JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

ELSEVIER Journal of Computational and Applied Mathematics 78 (1997) 161–177

A mono-implicit Runge–Kutta–Nyström modification of the Numerov method

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Received 1 March 1996; revised 24 July 1996

Abstract

We present two two-parameter families of fourth-order mono-implicit Runge–Kutta–Nyström methods. Each member of these families can be considered as a modification of the Numerov method. We analyze the stability and periodicity properties of these methods. It is shown that (i) within one of these families there exist A-stable (even L-stable) and P-stable methods, and (ii) in both families there exist methods with a phase lag of order six.

Keywords: Second-order ODEs; Runge–Kutta–Nyström methods; Mono-implicit methods; Stability; Periodicity; Phase lag

AMS classification: 65L05, 65L06, 65L20

1. Introduction

The most popular code for solving problems of the form

$$y'' = f(x,y), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \tag{1.1}$$

is given by the Numerov method

$$y_{k+2} - 2y_{k+1} + y_k = \frac{h^2}{12}(f_{k+2} + 10 f_{k+1} + f_k), \tag{1.2}$$

where $f_i = f(x_i, y_i)$. This method is of fourth order, its phase lag is of fourth order and the interval of periodicity is $(0, H_p^2) = (0, 6)$. In the last decades, several authors (see [1–4, 6, 9, 11, 13–16, 18] for example) considered modifications of the Numerov method (making it an explicit method, a hybrid method or using exponential fitting for instance) to raise the order, to extend the interval of periodicity or to make the phase lag of the newly constructed method smaller.

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PII S0377-0427(96)00139-2

In this paper, we present two two-parameter families $M_{23}(t,s)$ and $M_{32}(t,s)$ of four-stage Runge–Kutta–Nyström (RKN) methods for which each member satisfies the following requirements:

(i) it can be regarded as a modification of Numerov's method,

(ii) its order is at least four,

(iii) it is a mono-implicit (or singly implicit [3]) RKN (MIRKN) method, i.e., the method contains only one implicit stage, and

(iv) the method only involves function evaluations at points $x = x_0 + nh$, $n = 0, 1, \ldots$

The last two requirements can be motivated as follows. In [17], it was shown that there exist L-stable MIRK methods with four stages of order four for solving first-order initial value problems of the form

$$y' = f(x, y), \qquad y(x_0) = y_0,$$

where the c-vector of the RK method is given by $c = (0, 1, 2, 3)^{\mathrm{T}}$. In the present paper, we want to investigate the stability properties of the RKN methods of this form.

The general form of an s-stage RKN method is

$$y_{k+1} = y_k + hy'_k + h^2 \sum_{i=1}^{s} \bar{b}_i f(x_k + c_i h, Y_i),$$

$$y'_{k+1} = y'_k + h \sum_{i=1}^{s} b_i f(x_k + c_i h, Y_i),$$

whereby

$$Y_i = y_k + c_i h y'_k + h^2 \sum_{j=1}^{s} a_{ij} f(x_k + c_j h, Y_j), \quad i = 1, 2 \ldots, s.$$

Clearly, a RKN method is a one-step method that provides approximate values for the unknown solution y and its first derivative y'. As is the case for RK methods, these methods can be presented in a more compact way as

$$\begin{array}{c|c} c & A \\ \hline & \bar{b}^{\mathrm{T}} \\ & b^{\mathrm{T}} \end{array}$$

In general, a RKN method involves the solution of a system of nonlinear equations. The dimension of this system is s times the dimension of the problem (1.1). We however consider MIRKN methods. This means that in each step, the dimension of the system of nonlinear equations to be solved is reduced to the dimension of the problem (1.1), as is the case for the Numerov method itself.

2. Two two-parameter families of MIRKN methods

We consider the following identities:

$$y(x+v) - y(x) = vy'(x) + \int_x^{x+v} (x+v-t)y''(t)\,\mathrm{d}t, \tag{2.1}$$

$$y'(x+v) - y'(x) = \int_x^{x+v} y''(t)\,\mathrm{d}t. \tag{2.2}$$

In these identities, we use $x = x_k$ and $v = h$ and we approximate $y''(x) = f(x,y)$ by the unique polynomial of degree q that interpolates $f(x,y)$ at $x_k, x_{k+1}, \ldots, x_{k+q}$. Using $q = 2$ in (2.1) and $q = 3$ in (2.2), we obtain

$$y_{k+1} = y_k + hy'_k + h^2(\tfrac{7}{24}f_k + \tfrac{1}{4}f_{k+1} - \tfrac{1}{24}f_{k+2}), \tag{2.3}$$

$$y'_{k+1} = y'_k + h(\tfrac{3}{8}f_k + \tfrac{19}{24}f_{k+1} - \tfrac{5}{24}f_{k+2} + \tfrac{1}{24}f_{k+3}). \tag{2.4}$$

Eliminating the y' from (2.3) and (2.4), one obtains the Numerov method (1.2), so (2.3) and (2.4) are suited to build modified Numerov schemes upon.

Our idea is to use these equations as parts of a RKN method, i.e., we propose RKN methods which have the following structure:

$$\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1 & \frac{7}{24} & \frac{1}{4} & -\frac{1}{24} & 0 \\
2 & a_{31} & a_{32} & a_{33} & a_{34} \\
3 & a_{41} & a_{42} & a_{43} & a_{44} \\
\hline
 & \frac{7}{24} & \frac{1}{4} & -\frac{1}{24} & 0 \\
 & \frac{3}{8} & \frac{19}{24} & -\frac{5}{24} & \frac{1}{24}
\end{array} \tag{2.5}$$

Further, our aim is to construct MIRKN methods, i.e., methods which contain only one implicit stage. This clearly requires $a_{33} = 0 = a_{44}$ and either $a_{34} = 0$ or $a_{43} = 0$. We will consider both cases, giving rise to two different classes of methods.

