Japan J. Indust. Appl. Math., 16 (1999), 25–46

A Four-stage Implicit Runge-Kutta-Nyström Method with Variable Coefficients for Solving Periodic Initial Value Problems

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Received August 1, 1996
Revised January 9, 1998

A new implicit Runge-Kutta-Nyström method with variable coefficients is developed for solving the periodic initial value problem of the differential equation $y'' = f(t, y)$. The proposed method, whose coefficients are functions of the frequency and the stepsize, integrates exactly the equation, if the solution is a periodic function with a single Fourier component and the frequency is known. On the other hand, the order of accuracy of the method is shown to be 4 for the case that an estimated frequency, instead of the exact one, is applied to evaluate the coefficients, as well as for that the solution is non-periodic.

Key words: Runge-Kutta-Nyström method, trigonometric order, periodic initial value problems

1. Introduction

An important class of initial value problems which can arise in practice consists of problems whose solutions are known to be periodic. A number of numerical methods for this class of problems have been developed (see e.g. [1], [5], [7], and [8]). Only few of them, however, take advantage of special properties of the solution that may be known in advance. If the frequency of the solution, or a reasonable estimate for it, is known in advance, then the methods which take it as a priori knowledge are advantageous.

The purpose of this paper is to construct the 4-stage implicit Runge-Kutta-Nyström method which takes the frequency of the solution as a priori knowledge. The Runge-Kutta-Nyström method proposed here, whose coefficients are functions of the frequency and the stepsize, gives the exact solutions of the initial value problems, if the solutions are periodic and their frequencies are known in advance. On the other hand, if the solutions are not periodic, then the order of accuracy of the method is shown to be 4, when the coefficients are real and analytic functions of $\nu = \omega h$. Moreover, we analyze the two errors, phase and amplification errors, of the Runge-Kutta-Nyström method for the case that the exact frequency is unknown. We discuss further the fixed coefficients implementation which reduces the computational cost.

2. Trigonometric Runge-Kutta-Nyström (TRKN) Method

2.1. Trigonometric order

Let us consider a special class of second-order initial value problem of the form

$$y'' = f(t, y), \quad y(t_0) = \zeta, \quad y'(t_0) = \eta. \tag{1}$$

For solving equation (1), instead of applying conventional Runge-Kutta or linear multistep methods to the equivalent 1st-order system, which has the dimension twice that of equation (1), the direct application of the Runge-Kutta-Nyström method to equation (1) is more efficient, particularly when the equation is stiff and therefore implicit methods are necessary to solve it.

The Runge-Kutta-Nyström method takes the form

$$\begin{aligned} y_{n+1} &= y_n + hy'_n + h^2 \sum_{j=1}^{s} \bar{b}_j f(t_n + c_j h, Y_j), \\ y'_{n+1} &= y'_n + h \sum_{j=1}^{s} b_j f(t_n + c_j h, Y_j), \\ Y_j &= y_n + c_j h y'_n + h^2 \sum_{k=1}^{s} a_{jk} f(t_n + c_k h, Y_k), \quad j = 1, 2, \ldots, s. \end{aligned} \tag{2}$$

As in the case of Runge-Kutta methods, this can be represented in the Butcher array

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \cdots & \cdots & \cdots & \cdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & \bar{b}_1 & \bar{b}_2 & \cdots & \bar{b}_s \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}.$$

Although various Runge-Kutta-Nyström methods have been proposed (see, e.g, [3]), none of the methods have been developed for the specialized situation that the solution of the problem is periodic and the frequency is known. For such problems, it is appropriate to discuss the accuracies using the notion of the *trigonometric order*, which was first introduced by Gautschi [1] for linear multistep methods. According to Gautschi [1] we describe briefly the trigonometric order of linear multistep methods. Consider the linear multistep method

$$\sum_{j=0}^{k} \alpha_j y_j = h \sum_{j=0}^{k} \beta_j f_j, \tag{3}$$

for solving the first order equation $y' = f(t, y)$. If the difference operator

$$L[y(t); h] := \sum_{j=0}^{k} \{\alpha_j y(t + jh) - h\beta_j y'(t + jh)\} \tag{4}$$

associated with the multistep method annihilates trigonometric polynomials up to degree r, i.e.,

$$L[\cos(q\omega t); h] = L[\sin(q\omega t); h] = 0, \quad q = 1, \ldots, r,$$

$$L[\cos((r + 1)\omega t); h] \neq 0, \quad L[\sin((r + 1)\omega t); h] \neq 0,$$

then the linear multistep method is said to be of trigonometric r. For the Runge-Kutta-Nyström method, the trigonometric order is defined in an obvious manner analogous to that for the linear multistep method.

DEFINITION 2.1. An s-stage Runge-Kutta-Nyström method is said to be of *trigonometric order r relative to the frequency ω*, if all the relations

$$\begin{cases} y(t + c_j h) = y(t) + c_j h y'(t) + h^2 \sum_{k=1}^{s} a_{jk} y''(t + c_k h), \quad j = 1, \ldots, s + 1, \\ y'(t + h) = y'(t) + h \sum_{k=1}^{s} b_k y''(t + c_k h) \end{cases} \tag{5}$$

are satisfied by the functions $y(t) = \cos(m\omega t)$ and $\sin(m\omega t)$ $(m = 1, \ldots, r)$, and not satisfied by $y(t) = \cos((r + 1)\omega t)$ and $\sin((r + 1)\omega t)$, where we set $a_{s+1,k} = \bar{b}_k$ $(k = 1, \ldots, s)$ and $c_{s+1} = 1$. In addition, if the method is of trigonometric order ≥ 1, we will call the method *trigonometric Runge-Kutta-Nyström (TRKN) method.*

Hereafter we are only concerned with the method of trigonometric order 1, and examine the order of accuracy of the method, when the coefficients, which are the functions of $\nu = \omega h$, are real and analytic in the neighborhood of $\nu = 0$. The order of accuracy of the TRKN method is also important in the sense that it tells us at what rate the numerical solution converges to the exact solution, when the solution of (1) is not periodic, or when the solution is periodic but the coefficients are evaluated using an approximate frequency.

2.2. Order of accuracy of TRKN method

The order of accuracy of the Runge-Kutta-Nyström method is defined to be $p = \min\{p_1, p_2\}$ for the integers p_1 and p_2 satisfying

$$y(t_{n+1}) - y_{n+1} = O(h^{p_1+1}), \qquad y'(t_{n+1}) - y'_{n+1} = O(h^{p_2+1}), \tag{6}$$

where y_{n+1} and y'_{n+1} are the numerical solutions given by the method under the conditions that $y_n = y(t_n)$ and $y'_n = y'(t_n)$. The order condition for conventional Runge-Kutta-Nyström methods has been thoroughly studied by Hairer and Wanner

[2] and Hairer, Nørsett and Wanner [3]. Here we will show that the order of accuracy of the TRKN method is at least 2.

