of the solution of the radial Schrödinger Eq. (1). Section 2 presents the scheme, order conditions and phase properties for TDRK methods. In Sect. 3, we derive two new optimized modified TDRK methods by nullifying the phase-lags and their first derivatives. In Sect. 4 we carry out the error analysis for the new methods and give the asymptotic expressions of the local errors. Numerical results are reported in Sect. 5 to show the effectiveness and competence of our new methods. Section 6 is devoted to conclusions.

2 Phase properties of modified TDRK methods

2.1 Modified two-derivative Runge-Kutta methods and order conditions

For the numerical solution of initial value problems of systems of first-order differential equations

$$y'(x) = f(x, y), \quad y(x_0) = y_0, \tag{2}$$

where $y \in \mathbb{R}^N$, $f : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$ is a smooth function, Chan et al. [36] proposed the TDRK methods and obtained the order conditions. Suppose the solution of the problem (2) is oscillatory and ω is an accurate estimate of the principal frequency of the solution. We consider the following special form of explicit *modified TDRK method*

$$\begin{cases} Y_1 = y_n, \\ Y_i = y_n + c_i h f(x_n, y_n) + h^2 \sum_{j=1}^{i-1} a_{ij} g(x_n + c_j h, Y_j), \quad i = 2, \ldots, s, \\ y_{n+1} = y_n + h\beta(v) f(x_n, y_n) + h^2 \sum_{i=1}^{s} b_i(v) g(x_n + c_i h, Y_i), \end{cases} \tag{3}$$

where $g(x, y) = y''(x) := \frac{\partial f(x,y)}{\partial x} + \frac{\partial f(x,y)}{\partial y} f(x, y)$, c_i, a_{ij} $(1 \le j < i \le s)$ are real constants, $\beta(v)$ and $b_i(v)$ $(1 \le i \le s)$ are real even functions of $v = h\omega$. In

Kronecker's product, the scheme (3) has the form

$$\begin{cases} Y = e \otimes y_n + hc \otimes f(x_n, y_n) + h^2(A \otimes I_N)G(Y), \\ y_{n+1} = y_n + h\beta(v) f(x_n, y_n) + h^2(b(v)^T \otimes I_N)G(Y), \end{cases} \tag{4}$$

where I_N is the $N \times N$ identity matrix and

$$\begin{aligned} Y &= (Y_1^T, \ldots, Y_s^T)^T, G(Y) = (g(x_n, Y_1)^T, g(x_n + c_2 h, Y_2)^T, \ldots, \\ &\quad g(x_n + c_s h, Y_s)^T)^T, \\ A &= (a_{ij})_{s\times s}, \quad a_{ij} = 0, \text{ for } i < j, c = (0, c_2, \ldots, c_s)^T, \\ b(v) &= (b_1(v), \ldots, b_s(v))^T, e = (1, \ldots, 1)^T. \end{aligned}$$

The scheme (3) can also be expressed compactly by the Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline \beta(v) & b^T(v) \end{array} = \begin{array}{c|ccc} 0 & & & \\ c_2 & a_{21} & & \\ \vdots & \vdots & \cdots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss-1} \\ \hline \beta(v) & b_1(v) & \cdots & b_{s-1}(v) \quad b_s(v) \end{array}$$

or simply by $(c, A, b(v))$. We assume that as $\beta(v) \to 1$ as $\omega \to 0$ so that when $\omega \to 0$ the modified RK method (3) reduces to a traditional two-derivative RK method with constant coefficients (see [36]). The exact solution of the IVP (2) has the series expansion

$$y(x_n + h) = y_n + \sum_{t\in T} \frac{h^{r(t)}}{\sigma(t)} \frac{1}{\gamma(t)} \mathcal{F}(t)(y_n), \tag{5}$$

where the set of rooted trees T, order $r(t)$, symmetry $\sigma(t)$, density $\gamma(t)$ and the elementary differential $\mathcal{F}(t)(y_n)$ are defined in Butcher [37]. On the other hand, the numerical solution y_{n+1} given by the scheme (3) has the series expansion

$$y(x_n+h) = y_n + h\sum_{j=0}^{\infty} \frac{v^j \beta^{(j)}(0)}{j!} f(x_n, y_n) + \sum_{t\in T,\ r(t)\geq 2} \frac{h^{r(t)}}{\sigma(t)} b(v)^T \Phi(t) \mathcal{F}(t)(y_n), \tag{6}$$

where the vector of elementary weights $\Phi(t) = (\Phi_1(t), \ldots, \Phi_s(t))^T$ is defined in [39].

