Structure-Preserving Algorithms for Oscillatory Differential Equations

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Chapter 2
ARKN Methods

In this chapter, we study the adapted Runge–Kutta–Nyström (ARKN) methods, proposed by Franco (2002), for the system of second-order oscillatory differential equations $y'' + \omega^2 y = f(y, y')$, where $\omega > 0$. Based on the internal stages of the traditional RKN methods, ARKN methods adopt a new form of updates, where the special oscillatory structure of the system is incorporated. Order conditions are derived by means of the Nyström tree theory. The symplecticity conditions for ARKN methods are obtained. It is shown that ARKN methods cannot be symmetric. Finally, on the basis of the matrix-variation-of-constants formula, we develop multidimensional ARKN methods for more general equations $y'' + My = f(y, y')$ with a positive semi-definite (not necessarily symmetric) principal frequency matrix M. A notable feature of multidimensional ARKN methods is that they integrate exactly the homogeneous system $y'' + My = \mathbf{0}$. These methods do not rely on the decomposition of M so that they are applicable to the oscillatory systems with a positive semi-definite (but not symmetric) matrix M.

2.1 Traditional ARKN Methods

It is now conventional to require numerical algorithms to preserve the qualitative behavior of the true solution as much as possible when applied to a differential equation. However, for a second-order differential equation with an oscillatory solution, classical RKN methods often produce unsatisfactory numerical behavior since they fail to take account of the particular structure of the problem. In this section, we investigate ARKN methods for systems of second-order perturbed oscillators.

We start with the second-order initial value problem

$$\begin{cases} y'' + \omega^2 y = f(y, y'), \quad \omega > 0, \quad x \in [x_0, x_{\mathrm{end}}], \\ y(x_0) = y_0, \quad y'(x_0) = y_0', \end{cases} \tag{2.1}$$

where $y \in \mathbb{R}^d$ and $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$. We assume that the principal frequency ω is known or can be accurately estimated in advance. In the pioneering work [7],

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González et al. propose the idea of adapting RKN methods to the special structure of the system (2.1). Franco [5] continues to reform the updates of the classical RKN methods and proposes the so-called ARKN methods (Runge–Kutta–Nyström methods adapted to perturbed oscillators (2.1), see (2.3)). The following work can be found in [1, 3, 4, 15].

2.1.1 Formulation of the Scheme

Applying the well-known variation-of-constants formula to (2.1) gives the following integral equations:

$$\begin{cases} y(x_n+h) = \phi_0(\nu)y(x_n) + \phi_1(\nu)hy'(x_n) \\ \qquad\qquad + \displaystyle\int_{x_n}^{x_n+h} (x_n+h-z)\phi_1\big((x_n+h-z)\omega\big) f\big(y(z), y'(z)\big)\,\mathrm{d}z, \\ hy'(x_n+h) = -\nu^2\phi_1(\nu)y(x_n) + \phi_0(\nu)hy'(x_n) \\ \qquad\qquad + h\displaystyle\int_{x_n}^{x_n+h} \phi_0\big((x_n+h-z)\omega\big) f\big(y(z), y'(z)\big)\,\mathrm{d}z, \end{cases} \tag{2.2}$$

where

$$\phi_0(\xi) = \cos(\xi), \qquad \phi_1(\xi) = \frac{\sin(\xi)}{\xi}, \qquad \nu = h\omega.$$

Approximating the integrals in (2.2) by quadrature formulae leads to Franco's definition of ARKN methods.

Definition 2.1 *An s-stage ARKN method* for the initial value problem (2.1) is defined by the following scheme:

$$\begin{cases} Y_i = y_n + c_i hy'_n + h^2 \displaystyle\sum_{j=1}^{s} \bar{a}_{ij}\big(f\big(Y_j, Y'_j\big) - \omega^2 Y_j\big), \quad i = 1, \ldots, s, \\ Y'_i = y'_n + h \displaystyle\sum_{j=1}^{s} a_{ij}\big(f\big(Y_j, Y'_j\big) - \omega^2 Y_j\big), \quad i = 1, \ldots, s, \\ y_{n+1} = \phi_0(\nu)y_n + h\phi_1(\nu)y'_n + h^2 \displaystyle\sum_{i=1}^{s} \bar{b}_i(\nu) f\big(Y_i, Y'_i\big), \\ y'_{n+1} = -\omega\nu\phi_1(\nu)y_n + \phi_0(\nu)y'_n + h \displaystyle\sum_{i=1}^{s} b_i(\nu) f\big(Y_i, Y'_i\big), \end{cases} \tag{2.3}$$

where $c_i, \bar{a}_{ij}, a_{ij}, i, j = 1, \ldots, s$ are real constants and $\bar{b}_i(\nu), b_i(\nu), i = 1, \ldots, s$ are even functions of $\nu = h\omega$.

The ARKN method (2.3) can also be expressed in the Butcher tableau as

$$\begin{array}{c|cc} c & \bar{A} & A \\ \hline & \bar{b}^{\mathrm{T}}(\nu) & b^{\mathrm{T}}(\nu) \end{array} = \begin{array}{c|ccc ccc} c_1 & \bar{a}_{11} & \cdots & \bar{a}_{1s} & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1} & \cdots & \bar{a}_{ss} & a_{s1} & \cdots & a_{ss} \\ \hline & \bar{b}_1(\nu) & \cdots & \bar{b}_s(\nu) & b_1(\nu) & \cdots & b_s(\nu) \end{array}$$

2.1.2 Order Conditions

The ARKN method (2.3) is said to be of order p, if for the sufficiently smooth problem (2.1) the following conditions are satisfied:

$$e_{n+1} = y(x_n+h) - y_{n+1} = \mathscr{O}\big(h^{p+1}\big) \quad \text{and} \quad e'_{n+1} = y'(x_n+h) - y'_{n+1} = \mathscr{O}\big(h^{p+1}\big),$$

where $y(x_n + h)$ and $y'(x_n + h)$ are the exact solution of (2.1) and its derivative at $x_n + h$, respectively, and y_{n+1} and y'_{n+1} are the numerical results obtained by the method from the exact starting values $y_n = y(x_n)$ and $y'_n = y'(x_n)$.