We assume here that the abscissae c_j are independent of ω, and that the coefficients a_{jk} and b_k are real functions of $\nu = \omega h$ and analytic in the neighborhood of $\nu = 0$. Let the Taylor series expansions of the coefficients be

$$a_{jk} = a_{jk}^{(0)} + a_{jk}^{(1)}\nu + a_{jk}^{(2)}\nu^2 + \cdots,$$
$$b_k = b_k^{(0)} + b_k^{(1)}\nu + b_k^{(2)}\nu^2 + \cdots.$$

Then for these expansions we have the following lemma:

LEMMA 2.2. *For the coefficients a_{jk} and b_k of the TRKN method, there exist the relations*

$$\begin{aligned} \sum_{k=1}^{s} a_{jk}^{(0)} c_k^{l-1} &= \frac{c_j^{l+1}}{l(l+1)}, \quad l = 1,2, \quad j = 1,2,\ldots,s+1, \\ \sum_{k=1}^{s} b_k^{(0)} c_k^{l-1} &= \frac{1}{l}, \qquad l = 1,2. \end{aligned} \tag{7}$$

Proof. First we show the relation on a_{jk}. The substitutions $y(t) = \cos(\omega t)$ and $y(t) = \sin(\omega t)$ in the first of (5) yield

$$\begin{aligned} \frac{1-\cos(c_j\nu)}{\nu^2} &= \sum_{l=0}^{\infty}\sum_{k=1}^{s} a_{jk}^{(l)}\nu^l \cos(c_k\nu), \\ \frac{c_j\nu - \sin(c_j\nu)}{\nu^2} &= \sum_{l=0}^{\infty}\sum_{k=1}^{s} a_{jk}^{(l)}\nu^l \sin(c_k\nu), \end{aligned} \quad j = 1,\ldots,s+1, \tag{8}$$

which means that $a_{jk}^{(l)} = 0$ for odd l. Expanding $\cos(c_j\nu)$ and $\sin(c_j\nu)$ into the Taylor series, and collecting the same powers of ν, we have

$$\begin{aligned} A_{0,j} + A_{1,j}\nu^2 + A_{2,j}\nu^4 + \cdots &= 0, \\ B_{0,j}\nu + B_{1,j}\nu^3 + B_{2,j}\nu^5 + \cdots &= 0, \end{aligned} \tag{9}$$

where $A_{m,j}$ and $B_{m,j}$ are the constants given by

$$\begin{aligned} A_{m,j} &= \frac{(-1)^m c_j^{2m+2}}{(2m+2)!} - \sum_{l=0}^{m}\sum_{k=1}^{s} \frac{(-1)^l}{(2l)!} a_{jk}^{(2m-2l)} c_k^{2l}, \\ B_{m,j} &= \frac{(-1)^m c_j^{2m+3}}{(2m+3)!} - \sum_{l=0}^{m}\sum_{k=1}^{s} \frac{(-1)^l}{(2l+1)!} a_{jk}^{(2m-2l)} c_k^{2l+1}. \end{aligned} \tag{10}$$

The first relation of (7) is derived from $A_{0,j} = 0$ and $B_{0,j} = 0$.

Next we show the relation on b_k in the same way. The substitutions $y(t) = \cos(\omega t)$ and $y(t) = \sin(\omega t)$ in the second of (5) yield

$$\begin{aligned} \frac{\sin \nu}{\nu} &= \sum_{k=1}^{s} \sum_{l=0}^{\infty} b_k^{(l)} \nu^l \cos(c_k \nu), \\ \frac{1-\cos \nu}{\nu} &= \sum_{k=1}^{s} \sum_{l=0}^{\infty} b_k^{(l)} \nu^l \sin(c_k \nu), \end{aligned} \tag{11}$$

from which we have $b_k^{(l)} = 0$ for odd l. As before, expanding $\cos(c_k\nu)$ and $\sin(c_k\nu)$ into Taylor series and collecting the same powers of ν, we have

$$\begin{aligned} C_0 + C_1\nu^2 + C_2\nu^4 + \cdots &= 0, \\ D_0\nu + D_1\nu^3 + D_2\nu^5 + \cdots &= 0, \end{aligned} \tag{12}$$

where C_m and B_m are the constants given by

$$\begin{aligned} C_m &= \frac{(-1)^m}{(2m+1)!} - \sum_{l=0}^{m} \sum_{k=1}^{s} \frac{(-1)^l}{(2l)!} b_k^{(2m-2l)} c_k^{2l}, \\ D_m &= \frac{(-1)^m}{(2m+2)!} - \sum_{l=0}^{m} \sum_{k=1}^{s} \frac{(-1)^l}{(2l+1)!} b_k^{(2m-2l)} c_k^{2l+1}. \end{aligned} \tag{13}$$

The relation on b_k is derived from $C_0 = 0$ and $D_0 = 0$. ■

To analyze the local error, it is convenient to associate the difference operators

$$L_j\{y(t);h\} := y(t+c_jh) - y(t) - c_jhy'(t) - h^2 \sum_{k=1}^{s} a_{kj} y''(t+c_jh), \tag{14}$$

$$j = 1, \ldots, s+1,$$

$$M\{y(t);h\} := y'(t+h) - y'(t) - h \sum_{k=1}^{s} y''(t+c_kh), \tag{15}$$

with the TRKN method, where $y(t)$ is assumed to be not necessary periodic but sufficiently often differentiable. If $y(t)$ is the solution of (1) then between the operators and the local errors there exist the relations

$$\begin{aligned} T_j &:= y(t+c_jh) - Y_j = L_j\{y(t);h\} \\ &\quad + h^2 \sum_{k=1}^{s} a_{jk} (f(t+c_kh, y(t+c_kh)) - f(t, Y_k)), \quad j = 1, 2, \ldots, s+1, \\ T' &:= y'(t+h) - y'_{n+1} = M\{y(t);h\} \\ &\quad + h \sum_{k=1}^{s} b_k (f(t+c_kh, y(t+c_kh)) - f(t, Y_k)), \end{aligned} \tag{16}$$

where we set $Y_{s+1} = y_{n+1}$. We have therefore the inequalities

$$
\begin{aligned}
|T_j| &\le (1 - h^2 L\ |a_{jj}|)^{-1}\Big(|L_j\{y(t);h\}| + h^2 L \sum_{k\neq j}^{s} |a_{jk}|\ |T_k|\Big),\\
|T_{s+1}| &\le |L_{s+1}\{y(t);h\}| + h^2 L \sum_{k=1}^{s} |\bar{b}_k|\ |T_k|, \qquad (17)\\
|T'| &\le |M\{y(t);h\}| + hL \sum_{k=1}^{s} |b_k|\ |T_k|,
\end{aligned}
$$

where we assume that function $f(t, y)$ satisfies the Lipschitz condition with respect to y, and L is the Lipschitz constant. Using the inequalities we will analyze the orders of the local errors.

Let ρ_j and σ denote the orders of local errors T_j and T', respectively, i.e.,

$$T_j = O(h^{\rho_j}), \qquad T' = O(h^{\sigma}).$$

Note that p_1 and p_2 in (6) can be expressed in terms of ρ_j and σ as

$$p_1 = \rho_{s+1} - 1, \qquad p_2 = \sigma - 1. \qquad (18)$$

Moreover, let λ_j and μ denote the orders of operators L_j and M, respectively, i.e.,

$$L_j\{y(t);h\} = O(h^{\lambda_j}), \qquad M\{y(t);h\} = O(h^{\mu}).$$

Then we find from (17) that

$$
\begin{aligned}
\rho_j &= \min\Big\{\lambda_j,\ \min_{\substack{k\neq j\\ 1\le k\le s}} \{\rho_k\} + 2\Big\}, \quad j = 1, 2, \ldots, s+1,\\
\sigma &= \min\Big\{\mu,\ \min_{1\le k\le s} \{\rho_k\} + 1\Big\}.
\end{aligned} \qquad (19)
$$

We have immediately from (19) that $\rho_j \le \lambda_j$ for all j, so that

$$\min_j\{\rho_j\} \le \min_j\{\lambda_j\}.$$

For the minimum of ρ_j, denoted by ρ_m, we have

$$\min_j\{\rho_j\} = \rho_m = \lambda_m,$$

since if this is not the case we have from (19) the contradiction that

$$\rho_m = \min_{k\neq m}\{\rho_k\} + 2 \ge \rho_m + 2 > \rho_m.$$

The fact that $\min_j\{\rho_j\} = \lambda_m$, together with $\min_j\{\rho_j\} \le \min_j\{\lambda_j\}$, imply

$$\min_{1\le j\le s+1}\{\rho_j\} = \min_{1\le j\le s+1}\{\lambda_j\}. \qquad (20)$$

Next we will analyze the orders of operators L_j and M using the result.