Following the line of You [38], we have the following theorem on order conditions.

Theorem 2.1 *The modified TDRK method* (3) *has order p if and only if*

$$\beta^{(j)}(0) = 0, \quad \text{for} \quad j = 1, \ldots, p-1, \tag{7}$$

and

$$b(v)^T \Phi(t) = \frac{1}{\gamma(t)} + \mathcal{O}(h^{p-r(t)+1}), \quad \text{for all trees with } r(t) = 2, \ldots, p. \tag{8}$$

For example, the fourth-order conditions are given by

$$\begin{aligned} &\beta^{(j)}(0) = 0 \quad \text{for} \quad j = 1, 2, 3, \\ &b^T(v)e = \frac{1}{2} + \mathcal{O}(h^3), \quad b^T(v)c = \frac{1}{6} + \mathcal{O}(h^2), \quad b^T(v)c^2 = \frac{1}{12} + \mathcal{O}(h), \end{aligned} \tag{9}$$

where $c^2 = (0, c_2^2, \ldots, c_s^2)$.

2.2 Phase properties of modified TDRK methods

For the purpose of phase analysis, we consider the following scalar ideal equation

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

where $\omega > 0$ is an estimate of the principal frequency of the problem. Applying the TDRK method (3)–(10) yields

$$y_{n+1} = M(v) y_n, \tag{11}$$

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

Definition 2.1 (see [29]) For the modified TDRK method (3) with stability function $M(v)$, the quantities

$$PL(v) = v - \arg(M(v)), \; d(v) = 1 - |M(v)|$$

are called *phase-lag* or *dispersion* and *dissipation* or *error of amplification factor*, respectively. If

$$PL(v) = c_\phi v^{q+1} + \mathcal{O}(v^{q+3}), \quad d(v) = c_d v^{r+1} + \mathcal{O}(v^{r+3}),$$

the method is said to be of *phase-lag order q* and *dissipation order r*, respectively, where the c_ϕ and c_d are called the *phase-lag constant* and *dissipation constant*, respectively. If $PL(v) = 0$ and $\phi(v) = 0$, then the method is called *phase-fitted* and *amplification-fitted*, respectively.

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

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

and the phase-lag and dissipation become

$$PL(v) = v - \arccos \frac{U(v)}{\sqrt{U(v)^2 + V(v)^2}}, \; d(v) = 1 - \sqrt{U(v)^2 + V(v)^2}.$$

In particular, if (3) is an s-stage explicit TDRK method, that is, the coefficient matrix A is strictly lower-diagonal, then $A^s = 0$ and

$$\begin{aligned} U(v) &= 1 - v^2 b^T e + v^4 b^T Ae - \ldots + (-1)^s v^{2s} A^{s-1} e, \\ V(v) &= v1 - v^3 b^T c + v^5 b^T Ac - \ldots + (-1)^s v^{2s+1} A^{s-1} c. \end{aligned}$$

In the next section, we will derive two modified TDRK methods by nullifying their phase-lags and the first derivatives of the phase-lags.

3 Construction of the new methods

We begin by considering the two-stage TDRK methods given by the following Butcher tableau of coefficients

$$\begin{array}{c|cc} 0 & & \\ \frac{1}{2} & \frac{1}{8} & \\ \hline \beta(v) & b_1(v) & b_2(v) \end{array} \tag{12}$$

If we choose $\{\beta(v), b_1(v), b_2(v)\} = \left\{1, \frac{1}{2}, \frac{1}{8}\right\}$, a classical fourth-order TDRK method in [36] is recovered. Our task is to select proper parameters $\beta(v), b_1(v), b_2(v)$ so that the phase-lag property is optimized.