In order to express order conditions for ARKN methods, we define the *scalar ϕ-functions* (see [5])

$$\phi_j(\nu) = \sum_{k=0}^{\infty} (-1)^k \frac{\nu^{2k}}{(2k+j)!} \quad \text{for } j = 0, 1, \ldots. \tag{2.4}$$

It can be seen that

$$\begin{aligned} &\lim_{\nu \to 0} \phi_j(\nu) = \frac{1}{j!}, \quad \text{for } j = 0, 1, \ldots, \\ &\phi_j(\nu) = \frac{1}{\nu^2}\left(\frac{1}{(j-2)!} - \phi_{j-2}(\nu)\right), \quad \text{for } j = 2, 3, \ldots. \end{aligned} \tag{2.5}$$

Theorem 2.1 *The necessary and sufficient conditions for an ARKN method to be of order p are given by*

$$\bar{b}^{\mathrm{T}}(\nu)\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)}(\nu) = \mathscr{O}\big(h^{p-\rho(t)+1}\big), \quad \textit{for } t \in \bigcup_{q=2}^{p} NT_q, \tag{2.6}$$

$$\bar{b}^{\mathrm{T}}(\nu)\bar{A}\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)+2}(\nu) = \mathscr{O}\big(h^{p-\rho(t)-1}\big), \quad \textit{for } t \in \bigcup_{q=2}^{p-2} NT_q, \tag{2.7}$$

$$b^{\mathrm{T}}(\nu)\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)-1}(\nu) = \mathscr{O}\big(h^{p-\rho(t)+2}\big), \quad \textit{for } t \in \bigcup_{q=2}^{p+1} NT_q, \tag{2.8}$$

$$b^{\mathrm{T}}(\nu)\bar{A}\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)+1}(\nu) = \mathscr{O}\big(h^{p-\rho(t)}\big), \quad \textit{for } t \in \bigcup_{q=2}^{p-1} NT_q. \tag{2.9}$$

Theorem 2.2 *The condition* (2.6) *in Theorem* 2.1 *implies the condition* (2.7) *and the condition* (2.8) *implies the condition* (2.9).

The proofs of Theorem 2.1 and Theorem 2.2 can be found in [18]. From these theorems, we arrive at the following conclusive theorem.

Theorem 2.3 *An ARKN method has order* p *if and only if the following conditions are satisfied*:

$$\bar{b}^{\mathrm{T}}(\nu)\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)}(\nu) = \mathscr{O}(h^{p-\rho(t)+1}), \quad \textit{for } t \in \bigcup_{q=2}^{p} NT_q \tag{2.10}$$

and

$$b^{\mathrm{T}}(\nu)\Phi(t) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)-1}(\nu) = \mathscr{O}(h^{p-\rho(t)+2}), \quad \textit{for } t \in \bigcup_{q=2}^{p+1} NT_q. \tag{2.11}$$

Remark 2.1 It is obvious that, when $\omega \to 0$ ($\nu \to 0$), the scheme (2.3) reduces to the classical RKN scheme and $\phi_{\rho(t)}(\nu) \to \frac{1}{\rho(t)!}$. Accordingly, (2.10) and (2.11) become

$$\bar{b}^{\mathrm{T}}(0)\Phi(t) = \frac{1}{\gamma(t)}, \quad \text{for } t \in \bigcup_{q=2}^{p} NT_q,$$

$$b^{\mathrm{T}}(0)\Phi(t) = \frac{\rho(t)}{\gamma(t)}, \quad \text{for } t \in \bigcup_{q=2}^{p+1} NT_q,$$

which are exactly the order conditions for the classical RKN methods (see Chap. 1).

Here and hereafter, when order conditions are used to derive the coefficients of a method, the higher-order terms are usually omitted.

We also note that the ARKN method (2.3) for the autonomous equation (2.1) is applicable to the non-autonomous equation

$$\begin{cases} y'' + \omega^2 y = f\big(x, y, y'\big), & x \in [x_0, x_{\mathrm{end}}], \\ y(x_0) = y_0, & y'(x_0) = y_0'. \end{cases} \tag{2.12}$$

In fact, by appending x to the dependent variables, we can transform Eq. (2.12) into a system of the autonomous form (2.1) as follows:

$$\begin{cases} u'' + \omega^2 u = g\big(u, u'\big), & x \in [x_0, x_{\mathrm{end}}], \\ u(x_0) = (x_0, y_0)^{\mathrm{T}}, & u'(x_0) = \big(1, y_0'\big)^{\mathrm{T}}, \end{cases} \tag{2.13}$$

where $u(x) = (x, y(x)^{\mathrm{T}})^{\mathrm{T}}$ and $g(u, u') = (\omega^2 x, f(x, y, y')^{\mathrm{T}})^{\mathrm{T}}$. Applying the method (2.3) of order p ($p \geq 2$) to the autonomous differential equation (2.13) yields

$$\begin{cases} X_i = x_n + c_i h, \\ Y_i = y_n + c_i h y_n' + h^2 \sum\limits_{j=1}^{s} \bar{a}_{ij}\big(f\big(X_j, Y_j, Y_j'\big) - \omega^2 Y_j\big), \\ X_i' = 1, \\ Y_i' = y_n' + h \sum\limits_{j=1}^{s} a_{ij}\big(f\big(X_j, Y_j, Y_j'\big) - \omega^2 Y_j\big), \\ \quad i = 1, \dots, s, \end{cases} \tag{2.14}$$

and

$$\begin{cases} x_{n+1} = \phi_0(\nu) x_n + h\phi_1(\nu) + h^2 \sum\limits_{i=1}^{s} \bar{b}_i(\nu)\big(\omega^2 X_i\big), \\ y_{n+1} = \phi_0(\nu) y_n + h\phi_1(\nu) y_n' + h^2 \sum\limits_{i=1}^{s} \bar{b}_i(\nu) f\big(X_i, Y_i, Y_i'\big), \\ x_{n+1}' = -\omega\nu\phi_1(\nu) x_n + \phi_0(\nu) + h \sum\limits_{i=1}^{s} b_i(\nu)\big(\omega^2 X_i\big), \\ y_{n+1}' = -\omega\nu\phi_1(\nu) y_n + \phi_0(\nu) y_n' + h \sum\limits_{i=1}^{s} b_i(\nu) f\big(X_i, Y_i, Y_i'\big). \end{cases} \tag{2.15}$$