Assuming that the Taylor series expansion of $y(t)$ and those of the coefficients a_{jk} and b_k have a common interval of convergence, and using the results of Lemma 2.2, we have in the interval

$$\begin{aligned} L_j\{y(t);h\} &= \sum_{l=1}^{\infty} \frac{1}{(l-1)!} \left\{ \frac{c_j^{l+1}}{l(l+1)} - \sum_{k=1}^{s} \sum_{m=0}^{\infty} a_{jk}^{(2m)} c_k^{l-1} \nu^{2m} \right\} h^{l+1} y^{(l+1)}(t) \\ &= \left\{ \frac{c_j^2}{2} - \sum_{k=1}^{s} (a_{jk}^{(0)} + a_{jk}^{(2)} \nu^2 + \cdots) \right\} h^2 y^{(2)}(t) \\ &\quad + \left\{ \frac{c_j^3}{2\cdot 3} - \sum_{k=1}^{s} (a_{jk}^{(0)} c_k + a_{jk}^{(2)} c_k \nu^2 + \cdots) \right\} h^3 y^{(3)}(t) + \cdots \\ &= -\left(\sum_{k=1}^{s} a_{jk}^{(2)} \right) \nu^2 h^2 y^{(2)}(t) - \left(\sum_{k=1}^{s} a_{jk}^{(2)} c_k \right) \nu^2 h^3 y^{(3)}(t) + \cdots, \end{aligned} \tag{21}$$

$$\begin{aligned} M\{y(t);h\} &= \sum_{l=1}^{\infty} \frac{1}{(l-1)!} \left\{ \frac{1}{l} - \sum_{k=1}^{s} \sum_{m=0}^{\infty} b_k^{(2m)} c_k^{l-1} \nu^{2m} \right\} h^l y^{(l+1)}(t) \\ &= \left\{ 1 - \sum_{k=1}^{s} (b_k^{(0)} + b_k^{(2)} \nu^2 + \cdots) \right\} h y^{(2)}(t) \\ &\quad + \left\{ \frac{1}{2} - \sum_{k=1}^{s} (b_k^{(0)} c_k + b_k^{(2)} c_k \nu^2 + \cdots) \right\} h^2 y^{(3)}(t) + \cdots \\ &= -\left(\sum_{k=1}^{s} b_k^{(2)} \right) \nu^2 h y^{(2)}(t) - \left(\sum_{k=1}^{s} b_k^{(2)} c_k \right) \nu^2 h^2 y^{(3)}(t) + \cdots. \end{aligned} \tag{22}$$

This means that the orders of $L_j\{y(t);h\}$ and $M\{y(t);h\}$ are at least 4 and 3, respectively, i.e., $\lambda_j \geq 4$ and $\mu \geq 3$. Therefore we have from (19) and (20) that $\rho_j \geq 4$ $(j = 1, \ldots, s+1)$ and $\sigma \geq 3$, so that $p_1 \geq 3$ and $p_2 \geq 2$ in (6). We have thus proved the following theorem:

THEOREM 2.3. *Let p be the order of accuracy of the TRKN method, then $p \geq 2$.*

Although Theorem 2.3 shows that the order of accuracy p of any TRKN method is at least 2, it is not clear that the method can have $p \geq 3$. Next we will show that $p = 3$ and 4 can be attained by imposing additional conditions on the coefficients, and present the method that has $p = 4$. First we will prove two lemmas.

LEMMA 2.4. *For some integer $q > 0$, if the coefficients a_{jk} of the TRKN satisfy the condition*

$$\sum_{k=1}^{s} a_{jk} c_k^{2l} = \frac{c_j^{2l+2}}{(2l+1)(2l+2)}, \quad l = 0, 1, \ldots, q-1, \tag{23}$$

then

$$\sum_{k=1}^{s} a_{jk}^{(0)} c_k^{2q} = \frac{c_j^{2q+2}}{(2q+1)(2q+2)}.$$

Similarly, if for some integer $q > 0$

$$\sum_{k=1}^{s} a_{jk} c_k^{2l+1} = \frac{c_j^{2l+3}}{(2l+2)(2l+3)}, \quad l = 0, 1, \ldots, q-1, \tag{24}$$

then

$$\sum_{k=1}^{s} a_{jk}^{(0)} c_k^{2q+1} = \frac{c_j^{2q+3}}{(2q+2)(2q+3)}.$$

Proof. We will show only the first part of this lemma, since the second part can be proved in a straightforward manner. It is easily seen that (23) means

$$\sum_{k=1}^{s} a_{jk}^{(0)} c_k^{2l} = \frac{c_j^{2l+2}}{(2l+1)(2l+2)}, \quad l = 0, 1, \ldots, q-1,$$

$$\sum_{k=1}^{s} a_{jk}^{(2\kappa)} c_k^{2l} = 0, \quad \kappa > 0, \quad l = 0, 1, \ldots, q-1,$$

so that the value of $A_{m,j}$, which is defined by (10), at $m = q$ is given by

$$\begin{aligned} A_{q,j} &= \frac{(-1)^q c_j^{2q+2}}{(2q+2)!} - \sum_{l=0}^{q} \frac{(-1)^l}{(2l)!} \sum_{k=1}^{s} a_{jk}^{(2q-2l)} c_k^{2l} \\ &= \frac{(-1)^q c_j^{2q+2}}{(2q+2)!} - \frac{(-1)^q}{(2q)!} \sum_{k=1}^{s} a_{jk}^{(0)} c_k^{2q}. \end{aligned}$$

The first assertion thus holds, since $A_{q,j} = 0$. From $B_{q,j} = 0$ we can also show that the second assertion holds. ■

The next lemma can be proved in the same way.

LEMMA 2.5. *For some integer $q > 0$, if coefficients b_k satisfy*

$$\sum_{k=1}^{s} b_k c_k^{2l} = \frac{1}{2l+1}, \quad l = 0, 1, \ldots, q-1,$$

then

$$\sum_{k=1}^{s} b_k^{(0)} c_k^{2q} = \frac{1}{2q+1}.$$

Similarly, if for some integer $q > 0$

$$\sum_{k=1}^{s} b_k c_k^{2l+1} = \frac{1}{2l+2}, \quad l = 0, 1, \ldots, q-1,$$

then

$$\sum_{k=1}^{s} b_k^{(0)} c_k^{2q+1} = \frac{1}{2q+2}.$$

The next theorem provides a sufficient condition for the TRKN method has order of accuracy ≥ 3.