In each case, the five remaining parameters are chosen in such a way that the resulting RKN method is of order four, as is the case for the Numerov method. We recall [7] that a RKN method is of order p if

$$\begin{aligned} y(x_0+h) - y_1 &= \mathcal{O}(h^{p+1}), \\ y'(x_0+h) - y'_1 &= \mathcal{O}(h^{p+1}). \end{aligned} \tag{2.6}$$

In order to have order p, the so-called order conditions [5, 7, 8] have to be fulfilled by the coefficients in (2.5). These conditions are:

$p=1$	$b^{\mathrm{T}}\cdot e=1$	
$p=2$	$b^{\mathrm{T}}\cdot c=\frac{1}{2}$	$\bar{b}^{\mathrm{T}}\cdot e=\frac{1}{2}$
$p=3$	$b^{\mathrm{T}}\cdot c^2=\frac{1}{3}$	$\bar{b}^{\mathrm{T}}\cdot c=\frac{1}{6}$
	$b^{\mathrm{T}}\cdot A\cdot e=\frac{1}{6}$	
$p=4$	$b^{\mathrm{T}}\cdot c^3=\frac{1}{4}$	$\bar{b}^{\mathrm{T}}\cdot c^2=\frac{1}{12}$
	$b^{\mathrm{T}}\cdot (cA\cdot e)=\frac{1}{8}$	$\bar{b}^{\mathrm{T}}\cdot A\cdot e=\frac{1}{24}$
	$b^{\mathrm{T}}\cdot A\cdot c=\frac{1}{24}$	

Hereby $c^q=(c_1^q,c_2^q,\ldots,c_s^q)^{\mathrm{T}}$ and $e=(1,1,\ldots,1)^{\mathrm{T}}$.

The number of equations to be solved can however be reduced by imposing the condition $C(r)$:

$$C(r):\ A\cdot c^q=\frac{c^{q+2}}{(q+2)(q+1)},\quad q=0,1,2,\ldots,r. \tag{2.7}$$

This condition ensures that the order of the internal stages is at least $r+2$, i.e.,

$$Y_i=y(x_k+c_ih)+\mathcal{O}(h^{r+3}),\quad i=1,2,\ldots,s.$$

In case the c-vector contains positive integers, then this means that approximations are available at these knot-points (which may be overwritten in subsequent steps).

Case I: $M_{23}(t,s)$. Starting from (2.5) with $a_{34}=0$, one finds the following two-parameter family $M_{23}(t,s)$:

0	0	0	0	0
1	$\frac{7}{24}$	$\frac{1}{4}$	$-\frac{1}{24}$	0
2	$2-t$	t	0	0
3	$\frac{20}{3}-5t+s$	$-\frac{13}{6}+5t-2s$	s	0
	$\frac{7}{24}$	$\frac{1}{4}$	$-\frac{1}{24}$	0
	$\frac{3}{8}$	$\frac{19}{24}$	$-\frac{5}{24}$	$\frac{1}{24}$

Written down explicitly, these methods read

$$y_{k+1}=y_k+hy_k'+h^2(\tfrac{7}{24}f_k+\tfrac{1}{4}f_{k+1}-\tfrac{1}{24}\hat{f}_{k+2}), \tag{2.8}$$

$$y_{k+1}'=y_k'+h(\tfrac{3}{8}f_k+\tfrac{19}{24}f_{k+1}-\tfrac{5}{24}\hat{f}_{k+2}+\tfrac{1}{24}\hat{f}_{k+3}), \tag{2.9}$$

where $\hat{f}_{k+2} = f(x_{k+2}, \hat{y}_{k+2})$ and $\hat{f}_{k+3} = f(x_{k+3}, \hat{y}_{k+3})$ with

$$\hat{y}_{k+2} = y_k + 2hy'_k + h^2[(2-t)f_k + tf_{k+1}], \tag{2.10}$$

$$\hat{y}_{k+3} = y_k + 3hy'_k + h^2\left[(\tfrac{20}{3} - 5t + s)f_k + (-\tfrac{13}{6} + 5t - 2s)f_{k+1} + s\hat{f}_{k+2}\right].$$

For general t and s, the order of the internal stages is 2, i.e., $C(0)$ is fulfilled. However, for $t = \frac{4}{3}$, the order of the internal stages is raised to 3 and, if in addition $s = \frac{9}{8}$, condition $C(r)$ is fulfilled with $r = 2$. Note that $M_{23}(\frac{4}{3}, \frac{9}{8})$ corresponds to the situation in which $Y_3 = \hat{y}_{k+2}$ and $Y_4 = \hat{y}_{k+3}$ are obtained by putting in (2.1) $x = x_k$, $v = 2h$ and $v = 3h$, resp., and by approximating $y''(x) = f(x, y)$ by the unique polynomials of degree 1 and 2 that interpolate $f(x, y)$ at x_k, x_{k+1} and x_k, x_{k+1}, x_{k+2} respectively.

Case II: $M_{32}(t,s)$. Starting from (2.5) with $a_{43} = 0$, one obtains the two-parameter family $M_{32}(t,s)$:

$$\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1 & \frac{7}{24} & \frac{1}{4} & -\frac{1}{24} & 0 \\
2 & \frac{47}{30} + 2t - \frac{1}{5}s & \frac{13}{30} - 3t + \frac{1}{5}s & 0 & t \\
3 & \frac{9}{2} - s & s & 0 & 0 \\
\hline
 & \frac{7}{24} & \frac{1}{4} & -\frac{1}{24} & 0 \\
 & \frac{3}{8} & \frac{19}{24} & -\frac{5}{24} & \frac{1}{24}
\end{array}$$

The order of the internal stages is two for $s \neq \frac{9}{2}$ and three if $s = \frac{9}{2}$. Stage-order four is however impossible.

Finally, we want to remark that each scheme indeed corresponds to a MIRKN method. For $M_{23}(t,s)$, e.g., after substituting (2.10) into (2.8), one generally obtains a nonlinear equation in y_{k+1}, which can be solved by Newton iteration. Once this value is found, y'_{k+1} can be calculated explicitly from (2.9). One should however notice that for MIRKN methods, the Newton iteration matrix is nonlinear in the Jacobian such that this process becomes more expensive than the Newton iteration of one stage of a diagonal-implicit Runge–Kutta–Nyström method, for which the Newton iteration matrix is linear in the Jacobian.

3. Linear stability analysis

To investigate the stability properties, the scalar test equation

$$y'' + \lambda^2 y = 0 \tag{3.1}$$

is introduced [11, 14, 19]. The application of a RKN method to this problem leads to

$$\begin{pmatrix} y_{k+1} \\ y'_{k+1} \end{pmatrix} = M \begin{pmatrix} y_k \\ y'_k \end{pmatrix},$$

where

$$M = \begin{pmatrix} 1 - H^2\bar{b}^{\mathrm{T}} \cdot (I + H^2A)^{-1} \cdot e & h[1 - H^2\bar{b}^{\mathrm{T}} \cdot (I + H^2A)^{-1} \cdot c] \\ -\lambda H b^{\mathrm{T}} \cdot (I + H^2A)^{-1} \cdot e & 1 - H^2 b^{\mathrm{T}} \cdot (I + H^2A)^{-1} \cdot c \end{pmatrix} \tag{3.2}$$

with $H = \lambda h$. Eliminating y'_k and y'_{k+1}, one obtains the following relation:

$$y_{k+2} - \mathrm{tr}(M) y_{k+1} + \det(M) y_k = 0. \tag{3.3}$$

The characteristic equation associated with (3.3) is

$$r^2 - \mathrm{tr}(M) r + \det(M) = 0. \tag{3.4}$$

Let r_1 and r_2 be the roots of this characteristic equation.