Then the following order conditions from Theorem 2.3:

$$\sum_{i=1}^{s} \bar{b}_i(\nu) = \phi_2(\nu) + \mathscr{O}\big(h^{p-1}\big), \qquad \sum_{i=1}^{s} \bar{b}_i(\nu) c_i = \phi_3(\nu) + \mathscr{O}\big(h^{p-2}\big),$$

$$\sum_{i=1}^{s} b_i(\nu) = \phi_1(\nu) + \mathscr{O}\big(h^{p}\big), \qquad \sum_{i=1}^{s} b_i(\nu) c_i = \phi_2(\nu) + \mathscr{O}\big(h^{p-1}\big)$$

imply that

$$\begin{aligned}
x_{n+1} &= \left(\phi_0(\nu) + \nu^2 \sum_{i=1}^{s} \bar{b}_i(\nu)\right) x_n + h\left(\phi_1(\nu) + \nu^2 \sum_{i=1}^{s} \bar{b}_i(\nu) c_i\right), \\
&= \left(\phi_0(\nu) + \nu^2\left(\phi_2(\nu) + \mathscr{O}\left(h^{p-1}\right)\right)\right) x_n + h\left(\phi_1(\nu) + \nu^2\left(\phi_3(\nu) + \mathscr{O}\left(h^{p-2}\right)\right)\right) \\
&= x_n + h + \mathscr{O}\left(h^{p+1}\right), \\
x'_{n+1} &= -\omega\nu\left(\phi_1(\nu) - \sum_{i=1}^{s} b_i(\nu)\right) x_n + \left(\phi_0(\nu) + \nu^2 \sum_{i=1}^{s} b_i(\nu) c_i\right), \\
&= -\omega\nu\left(\phi_1(\nu) - \left(\phi_1(\nu) + \mathscr{O}\left(h^{p}\right)\right)\right) x_n + \left(\phi_0(\nu) + \nu^2\left(\phi_2(\nu) + \mathscr{O}\left(h^{p-1}\right)\right)\right) \\
&= 1 + \mathscr{O}\left(h^{p+1}\right),
\end{aligned}$$

where the property $\phi_0(\nu) + \nu^2\phi_2(\nu) = \phi_1(\nu) + \nu^2\phi_3(\nu) = 1$ is used. Thus we have $y_{n+1} = y(x_n + h) + \mathscr{O}(h^{p+1})$ and $y'_{n+1} = y'(x_n + h) + \mathscr{O}(h^{p+1})$ since the method considered is of order p.

2.2 Symplectic ARKN Methods

In a wide range of physical applications from molecular dynamics to nonlinear wave propagation (after semi-discretization), an important class of problems has the form

$$\begin{cases} \ddot{q} + \omega^2 q = f(q), & t \in [t_0, t_{\text{end}}], \\ q(t_0) = q_0, & \dot{q}(t_0) = \dot{q}_0, \end{cases} \tag{2.16}$$

where "$\dot{q}$" and "$\ddot{q}$" denote time derivatives. The solution to the system (2.16) is oscillatory. Assume that the function f has the form $f(q) = -\nabla U(q)$ for some smooth function $U(q)$. Then the system (2.16) is a Hamiltonian system with the Hamiltonian

$$H(p, q) = \frac{1}{2} p^{\mathrm{T}} p + \frac{\omega^2}{2} q^{\mathrm{T}} q + U(q),$$

where $p = \dot{q}$.

In this section we focus on the symplecticity conditions of ARKN methods for separable Hamiltonian systems. It turns out that symplectic ARKN (SARKN) methods cannot have algebraic order greater than two, and explicit SARKN methods can have only one stage.

2.2.1 Symplecticity Conditions for ARKN Integrators

For the system (2.16), the ARKN method (2.3) takes the form

$$\begin{cases} Q_i = q_n + c_i h\dot{q}_n + h^2 \sum_{j=1}^{s} \bar{a}_{ij}\big(f(Q_j) - \omega^2 Q_j\big), \quad i = 1, \ldots, s, \\ q_{n+1} = \phi_0(\nu) q_n + h\phi_1(\nu)\dot{q}_n + h^2 \sum_{i=1}^{s} \bar{b}_i(\nu) f(Q_i), \\ h\dot{q}_{n+1} = -\nu^2 \phi_1(\nu) q_n + \phi_0(\nu) h\dot{q}_n + h^2 \sum_{i=1}^{s} b_i(\nu) f(Q_i). \end{cases} \tag{2.17}$$

Its Butcher tableau is given by

$$\begin{array}{c|c} c & \bar{A} \\ \hline & \bar{b}^{\mathrm{T}}(\nu) \\ \hline & b^{\mathrm{T}}(\nu) \end{array} = \begin{array}{c|ccc} c_1 & \bar{a}_{11} & \cdots & \bar{a}_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1} & \cdots & \bar{a}_{ss} \\ \hline & \bar{b}_1(\nu) & \cdots & \bar{b}_s(\nu) \\ \hline & b_1(\nu) & \cdots & b_s(\nu) \end{array}$$

The following theorem presents the symplecticity conditions for ARKN methods.

Theorem 2.4 (Shi and Wu [14]) *An s-stage ARKN method (2.17) is symplectic if its coefficients satisfy the following conditions*:

$$\begin{aligned} &\bar{b}_i(\nu)\big(\phi_0(\nu) + \nu^2 c_i \phi_1(\nu)\big) = b_i(\nu)\big(\phi_1(\nu) - c_i \phi_0(\nu)\big), \\ &b_i(\nu)\big(\bar{b}_j(\nu) - \bar{a}_{ij}\phi_0(\nu)\big) - \nu^2 \bar{b}_i(\nu)\bar{a}_{ij}\phi_1(\nu) \\ &\quad = b_j(\nu)\big(\bar{b}_i(\nu) - \bar{a}_{ji}\phi_0(\nu)\big) - \nu^2 \bar{b}_j(\nu)\bar{a}_{ji}\phi_1(\nu), \\ &\big(b_i(\nu)\phi_0(\nu) + \nu^2 \bar{b}_i(\nu)\phi_1(\nu)\big)\bar{a}_{ij} = \big(b_j(\nu)\phi_0(\nu) + \nu^2 \bar{b}_j(\nu)\phi_1(\nu)\big)\bar{a}_{ji} \end{aligned} \tag{2.18}$$

for $i, j = 1, \ldots, s$.

In the sequel to this and the next subsections, the variable (ν) in $\bar{b}$ and b is suppressed for convenience.

Proof The argument is similar to that of Sanz-Serna and Calvo in [13] in the proof of symplecticity conditions for the classical RKN methods. To show the symplecticity of the method (2.3), it suffices to verify

$$\sum_{J=1}^{d} \mathrm{d}q_{n+1}^J \wedge \mathrm{d}\dot{q}_{n+1}^J = \sum_{J=1}^{d} \mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J,$$

where the symbol "$\wedge$" is the exterior product, and the superscript "J" indicates component indices.