THEOREM 2.6. *In addition to condition* (5), *if we impose the condition*

$$\sum_{k=1}^{s} b_k = 1, \tag{25}$$

on b_k, *then the order of accuracy* p *satisfies* $p \geq 3$.

Proof. From the result of Lemma 2.5 we have

$$\sum_{k=1}^{s} b_k^{(0)} c_k^2 = \frac{1}{3}.$$

Applying the result and that of Lemma 2.2 to operator M, we can find that the order of operator M is at least 4, i.e., $\mu \geq 4$, so that we have from (18) and (19) that $\sigma \geq 4$ and $p_2 \geq 3$, since in this case λ_j's remain fixed. Thus the assertion holds. ■

The next theorem provides a sufficient condition for the existence of the TRKN method of order of accuracy ≥ 4.

THEOREM 2.7. *In addition to condition* (5), *if we impose the conditions*

$$\sum_{k=1}^{s} b_k = 1, \qquad \sum_{k=1}^{s} \bar{b}_k = \frac{1}{2}, \qquad \sum_{k=1}^{s} b_k c_k = \frac{1}{2}, \tag{26}$$

on b_k *and* $\bar{b}_k$, *then* $p \geq 4$.

Proof. It suffices to prove that operators L_{s+1} and M are of orders at least 5. First we show $\rho_{s+1} \geq 5$. From the result of Lemma 2.4 for $j = s+1$, we have

$$\sum_{k=1}^{s} \bar{b}_k^{(0)} c_k^2 = \frac{1}{3 \cdot 4}.$$

This result and that of Lemma 2.2 lead to $\rho_{s+1} \geq 5$, since

$$\begin{aligned} L_{s+1} &= \left(\frac{1}{2\cdot 3} - \sum_{k=1}^{s} \bar{b}_k c_k\right) h^3 y^{(3)}(t) + \frac{1}{2}\left(\frac{1}{3\cdot 4} - \sum_{k=1}^{s} \bar{b}_k c_k^2\right) h^4 y^{(4)}(t) + \cdots \\ &= -\left(\sum_{k=1}^{s} \bar{b}_k^{(2)} c_k\right) \nu^2 h^3 y^{(3)}(t) - \frac{1}{2}\left(\sum_{k=1}^{s} \bar{b}_k^{(2)} c_k^2\right) \nu^2 h^4 y^{(4)}(t) + \cdots \end{aligned}$$

Next we show $\mu \geq 5$. From the result of Lemma 2.5, we have

$$\sum_{k=1}^{s} b_k^{(0)} c_k^2 = \frac{1}{3}, \qquad \sum_{k=1}^{s} b_k^{(0)} c_k^3 = \frac{1}{4},$$

and therefore

$$\begin{aligned} M &= \frac{1}{2}\left(\frac{1}{3} - \sum_{k=1}^{s} b_k c_k^2\right) h^3 y^{(4)}(t) + \frac{1}{3!}\left(\frac{1}{4} - \sum_{k=1}^{s} b_k c_k^3\right) h^4 y^{(5)}(t) + \cdots \\ &= -\frac{1}{2}\left(\sum_{k=1}^{s} b_k^{(2)} c_k^2\right) \nu^2 h^3 y^{(4)}(t) - \frac{1}{3!}\left(\sum_{k=1}^{s} b_k^{(2)} c_k^3\right) \nu^2 h^4 y^{(5)}(t) + \cdots \end{aligned}$$

The assertion of the theorem thus holds. ■

Next we will propose the implicit TRKN method of trigonometric order 1 satisfying condition (26). In order to construct such a method it is necessary that $s \geq 4$, since there exist four equations to be satisfied with b_k's. Here we propose the 4-stage implicit TRKN method of this class, which will be called TRKN41.

We can easily see from the discussions above that the condition

$$\sum_{k=1}^{4} \bar{b}_k^{(2)} c_k = \sum_{k=1}^{4} b_k^{(2)} c_k^2 = 0 \tag{27}$$

is necessary for TRKN41 to have $p > 4$. We will make it clear in the later section that this condition does not hold for TRKN41, i.e., the order of accuracy of the method is exactly 4.

3. Derivation of TRKN41 Method

3.1. Coefficients of TRKN41 method

If we write down condition (5) for $s = 4$ and $r = 1$, then we have

$$\begin{cases} \cos(c_i\nu) - 1 + \nu^2 \sum_{j=1}^{4} a_{ij}\cos(c_j\nu) = 0, & i = 1,\dots,4, \\ \sin(c_i\nu) - c_i\nu + \nu^2 \sum_{j=1}^{4} a_{ij}\sin(c_j\nu) = 0, & i = 1,\dots,4, \\ \cos\nu - 1 + \nu^2 \sum_{j=1}^{4} \bar{b}_j\cos(c_j\nu) = 0, \\ \sin\nu - \nu + \nu^2 \sum_{j=1}^{4} \bar{b}_j\sin(c_j\nu) = 0, \\ \sin\nu - \nu \sum_{j=1}^{4} b_j\cos(c_j\nu) = 0, \\ \cos\nu - 1 + \nu \sum_{j=1}^{4} b_j\sin(c_j\nu) = 0. \end{cases} \tag{28}$$

The coefficients b_j's are uniquely determined by conditions (26) and (28), if c_j's are different from each other, since there exist four equations for four unknowns. For c_j's it will be natural to take the equally spaced abscissae such that

$$c_1 = 0,\ c_2 = 1/3,\ c_3 = 2/3,\ c_4 = 1. \tag{29}$$

In our case, this choice of c_j's leads to that $a_{1j} = 0$ ($j = 1,\dots,4$), and therefore we can reduce the total cost of evaluating stages, since the 1st stage becomes explicit. For other a_{ij} ($i > 1$), on the other hand, there exist only two equations for four unknowns, so that we set $a_{ij} = 0$ except for a_{i1} and a_{ii}; this choice of a_{ij}'s enables us to evaluate the second, third and fourth stages in parallel after the evaluation of the first stage, if parallel computers are available.

For $\bar{b}_j$'s, there exist three equations for four unknowns, so that we take $\bar{b}_4$ as a free parameter, say $\bar{b}_4 = \alpha$.

We show the coefficients derived in this way, which are analytic at $\nu = 0$, together with their power series expansions. These expansions are useful to avoid the losses of significance by cancellation which arises in the evaluations of the coefficients for small ν.