3.1. *Stability*

Definition 3.1. The method (3.3) has an interval of stability $(0, H_s^2)$ if $|r_1| < 1$ and $|r_2| < 1$ or $|r_1| \leqslant 1$ and $|r_2| \leqslant 1$ and the roots on the unit disk are simple for all $H^2 \in (0, H_s^2)$. If the interval of stability is $(0, \infty)$, the method is said to be absolutely stable (A-stable). Moreover if $\lim_{H^2 \to +\infty} r_1 = \lim_{H^2 \to +\infty} r_2 = 0$, then the method is called L-stable [19].

Case I: $M_{23}(t,s)$. From (3.4) if follows that $r_1 r_2 = \det(M)$. Since

$$\det(M) = 1 - \frac{22 - 96s - 21t + 72st}{72(24 + 6H^2 + H^4 t)} H^6, \tag{3.5}$$

it follows that $|\det(M)| < 1$, $\forall H^2 > 0$ iff $-N(H^2) < T(H^2) < N(H^2)$, with $\det(M) = T(H^2)/N(H^2)$. One finds

$$N(H^2) - T(H^2) = (22 - 96s - 21t + 72st) H^6,$$

and

$$N(H^2) + T(H^2) = 3456 + 864H^2 + 144tH^4 - (22 - 96s - 21t + 72st) H^6.$$

If $T(H^2) + N(H^2) > 0$, $\forall H^2 > 0$, then $N(H^2) - T(H^2)$ has a positive real zero so that there exist no A-stable methods.

Case II: $M_{32}(t,s)$. Following the Routh–Hurwitz criterium, one finds $|r_{1,2}| < 1$ iff

$$\det(M) < 1, \qquad \det(M) - \mathrm{tr}(M) > -1, \qquad \det(M) + \mathrm{tr}(M) > -1. \tag{3.6}$$

where

$$\det(M) = 1 - \frac{43 - 14s + 3480t - 1200st}{8(720 + 180H^2 + (13 + 6s - 90t)H^4 - 30stH^6)} H^6.$$

It turns out that the conditions (3.6) are fulfilled for a wide range of (t,s)-pairs. Within these are included two L-stable methods $M_{32}(t_{L_1},s_{L_1})$ and $M_{32}(t_{L_2},s_{L_2})$:

$$\begin{cases} s_{L_1} = \dfrac{175-\sqrt{11\,641}}{28}, \\ t_{L_1} = \dfrac{-329+\sqrt{11\,641}}{27\,600}, \end{cases} \qquad \begin{cases} s_{L_2} = \dfrac{175+\sqrt{11\,641}}{28}, \\ t_{L_2} = \dfrac{-329-\sqrt{11\,641}}{27\,600}. \end{cases}$$

3.2. Periodicity

Definition 3.2. A numerical method has an interval of periodicity $(0,H_p^2)$ if, for all $H^2 \in (0,H_p^2)$, r_1 and r_2 satisfy $r_1 = e^{i\theta(H)}$ and $r_2 = e^{-i\theta(H)}$, where $\theta(H)$ is a real function of H. If the interval of periodicity is $(0,\infty)$, the method is said to be P-stable.

In order to have complex conjugate roots r_1 and r_2 with modulus 1, the necessary and sufficient conditions are given by

$$\det(M)=1 \quad \text{and} \quad D(H^2)=\mathrm{tr}(M)^2-4\det(M)<0.$$

Case I: $M_{23}(t,s)$. It follows from (3.5) and $\det(M)=1$ that $M(t,s)$ only has a nonvanishing interval of periodicity if $t \neq \frac{4}{3}$ and

$$s=\frac{22-21t}{24(4-3t)}. \tag{3.7}$$

In that case $D(H^2)$ is given by

$$D(H^2)=\frac{H^2D_1(H^2)D_2(H^2)}{144(4-3t)^2(24+6H^2+H^4t)^2}, \tag{3.8}$$

with

$$D_1(H^2)=288(3t-4)+48(3t-4)H^2+(6t-5)H^4$$

and

$$D_2(H^2)=1152(4-3t)+48(1-t)(3t-4)H^4+(6t-5)H^6,$$

so that H_p^2 corresponds to the smallest positive real root of $D_1(H^2)D_2(H^2)=0$. For $t \neq \frac{5}{6}$, $D_2(H^2)$ is a cubic function in H^2 which has three real zeros whenever $t \leqslant t_1 \approx 0.8728$ ($s \geqslant s_1 \approx 0.1107$) where t_1 is the unique real root of

$$-1823+8676t-16188t^2+14720t^3-6528t^4+1152t^5=0.$$

For $t>t_1$, $D_2(H^2)$ only has one real zero. This causes a discontinuity for H_p^2 at t_1.

A detailed analysis shows that for every real t there is at least one positive real root of $D(H^2)=0$ and that the following cases have to be considered (see Fig. 1):

(i) for $t \leqslant t_1$, H_p^2 is equal to the smallest positive zero of $D_2(H^2)$. H_p^2 increases as t approaches t_1 and reaches approximately 23.787.

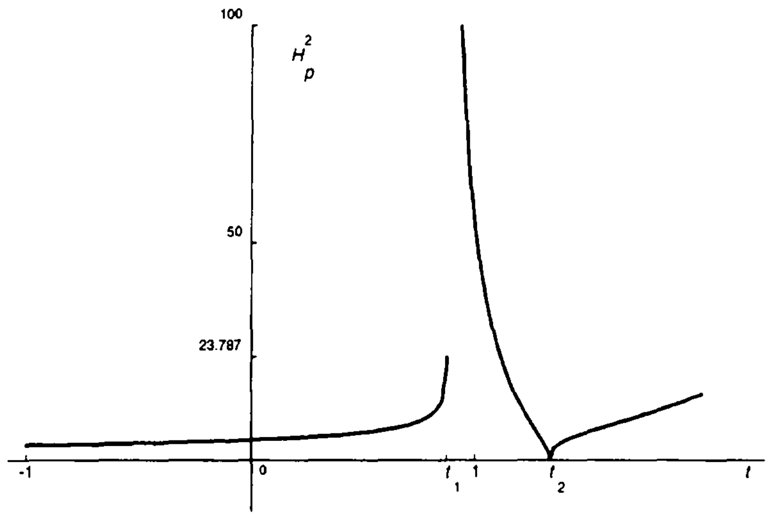

Fig. 1. H_p^2 as a function of t for $M_{23}(t,s)$.