In fact, by direct computation, we obtain

$$\begin{aligned} \mathrm{d}q_{n+1}^J \wedge \mathrm{d}\dot{q}_{n+1}^J = {} & \big(\phi_0^2(\nu) + \nu^2\phi_1^2(\nu)\big)\,\mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J \\ & + h\sum_{i=1}^{s}\big(b_i\phi_0(\nu) + \bar{b}_i\nu^2\phi_1(\nu)\big)\,\mathrm{d}q_n^J \wedge \mathrm{d}f_i^J \\ & + h^2\sum_{i=1}^{s}\big(\phi_1(\nu)b_i - \phi_0(\nu)\bar{b}_i\big)\,\mathrm{d}\dot{q}_n^J \wedge \mathrm{d}f_i^J \\ & + h^3\sum_{i,j=1}^{s}\bar{b}_i b_j\,\mathrm{d}f_i^J \wedge \mathrm{d}f_j^J, \end{aligned} \tag{2.19}$$

where $f_i^J = f^J(Q_i)$. From the definition of $\phi_0(\nu)$ and $\phi_1(\nu)$, we have

$$\phi_0^2(\nu) + \nu^2\phi_1^2(\nu) = 1$$

and hence

$$\begin{aligned} \mathrm{d}q_{n+1}^J \wedge \mathrm{d}\dot{q}_{n+1}^J = {} & \mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J + h\sum_{i=1}^{s}\big(b_i\phi_0(\nu) + \bar{b}_i\nu^2\phi_1(\nu)\big)\,\mathrm{d}q_n^J \wedge \mathrm{d}f_i^J \\ & + h^2\sum_{i=1}^{s}\big(\phi_1(\nu)b_i - \phi_0(\nu)\bar{b}_i\big)\,\mathrm{d}\dot{q}_n^J \wedge \mathrm{d}f_i^J \\ & + h^3\sum_{i,j=1}^{s}\bar{b}_i b_j\,\mathrm{d}f_i^J \wedge \mathrm{d}f_j^J. \end{aligned} \tag{2.20}$$

Differentiating the first equation of (2.17) yields

$$\mathrm{d}Q_i^J = \mathrm{d}q_n^J + c_i h\,\mathrm{d}\dot{q}_n^J + h^2\sum_{j=1}^{s}\bar{a}_{ij}\big(\mathrm{d}f_j^J - \omega^2\,\mathrm{d}Q_j^J\big), \quad i = 1, \ldots, s.$$

Then, we have

$$\mathrm{d}q_n^J = \mathrm{d}Q_i^J - c_i h\,\mathrm{d}\dot{q}_n^J - h^2\sum_{j=1}^{s}\bar{a}_{ij}\big(\mathrm{d}f_j^J - \omega^2\,\mathrm{d}Q_j^J\big), \quad i = 1, \ldots, s.$$

Therefore

$$\mathrm{d}q_n^J \wedge \mathrm{d}f_i^J = \mathrm{d}Q_i^J \wedge \mathrm{d}f_i^J - c_i h\,\mathrm{d}\dot{q}_n^J \wedge \mathrm{d}f_i^J - h^2\sum_{j=1}^{s}\bar{a}_{ij}\big(\mathrm{d}f_j^J - \omega^2\,\mathrm{d}Q_j^J\big) \wedge \mathrm{d}f_i^J. \tag{2.21}$$

With (2.21), the formula (2.20) becomes

$$
\begin{aligned}
&\mathrm{d}q_{n+1}^J \wedge \mathrm{d}\dot{q}_{n+1}^J \\
&\quad = \mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J + h\sum_{i=1}^{s}\big(b_i\phi_0(\nu) + \bar{b}_i\nu^2\phi_1(\nu)\big)\,\mathrm{d}Q_i^J \wedge \mathrm{d}f_i^J \\
&\qquad + h\sum_{i,j=1}^{s}\big(\nu^2 b_i\bar{a}_{ij}\phi_0(\nu) + \nu^4\bar{b}_i\bar{a}_{ij}\phi_1(\nu)\big)\,\mathrm{d}Q_j^J \wedge \mathrm{d}f_i^J \\
&\qquad + h^2\sum_{i=1}^{s}\big(b_i\phi_1(\nu) - \bar{b}_i c_i\nu^2\phi_1(\nu) - b_i c_i\phi_0(\nu) - \bar{b}_i\phi_0(\nu)\big)\,\mathrm{d}\dot{q}_n^J \wedge \mathrm{d}f_i^J \\
&\qquad + h^3\sum_{i,j=1}^{s}\big(b_i\bar{a}_{ij}\phi_0(\nu) + \bar{b}_i\bar{a}_{ij}\nu^2\phi_1(\nu) + \bar{b}_i b_j\big)\,\mathrm{d}f_i^J \wedge \mathrm{d}f_j^J \\
&\quad = \mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J + h\sum_{i=1}^{s}\big(b_i\phi_0(\nu) + \bar{b}_i\nu^2\phi_1(\nu)\big)\,\mathrm{d}Q_i^J \wedge \mathrm{d}f_i^J \\
&\qquad + h\sum_{i<j}\big(\nu^2 b_i\bar{a}_{ij}\phi_0(\nu) + \nu^4\bar{b}_i\bar{a}_{ij}\phi_1(\nu) - \nu^2 b_j\bar{a}_{ji}\phi_0(\nu) \\
&\qquad - \nu^4\bar{b}_j\bar{a}_{ji}\phi_1(\nu)\big)\,\mathrm{d}Q_j^J \wedge \mathrm{d}f_i^J \\
&\qquad + h^2\sum_{i=1}^{s}\big(b_i\phi_1(\nu) - \bar{b}_i c_i\nu^2\phi_1(\nu) - b_i c_i\phi_0(\nu) - \bar{b}_i\phi_0(\nu)\big)\,\mathrm{d}\dot{q}_n^J \wedge \mathrm{d}f_i^J \\
&\qquad + h^3\sum_{i<j}\big(b_i\bar{a}_{ij}\phi_0(\nu) + \bar{b}_i\bar{a}_{ij}\nu^2\phi_1(\nu) + \bar{b}_i b_j - b_j\bar{a}_{ji}\phi_0(\nu) \\
&\qquad - \bar{b}_j\bar{a}_{ji}\nu^2\phi_1(\nu) - \bar{b}_j b_i\big)\,\mathrm{d}f_i^J \wedge \mathrm{d}f_j^J,
\end{aligned}
\tag{2.22}
$$