$$\begin{aligned} b_1 &= \frac{-6\cos\left(\frac{\nu}{3}\right) + 2\nu\sin\left(\frac{\nu}{3}\right) + 6\cos\left(\frac{2\nu}{3}\right) - \nu\sin\left(\frac{2\nu}{3}\right) - 2\cos\nu + 2}{2\nu\left(5\sin\left(\frac{\nu}{3}\right) - 4\sin\left(\frac{2\nu}{3}\right) + \sin\nu\right)} \\ &= \frac{1}{8} + \frac{1}{1440}\nu^2 + \frac{1}{181440}\nu^4 + \frac{31}{587865600}\nu^6 + \cdots \end{aligned} \tag{30}$$

$$b_2 = \frac{1}{2} - b_1 = \frac{3}{8} - \frac{1}{1440}\nu^2 - \frac{1}{181440}\nu^4 - \frac{31}{587865600}\nu^6 + \cdots \tag{31}$$

$$b_3 = b_2 \tag{32}$$

$$b_4 = b_1 \tag{33}$$

$$\begin{aligned}
\bar{b}_1 &= \frac{\cos\left(\frac{\nu}{3}\right) + (2\alpha - 1/2)\nu \sin\left(\frac{\nu}{3}\right) - \cos\left(\frac{2\nu}{3}\right) - \alpha\nu \sin\left(\frac{2\nu}{3}\right)}{2\nu \sin\left(\frac{\nu}{3}\right)\left(\cos\left(\frac{\nu}{3}\right) - 1\right)} \\
&= \frac{-8\alpha + 1}{8} + \frac{1}{1440}\nu^2 + \frac{1}{181440}\nu^4 + \frac{31}{587865600}\nu^6 + \cdots \qquad (34)
\end{aligned}$$

$$\begin{aligned}
\bar{b}_2 &= \frac{-(1 + \alpha\nu^2)\sin\left(\frac{\nu}{3}\right) + ((-\alpha + 1/2)\nu^2 - 1)\sin\left(\frac{2\nu}{3}\right) + \nu\cos\left(\frac{2\nu}{3}\right) + (\alpha\nu^2 + 1)\sin\nu - \nu}{2\nu^2 \sin\left(\frac{\nu}{3}\right)\left(\cos\left(\frac{\nu}{3}\right) - 1\right)} \\
&= \frac{12\alpha + 1}{4} + \frac{-240\alpha + 1}{2160}\nu^2 + \frac{168\alpha - 1}{163296}\nu^4 - \frac{3360\alpha + 1}{881798400}\nu^6 + \cdots \qquad (35)
\end{aligned}$$

$$\begin{aligned}
\bar{b}_3 &= \frac{((\alpha - 1/2)\nu^2 + 1)\sin\left(\frac{\nu}{3}\right) - \nu\cos\left(\frac{\nu}{3}\right) + (\alpha\nu^2 + 1)\sin\left(\frac{2\nu}{3}\right) - (\alpha\nu^2 + 1)\sin\nu + \nu}{2\nu^2 \sin\left(\frac{\nu}{3}\right)\left(\cos\left(\frac{\nu}{3}\right) - 1\right)} \\
&= \frac{-24\alpha + 1}{8} + \frac{96\alpha - 1}{864}\nu^2 + \frac{-1680\alpha + 1}{1632960}\nu^4 + \frac{960\alpha - 13}{251942400}\nu^6 + \cdots \qquad (36)
\end{aligned}$$

$$\bar{b}_4 = \alpha \text{ (free parameter)} \qquad (37)$$

$$\begin{aligned}
a_{21} &= \frac{-\nu\cot\left(\frac{\nu}{3}\right) + 3}{3\nu^2} \\
&= \frac{1}{27} + \frac{1}{3645}\nu^2 + \frac{2}{688905}\nu^4 + \frac{1}{31000725}\nu^6 + \cdots \qquad (38)
\end{aligned}$$

$$\begin{aligned}
a_{22} &= \frac{-3\sin\left(\frac{\nu}{3}\right) + \nu}{3\nu^2 \sin\left(\frac{\nu}{3}\right)} \\
&= \frac{1}{54} + \frac{7}{29160}\nu^2 + \frac{31}{11022480}\nu^4 + \frac{127}{3968092800}\nu^6 + \cdots \qquad (39)
\end{aligned}$$

$$\begin{aligned}
a_{31} &= \frac{-2\nu\cot\left(\frac{2\nu}{3}\right) + 3}{3\nu^2} \\
&= \frac{4}{27} + \frac{16}{3645}\nu^2 + \frac{128}{688905}\nu^4 + \frac{256}{31000725}\nu^6 + \cdots \qquad (40)
\end{aligned}$$

$$a_{32} = 0 \qquad (41)$$

$$\begin{aligned}
a_{33} &= \frac{-3\sin\left(\frac{2\nu}{3}\right) + 2\nu}{3\nu^2 \sin\left(\frac{2\nu}{3}\right)} \\
&= \frac{2}{27} + \frac{14}{3645}\nu^2 + \frac{124}{688905}\nu^4 + \frac{254}{31000725}\nu^6 + \cdots \qquad (42)
\end{aligned}$$

$$\begin{aligned}
a_{41} &= \frac{-\nu\cot\nu + 1}{\nu^2} \\
&= \frac{1}{3} + \frac{1}{45}\nu^2 + \frac{2}{945}\nu^4 + \frac{1}{4725}\nu^6 + \cdots \qquad (43)
\end{aligned}$$

$$a_{42} = 0 \qquad (44)$$

$$a_{43} = 0 \qquad (45)$$

$$\begin{aligned} a_{44} &= \frac{-\sin\nu+\nu}{\nu^2\sin\nu} \\ &= \frac{1}{6}+\frac{7}{360}\nu^2+\frac{31}{15120}\nu^4+\frac{127}{604800}\nu^6+\cdots \end{aligned} \quad (46)$$

From the expressions above we have

$$\sum_{k=1}^{4} b_k^{(2)} c_k^2 = \frac{1}{3240} \neq 0,$$

therefore $M = O(h^5)$, which means that TRKN41 has $p = 4$.

3.2. Numerical example

The following examples show the power of TRKN41 for periodic or approximately periodic problems.

Example 3.1. Let us consider the equation

$$y''(t) = -y(t) + \varepsilon \cos t, \quad (47)$$

$$y(0) = 1, \quad y'(0) = 0,$$

whose solution is given by

$$y(t) = \cos t + 0.5\varepsilon t \sin t. \quad (48)$$

We integrate this equation from $t = 0$ to 10 by TRKN41 with $\omega = 1$ and $\alpha = 0$, by using the double precision IEEE arithmetic. The errors at $t = 10$ for various values of ε are shown in Table 1.

Table 1. Errors at $t = 10$ of TRKN41 with $\omega = 1$ and $\alpha = 0$.

ε	$h = 0.200$	$h = 0.100$	$h = 0.050$
10^{-5}	-4.108e-10	-2.378e-11	-1.317e-12
10^{-4}	-4.108e-09	-2.379e-10	-1.315e-11
10^{-3}	-4.108e-08	-2.379e-09	-1.314e-10
10^{-2}	-4.108e-07	-2.379e-08	-1.314e-09
10^{-1}	-4.108e-06	-2.379e-07	-1.314e-08

The first term on the right-hand side of (48) can be represented exactly by TRKN41 for any stepsize $h > 0$, but the second term, which is proportional to ε, can never be represented exactly. Therefore, the errors of the method are proportional to ε, as shown in Table 1.

Example 3.2. Let us consider the well-known two-body problem (see [4] or [6]):

$$y_1'' = -y_1/(y_1^2+y_2^2)^{3/2}, \qquad y_2'' = -y_2/(y_1^2+y_2^2)^{3/2}, \quad (49)$$

$$y_1(0) = 1 - e, \quad y_1'(0) = 0, \quad y_2(0) = 0, \quad y_2'(0) = \sqrt{\frac{1+e}{1-e}},$$

where e is an eccentricity. The exact solution of the problem is given by

$$y_1(t) = \cos u - e, \qquad y_2(t) = \sqrt{1-e^2}\sin u, \tag{50}$$

where u is the solution of Kepler's equation

$$u = t + e \sin u.$$

When $e = 0$

$$y_1(t) = \cos t, \quad y_2(t) = \sin t,$$

so that the method with $\omega = 1$ is expected to be particularly accurate for the problems with small e. Here we integrate equation (49) from $t = 0$ to 20 for $e = 0,\ 0.01,\ 0.1$, and 0.5, by using TRKN41 with $\omega = 1$. We evaluate the maximum errors

$$\max_{0 \le nh \le 20} (|y_{1,n} - y_1(nh)| + |y_{2,n} - y_2(nh)|),$$

where $y_{1,n}$ and $y_{2,n}$ are the numerical approximations to $y_1(nh)$ and $y_2(nh)$, respectively. The results are compared with those of the 2-stage Gauss Runge-Kutta method (see Table 2, 3).

