TrigonometricRunge－Kutta－Nyström Method for Solving Periodic Initial Value Problems<br>小澤一文（東北大学情報処理教育センター）${ }^{1}$

## 1 Introduction

A number of numerical methods for the solution of periodic initial value 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 it will be advantageous to take it as a priori knowledge for the solution of the problem．

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 the 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 method is shown to be of（algebraic）order 4.

## 2 Runge－Kutta－Nyström Method and Trigonometric Order

Let us consider the second－order initial value problem of the type

$$
\begin{equation*}
y^{\prime \prime}=f(t, y), \quad y\left(t_{0}\right)=\zeta, \quad y^{\prime}\left(t_{0}\right)=\eta . \tag{1}
\end{equation*}
$$

For solving equation（1），instead of applying conventional Runge－Kutta or linear multi－ step methods to the equivalent 1st－order system，which has the dimension twice that of equation（1），the direct application of Runge－Kutta－Nyström methods 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

$$
\begin{align*}
& y_{n+1}=y_{n}+h y_{n}^{\prime}+h^{2} \sum_{j=1}^{s} \bar{b}_{j} f\left(t_{n}+c_{j} h, Y_{j}\right),  \tag{2}\\
& y_{n+1}^{\prime}=y_{n}^{\prime}+h \sum_{j=1}^{s} \dot{b}_{j} f\left(t_{n}+c_{j} h, Y_{j}\right), \\
& Y_{j}=y_{n}+c_{j} h y_{n}^{\prime}+h^{2} \sum_{k=1}^{s} a_{j k} f\left(t_{n}+c_{k} h, Y_{k}\right), \quad j=1,2, \ldots, s .
\end{align*}
$$

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

[^0]| $c_{1}$ | $a_{11}$ | $a_{12}$ | $\cdots$ | $a_{1 s}$ |
| :---: | :---: | :---: | :---: | :---: |
| $c_{2}$ | $a_{21}$ | $a_{22}$ | $\cdots$ | $a_{2 s}$ |
| $\vdots$ | $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |
| $c_{s}$ | $a_{s 1}$ | $a_{s 2}$ | $\cdots$ | $a_{s s}$ |
|  | $\bar{b}_{1}$ | $\bar{b}_{2}$ | $\cdots$ | $\bar{b}_{s}$ |
|  | $b_{1}$ | $b_{2}$ | $\cdots$ | $b_{s}$ |

Fig.1. Butcher array of Runge-Kutta-Nyström method (2).
The order of the Runge-Kutta-Nyström method is defined to be $p=\min \left\{p_{1}, p_{2}\right\}$ for the integers $p_{1}$ and $p_{2}$ satisfying

$$
\begin{equation*}
y\left(t_{n+1}\right)-y_{n+1}=O\left(h^{p_{1}+1}\right), \quad y^{\prime}\left(t_{n+1}\right)-y_{n+1}^{\prime}=O\left(h^{p_{2}+1}\right) \tag{3}
\end{equation*}
$$

where $y_{n+1}$ and $y_{n+1}^{\prime}$ are the numerical solutions given by the method under the conditions that $y_{n}=y\left(t_{n}\right)$ and $y_{n}^{\prime}=y^{\prime}\left(t_{n}\right)$. The order condition for the Runge-Kutta-Nyström method has been thoroughly studied by Hairer, Nørsett and Wanner[2].

Although we would, in general, expect that the higher the order of the method the greater the accuracy, it is not necessarily sufficient to use higher order formulae, if the solution of the problem is oscillatory. For such problems, it is particularly 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

$$
\begin{equation*}
\sum_{j=0}^{k} \alpha_{j} y_{j}=h \sum_{j=0}^{k} \beta_{j} f_{j} \tag{4}
\end{equation*}
$$

for solving the first order equation $y^{\prime}=f(t, y)$. If the difference operator

$$
\begin{equation*}
L[y(t) ; h]:=\sum_{j=0}^{k}\left\{\alpha_{j} y(t+j h)-h \beta_{j} y^{\prime}(t+j h)\right\} \tag{5}
\end{equation*}
$$

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

$$
\begin{gathered}
L[\cos (q \omega t) ; h]=L[\sin (q \omega t) ; h]=0, \quad q=1, \ldots, r \\
L[\cos ((r+1) \omega t) ; h] \neq 0, \quad L[\sin ((r+1) \omega t) ; h] \neq 0
\end{gathered}
$$