(ii) for $t_1 < t < t_2 = \frac{4}{3}$, H_p^2 is equal to the positive zero of $D_1(H^2)$. In t_1 there is a discontinuity: H_p^2 reaches approximately 286.285 near t_1 and decreases down to 0 as t approaches t_2.

(iii) for $t > t_2$, H_p^2 is equal to the unique real zero of $D_2(H^2)$. H_p^2 turns out to be an approximately linearly increasing function of t.

Case II: $M_{32}(t,s)$. In order to have $\det(M) = 1$ we require $s = \dfrac{43 + 3480t}{2(7 + 600t)}$. We then obtain

$$D(H^2) = \frac{3H^2(7 + 600t)D_1(H^2)D_2(H^2)}{16N^2(H^2)}$$

with

$$N(H^2) = 144(7 + 600t) + 36(7 + 600t)H^2 + 2(22 + 1761t - 5400t^2)H^4 - 3t(43 + 3370t)H^6,$$

$$D_1(H^2) = -192 - 32H^2 + (1 + 144t)H^4,$$

$$D_2(H^2) = 2304(7 + 600t) + 32(1 - 39t - 5400t^2)H^4 + 3(7 + 920t + 30720t^2)H^6.$$

The following cases have to be considered:

(i) for $t < t_1 = -\frac{7}{600}$ (or equivalently $s < s_1 = \frac{29}{10}$), H_p^2 is equal to the smallest positive zero of $D_2(H^2)$ which tends to $\frac{15}{8}$ as $t \to -\infty$ (as $s \xrightarrow{<} s_1$),

(ii) for $t = t_1$ (s undefined), $H_p^2 = 0$,

(iii) for $t_1 < t \leqslant t_2 = -\frac{1}{144}$ ($s \geqslant s_2 = \frac{113}{34}$), the method is P-stable,

(iv) for $t > t_2$ ($s_1 < s < s_2$) H_p^2 is the positive root of $D_1(H^2)$, which tends to zero as $t \to +\infty$ ($s \xrightarrow{>} s_1$).

The endpoint of the interval of periodicity as a function of t, resp. s, is depicted in Figs 2 and 3.

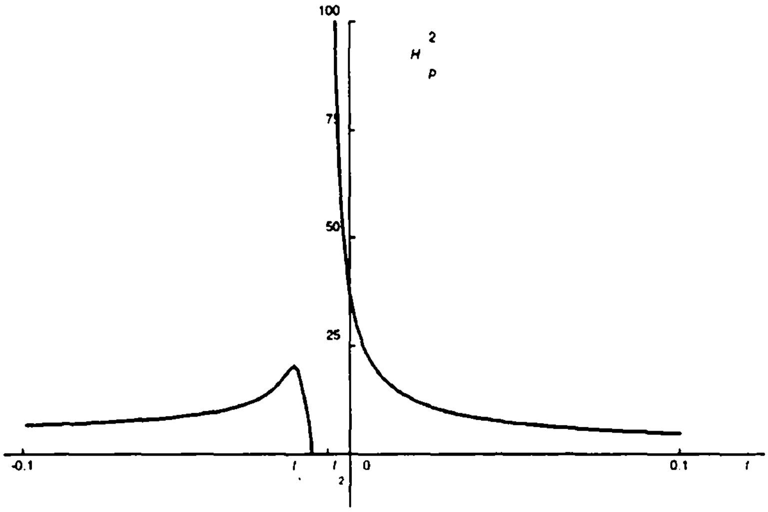

Fig. 2. H_p^2 as a function of t for $M_{32}(t,s)$.

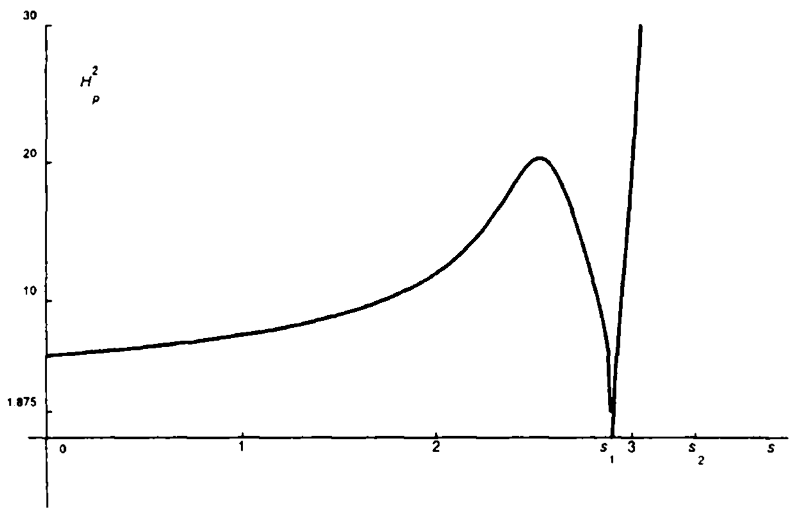

Fig. 3. H_p^2 as a function of s for $M_{32}(t,s)$.

3.3. Phase lag

We consider the case for which there is a nonvanishing interval of periodicity. In that case, the characteristic equation (3.4) becomes

$$r^2 - \mathrm{tr}(M)r + 1 = 0. \tag{3.9}$$

Following [18], we give the next definition.

Table 1
Overview of the stability properties of some members of $M_{23}(t,s)$

t	s	Phase lag	H_p^2
$\frac{1}{2}$	$\frac{23}{120}$	$\frac{11}{20160}H^7$	6.299
$\frac{43}{30}$	$\frac{9}{8}$	$\frac{131}{60480}H^7$	5.234
$t_1 \approx 0.8728$	$s_1 \approx 0.1107$	$-0.945\ 10^{-2}H^5$	$\lim_{t \to t_1^<} H_p^2 = 23.787$; $\lim_{t \to t_1^>} H_p^2 = 286.285$

Definition 3.3. For any method corresponding to the characteristic equation (3.9), the phase lag is defined as the leading term in the expansion of $\phi(H) = H - \theta(H)$. The order of the phase lag is said to be q if $\phi(H) = \mathcal{O}(H^{q-1})$ as $H \to 0$.