Table 2. Maximum errors of TRKN41 with $\omega = 1$ and $\alpha = 0$.

	h =0.200	h =0.100	h =0.050
e =0.00	1.209e-14	4.638e-14	2.169e-13
e =0.01	9.668e-05	6.210e-06	3.919e-07
e =0.10	7.646e-04	6.030e-05	4.150e-06
e =0.50	3.003e-01	6.445e-03	1.486e-04

Table 3. Maximum errors of the 2-stage Gauss Runge-Kutta method.

	h =0.200	h =0.100	h =0.050
e =0.00	5.839e-04	3.658e-05	2.290e-06
e =0.01	5.939e-04	3.623e-05	2.266e-06
e =0.10	8.345e-04	5.238e-05	3.278e-06
e =0.50	2.121e-02	1.493e-03	9.551e-05

As the tables show, TRKN41 always yields the exact results for the problem with $e = 0.00$; the values corresponding to $e = 0.00$ in Table 2 must be the accumulations of roundoff errors. In addition, as has been expected, for the problem with $e = 0.01$, the results by the TRKN41 are more accurate than those by the 2-stage Gauss Runge-Kutta.

4. Phase and Amplification Errors of TRKN41

From the point of view of algebraic errors, the result given by TRKN41 will be satisfactory for any periodic problem, even if an inexact value of ω is used to evaluate the coefficients, since the order of accuracy of the method is proved to be 4. However, it is often the case that high accuracies in the phase and/or amplitude of the solution are required, when the solution is periodic. In this section we investigate the orders concerning the two errors, the phase and amplification errors, when an inexact value of ω is used to evaluate the coefficients. Hereafter, we denote the coefficients of the Runge-Kutta-Nyström method by $a_{ij}(\nu^2)$, $\bar{b}_i(\nu^2)$, and $b_i(\nu^2)$ to emphasize the dependences on ν^2.

Let us consider the test equation

$$y'' = -\omega^2 y, \quad y(0) = y_0, \quad y'(0) = y_0', \tag{51}$$

where the exact solution is given by

$$y(t) = y_0 \cos \omega t + \left(\frac{y_0'}{\omega}\right) \sin \omega t.$$

Here we assume that we can never know the exact frequency ω, but know an estimate, say $\widehat{\omega}$. If we integrate the test equation by TRKN41, whose coefficients are evaluated by using $\widehat{\omega}$, then the numerical solution satisfies

$$\begin{pmatrix} y_n \\ hy_n' \end{pmatrix} = R^n(\nu^2, \widehat{\nu}^2) \begin{pmatrix} y_0 \\ hy_0' \end{pmatrix}, \tag{52}$$

where

$$R(\nu^2, \widehat{\nu}^2) = P - \nu^2 \begin{pmatrix} \bar{\boldsymbol{b}}^{\mathrm{T}}(\widehat{\nu}^2) \\ \boldsymbol{b}^{\mathrm{T}}(\widehat{\nu}^2) \end{pmatrix} \left(I + \nu^2 A(\widehat{\nu}^2)\right)^{-1} V \tag{53}$$

$$P = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A = \begin{pmatrix} a_{11} & \cdots & a_{14} \\ \vdots & & \vdots \\ a_{41} & \cdots & a_{44} \end{pmatrix}, \quad V = \begin{pmatrix} 1 & c_1 \\ 1 & c_2 \\ 1 & c_3 \\ 1 & c_4 \end{pmatrix},$$

$$\nu = \omega h, \quad \widehat{\nu} = \widehat{\omega} h,$$

$$\boldsymbol{b}(\widehat{\nu}^2) = (b_1(\widehat{\nu}^2),\ b_2(\widehat{\nu}^2),\ b_3(\widehat{\nu}^2),\ b_4(\widehat{\nu}^2))^{\mathrm{T}},$$

$$\bar{\boldsymbol{b}}(\widehat{\nu}^2) = (\bar{b}_1(\widehat{\nu}^2),\ \bar{b}_2(\widehat{\nu}^2),\ \bar{b}_3(\widehat{\nu}^2),\ \bar{b}_4(\widehat{\nu}^2))^{\mathrm{T}}.$$

Notice that the amplification factor $R(\nu^2, \widehat{\nu}^2)$ satisfies

$$R(\nu^2, \nu^2) = \begin{pmatrix} \cos\nu & \nu^{-1}\sin\nu \\ -\nu\sin\nu & \cos\nu \end{pmatrix}, \tag{54}$$

since the method gives the exact solution for (51) if $\widehat{\nu} = \nu$.

Assuming that the eigenvalues of $R(\nu^2, \widehat{\nu}^2)$, say λ_1 and λ_2, are complex conjugate for small h, then we have

$$|\lambda_1|^2 = |\lambda_2|^2 = \det R(\nu^2, \widehat{\nu}^2)$$

$$\mathrm{Re}(\lambda_1) = \mathrm{Re}(\lambda_2) = \frac{1}{2}\mathrm{trace}\, R(\nu^2, \widehat{\nu}^2).$$

Therefore, the quantities $\phi(\nu^2, \widehat{\nu}^2)$ and $\psi(\nu^2, \widehat{\nu}^2)$ defined by

$$\phi(\nu^2, \widehat{\nu}^2) = 1 - \left\{\det R(\nu^2, \widehat{\nu}^2)\right\}^{1/2}, \tag{55}$$

$$\psi(\nu^2, \widehat{\nu}^2) = \nu - \arccos\left(\frac{\mathrm{trace}\, R(\nu^2, \widehat{\nu}^2)}{2\left\{\det R(\nu^2, \widehat{\nu}^2)\right\}^{1/2}}\right) \tag{56}$$

denote the amplification and phase errors, respectively. According to van der Houwen and Sommeijer [8] we define the orders of these two errors:

DEFINITION 4.1. For TRKN41, assuming $0 \le \widehat{\nu}/\nu < \infty$, if $\phi(\nu^2, \widehat{\nu}^2) = O(h^{q+1})$ and $\psi(\nu^2, \widehat{\nu}^2) = O(h^{r+1})$, then the method is said to be *dissipative of order q* and *dispersive of order r*.