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

Definition 1. Runge-Kutta-Nyström method (2) is said to be of trigonometric order $\mu$ relative to the frequency $\omega$, if all the relations

$$
\left\{\begin{array}{l}
y\left(t+c_{j} h\right)=y(t)+c_{j} h y^{\prime}(t)+h^{2} \sum_{k=1}^{s} a_{j k} y^{\prime \prime}\left(t+c_{k} h\right), \quad j=1, \ldots, s+1  \tag{6}\\
y^{\prime}(t+h)=y^{\prime}(t)+h \sum_{k=1}^{s} b_{k} y^{\prime \prime}\left(t+c_{k} h\right)
\end{array}\right.
$$

are satisfied by the functions $y(t)=\cos (m \omega t)$ and $\sin (m \omega t)(m=1, \ldots, \mu)$, 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 $\geq 1$, we will say that the Runge-Kutta-Nyström method is trigonometric.

For the coefficients of trigonometric Runge-Kutta-Nyström methods we have the following lemma:

Lemma 2. Let us assume that the coefficients $a_{j k}$ 's of trigonometric Runge-KuttaNyström methods, which are functions of $\nu=\omega$, are determined to be analytic at $\nu=0$ for given $c_{j}$ 's. Then the coefficients $a_{j k}$ 's satisfy the relation

$$
\begin{equation*}
\sum_{k=1}^{s} a_{j k}=\frac{1}{2} c_{j}^{2}+O\left(h^{2}\right), \quad j=1,2, \ldots, s \tag{7}
\end{equation*}
$$

Proof. Since $a_{j k}$ is assumed to be analytic at $\nu=0$, it has the power series expansion of the form

$$
a_{j k}=a_{j k}^{(0)}+a_{j k}^{(1)} \nu+a_{j k}^{(2)} \nu^{2}+\cdots
$$

Using the expansion, we have

$$
\begin{equation*}
\frac{1-\cos \left(c_{j} \nu\right)}{\nu^{2}}=\sum_{m=0}^{\infty} \sum_{k=1}^{s} a_{j k}^{(m)} \nu^{m} \cos \left(c_{k} \nu\right) \tag{8}
\end{equation*}
$$

since the relation

$$
\begin{equation*}
y\left(t+c_{j} h\right)=y(t)+c_{j} h y^{\prime}(t)+h^{2} \sum_{k=1}^{s} a_{j k} y^{\prime \prime}\left(t+c_{k} h\right), \quad j=1, \ldots, s \tag{9}
\end{equation*}
$$

holds when $y(t)=\cos (\omega t)$. By equating the coefficients of the same power of $\nu$ on both sides of (8), we have for $j=1,2, \ldots, s$

$$
\sum_{k=1}^{s} a_{j k}^{(0)}=\frac{1}{2} c_{j}^{2}, \quad \sum_{k=1}^{s} a_{j k}^{(2 m+1)}=0, \quad m=0,1, \ldots
$$

which implies (7).
Here we will call the order defined by (3) algebraic order to distinguish it from the trigonometric order. For the bound on the trigonometric order $\mu$, we have immediately

$$
\begin{equation*}
\mu \leq\lfloor s / 2\rfloor \tag{10}
\end{equation*}
$$

since each of conditions (6) denotes two equations. The bound given by (10) is the one derived by imposing no restrictions on the algebraic order. However, Runge-KuttaNyström methods of algebraic order> 1 are generally recommended for integrating the equation with reasonable accuracy, when the solution is non-periodic. Here we consider the trigonometric Runge-Kutta-Nyström method of algebraic order 2. The condition for the Runge-Kutta-Nyström method to have algebraic order 2 is given by [2]

$$
\begin{equation*}
\sum_{j=1}^{s} b_{j}=1, \quad \sum_{j=1}^{s} \bar{b}_{j}=1 / 2, \quad \sum_{j=1}^{s} b_{j} c_{j}=1 / 2 \tag{11}
\end{equation*}
$$

For the trigonometric Runge-Kutta-Nyström method satisfying (11) we have the following theorem:

Theorem 3. Suppose that an s-stage trigonometric Runge-Kutta-Nyström method satisfies condition (11), which merely ensures that the algebraic order of the method is at least 2, and that the coefficients $a_{j k}$ 's are analytic at $\nu=0$, then the algebraic order of the method is raised up to 4.
Proof. It suffices to prove that the assertion of the theorem is true for any problems whose solutions $y(t)$ are the elements of $\operatorname{span}\left\{1, t, t^{2}, \cos (\omega t), \sin (\omega t)\right\}$, since polynomials of any degree can be approximated by the elements with errors of $O\left(t^{5}\right)$ for small $t$; the monomials $t^{3}$ and $t^{4}$ can be expressed by

$$
\begin{aligned}
t^{3} & =\left(6 / \omega^{2}\right) t-\left(6 / \omega^{3}\right) \sin (\omega t)+O\left(t^{5}\right) \\
t^{4} & =-24 / \omega^{4}+\left(12 / \omega^{2}\right) t^{2}+\left(24 / \omega^{4}\right) \cos (\omega t)+O\left(t^{6}\right)
\end{aligned}
$$

Let us consider the locally exact solution of (1), i.e., the solution satisfying $y_{n}=y\left(t_{n}\right)$ and $y_{n}^{\prime}=y^{\prime}\left(t_{n}\right)$. For the case that $y(t)=t^{2}$, we have

$$
\begin{align*}
Y_{i} & =y_{n}+c_{i} h y_{n}^{\prime}+h^{2} \sum_{k=1}^{s} a_{i k} f\left(t_{n}+c_{k} h, Y_{k}\right) \\
& =y\left(t_{n}+c_{i} h\right)+O\left(h^{4}\right) \tag{12}
\end{align*}
$$

since (7) holds. In addition, for the cases that $y(t)=\cos (\omega t)$ and $\sin (\omega t)$, we have

$$
\begin{align*}
Y_{i} & =y_{n}+c_{i} h y_{n}^{\prime}+h^{2} \sum_{k=1}^{s} a_{i k} f\left(t_{n}+c_{k} h, Y_{k}\right) \\
& =y\left(t_{n}+c_{i} h\right) \tag{13}
\end{align*}
$$

since the method is trigonometric. This relation is of course true for $y(t)=1$ and $t$. Thus for the functions $y(t) \in \operatorname{span}\left\{1, t, t^{2}, \cos (\omega t), \sin (\omega t)\right\}$, we have

$$
\begin{align*}
y_{n+1} & =y_{n}+h y_{n}^{\prime}+h^{2} \sum_{i=1}^{s} \bar{b}_{i} f\left(t_{n}+c_{i} h, Y_{i}\right) \\
& =y_{n}+h y_{n}^{\prime}+h^{2} \sum_{i=1}^{s} \bar{b}_{i} y^{\prime \prime}\left(t_{n}+c_{i} h\right)+O\left(h^{6}\right) \\
& =y\left(t_{n}+h\right)+O\left(h^{6}\right) \tag{14}
\end{align*}
$$

and

$$
\begin{align*}
y_{n+1}^{\prime} & =y_{n}^{\prime}+h \sum_{i=1}^{s} b_{i} f\left(t_{n}+c_{i} h, Y_{i}\right) \\
& =y_{n}^{\prime}+h \sum_{i=1}^{s} b_{i} y^{\prime \prime}\left(t_{n}+c_{i} h\right)+O\left(h^{5}\right) \\
& =y^{\prime}\left(t_{n}+h\right)+O\left(h^{5}\right) \tag{15}
\end{align*}
$$

where we have assumed that $f(t, y)$ satisfies the Lipschitz condition with respect to $y$. Thus the assertion of the theorem holds.

Note that although the trigonometric Runge-Kutta-Nyström method satisfying the condition of Theorem 3 is shown to be of algebraic order 4, the method does not give the exact results for the problems whose solutions are algebraic polynomials of degree 3 or 4; compare the fact that conventional Runge-Kutta or Runge-Kutta-Nyström methods of algebraic order 4 integrate such problems exactly. Using the fact that any sinusoidal functions, i.e., $\cos (\lambda t)$ and $\sin (\lambda t)$, can also be approximated by the elements of $\operatorname{span}\left\{1, t, t^{2}, \cos (\omega t), \sin (\omega t)\right\}$ with errors of $O\left(t^{5}\right)$, we have the following corollary:

Corollary 4. The algebraic order of the trigonometric Runge-Kutta-Nyström method is 4 also for periodic problems with unknown frequencies, if the method satisfies the condition of Theorem 3.