for $J = 1, \ldots, d$. Summing over all J gives

$$
\begin{aligned}
&\sum_{J=1}^{d}\mathrm{d}q_{n+1}^J \wedge \mathrm{d}\dot{q}_{n+1}^J \\
&\quad = \sum_{J=1}^{d}\mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J + h\sum_{i=1}^{s}\big(b_i\phi_0(\nu) + \bar{b}_i\nu^2\phi_1(\nu)\big)\sum_{J=1}^{d}\mathrm{d}Q_i^J \wedge \mathrm{d}f_i^J \\
&\qquad + h\sum_{i<j}\big(\nu^2 b_i\bar{a}_{ij}\phi_0(\nu) + \nu^4\bar{b}_i\bar{a}_{ij}\phi_1(\nu) - \nu^2 b_j\bar{a}_{ji}\phi_0(\nu)
\end{aligned}
$$

$$
\begin{aligned}
&- \nu^4 \bar{b}_j \bar{a}_{ji} \phi_1(\nu)\big) \sum_{J=1}^{d} \mathrm{d}Q_j^J \wedge \mathrm{d}f_i^J \\
&+ h^2 \sum_{i=1}^{s} \big(b_i \phi_1(\nu) - \bar{b}_i c_i \nu^2 \phi_1(\nu) - b_i c_i \phi_0(\nu) \\
&- \bar{b}_i \phi_0(\nu)\big) \sum_{J=1}^{d} \mathrm{d}\dot{q}_n^J \wedge \mathrm{d}f_i^J \\
&+ h^3 \sum_{i<j} \big(b_i \bar{a}_{ij} \phi_0(\nu) + \bar{b}_i \bar{a}_{ij} \nu^2 \phi_1(\nu) + \bar{b}_i b_j - b_j \bar{a}_{ji} \phi_0(\nu) \\
&- \bar{b}_j \bar{a}_{ji} \nu^2 \phi_1(\nu) - \bar{b}_j b_i\big) \sum_{J=1}^{d} \mathrm{d}f_i^J \wedge \mathrm{d}f_j^J.
\end{aligned} \tag{2.23}
$$

From

$$
\mathrm{d}f_i^J \wedge \mathrm{d}Q_i^J = \left(\sum_{I=1}^{d} \frac{\partial f^J}{\partial q^I}(Q_i)\, \mathrm{d}Q_i^I \right) \wedge \mathrm{d}Q_i^J = \sum_{I=1}^{d} \frac{\partial f^J}{\partial q^I}(Q_i)\, \mathrm{d}Q_i^I \wedge \mathrm{d}Q_i^J
$$

and

$$
f(q) - \omega^2 q = -\frac{\partial U}{\partial q},
$$

it follows that

$$
\begin{aligned}
\sum_{J=1}^{d} \mathrm{d}f_i^J \wedge \mathrm{d}Q_i^J &= \sum_{J=1}^{d} \left(\omega^2 \mathrm{d}Q_i^J - \sum_{I=1}^{d} \frac{\partial^2 U}{\partial q^J \partial q^I}(Q_i)\, \mathrm{d}Q_i^I \right) \wedge \mathrm{d}Q_i^J \\
&= -\sum_{I=1}^{d} \frac{\partial^2 U}{\partial q^J \partial q^I}(Q_i)\, \mathrm{d}Q_i^I \wedge \mathrm{d}Q_i^J \\
&= -\sum_{I<J} \left(\frac{\partial^2 U}{\partial q^J \partial q^I}(Q_i) - \frac{\partial^2 U}{\partial q^I \partial q^J}(Q_i) \right) \mathrm{d}Q_i^I \wedge \mathrm{d}Q_i^J \\
&= 0.
\end{aligned} \tag{2.24}
$$

The last equality follows from the symmetry of the partial derivatives. Consequently, the formula (2.23) becomes

$$
\sum_{J=1}^{d} \mathrm{d}q_{n+1}^J \wedge \mathrm{d}\dot{q}_{n+1}^J = \sum_{J=1}^{d} \mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J + h \sum_{i<j} \big(\nu^2 b_i \bar{a}_{ij} \phi_0(\nu) + \nu^4 \bar{b}_i \bar{a}_{ij} \phi_1(\nu)
$$

$$
\begin{aligned}
&- \nu^2 b_j \bar{a}_{ji} \phi_0(\nu) - \nu^4 \bar{b}_j \bar{a}_{ji} \phi_1(\nu)\big) \sum_{J=1}^{d} \mathrm{d}Q_j^J \wedge \mathrm{d}f_i^J \\
&+ h^2 \sum_{i=1}^{s} \big(b_i \phi_1(\nu) - \bar{b}_i c_i \nu^2 \phi_1(\nu) - b_i c_i \phi_0(\nu) \\
&- \bar{b}_i \phi_0(\nu)\big) \sum_{J=1}^{d} \mathrm{d}\dot{q}_n^J \wedge \mathrm{d}f_i^J \\
&+ h^3 \sum_{i<j} \big(b_i \bar{a}_{ij} \phi_0(\nu) + \bar{b}_i \bar{a}_{ij} \nu^2 \phi_1(\nu) + \bar{b}_i b_j - b_j \bar{a}_{ji} \phi_0(\nu) \\
&- \bar{b}_j \bar{a}_{ji} \nu^2 \phi_1(\nu) - \bar{b}_j b_i\big) \sum_{J=1}^{d} \mathrm{d}f_i^J \wedge \mathrm{d}f_j^J. \qquad (2.25)
\end{aligned}
$$

The conditions (2.18) yield

$$
\sum_{J=1}^{d} \mathrm{d}q_{n+1}^J \wedge \mathrm{d}\dot{q}_{n+1}^J = \sum_{J=1}^{d} \mathrm{d}q_n^J \wedge \mathrm{d}\dot{q}_n^J.
$$

This completes the proof. □

It is noted that, when $\omega \to 0$ ($v \to 0$), the symplecticity conditions (2.18) for ARKN integrators become those for the classical RKN methods. Consequently, an SARKN integrator reduces to a classical symplectic RKN method.