We will analyze these two orders. Let us denote $R(\nu^2, \widehat{\nu}^2)$ by

$$R(\nu^2, \widehat{\nu}^2) = P - \nu^2 Q(\nu^2, \widehat{\nu}^2), \tag{57}$$

where

$$Q(\nu^2, \widehat{\nu}^2) = \begin{pmatrix} \overline{b}^{\mathrm{T}}(\widehat{\nu}^2) \\ b^{\mathrm{T}}(\widehat{\nu}^2) \end{pmatrix} \left(I + \nu^2 A(\widehat{\nu}^2)\right)^{-1} V$$

Then q_{ij}, the ijth element of $Q(\nu^2, \widehat{\nu}^2)$, is given by

$$\begin{aligned} q_{11} &= \overline{b}_1 + \overline{b}_2 \frac{1 - \nu^2 a_{21}}{1 + \nu^2 a_{22}} + \overline{b}_3 \frac{1 - \nu^2 a_{31}}{1 + \nu^2 a_{33}} + \overline{b}_4 \frac{1 - \nu^2 a_{41}}{1 + \nu^2 a_{44}} \\ &= \frac{1}{2} - \frac{\omega^2}{24}h^2 + \frac{\omega^2\left(80\alpha(\omega^2 - \widehat{\omega}^2) + 5\omega^2 - 2\widehat{\omega}^2\right)}{2160}h^4 + O(h^6), \end{aligned} \tag{58}$$

$$q_{12} = \frac{\overline{b}_2 c_2}{1 + \nu^2 a_{22}} + \frac{\overline{b}_3 c_3}{1 + \nu^2 a_{33}} + \frac{\overline{b}_4 c_4}{1 + \nu^2 a_{44}}$$

$$= \frac{1}{6} + \frac{-5\omega^2(24\alpha+5) + 2\widehat{\omega}^2(60\alpha-1)}{3240}h^2 \tag{59}$$
$$+ \frac{35\omega^4(600\alpha+17) - 70\omega^2\widehat{\omega}^2(294\alpha+5) - 2\widehat{\omega}^4(210\alpha+1)}{1224720}h^4 + O(h^6),$$

$$q_{21} = b_1 + b_2\frac{1-\nu^2 a_{21}}{1+\nu^2 a_{22}} + b_3\frac{1-\nu^2 a_{31}}{1+\nu^2 a_{33}} + b_4\frac{1-\nu^2 a_{41}}{1+\nu^2 a_{44}}$$
$$= 1 - \frac{\omega^2}{6}h^2 + \frac{\omega^2(55\omega^2 - 28\widehat{\omega}^2)}{3240}h^4 + O(h^6), \tag{60}$$

$$q_{22} = \frac{b_2 c_2}{1+\nu^2 a_{22}} + \frac{b_3 c_3}{1+\nu^2 a_{33}} + \frac{b_4 c_4}{1+\nu^2 a_{44}}$$
$$= \frac{1}{2} - \frac{\omega^2}{24}h^2 + \frac{\omega^2(95\omega^2 - 68\widehat{\omega}^2)}{19440}h^4 + O(h^6). \tag{61}$$

Using from (57) to (61), we have

$$1 - \det R(\nu^2, \widehat{\nu}^2) = (q_{11} + q_{22} - q_{21})\nu^2 - (q_{11}q_{22} - q_{21}q_{12})\nu^4$$
$$= \frac{1}{12}\omega^4 h^4 + \frac{(360\alpha(\omega^2 - \widehat{\omega}^2) - 95\omega^2 + 41\widehat{\omega}^2)}{9720}\omega^4 h^6$$
$$- \frac{1}{12}\omega^4 h^4 - \frac{60\alpha(\omega^2 - \widehat{\omega}^2) - 10\omega^2 + \widehat{\omega}^2}{1620}\omega^4 h^6 + O(h^8),$$
$$= \frac{7}{1944}\left\{\left(\frac{\widehat{\omega}}{\omega}\right)^2 - 1\right\}\omega^6 h^6 + O(h^8), \tag{62}$$

which leads to that

$$1 - \left\{\det R(\nu^2, \widehat{\nu}^2)\right\}^{1/2} = \frac{7}{3888}(\kappa^2 - 1)\omega^6 h^6 + O(h^8), \tag{63}$$

where we set $\kappa = \widehat{\omega}/\omega$. Thus we have proved the following theorem:

THEOREM 4.2. *TRKN41 with the coefficients evaluated at $\widehat{\omega}$ is dissipative of order 5, if $\widehat{\omega} \neq \omega$.*

Next we consider the phase error of the numerical solution by TRKN41 method. At first we set

$$\cos\overline{\nu} = \frac{\frac{1}{2}\mathrm{trace}R(\nu^2, \widehat{\nu}^2)}{\left\{\det R(\nu^2, \widehat{\nu}^2)\right\}^{1/2}}.$$

Using from (57) to (61), we have

$$\frac{1}{2}\mathrm{trace}R(\nu^2, \widehat{\nu}^2) = 1 - \frac{1}{2}\nu^2(q_{11} + q_{22})$$
$$= 1 - \frac{1}{2}\omega^2 h^2 + \frac{1}{24}\omega^4 h^4$$
$$- \frac{1}{19440}\left\{360\alpha(1-\kappa^2) + 70 - 43\kappa^2\right\}\omega^6 h^6 + O(h^8), \tag{64}$$

and using this and (63), we have

$$\cos\overline{\nu} = 1 - \frac{1}{2}\omega^2h^2 + \frac{1}{24}\omega^4h^4 - \frac{120\alpha(1-\kappa^2)+35-26\kappa^2}{6480}\omega^6h^6 + O(h^8), \quad (65)$$

which leads to that

$$\cos\nu - \cos\overline{\nu} = \frac{1}{3240}(60\alpha+13)(1-\kappa^2)\omega^6h^6 + O(h^8). \quad (66)$$

Taking into account the expansion

$$\nu - \overline{\nu} = -\frac{1}{\sin\nu}(\cos\nu - \cos\overline{\nu}) + \frac{\cos\nu}{2\sin^3\nu}(\cos\nu - \cos\overline{\nu})^2 + \cdots, \quad (67)$$

we have

$$\psi(\nu^2, \widehat{\nu}^2) = -\frac{1}{3240}(60\alpha+13)(1-\kappa^2)\omega^5h^5 + O(h^7). \quad (68)$$

In this expression, if $\alpha = -13/60$ the order of $\psi(\nu^2, \widehat{\nu}^2)$ is improved by 2, and then the result, which is derived by tedious manipulation, is given by

$$\psi(\nu^2, \widehat{\nu}^2) = \frac{1}{272160}(296 - 103\kappa^2)(1-\kappa^2)\omega^7h^7 + (h^9). \quad (69)$$

Thus we have proved the following theorem:

THEOREM 4.3. *TRKN41 with the coefficients evaluated at $\widehat{\omega}$ is dispersive of order 4 and 6, if $\alpha \neq -13/60$ and $\alpha = -13/60$, respectively.*

Example 4.1. Let us consider the equation

$$y'' = -(1 + 0.01y^2)y + 0.01\cos^3 t, \quad (70)$$

$$y(0) = 1, \qquad y'(0) = 0,$$

Table 4. Errors E of TRKN41 with $\alpha = 0$ and $\alpha = -13/60$.