The error analysis in case of unknown frequency is appeared in detail in [4]. Hereafter we will consider the $s$-stage trigonometric Runge-Kutta-Nyström method satisfying condition (11). For such method, the bound for the trigonometric order is given by

$$
\begin{equation*}
\mu \leq\left\lfloor\frac{s-2}{2}\right\rfloor, \tag{16}
\end{equation*}
$$

since two equations for $b_{j}$ are included in (11). This shows that it is necessary $s \geq 4$ to construct a Runge-Kutta-Nyström method of trigonometric order 1. In this paper we will develop an implicit 4-stage Runge-Kutta-Nyström method of trigonometric order 1.

## 3 Runge-Kutta-Nyström Method of Trigonometric Order 1

### 3.1 Implicit 4-stage Runge-Kutta-Nyström Method

If we write down condition (6) for $s=4$ and $\mu=1$, then we have

$$
\left\{\begin{array}{l}
\cos \left(c_{i} \nu\right)-1+\nu^{2} \sum_{j=1}^{4} a_{i j} \cos \left(c_{j} \nu\right)=0,  \tag{17}\\
\sin \left(c_{i} \nu\right)-c_{i} \nu \cos \left(c_{i} \nu\right)+\nu^{2} \sum_{j=1}^{4} a_{i j} \sin \left(c_{j} \nu\right)=0, \quad i=1, \ldots, 4, \\
\cos \nu-1+\nu^{2} \sum_{j=1}^{4} \bar{b}_{j} \cos \left(c_{j} \nu\right)=0, \\
\sin \nu-\nu \cos \nu+\nu^{2} \sum_{j=1}^{4} \bar{b}_{j} \sin \left(c_{j} \nu\right)=0, \\
\sin \nu-\nu \sum_{j=1}^{4} b_{j} \cos \left(c_{j} \nu\right)=0 \\
\cos \nu-1+\nu \sum_{j=1}^{4} b_{j} \sin \left(c_{j} \nu\right)=0
\end{array}\right.
$$

where $\nu=\omega h$. The coefficients $b_{j}$ 's are uniquely determined by conditions (11) and (17), 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

$$
\begin{equation*}
c_{1}=0, c_{2}=1 / 3, c_{3}=2 / 3, c_{4}=1 \tag{18}
\end{equation*}
$$

because our main interest here is not in deriving higher algebraic order methods.
In our case, this choice of $c_{j}$ 's leads to that $a_{1 j}=0(j=1, \ldots, 4)$, and therefore we can reduce the total cost of evaluating stages, since the 1st stage becomes explicit. For other $a_{i j}(i>1)$, on the other hand, there exist only two equations for four unknowns, so that we set $a_{i j}=0$ except for $a_{i 1}$ and $a_{i i}$; this choice of $a_{i j}$ 's enables us to evaluate the second, third and fourth stages in parallel on parallel processors after the evaluation of the first stage.

For $\bar{b}_{j}$ 's, there exist three equations for four unknowns, so that we take $\bar{b}_{4}$ as a free parameter, say $\bar{b}_{4}=\alpha$.

The coefficients derived in this way, which are analytic at $\nu=0$, are shown in [4].

### 3.2 Numerical Experiments

The following examples show the power of the trigonometric Runge-Kutta-Nyström method for periodic or approximately periodic problems.

Example 1. Let us consider the equation

$$
\begin{gather*}
y^{\prime \prime}(t)=-y(t)+\varepsilon \cos t  \tag{19}\\
y(0)=1, \quad y^{\prime}(0)=0
\end{gather*}
$$

whose solution is given by

$$
\begin{equation*}
y(t)=\cos t+0.5 \varepsilon t \sin t \tag{20}
\end{equation*}
$$

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

Table 1. Errors at $t=10$ of the trigonometric Runge-Kutta-Nyström method with $\omega=1$ and $\alpha=0$.

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

The first term on the right-hand side of (20) can be represented exactly by the trigonometric Runge-Kutta-Nyström method for any stepsize $h>0$, but the second term, which is proportional to $\varepsilon$, can never be represented exactly. Therefore, the errors of the method are proportional to $\varepsilon$, as shown in Table 1.