2.2.2 Existence of Symplectic ARKN Integrators

With the symplecticity conditions (2.18), in order to determine SARKN methods, we assume that no b_i or $\bar{b}_i$ in (2.17) vanishes. The reason for the assumptions will be clarified below. If $b_j = 0$ for some $j \in \{1, \dots, s\}$, then the first equation in (2.18) implies that $\bar{b}_j = 0$, and from the third equation in (2.18) we have

$$
\big(b_i \phi_0(\nu) + \nu^2 \bar{b}_i \phi_1(\nu)\big) \bar{a}_{ij} = 0, \qquad (2.26)
$$

for $i = 1, \dots, s$.

From the first equation in (2.18), it follows that

$$
\bar{b}_i = \frac{\phi_1(\nu) - c_i \phi_0(\nu)}{\phi_0(\nu) + c_i \nu^2 \phi_1(\nu)} b_i, \qquad (2.27)
$$

and then

$$
b_i \phi_0(\nu) + \nu^2 \bar{b}_i \phi_1(\nu) = b_i \phi_0(\nu) + \nu^2 \frac{\phi_1(\nu) - c_i \phi_0(\nu)}{\phi_0(\nu) + c_i \nu^2 \phi_1(\nu)} \phi_1(\nu) b_i
$$

$$= \frac{b_i}{\phi_0(\nu) + c_i\nu^2\phi_1(\nu)} = \frac{\bar{b}_i}{\phi_1(\nu) - c_i\phi_0(\nu)},$$

which, together with (2.26), implies $\bar{a}_{ij} = 0$ for i such that $b_i \neq 0$ and $\bar{b}_i \neq 0$. Hence, the jth stage has no contribution to the updates in (2.17), or to the ith internal stages with nontrivial b_i and $\bar{b}_i$. Therefore, the method becomes one with fewer stages. Moreover, we have the following result.

Theorem 2.5 *An s-stage symplectic ARKN method has a Butcher tableau of coefficients of the form*

$$\begin{array}{c|ccccc}
c_s & \bar{a}_{11} & \bar{a}_{12} & \bar{a}_{13} & \cdots & \bar{a}_{1s} \\
c_s & \frac{b_1}{b_2}\bar{a}_{12} & \bar{a}_{22} & \bar{a}_{23} & \cdots & \bar{a}_{2s} \\
c_s & \frac{b_1}{b_3}\bar{a}_{13} & \frac{b_2}{b_3}\bar{a}_{23} & \bar{a}_{33} & \cdots & \bar{a}_{3s} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & \frac{b_1}{b_s}\bar{a}_{1s} & \frac{b_2}{b_s}\bar{a}_{2s} & \frac{b_3}{b_s}\bar{a}_{3s} & \cdots & \bar{a}_{ss} \\
\hline
\bar{b} & Kb_1 & Kb_2 & Kb_3 & \cdots & Kb_s \\
\hline
b & b_1 & b_2 & b_3 & \cdots & b_s
\end{array}$$

where $b_i \neq 0,\ i = 1, \ldots, s$, *and* $K = \frac{\phi_1(\nu) - c_s\phi_0(\nu)}{\phi_0(\nu) + c_s\nu^2\phi_1(\nu)}$.

Proof From the second equation in (2.18), it follows that

$$b_i\bar{b}_j - \big(b_i\phi_0(\nu) + \nu^2\bar{b}_i\phi_1(\nu)\big)\bar{a}_{ij} = b_j\bar{b}_i - \big(b_j\phi_0(\nu) + \nu^2\bar{b}_j\phi_1(\nu)\big)\bar{a}_{ji}, \quad i, j = 1, \ldots, s. \tag{2.28}$$

Comparing (2.28) with the third equation in (2.18) yields

$$b_i\bar{b}_j = b_j\bar{b}_i, \quad i, j = 1, \ldots, s. \tag{2.29}$$

Multiplying both sides of the first equation in (2.18) by b_s, we have

$$\bar{b}_i b_s\big(\phi_0(\nu) + \nu^2 c_i\phi_1(\nu)\big) = b_i b_s\big(\phi_1(\nu) - c_i\phi_0(\nu)\big), \quad i = 1, \ldots, s. \tag{2.30}$$

Substituting (2.29) with $j = s$ into (2.30) gives

$$\bar{b}_s\big(\phi_0(\nu) + \nu^2 c_i\phi_1(\nu)\big) = b_s\big(\phi_1(\nu) - c_i\phi_0(\nu)\big). \tag{2.31}$$

On the other hand, the first equation in (2.18) gives

$$\bar{b}_s\big(\phi_0(\nu) + \nu^2 c_s\phi_1(\nu)\big) = b_s\big(\phi_1(\nu) - c_s\phi_0(\nu)\big). \tag{2.32}$$

Denoting

$$M_i = \phi_0(\nu) + \nu^2 c_i \phi_1(\nu), \qquad N_i = \phi_1(\nu) - c_i \phi_0(\nu), \quad i = 1, \ldots, s,$$

(2.31) and (2.32) then become

$$\begin{cases} \bar{b}_s M_i = b_s N_i, \\ b_s N_s = \bar{b}_s M_s. \end{cases} \tag{2.33}$$

Since $b_s \neq 0$ and $\bar{b}_s \neq 0$, the multiplication of the two equations in (2.33) leads to

$$N_s M_i = M_s N_i,$$

i.e.,

$$\big(\phi_1(\nu) - c_s\phi_0(\nu)\big)\big(\phi_0(\nu) + \nu^2 c_i \phi_1(\nu)\big) = \big(\phi_0(\nu) + \nu^2 c_s \phi_1(\nu)\big)\big(\phi_1(\nu) - c_i \phi_0(\nu)\big),$$

which implies that

$$(c_i - c_s)\big(\phi_0^2(\nu) + \nu^2 \phi_1^2(\nu)\big) = 0.$$

From $\phi_0^2(\nu) + \nu^2\phi_1^2(\nu) = 1$, it follows that $c_i = c_s$, $i = 1, \ldots, s-1$. By (2.27), we obtain

$$\bar{b}_i = K b_i$$

with

$$K = \frac{\phi_1(\nu) - c_s\phi_0(\nu)}{\phi_0(\nu) + c_s \nu^2 \phi_1(\nu)}$$

and the third equation in (2.18) becomes

$$b_i\big(\phi_0(\nu) + \nu^2 K \phi_1(\nu)\big)\bar{a}_{ij} = b_j\big(\phi_0(\nu) + \nu^2 K \phi_1(\nu)\big)\bar{a}_{ji}, \tag{2.34}$$

for $i, j = 1, \ldots, s$. Since $\phi_0(\nu) + \nu^2 K \phi_1(\nu) \neq 0$, we have $\bar{a}_{ji} = \frac{b_i}{b_j}\bar{a}_{ij}$ for all $i \leq j$. □