Case I: $M_{23}(t,s)$. We find that for $M_{23}(t,s)$ with s given by (3.7), $\phi(H)$ is given by

$$\phi(H) = \frac{(43-30t)(2t-1)}{960(3t-4)}H^5 + \frac{81-290t+168t^2}{16\,128(3t-4)}H^7 + \mathcal{O}(H^9). \tag{3.10}$$

This means that for $t = \frac{1}{2}$ and $t = \frac{43}{30}$ the phase lag is of order six, while for all other t-values the phase lag is of order four. To conclude the discussion of $M_{23}(t,s)$ we present Table 1, which includes all discussed methods.

Case II: $M_{32}(t,s)$. $\phi(H)$ is given by

$$\phi(H) = -\frac{69+7040t+120\,000t^2}{640(7+600t)}H^5 + \frac{1883+211\,944t+4\,717\,440t^2}{96\,768(7+600t)}H^7 + \mathcal{O}(H^9).$$

The phase lag is of order 6 for $(t_{\mathrm{ph}_1}, s_{\mathrm{ph}_1})$ and $(t_{\mathrm{ph}_2}, s_{\mathrm{ph}_2})$, with

$$\begin{cases} t_{\mathrm{ph}_1} = \dfrac{-88-\sqrt{2569}}{3000}, \\ s_{\mathrm{ph}_1} = \dfrac{1477+29\sqrt{2569}}{10(53+\sqrt{2569})}, \end{cases} \qquad \begin{cases} t_{\mathrm{ph}_2} = \dfrac{-88+\sqrt{2569}}{3000}, \\ s_{\mathrm{ph}_2} = \dfrac{-1477+29\sqrt{2569}}{10(-53+\sqrt{2569})}, \end{cases}$$

and $\phi(H)$ takes the value $\phi(H)_{\mathrm{ph}_1}$, resp. $\phi(H)_{\mathrm{ph}_2}$, with

$$\phi(H)_{\mathrm{ph}_1} = \frac{-3\,348\,869 - 67\,513\sqrt{2569}}{60\,480\,000(53+\sqrt{2569})}H^7 + \mathcal{O}(H^9),$$

$$\phi(H)_{\mathrm{ph}_2} = \frac{3\,348\,869 - 67513\sqrt{2569}}{60\,480\,000(-53+\sqrt{2569})}H^7 + \mathcal{O}(H^9).$$

From the leading term of $\phi(H)$, it is clear that P-stable methods $M_{32}(t,s)$ with t very close to $-\frac{7}{600}$ are not to be preferred. This is illustrated in Table 2.

Table 2
Overview of the stability properties of some members of $M_{32}(t,s)$

t	s	Phase lag	H_p^2
t_{ph_1}	s_{ph_1}	$-0.111\cdot10^{-2}\,H^7$	9.260
t_{ph_2}	s_{ph_2}	$0.522\cdot10^{-3}H^7$	6.345
−0.011666666	30000029/10	$-0.125\cdot10^5H^5$	∞
−0.0116	329/10	$-0.136H^5$	∞
−0.01	41/10	$-0.166\cdot10^{-1}H^5$	∞
−1/144	113/34	$-0.143\cdot10^{-1}H^5$	∞

4. Some illustrations

We will illustrate the importance of the phase lag and P-stability of the methods considered by means of four test problems.

4.1. Example 1

We consider the testcase

$$y'' + y = 0, \qquad y(0) = 1, \quad y'(0) = 0 \quad \text{and} \quad x \in [0, 10]. \tag{4.1}$$

Four methods are applied with stepsize $h = \frac{1}{10}$:
(1) $M_{32}(t_{ph_1}, s_{ph_1})$ for which the phase lag is of order 6,
(2) $M_{32}(t_{ph_2}, s_{ph_2})$ for which the phase lag is of order 6,
(3) the P-stable method $M_{32}(-\frac{1}{100}, \frac{41}{10})$,
(4) the Numerov method.
For the Numerov method, it is assumed that y_1 instead of y'_0 is given as input.

In Fig. 4 we plot the absolute errors in y in logarithmic scale. We recall that the first three methods have a local truncation error that starts with a $\mathcal{O}(H^5)$ term. One notices that $M_{32}(t_{ph_1}, s_{ph_1})$ and $M_{32}(t_{ph_2}, s_{ph_2})$ behave better than the Numerov method and the P-stable method since the phase lag of the former methods is smaller. It should also be noted that, although the local truncation error of the Numerov method starts with a $\mathcal{O}(H^6)$ term, for all methods considered the global error is of order four. Table 3 illustrates that one should not choose t very close to $-\frac{7}{600}$ (s then also tends to $+\infty$).

4.2. Example 2

We use the same methods to solve the IVP [4, 10, 19]:

$$\begin{aligned} y'' &= \begin{pmatrix} \mu - 2 & 2\mu - 2 \\ 1 - \mu & 1 - 2\mu \end{pmatrix} y, \qquad x \in [0, 10], \\ y(0) &= \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \qquad y'(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \end{aligned} \tag{4.2}$$

which has the exact solution $y(x) = (2\cos x, -\cos x)^{\mathrm{T}}$ for all real $\mu > 0$.

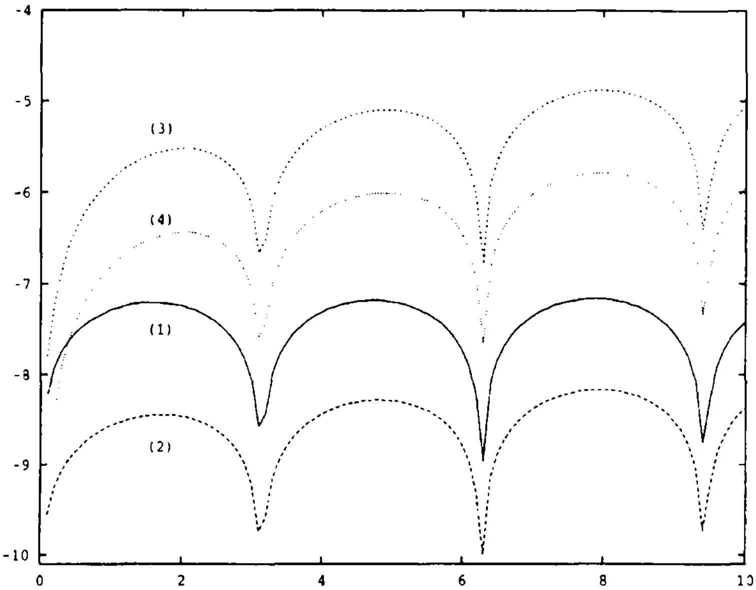

Fig. 4. Absolute errors in y in logarithmic scale for the four methods considered when applied to (4.1) with $h = \frac{1}{10}$.