3.1 A TDRK method with zero phase-lag

In order to construct the first optimized method, we require the phase-lag $PL(v)$ to be zero and get the following relation

$$\beta(v)v - \frac{b_2(v)v^3}{2} - \left(1 - b_1(v)v^2 + b_2(v)v^2 - \frac{b_2(v)v^4}{8}\right)\tan(v) = 0. \tag{13}$$

On the other hand we pick two of the fourth-order conditions in (9) for $s = 2$

$$b_1(v) + b_2(v) = \frac{1}{2} + \mathcal{O}(h^3), \quad b_2(v)c_2 = \frac{1}{6} + \mathcal{O}(h^2). \tag{14}$$

Solving the Eqs. (13) and (14) with the higher order terms omitted yields

$$\beta(v) = \frac{4v^3 + \tan(24 - 12v^2 + v^4)}{24v}, \; b_1(v) = \frac{1}{6}, \; b_2(v) = \frac{1}{3}. \tag{15}$$

For small values of $|v|$, $\beta(v)$ has the following Taylor series

$$\beta(v) = 1 + \frac{v^4}{120} + \frac{v^6}{840} + \frac{v^8}{2268} + \frac{221v^{10}}{6227020800} + \frac{349v^{12}}{4864860} + \cdots.$$

It is easy to verify that the coefficients $\beta(v)$, $b_1(v)$ and $b_2(v)$ satisfy the other two equations in (9). Therefore, the modified TDRK method defined by (12) and (15) has order four and we denote this method as MTDRKA. From the Taylor series, the local truncation error of the method is

$$\begin{aligned} LTE = h^5\Big(&-6\omega^4 f + g_{xxx} + g_{yyy}(f,f,f) + 3g_{xxy}f + 3g_{xyy}(f,f) + 3g_{xy}g \\ &+3g_{yy}(f,g) + 18g_y g_x + 18g_y g_y f\Big)/720 + \mathcal{O}(h^6), \end{aligned} \tag{16}$$

where all the functions and derivatives are evaluated at $(x, y) = (x_n, y_n)$.

3.2 A TDRK method with zero phase-lag and zero derivative of phase-lag

Now we assume that the phase-lag $PL(v)$ has been zero. We require further the first derivative $DPL(v)$ of $PL(v)$ with respect to v to be also zero. Then we have the following equation

$$\begin{aligned} &\beta(v) - \frac{3b_2(v)v^2}{2} - \left(1 - v^2\left(b_1(v) + b_2(v) - \frac{b_2(v)v^2}{8}\right)\right)\sec(v)^2 \\ &- \left(\frac{b_2(v)v^3}{4} - 2v\left(b_1(v) + b_2(v) - \frac{b_2(v)v^2}{8}\right)\right)\tan(v) = 0. \end{aligned} \tag{17}$$

Solving the Eqs. (13) and (17) and a fourth-order condition $b_1(v) + b_2(v) = \frac{1}{2}$, we obtain the following coefficients

$$\begin{aligned} \beta(v) &= \frac{v(v^2-4) + 2(6-v^2)\tan(v) + v^3\sec^2(v)}{v(8 + v^2\sec(v)^2 + 3v\tan(v))}, \\ b_2(v) &= \frac{4(v(v^2-2)\sec(v)^2 + \tan(v)(v^2+2))}{v^3(8 + v^2\sec(v)^2 + 3v\tan(v))}, \\ b_1(v) &= \frac{1}{2} - b_2(v). \end{aligned} \tag{18}$$

For small values of $|v|$, $\beta(v)$ has the following Taylor series

$$\beta(v) = 1 - \frac{v^4}{120} + \frac{v^6}{560} + \frac{v^8}{3780} + \frac{317v^{10}}{1995840} + \frac{1411v^{12}}{51891840} + \cdots.$$

It is easy to verify that the coefficients $\beta(v)$, $b_1(v)$ and $b_2(v)$ satisfy the other two equations in (9). Therefore, the modified TDRK method defined by (12) and (18) has order four and we denote this method as MTDRKB. The local truncation error of the method is given by

$$\begin{aligned} LTE = h^5\Big(&6\omega^4 f + 24\omega^2(g_x + g_y f) + g_{xxx} + g_{yyy}(f,f,f) \\ &+3g_{xxy}f + 3g_{xyy}(f,f) + 3g_{xy}g + 3g_{yy}(f,g) + 18g_y g_x \\ &+18g_y g_y f\Big)/720 + \mathcal{O}(h^6). \end{aligned} \tag{19}$$