Theorem 2.6 *The order of an SARKN method cannot exceed two.*

Proof From Theorem 2.3, an s-stage ARKN method has order two if and only if

$$\sum_{i=1}^{s} b_i = \phi_1(\nu) + \mathscr{O}\big(h^2\big), \tag{2.35}$$

$$\sum_{i=1}^{s} b_i c_i = \phi_2(\nu) + \mathscr{O}(h), \tag{2.36}$$

$$\sum_{i=1}^{s} \bar{b}_i = \phi_2(\nu) + \mathscr{O}(h). \tag{2.37}$$

The condition (2.36) means

$$\sum_{i=1}^{s} b_i c_i = c_s \sum_{i=1}^{s} b_i = c_s\big(\phi_1(\nu) + \mathscr{O}\big(h^2\big)\big) = \phi_2(\nu) + \mathscr{O}(h),$$

which implies $c_s = \frac{1}{2}$.

From the proof of Theorem 2.5, we have $c_i = c_s = \frac{1}{2}$ for $i < s$. Thus, (2.37) contradicts the following third-order condition:

$$\sum_{i=1}^{s} \bar{b}_i c_i = \phi_3(\nu) + \mathscr{O}(h).$$

Therefore, an SARKN method cannot be of order three. □

Theorem 2.7 *An explicit SARKN method can only have one stage.*

Proof For an explicit method, $\bar{a}_{ij} = 0$ for all $i \le j$. Then from Theorem 2.5 it follows that $\bar{a}_{ji} = \frac{b_i}{b_j}\bar{a}_{ij} = 0$ for all $i \le j$, implying that $\bar{a}_{ij} = 0$ for $i, j = 1, \dots, s$.

On the other hand, Theorem 2.5 shows $c_i = c_s$ for all i. Therefore, an arbitrary s-stage explicit SARKN method is equivalent to a one-stage method. The proof is complete. □

From the second-order conditions (2.35)–(2.37) and the symplecticity conditions (2.18), we obtain a one-stage explicit SARKN method of order two:

$$\begin{array}{c|c} 1/2 & 0 \\ \hline \bar{b} & K\phi_1(\nu) \\ \hline b & \phi_1(\nu) \end{array} \tag{2.38}$$

where

$$K = \frac{\phi_1(\nu) - \frac{1}{2}\phi_0(\nu)}{\phi_0(\nu) + \frac{1}{2}\nu^2\phi_1(\nu)}.$$

This method (2.38) is denoted SARKN1s2.

When $\nu \to 0$, the scheme reduces to the Störmer–Verlet method:

$$\begin{array}{c|c} 1/2 & 0 \\ \hline \bar{b} & 1/2 \\ \hline b & 1 \end{array} \tag{2.39}$$

Furthermore, by the second-order conditions (2.35)–(2.37), the symplecticity conditions (2.18) and one of the third-order conditions

$$\sum_{i=1}^{s} b_i \bar{a}_{ij} = \phi_3(\nu) + \mathscr{O}(h),$$

we obtain a one-stage implicit SARKN method of order two:

$$\begin{array}{c|c} 1/2 & 1/6 \\ \hline \bar{b} & K\phi_1(\nu) \\ \hline b & \phi_1(\nu) \end{array}$$

where

$$K = \frac{\phi_1(\nu) - \frac{1}{2}\phi_0(\nu)}{\phi_0(\nu) + \frac{1}{2}\nu^2\phi_1(\nu)}.$$

2.2.3 Phase and Stability Properties of Method SARKN1s2

In what follows, we are concerned with the phase and stability properties of the method SARKN1s2.

For classical RKN methods, the stability properties are analyzed usually by applying the methods to the second-order homogeneous linear test model

$$\ddot{q} = -\lambda^2 q, \quad \lambda > 0.$$

Since ARKN methods are frequency-dependent, similar to Van der Houwen et al.'s approach in [12], we consider the reformed linear test equation

$$\ddot{q} + \omega^2 q = -\varepsilon q, \quad \omega^2 + \varepsilon > 0, \tag{2.40}$$

where $\varepsilon = \lambda^2 - \omega^2$ represents the error of an estimate ω of the frequency λ. An application of the ARKN method (2.3) to (2.40) yields

$$\begin{cases} Q = eq_n + hc\dot{q}_n - \left(\nu^2 + z\right)\bar{A}Q, \quad z = \varepsilon h^2,\ \nu = \omega h, \\ q_{n+1} = \phi_0(\nu)q_n + \phi_1(\nu)h\dot{q}_n - z\bar{b}^{\mathrm{T}}(\nu)Q, \\ h\dot{q}_{n+1} = -\nu^2\phi_1(\nu)q_n + \phi_0(\nu)h\dot{q}_n - zb^{\mathrm{T}}(\nu)Q. \end{cases} \tag{2.41}$$

The numerical solution gives the recursion

$$\begin{pmatrix} q_{n+1} \\ h\dot{q}_{n+1} \end{pmatrix} = R\left(\nu^2, z\right)\begin{pmatrix} q_n \\ h\dot{q}_n \end{pmatrix},$$

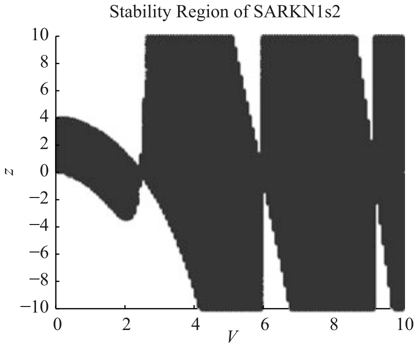

Fig. 2.1 Stability region of the symplectic explicit ARKN method SARKN1s2. Reprinted from Ref. [14], Copyright 2012, with permission from Elsevier

where the stability matrix

$$R(\nu^2, z) = \begin{pmatrix} \phi_0(\nu) - z\bar{b}^{\mathrm{T}}(\nu)N^{-1}e & \phi_1(\nu) - z\bar{b}^{\mathrm{T}}(\nu)N^{-1}c \\ -\nu^2\phi_1(\nu) - zb^{\mathrm{T}}(\nu)N^{-1}e & \phi_0(\nu) - zb^{\mathrm{T}}(\nu)N^{-1}c \end{pmatrix},$$
$$N = I + (\nu^2 + z)\bar{A}. \tag{2.42}$$

The phase and stability properties of the numerical solution are characterized by the eigenvalues or the spectrum of the matrix $R(\nu^2, z)$. Thus we consider the characteristic equation

$$\xi^2 - \mathrm{tr}(R(\nu^2, z))\xi + \det(R(\nu^2, z)) = 0.$$

Definition 2.2 For an ARKN method with $R(\nu^2, z)$ given by (2.42), the set in the ν–z plane

$$R_s = \{(v, z) | v > 0, \rho(R(\nu^2, z)) < 1\}$$

is called the *stability region* of the method.