Table 3
Absolute errors in y at $x=10$ in logarithmic scale for some members of $M_{32}(t,s)$ when applied to (4.1) with $h = \frac{1}{10}$

t	s	$\log \lVert \Delta \rVert_\infty$
t_{ph_1}	s_{ph_1}	−7.41
t_{ph_2}	s_{ph_2}	−8.32
−0.011666666	30 000 029/10	0.16
−0.0116	329/10	−4.09
−0.01	41/10	−5.05
−1/144	113/34	−5.11

The eigenvalues of $\partial f/\partial y$ are given by -1 and $-\mu$, so for large values of μ, methods with a large interval of periodicity are required. In Fig. 5, which presents the maximum norm errors in logarithmic scale for the four methods considered, we use the value $\mu = 2500$ and fixed stepsize $h = \frac{1}{60}\pi$.

We also apply some members of $M_{23}(t,s)$, with s as in (3.7), to the same test case (4.2) with stepsize $h=\frac{1}{60}\pi$. In Table 4 one finds the maximum norm errors at the endpoint $x=10$ in logarithmic scale, together with the endpoint H_p^2 of the interval of periodicity. As expected from Fig. 1, some methods are unstable for the stepsize considered.

4.3. Example 3

As a third example we consider the following stiff linear nonhomogeneous problem of Prothero and Robinson type:

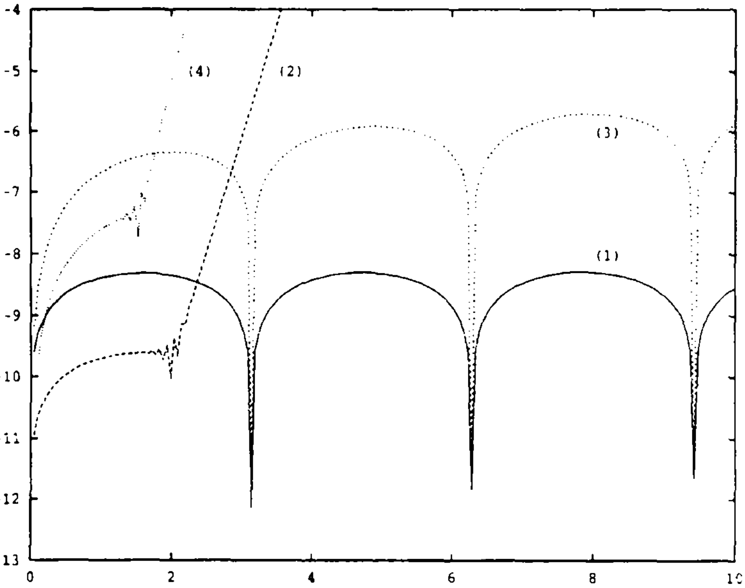

Fig. 5. Maximum-norm errors in y in logarithmic scale for the four methods considered when applied to (4.2) with $h = \frac{1}{60}\pi$.

Table 4
Maximum-norm errors in y in logarithmic scale at $x = 10$ for three members of $M_{23}(t,s)$ when applied to (4.2) with $h = \frac{1}{60}\pi$. For these methods, we also indicate the endpoint of the interval of periodicity

t	H_p^2	$\mu = 1$	$\mu = 1000$	$\mu = 3000$	$\mu = 5000$
0	4.628	−6.04	−6.04	Unstable	Unstable
$\frac{9}{10}$	161.785	−6.08	−6.08	−6.08	−6.08
$\frac{6}{5}$	12.814	−5.68	−5.68	−5.68	Unstable

$$y'' + J(y - g) = g'', \qquad J = \mathrm{diag}(100^{j-1}), \qquad g(x) = (1 + \sin jx), \quad j = 1,\dots,6$$
$$y(0) = g(0), \qquad y'(0) = g'(0), \tag{4.3}$$

which has exact solution $y(x) = g(x)$.

We integrated problem (4.3) with a P-stable method, e.g., $M_{32}(-\frac{1}{96}, \frac{9}{2})$, and fixed steplength from 0 to the endpoint $x_{\mathrm{end}} = 10$.

Due to the linearity of the problem and the diagonal form of the matrix J, it is possible to rewrite the numerical method for the ith equation of the problem considered in the following way:

$$\begin{pmatrix} y_{k+1}^{[i]} \\ y'^{[i]}_{k+1} \end{pmatrix} = M_i \begin{pmatrix} y_k^{[i]} \\ y'^{[i]}_k \end{pmatrix} + \begin{pmatrix} h^2\bar{b}_\bullet^{\mathrm{T}}(I - H_i^2(I + H_i^2A)^{-1} \cdot A) \\ hb_\bullet^{\mathrm{T}}(I - H_i^2(I + H_i^2A)^{-1} \cdot A) \end{pmatrix} (G_k''^{[i]} + J_{ii}G_k^{[i]}),$$

with $H_i^2 = J_{ii}h^2$, M_i as in (3.2) with H replaced by H_i and with

$$G_k^{[i]} = (g^{[i]}(x_k + c_1 h), \ldots, g^{[i]}(x_k + c_s h))^{\mathrm{T}}$$

and

$$G_k''^{[i]} = (g''^{[i]}(x_k + c_1 h), \ldots, g''^{[i]}(x_k + c_s h))^{\mathrm{T}}.$$

A comparison is made with the P-stable fourth-order three-stage method in [12]:

$$\begin{array}{c|ccc}
\frac{2}{3} & \frac{2}{9} & & \\[4pt]
\frac{109+\alpha}{168} & \frac{(\alpha+221)(\alpha-3)}{56448} & \frac{2}{9} & \\[4pt]
\frac{28}{109+\alpha} & -\frac{2(67+\alpha)\gamma}{9(109+\alpha)^3(\alpha-3)} & -\frac{196(67+\alpha)\beta}{9(109+\alpha)^3(\alpha-3)} & \frac{2}{9} \\[4pt]
\hline
 & \frac{\alpha^2+50\alpha-1727}{4(\alpha-3)(67+\alpha)} & -\frac{784(\alpha-59)}{(\alpha-3)\beta} & \frac{(81+\alpha)(109+\alpha)^2}{4(67+\alpha)\beta} \\[4pt]
 & \frac{3(\alpha^2+50\alpha-1727)}{4(\alpha-3)(67+\alpha)} & \frac{131712}{(\alpha-3)\beta} & \frac{(109+\alpha)^3}{4(67+\alpha)\beta}
\end{array} \tag{4.4}$$

where $\alpha = 2473^{0.5}$, $\beta = \alpha^2 + 218\alpha + 7177$ and $\gamma = \alpha^3 + 159\alpha^2 - 5685\alpha - 752\,723$.