4 Error analysis for the new TDRK methods applied to the Schrödinger equations

In order to use the TDRK method (3) to solve the problem (1), we first rewrite (1) into a system of first-order ordinary differential equations of the form (2) as follows

$$\begin{cases} y'(x) = z(x), \\ z'(x) = (W(x) - E)y(x). \end{cases} \tag{20}$$

And accordingly

$$\begin{cases} y''(x) = (W(x) - E)y(x), \\ z''(x) = (W(x) - E)z(x) + W'(x)y(x). \end{cases} \tag{21}$$

Thus the TDRK method (3) applied to (20) yields

$$\begin{cases} Y_1 = y_n, \\ Z_1 = z_n, \\ Y_i = y_n + c_i h z_n + h^2 \sum_{j=1}^{i-1} a_{ij}\big(W(x_n) + c_j h - E\big)Y_j, \ i = 2, \ldots, s, \\ Z_i = z_n + c_i h\big(W(x_n) - E\big)y_n + h^2 \sum_{j=1}^{i-1} a_{ij}\big((W(x_n + c_j h) - E)Z_j \\ +W'(x_n + c_j h)Y_j\big), \ i = 2, \ldots, s, \\ y_{n+1} = y_n + h\beta(v)z_n + h^2 \sum_{j=1}^{s} b_i(v)\big(W(x_n + c_i h) - E\big)Y_i, \\ z_{n+1} = z_n + h\beta(v)\big(W(x_n) - E\big)y_n + h^2 \sum_{i=1}^{s} b_i(v)\big((W(x_n + c_i h) - E) \\ Z_i + W'(x_n + c_i h)Y_i\big). \end{cases} \tag{22}$$

In Ixaru and Rizea [34] put forward a procedure of finding the asymptotic expressions of errors of exponentially fitted Numerov methods solving Schrödinger equation for large values of energy. In this section, we follow the approach of Van de Vyver in [27,28] and adapt this procedure to the new methods derived in Sect. 3. It has been observed that the numerical performance of the method is crucially influenced by the fitting frequency v. As a recipe, we take the following strategy: we divide $[0, \infty]$ into subintervals $[x_i, x_{i+1}]$, $i = 0, 1, \ldots$, on each of which the $W(x)$ can be considered constant, denoted by $\bar{W}$. Then on each subinterval $[x_i, x_{i+1}]$ the Eq. (1) is approximated by the second-order linear equation $y_i'' = (\bar{W} - E)y_i$ with constant coefficients, which has the general solution

$$y_i(x) = A\exp(\sqrt{\bar{W} - E}x) + B\exp(-\sqrt{\bar{W} - E}x),$$

where A and B are complex constant. A reasonable choice for the fitting frequency on each subinterval $[x_i, x_{i+1}]$ is $\omega = \sqrt{E - \bar{W}}$. The Eq. (1) can be reformulated as $y''(x) = (W(x) - \bar{W} + D)y(x)$ where $D = -\omega^2$. Then the Schrödinger Eq. (1) is equivalent to the first-order system (2) with

$$f(x, y, z) = \begin{pmatrix} z \\ \big(W(x) - \bar{W} + D\big)y \end{pmatrix}.$$

The function g in the modified TDRK method (3) is then

$$g(x, y, z) = \begin{pmatrix} \big(W(x) - \bar{W} + D\big)y \\ \big(W(x) - \bar{W} + D\big)z + W'(x)y \end{pmatrix}.$$

Substituting the previous formulas of $f(x, y, z)$ and $g(x, y, z)$ into (16) and (19) we obtain the local truncation errors of the new methods MTDRKA and MTDRKB as follows:

$$LTE_{MTDRKA,y} = \frac{h^5}{720}\Big(\big(24y(x)W'(x) - 12y'(x)\Delta W\big)D + 24W'(x)y(x)\Delta W$$
$$-5y(x)W'(x)^2 - 6y'(x)\Delta W^2 + 3y'(x)W''(x) + y(x)W^{(3)}(x)\Big) + \mathcal{O}(h^6), \quad (23)$$

$$LTE_{MTDRKB,y} = \frac{h^5}{720}\Big(- 3y(x)W'(x)D + 9y(x)W'(x)\Delta W + 3y'(x)\big(2\Delta W^2$$
$$+W''(x) + y(x)W^{(3)}(x)\big)\Big) + \mathcal{O}(h^6), \quad (24)$$

where $\triangle W = W(x) - \bar{W}$. From (23) and (24), we can see that, for large values of $|D|$,

$$\|LTE_{MTDRKA,y}\| \approx \frac{h^5}{30}\|y(x)W'(x)D\|,$$
$$\|LTE_{MTDRKB,y}\| \approx \frac{h^5}{240}\|y(x)W'(x)D\|. \quad (25)$$

This explains the higher efficiency of the method MTDRKB compared to the method MTDRKA.