Example 2. Let us consider the well-known two-body problem (see [3] or [6]):

$$
\begin{align*}
& y_{1}^{\prime \prime}=-y_{1} / r^{3}, \quad y_{2}^{\prime \prime}=-y_{2} / r^{3} \\
& r=\sqrt{y_{1}^{2}+y_{2}^{2}} \tag{21}
\end{align*}
$$

$$
y_{1}(0)=1-e, y_{1}^{\prime}(0)=0, y_{2}(0)=0, y_{2}^{\prime}(0)=\sqrt{\frac{1+e}{1-e}}
$$

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

$$
\begin{equation*}
y_{1}(t)=\cos u-e, \quad y_{2}(t)=\sqrt{1-e^{2}} \sin u \tag{22}
\end{equation*}
$$

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 (21) from $t=0$ to 20 for $e=0,0.01,0.1$, and 0.5 , by using the trigonometric Runge-Kutta-Nyström method with $\omega=1$. We evaluate the maximum errors

$$
\max _{0 \leq n h \leq 20}\left(\left|y_{1, n}-y_{1}(n h)\right|+\left|y_{2, n}-y_{2}(n h)\right|\right)
$$

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

Table 2. Maximum errors of the trigonometric Runge-Kutta-Nyström method with $\omega=1$ and $\alpha=0$.

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

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

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

As the tables show, the trigonometric Runge-Kutta-Nyström method 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 trigonometric Runge-Kutta-Nyström method are more accurate than those by the 2-stage Gauss Runge-Kutta.

Example 3. (Coupled pendulum[2]) Let us consider the coupled pendulum of Fig. 2. The kinetic and potential energies of the system are

$$
\begin{aligned}
& T=\frac{m_{1} l_{1}^{2} \dot{\varphi}_{1}{ }^{2}}{2}+\frac{m_{2} l_{2}^{2} \dot{\varphi}_{2}{ }^{2}}{2} \\
& V=-m_{1} l_{1} \cos \varphi_{1}-m_{2} l_{2} \cos \varphi_{2}+\frac{c r^{2}\left(\sin \varphi_{1}-\sin \varphi_{2}\right)^{2}}{2}
\end{aligned}
$$

Using the well-known Lagrange theory, we have the equations of motion of the system

$$
\left\{\begin{array}{l}
\ddot{\varphi}_{1}=-\frac{\sin \varphi_{1}}{l_{1}}-\frac{c r^{2}}{m_{1} l_{1}^{2}}\left(\sin \varphi_{1}-\sin \varphi_{2}\right) \cos \varphi_{1}+f(t)  \tag{23}\\
\ddot{\varphi}_{2}=-\frac{\sin \varphi_{2}}{l_{2}}-\frac{c r^{2}}{m_{2} l_{2}^{2}}\left(\sin \varphi_{2}-\sin \varphi_{1}\right) \cos \varphi_{2}
\end{array}\right.
$$

In our experiment we set

$$
l_{1}=l_{2}=1, m_{1}=1, m_{2}=0.99, c=2, r=0.1
$$

For the parameters above we might expect that the solution of the system is approximately periodic with frequency $\omega=1$, and so that the method with $\omega=1$ is more accurate. We integrate (23) from $t=0$ to $100 \pi$ by the trigonometric Runge-Kutta-Nyström method under the condition that

$$
\varphi_{1}(0)=0, \quad \dot{\varphi}_{1}(0)=0, \quad \varphi_{2}(0)=0, \quad \dot{\varphi}_{2}(0)=0, \quad f(t)=\delta(t)
$$

and calculate numerically the Hamiltonian function $H(=T+V)$, which is ideally constant. For various $\omega$ 's, the maximum deviations $\max _{n}\left|H_{n}-H_{0}\right|$, where $H_{n}$ and $H_{0}$ are the values of $H$ at $t=n h$ and $t=0$, respectively, are shown in Table 4.

Table 4. Maximum deviations of Hamiltonian function.


From this table we can see that the deviation at $\omega=1$ is extremely small, so that we can conclude that the method with $\omega=1$ is most accurate.

## 4 Fixed Coefficient Implementation

If the trigonometric Runge-Kutta-Nyström method 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 must evaluate the coefficients at some $\hat{\nu}$ and fix them, even if the stepsize has been changed; we will refer to this implementation as "fixed coefficient mode." In this case, however, the algebraic order of the method is only 2. Here we will consider in detail the fixed coefficient mode.