	$\alpha = 0$	$\alpha = -13/60$
$-\log_2(h/\pi)$	E ($\log_2\|E\|$)	E ($\log_2\|E\|$)
2	-1.87e-02(-5.74)	1.07e-02(-6.54)
3	-1.54e-03(-9.35)	3.15e-04(-11.6)
4	-1.07e-04(-13.2)	7.86e-06(-17.0)
5	-7.01e-06(-17.1)	1.46e-07(-22.7)
6	-4.47e-07(-21.1)	-1.05e-09(-29.8)
7	-2.82e-08(-25.1)	-3.70e-10(-31.3)
8	-1.77e-09(-29.1)	-3.24e-11(-34.8)
9	-1.11e-10(-33.1)	-2.28e-12(-38.7)
10	-6.96e-12(-37.1)	-1.62e-13(-42.5)

$E := y_n - y(t_n)$, where $t_n = nh = 8.25\pi$

where the exact solution is $y(t) = \cos t$. Here we integrate the equation from $t = 0$ to $t = 8.25\pi$ by TRKN41 with $\alpha = 0$ and $\alpha = -13/60$, and evaluate the algebraic errors, since it seems to be difficult to detect the dispersive order from numerical experiments (see [8] and [9]). The algebraic errors evaluated at the point $t = 8.25\pi$ for varying stepsize $h = \pi/2^i$ $(i = 2, \ldots, 10)$ are shown in Table 4.

As mentioned above, although all the values in Table 4 are not the phase errors but the algebraic errors, we can easily find that the higher dispersive order method, the method with $\alpha = -13/60$, gives more accurate results than does the lower order dispersive method; the observed convergence rate of the algebraic error of the higher dispersive order method is initially almost $O(h^6)$.

5. Fixed Coefficient Implementation of TRKN41

If TRKN41 is implemented as a variable stepsize mode, then we must re-evaluate the coefficients once the stepsize has been changed. This leads to a considerable amount of work, if the stepsize is changed frequently. In order to avoid this re-evaluation, we could fix the values of the coefficients, even if the stepsize has been changed; we will refer to this implementation as "fixed coefficient mode." It should be noticed that in this mode, although trigonometric conditions (5) is invalid, condition (26) is still valid, since the latter condition does not include the stepsize h explicitly. Note also that this condition is the order condition for conventional Runge-Kutta-Nyström methods to have order 2 [3]. Therefore if the method is implemented in this mode, then the method is not trigonometric but has order of accuracy 2. Here we will consider in detail the fixed coefficient mode.

Let us assume that the coefficients of TRKN41 are evaluated at fixed $\widehat{\nu}$, say $\widehat{\nu}_0$. Here we denote by $T_n(\widehat{\nu}_0{}^2)$ the local truncation error at $t = t_{n+1}$ in this mode, i.e.,

$$T_n(\widehat{\nu}_0{}^2) := (y(t_{n+1}) - y_{n+1}, y'(t_{n+1}) - y'_{n+1})^{\mathrm{T}},$$

where $y_n = y(t_n)$ and $y'_n = y'(t_n)$ are assumed. If we expand $T_n(\widehat{\nu}_0{}^2)$ into the power series in h such as

$$T_n(\widehat{\nu}_0{}^2) = t_0^{(n)}(\widehat{\nu}_0^2) + t_1^{(n)}(\widehat{\nu}_0^2)h + t_2^{(n)}(\widehat{\nu}_0^2)h^2 + \cdots, \tag{71}$$

then the coefficients $t_i^{(n)}(\widehat{\nu}_0^2)$ $(i = 0, 1, \ldots)$ must satisfy

$$t_0^{(n)}(\widehat{\nu}_0^2) = t_1^{(n)}(\widehat{\nu}_0^2) = t_2^{(n)}(\widehat{\nu}_0^2) = 0, \quad \text{for all } \widehat{\nu}_0^2 \geq 0$$

and

$$t_3^{(n)}(\widehat{\nu}_0^2) = t_4^{(n)}(\widehat{\nu}_0^2) = O(\widehat{\nu}_0^2), \quad \widehat{\nu}_0^2 \to 0,$$

since, the method is effectively of algebraic order 4, if the method is implemented as "variable coefficient mode." The above result shows that although the order of accuracy of the method in the fixed coefficient mode is, in general, 2, it becomes 4 only when the coefficients are evaluated at $\widehat{\nu}_0 = 0$. Therefore, $\widehat{\omega} = 0$ is the best choice for the cases that the exact frequencies are unknown or the solutions are not periodic; if we take $\widehat{\omega} = 0$ then $\widehat{\nu}$ is always 0 for any stepsize h so that the re-evaluation of the coefficients is unnecessary, even in the case of variable coefficient mode.

In each of the power series expansions given by from (30) to (46), if we take the first term as the value of the coefficient corresponding to $\widehat{\nu} = 0$, then the Butcher array of the method corresponding to $\widehat{\omega} = 0$ is given by

$$\begin{array}{c|cccc}
0 & 0 & & & \\
1/3 & 1/27 & 1/54 & & \\
2/3 & 4/27 & & 2/27 & \\
1 & 1/3 & & & 1/6 \\
\hline
 & -\alpha + 1/8 & 3\alpha + 1/4 & -3\alpha + 1/8 & \alpha \\
\hline
 & 1/8 & 3/8 & 3/8 & 1/8
\end{array} .$$

This method is shown to be of order 4 also by the order condition derived from SN-trees [3].

Example 5.1. Let us consider again the two-body problem (49). Here we solve the problem with $e = 0$ for the following five cases:

1. Fixed coefficient mode:
   - $\widehat{\nu} = 0$ ($\widehat{\omega} = 0$)
   - $\widehat{\nu} = 0.125$
   - $\widehat{\nu} = 0.25$

Table 5. Errors of TRKN41 for the two-body problem (49) with $e = 0$.

$\log_2 h$	$\log_2 E$				
	$\widehat{\nu} = 0$	$\widehat{\nu} = 0.125$	$\widehat{\nu} = 0.25$	$\widehat{\nu} = h$	$\widehat{\nu} = 2h$
-2.00	-7.90	-8.31	-45.8	-45.8	-6.27
-3.00	-12.3	-45.9	-10.7	-45.9	-10.7
-4.00	-16.5	-14.9	-12.6	-44.5	-14.9
-5.00	-20.6	-16.7	-14.7	-43.4	-19.1
-6.00	-24.7	-18.7	-16.7	-44.4	-23.1
-7.00	-28.8	-20.8	-18.7	-44.8	-27.2
-8.00	-32.8	-22.8	-20.8	-41.8	-31.2
-9.00	-36.8	-24.8	-22.8	-41.5	-35.2

$E := \max_{0 \le nh \le 20}(|y_{1,n} - y_1(nh)| + |y_{2,n} - y_2(nh)|)$

2. Variable coefficient mode:
   - $\widehat{\nu} = h$ $(\widehat{\omega} = 1)$
   - $\widehat{\nu} = 2h$ $(\widehat{\omega} = 2)$

The errors for these two modes are shown in Table 5.

We can easily find from the table that the errors in the fixed coefficient mode behave like $O(h^4)$ only for the case $\widehat{\nu} = 0$.

6. Conclusion

In this paper we have proposed the implicit Runge-Kutta-Nyström method with variable coefficients for solving the periodic initial value problem. The method always gives the exact solution of the problem, when the solution consists of a single Fourier component with known frequency. Moreover, for the method we have analysed the errors in phase and amplitude. Finally we have investigated two types of implementations: the fixed coefficient and variable coefficient implementations. The order of accuracy of our method is 4 for the cases that the exact frequency is unknown, and for the cases that the coefficients of the method are evaluated at $\nu = 0$ and remain fixed. Higher trigonometric order Runge-Kutta-Nyström methods and the stepsize control strategy for the present method will be treated in future reports.

Acknowledgment. The author is very grateful to two anonymous referees, whose comments greatly improved this paper. He is also grateful to Dr. S. Yamada for his valuable comment.

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