5 Numerical results

In this section, we test the numerical performance of the new fourth-order modified TDRK methods in the integration of the radial Schrödinger equation with the Woods–

Saxon potential. We compare the new methods with some existing highly efficient methods in the literature. The methods we choose for comparison are as follows:

- RK4V: the optimized fourth-order RK method (CASEII) given by Van de Vyver in [27].
- MODRKB: the modified fourth-order RK method (CASEII) given by Van de Vyver in [28].
- EFRK4: the exponentially fitted fourth order RK method presented by Vanden Berghe et al. in [30].
- RK4S: the exponentially fitted fourth order RK method derived by Simos in [31].
- PHARK4: the phase fitted fourth order RK method presented by Simos and Vigo Aguiar in [33].
- MTDRKA: the first modified two-derivative RK method with one evaluation of function f and two evaluations of function g per step derived in Sect. 3.
- MTDRKB: the second modified two-derivative RK method with one evaluation of function f and two evaluations of function g per step derived in Sect. 3.

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

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

where $z = \Big(\exp\big(a(x-b)+1\big)\Big)^{-1}$, $c_0 = -50$, $a = 5/3$, $b = 7$. 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 [34] and it has been widely used to test the quality of a numerical method solving the Schrödinger equation. In the numerical experiments, we consider the so-called resonant-state problem $E > 0$, that is to find the energies (or resonances) $E \in [0, 1{,}000]$ for which the phase shift is equal to $\dfrac{\pi}{2}$. 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 [5,34] 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 Figs. 1, 2, 3, 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) required by each method for $E_{\text{analytical}} = 53.588872$, 163.215341, 341.495874, 989.701916, respectively. In Figs. 5, 6, 7, 8, we plot LOG(ERR) versus the CPU time consumed

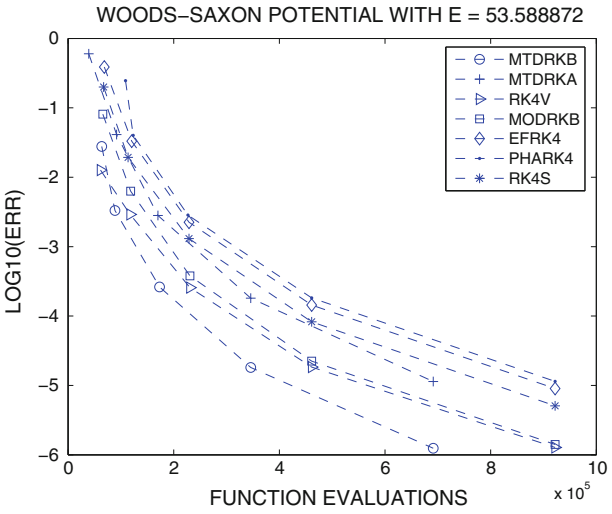

Fig. 1 Efficiency curves for $E = 53.588872$

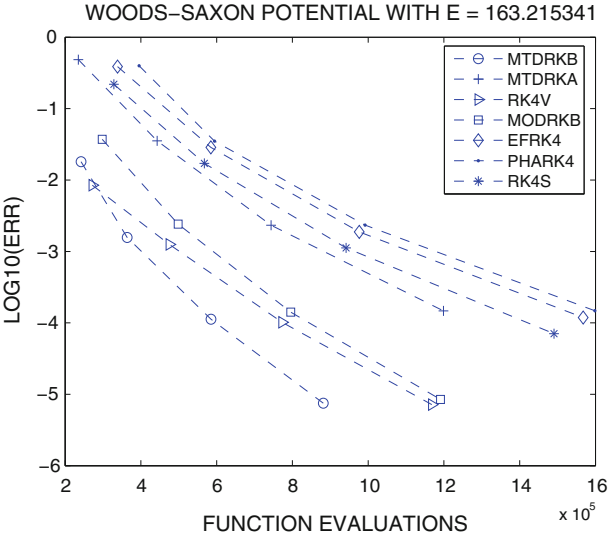

Fig. 2 Efficiency curves for $E = 163.215341$

by each method for $E_{\text{analytical}} = 53.588872, 163.215341, 341.495874, 989.701916$, respectively. The calculation are carried out on HP Z800 Workstation.