Let us assume that the coefficients of the trigonometric Runge-Kutta-Nyström method are evaluated by using some fixed $\hat{\nu}$, say $\hat{\nu}_{0}$. Here we denote by $T_{n}\left(\hat{\nu}_{0}{ }^{2}\right)$ the local truncation error at $t=t_{n+1}$ in this mode, i.e.,

$$
T_{n}\left({\hat{\nu_{0}}}^{2}\right):=\left(y\left(t_{n+1}\right)-y_{n+1}, y^{\prime}\left(t_{n+1}\right)-y_{n+1}^{\prime}\right)^{\mathrm{T}}
$$

where $y_{n}=y\left(t_{n}\right)$ and $y_{n}^{\prime}=y^{\prime}\left(t_{n}\right)$ are assumed. If we expand $T_{n}\left(\hat{\nu}_{0}{ }^{2}\right)$ into the power series in $h$ such as

$$
\begin{equation*}
T_{n}\left(\hat{\nu}_{0}^{2}\right)=t_{0}^{(n)}\left(\hat{\nu}_{0}^{2}\right)+t_{1}^{(n)}\left(\hat{\nu}_{0}^{2}\right) h+t_{2}^{(n)}\left(\hat{\nu}_{0}^{2}\right) h^{2}+\cdots \tag{24}
\end{equation*}
$$

then the coefficients $t_{i}^{(n)}\left(\hat{\nu}_{0}^{2}\right)(i=0,1, \ldots)$ must satisfy the conditions

$$
t_{0}^{(n)}\left(\hat{\nu}_{0}^{2}\right)=t_{1}^{(n)}\left(\hat{\nu}_{0}^{2}\right)=t_{2}^{(n)}\left(\hat{\nu}_{0}^{2}\right)=0, \quad \text { for all } \hat{\nu}_{0}^{2} \geq 0
$$

and

$$
t_{3}^{(n)}\left(\hat{\nu}_{0}^{2}\right)=t_{4}^{(n)}\left(\hat{\nu}_{0}^{2}\right)=O\left(\hat{\nu}_{0}^{2}\right), \quad \hat{\nu}_{0}^{2} \rightarrow 0
$$

since, as is shown in Theorem 3, the method is effectively of algebraic order 4, if the method is implemented as "variable coefficient mode." The above result shows that although the algebraic order of the method in the fixed coefficient mode is, in general, 2, it becomes 4 only when the coefficients are evaluated at $\hat{\nu_{0}}=0$. Therefore, $\hat{\omega}=0$ is the best choice for the cases that the exact frequencies are unknown or the solutions are not periodic; if we take $\hat{\omega}=0$ then $\hat{\nu}$ 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.

The method corresponding to $\hat{\nu}=0$ has the Butcher array given by

| 0 | 0 |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| $1 / 3$ | $1 / 27$ | $1 / 54$ |  |  |
| $2 / 3$ | $4 / 27$ |  | $2 / 27$ |  |
| 1 | $1 / 3$ |  |  | $1 / 6$ |
|  | $-\alpha+1 / 8$ | $3 \alpha+1 / 4$ | $-3 \alpha+1 / 8$ | $\alpha$ |
|  | $1 / 8$ | $3 / 8$ | $3 / 8$ | $1 / 8$ |

Fig.2. Butcher array of the trigonometric Runge-Kutta-Nyström method with $\hat{\omega}=0$.
This method is shown to be of algebraic order 4 also by the order condition derived from SN-trees [2].

Example 4. Let us consider again the two-body problem (21). Here we solve the problem with $e=0$ for the following five cases:

Table 5. Errors of the trigonometric Runge-Kutta-Nyström method for the two-body problem (21) with $e=0$, where $E=\max _{0 \leq n h \leq 20}\left(\left|y_{1, n}-y_{1}(n h)\right|+\left|y_{2, n}-y_{2}(n h)\right|\right)$.

| $\log _{2} h$ | $\log _{2} E$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\hat{\nu}=0$ | $\hat{\nu}=0.125$ | $\hat{\nu}=0.25$ | $\hat{\nu}=h$ | $\hat{\nu}=2 h$ |
| -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 |

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

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