In Fig. 6 the errors $\max_{i=1,\ldots,6}(|y^{[i]}(x_k) - y_k^{[i]}|, |y'^{[i]}(x_k) - y_k'^{[i]}|)$ are displayed in logarithmic-norm for different values of h at $x = \frac{1}{100}k$, $k = 1, \ldots, 1000$. The upper figure corresponds to the P-stable method $M_{32}(-\frac{1}{96}, \frac{9}{2})$, the lower one to the P-stable method (4.4). In both cases, one can detect the periodicity. However, in the lower figure this periodic behaviour is much more disturbed. For the P-stable method $M_{32}(-\frac{1}{96}, \frac{9}{2})$, the error displayed corresponds to the component $y'^{[6]}$ due to the large values in the stiffness matrix J. Indeed, we found that the errors in $y^{[i]}$ and $y'^{[i]}$ increase as i increases. This phenomenon is not so significant for the other method, such that it is not always the error in $y'^{[6]}$ that is displayed.

4.4. Example 4

We consider the nonlinear problem of Prothero and Robinson type:

$$y'' + v^2(y-g)^3 = g'', \quad v \gg 0, \; g(x) = \cos x, \tag{4.5}$$

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

which has exact solution $y(x) = g(x)$.

First, we integrated this problem with two different methods from 0 to $x_{\mathrm{end}} = 10$ with fixed steplength for $v = 10^4$ and $v = 10^5$.

Due to the large value of the stiffness parameter v, we again apply the P-stable method, $M_{32}(-\frac{1}{96}, \frac{9}{2})$, for which the stage order is three, the largest possible value in this family. In each time step, Newton-iteration (with a tolerance set to $\mathrm{TOL} = 10^{-10}$) is used to solve the nonlinear equation in y_{n+1}. As a

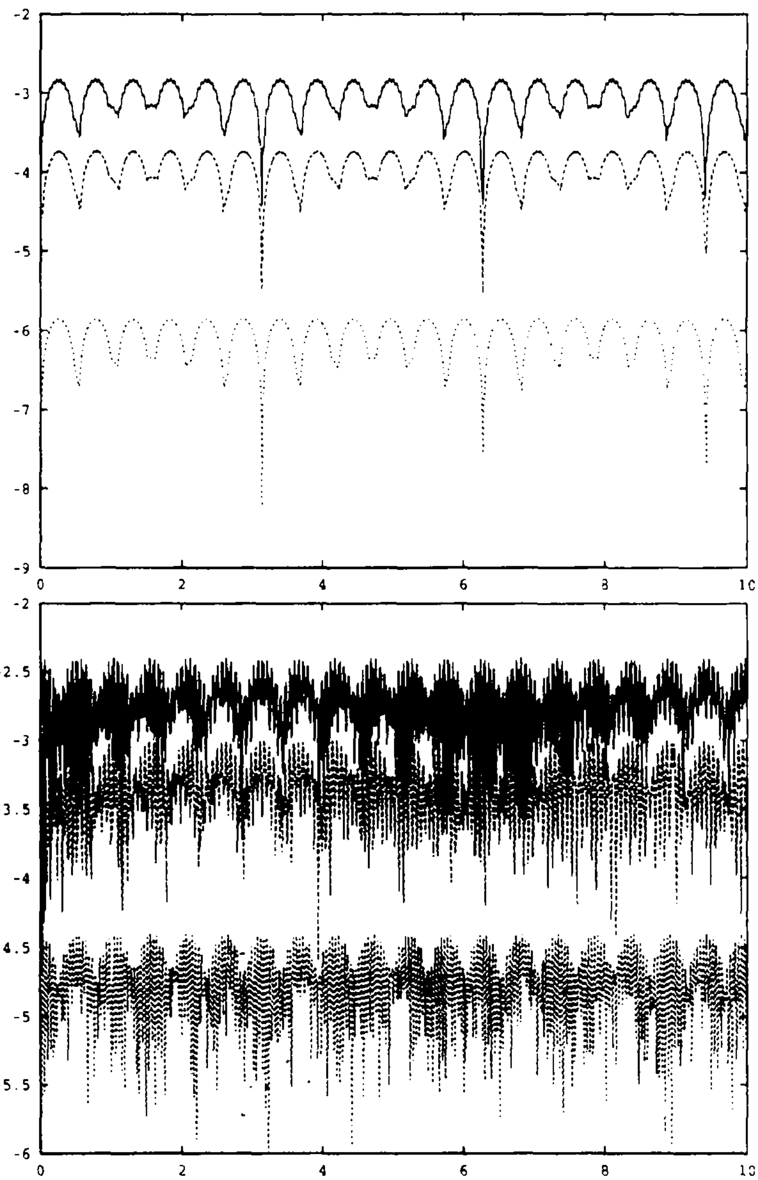

Fig. 6. Maximum-norm errors in logarithmic scale for method $M_{32}(-\frac{1}{96}, \frac{9}{2})$ (upper part) and the method (4.4) (lower part) when applied to (4.3) with $h = 0.01$, $h = 0.005$ and $h = 0.001$.

starting value, we use the value Y_2, obtained from the previous step (except for the first step, where we use the Euler method as predictor for y_1).

Again a comparison is made with method (4.4). When applied to (4.5) this diagonal-implicit method requires the solution of 3 nonlinear equations. Since no other predictor is available, we perform an explicit Euler step to start the iteration and the same value for TOL is used.