From Figs. 1, 2, 3, 4, 5, 6, 7, 8, it is seen that the new method MTDRKB outperform the methods PHARK4, EFRK4 and RK4S. Among all the methods we select the method MTDRKB is the most efficient.

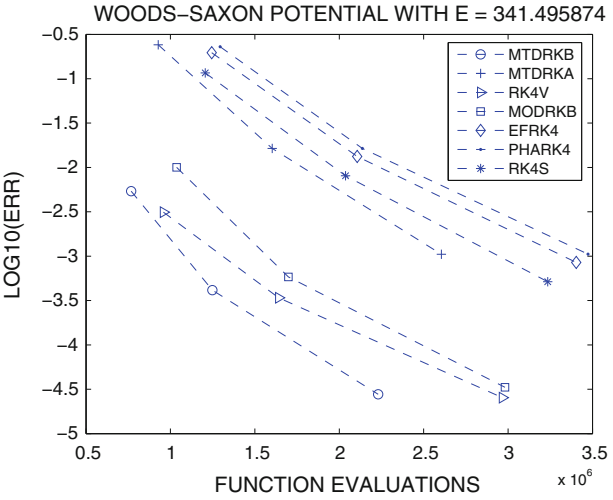

Fig. 3 Efficiency curves for $E = 341.495874$

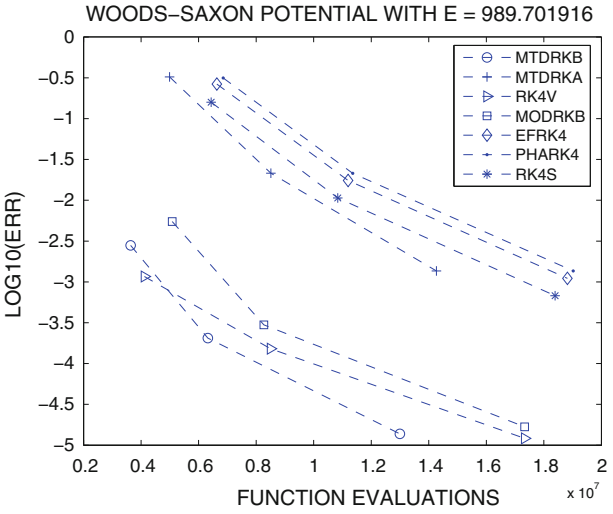

Fig. 4 Efficiency curves for $E = 989.701916$

6 Conclusions

In this paper, explicit two-derivative Runge–Kutta (TDRK) methods adapted to oscillatory initial-value problems are considered. Two practical optimized TDRK methods are constructed with vanished phase-lags and their first derivatives. We have compared our new methods with some optimized (exponentially fitted or phase-fitted) RK methods for the numerical solution of the Schrödinger equation. The analysis of the asymptotic expressions of the local errors for large energies suggests theoretical advantages

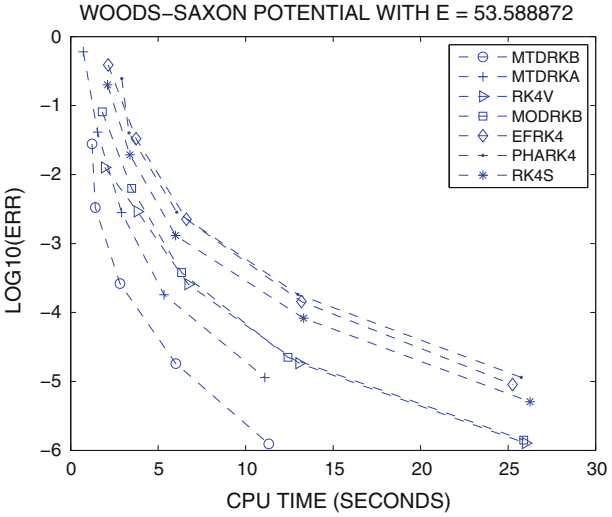

Fig. 5 Efficiency curves for $E = 53.588872$

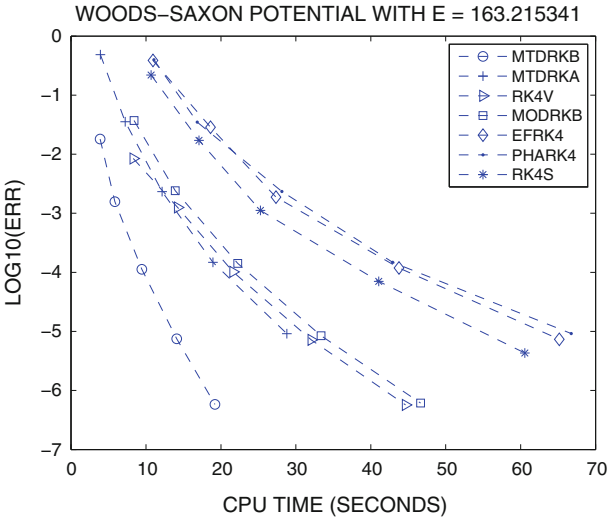

Fig. 6 Efficiency curves for $E = 163.215341$

of the newly constructed TDRK methods. When applied to the radial time-independent Schrödinger equation with the Woods–Saxon potential, the new methods are shown to outperform some highly effective codes in the literature, especially in the case of higher resonance. The special structure involving the second-order derivative and the optimized phase property are responsible to the excellent behavior of the new methods.

Finally, we note that, as in most integrators adapted to oscillatory problems, the coefficients of our new optimized TDRK methods depend on a fitting frequency ω, an estimate of the true frequency of the problem. In applications, the principal frequency

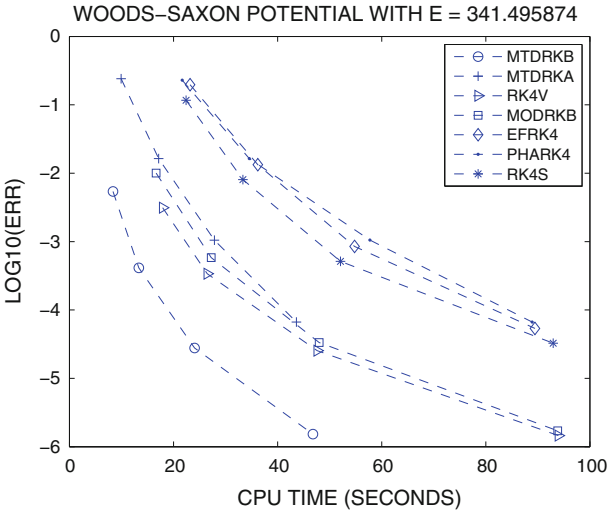

Fig. 7 Efficiency curves for $E = 341.495874$

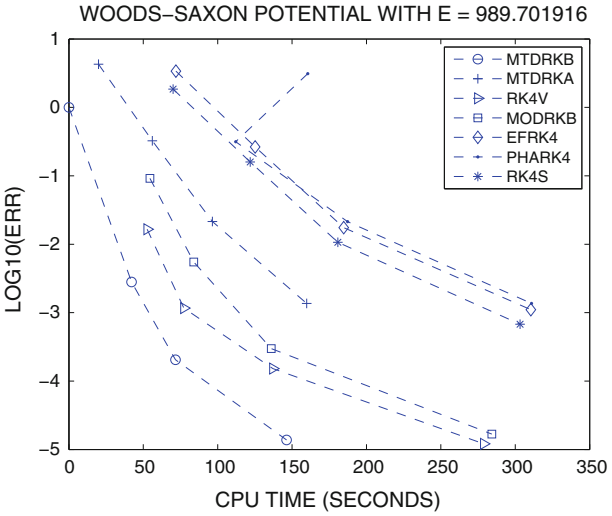

Fig. 8 Efficiency curves for $E = 989.701916$

is usually unknown, but we assume that a precise estimate ω has been obtained in advance. For techniques of estimating the principal frequency, we refer the reader to [15,45–47].

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