Table 5
Absolute errors $\max(|y(x_{end}) - y_{end}|, |y'(x_{end}) - y'_{end}|)$ in logarithmic norm and the number of iterations (in parantheses) at $x_{end} = 10$ for the nonlinear problem

	$\nu = 10^4$		$\nu = 10^5$	
h	Method (4.4)	$M_{32}(\frac{9}{2}, -\frac{1}{96})$	Method (4.4)	$M_{32}(\frac{9}{2}, -\frac{1}{96})$
0.1	−4.51 (3664)	−5.74 (321)	−3.88 (5347)	−4.57 (474)
0.05	−6.66 (5324)	−7.00 (485)	−5.21 (8580)	−7.18 (546)
0.025	−8.99 (7351)	−8.22 (847)	−7.86 (13007)	−8.22 (908)
0.0125	−11.00 (10484)	−9.44 (1549)	−9.65 (18744)	−9.44 (1610)

Table 6
The logarithm of the accuracy obtained in x_{end}, the number of iterations, rejected steps and accepted steps for several values of TOL when $M_{32}(-\frac{1}{96}, \frac{9}{2})$ is implemented in a variable-step mode with embedding and applied to the nonlinear problem

	TOL=10^{-6}		TOL=10^{-8}		TOL=10^{-10}	
	$\nu = 10^4$	$\nu = 10^5$	$\nu = 10^4$	$\nu = 10^5$	$\nu = 10^4$	$\nu = 10^5$
acc	−5.95	−6.47	−8.04	−8.04	−10.04	−10.05
niter	350	715	1051	1059	3285	3285
nreject	7	7	8	8	8	8
naccept	171	168	540	540	1703	1703

The results are summarized in Table 5. It can be seen that both methods produce acceptable results. Our method however needs much less iterations than the diagonal-implicit method. One should also take account of the fact that this diagonal-implicit method needs Newton iteration for each of the three stages.

Finally, we also implemented our method in a simple variable-step mode, which is only designed to show the usefulness of the formulae of this paper. Hence, we do not expect the implementation to be optimal.

To perform error control on y and y', we looked for an embedded third-order method. From the embedded third-order family for which

$$\bar{b}^{\mathrm{T}} = ((1+3u+6v)/4,\ (1-12u-18v)/6,\ u, v)^{\mathrm{T}},$$
$$b^{\mathrm{T}} = ((5-12w)/12,\ (2+9w)/3,\ -(1+36w)/12, w)^{\mathrm{T}},$$

we have chosen the method with $(u, v, w) = (-\frac{1}{20}, \frac{1}{30}, \frac{1}{15})$ to compute the embedded solutions $\tilde{y}$ and $\tilde{y}'$. In each time step, we computed the error err $= \max(|y_{n+1} - \tilde{y}_{n+1}|, |y'_{n+1} - \tilde{y}'_{n+1}|)$ and the new stepsize was determined by the expression

$$h_{new} = \max(0.1, \min(5, 0.9\,(\mathrm{err}/\mathrm{TOL})^{0.25})),$$

where TOL is the input value of the required accuracy. If err < TOL, the step is accepted. The stepsize is changed and an interpolating polynomial through y_n, y_{n+1}, Y_2 and Y_3 is used to predict the starting value in the Newton iteration in the next step. If the permitted change in the stepsize is less than 10%, the stepsize is left unchanged and Y_2 is used as starting value in the Newton process in the next step.

If err > TOL, the step is rejected, the stepsize is changed and the starting value for the iteration is obtained using the same interpolating polynomial. Finally, we mention that the tolerance of the Newton process is set to TOL/10.

The results obtained with our method are displayed in Table 6. Table 6 shows the logarithm of the accurary obtained, the number of iterations, the number of accepted steps and the number of rejected steps for different values of v and different values of TOL.

References

[1] J.R. Cash, High order P-stable formulae for the numerical integration of periodic initial value problems, *Numer. Math.* **37** (1981) 355–370.

[2] M.M. Chawla and P.S. Rao, A Numerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems, *J. Comput. Appl. Math.* **11** (1984) 277–281.

[3] J.P. Coleman, Numerical methods for $y'' = f(x, y)$ via rational approximations for the cosine, *IMA J. Numer. Anal.* **9** (1989) 145–165.

[4] J.M. Franco, An explicit hybrid method of Numerov type for second-order periodic initial-value problems, *J. Comput. Appl. Math.* **59** (1995) 79–90.

[5] E. Hairer, Méthodes de Nyström pour l'équation différentielle $y' = f(x, y)$, *Numer. Math.* **27** (1977) 283–300.

[6] E. Hairer, Unconditionally stable methods for second order differential equations, *Numer. Math.* **32** (1979) 373–379.

[7] E. Hairer, S.P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations I, Nonstiff Problems* (Springer, Heidelberg, 1987).

[8] E. Hairer and G. Wanner, A theory for Nyström methods, *Numer. Math.* **25** (1976) 383–400.

[9] L.Gr. Ixaru and M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies, *Comput. Phys. Commun.* **19** (1980) 23–27.

[10] L. Kramarz, Stability of collocation methods for the numerical solution of $y'' = f(x, y)$, *BIT* **20** (1980) 215–222.

[11] J.D. Lambert and I.A. Watson, Symmetric multistep methods for periodic initial value problems, *J. Inst. Math. Appl.* **18** (1976) 189–202.

[12] P.W. Sharp, J.M. Fine and K. Burrage, Two-stage and three-stage diagonally implicit Runge–Kutta–Nyström methods of orders three and four, *IMA J. Numer. Anal.* **10** (1990) 489–504.

[13] T.E. Simos and A.D. Raptis, Numerov-type methods with minimal phase-lag for the numerical integration of the one-dimensional Schrödinger equation, *Computing* **45** (1990) 175–181.

[14] R.M. Thomas, Phase properties of high order almost P-stable formulae, *BIT* **24** (1984) 225–238.

[15] G. Vanden Berghe, H. De Meyer and J. Vanthournout, A modified Numerov integration method for second order periodic initial-value problems, *J. Comput. Math.* **32** (1990) 233–242.

[16] M. Van Daele, H. De Meyer and G. Vanden Berghe, A modified Numerov integration method for general second order initial value problems, *Internat. J. Comput. Math.* **40** (1991) 117–127.

[17] M. Van Daele, G. Vanden Berghe and H. De Meyer, A general theory of stabilized extended one-step methods for ODEs, *Internat. J. Comput. Math.* **60** (1996) 253–263.

[18] P.J. van der Houwen and B.P. Sommeijer, Explicit Runge–Kutta(-Nyström) methods with reduced plase errors for computing oscillating solutions, *SIAM J. Numer. Anal.* **24** (1987) 595–617.

[19] P.J. van der Houwen, B.P. Sommeijer and Nguyen Huu Cong, Stability of collocation-based Runge–Kutta–Nyström methods, *BIT* **31** (1991) 469–481.