The stability region of the method SARKN1s2 (2.38) is depicted in Fig. 2.1.

For the integration of oscillatory problems, it is important to analyze the phase properties (dispersion and dissipation) of the numerical methods. See, e.g., [11] for details.

Definition 2.3 For the ARKN method (2.1) with the stability matrix $R(\nu^2, z)$ given by (2.42), the following two quantities are called the *dispersion* and the *dissipation* of the method, respectively:

$$P(\zeta) = \zeta - \arccos\left(\frac{\mathrm{tr}(R(\nu^2, z))}{2\sqrt{\det(R(\nu^2, z))}}\right), \qquad D(\zeta) = 1 - \sqrt{\det(R(\nu^2, z))},$$

where $\zeta = \sqrt{\nu^2 + z}$. The method is said to be *dispersive of order* q and *dissipative of order* r, if $P(\zeta) = \mathcal{O}(\zeta^{q+1})$ and $D(\zeta) = \mathcal{O}(\zeta^{r+1})$, respectively. If $P(\zeta) = 0$

and $D(\zeta) = 0$, then the method is said to be *zero-dispersive* and *zero-dissipative*, respectively.

For the symplectic ARKN method SARKN1s2 given by (2.38), we have

$$P(\zeta) = -\frac{\varepsilon^2\zeta^3}{24(\varepsilon^2 + \omega^2)} + \mathscr{O}(\zeta^5),$$

which shows that the method is dispersive of order two.

For symplectic ARKN methods, we have $\det(R) = 1$ and hence the method SARKN1s2 is zero-dissipative.

2.2.4 Nonexistence of Symmetric ARKN Methods

In Hairer et al. [9], it is shown that symmetric methods have excellent long-time behavior when solving reversible differential equations. Thus we would like to find ARKN methods that are symmetric. Unfortunately, it will be seen in this subsection that no ARKN method can be symmetric.

Definition 2.4 A numerical one-step method Φ_h is said to be *symmetric* or *time-reversible* if it satisfies

$$\Phi_h \circ \Phi_{-h} = id(\text{the identity map}) \quad \text{i.e.,} \quad \Phi_h = \Phi_{-h}^{-1}. \tag{2.43}$$

The map Φ_{-h}^{-1} is called the *adjoint method* of Φ_h and is denoted by Φ_h^* (see [9]).

Theorem 2.8 *The adjoint method* (*denoted by the coefficients* $a_{ij}^*, b_j^*, \bar{b}_j^*$ *and* c_j^*) *of an s-stage ARKN method* (2.3) *with stepsize h for* (2.16) *cannot be an ARKN method. That is to say, no symmetric ARKN method exists.*

Proof Exchanging $q_{n+1} \leftrightarrow q_n$, $\dot{q}_{n+1} \leftrightarrow \dot{q}_n$ and replacing h by $-h$ in the ARKN formula (2.17) yields

$$\begin{cases} Q_i^* = q_{n+1} - c_i h\dot{q}_{n+1} + h^2 \displaystyle\sum_{j=1}^{s} \bar{a}_{ij}\big(f\big(Q_j^*\big) - \omega^2 Q_j^*\big), \quad i = 1, \dots, s, \\ q_n = \phi_0(\nu)q_{n+1} - h\phi_1(\nu)\dot{q}_{n+1} + h^2 \displaystyle\sum_{i=1}^{s} \bar{b}_i(\nu)f\big(Q_i^*\big), \\ \dot{q}_n = \omega\nu\phi_1(\nu)q_{n+1} + \phi_0(\nu)\dot{q}_{n+1} - h \displaystyle\sum_{i=1}^{s} b_i(\nu)f\big(Q_i^*\big). \end{cases} \tag{2.44}$$

From (2.44), it follows that

$$\begin{cases} q_{n+1} = \phi_0(\nu)q_n + h\phi_1(\nu)\dot{q}_n + h^2 \sum_{i=1}^{s} \big(\phi_1(\nu)b_i(\nu) - \phi_0(\nu)\bar{b}_i(\nu)\big) f\big(Q_i^*\big), \\ \dot{q}_{n+1} = -\omega\nu\phi_1(\nu)q_n + \phi_0(\nu)\dot{q}_n + h \sum_{i=1}^{s} \big(\phi_0(\nu)b_i(\nu) + \nu^2\phi_1(\nu)\bar{b}_i(\nu)\big) f\big(Q_i^*\big), \\ Q_i^* = \big(\phi_0(\nu) + c_i\nu^2\phi_1(\nu)\big)q_n + \big(\phi_1(\nu) - c_i\phi_0(\nu)\big)h\dot{q}_n - h^2 \sum_{j=1}^{s} \bar{a}_{ij}\omega^2 Q_j^* \\ \qquad + h^2 \sum_{j=1}^{s} \big(\bar{a}_{ij} - c_i\big(\phi_0(\nu)b_j(\nu) + \nu^2\phi_1(\nu)\bar{b}_j(\nu)\big) \\ \qquad + \big(\phi_1(\nu)b_j(\nu) - \phi_0(\nu)\bar{b}_j(\nu)\big)\big) f\big(Q_j^*\big), \quad i = 1, \dots, s. \end{cases} \tag{2.45}$$

Replace all indices i and j in (2.45) by $s+1-i$ and $s+1-j$, respectively. If the adjoint method (2.45) of the s-stage ARKN method (2.3) were again an s-stage ARKN method, then the coefficients of (2.45) would satisfy the following conditions:

$$\begin{cases} \bar{b}_i^*(\nu) = \phi_1(\nu)b_{s+1-i}(\nu) - \phi_0(\nu)\bar{b}_{s+1-i}(\nu), \\ b_i^*(\nu) = \phi_0(\nu)b_{s+1-i}(\nu) + \nu^2\phi_1(\nu)\bar{b}_{s+1-i}(\nu), \\ 1 = \phi_0(\nu) + c_{s+1-i}\nu^2\phi_1(\nu), \\ c_i^* = \phi_1(\nu) - c_{s+1-i}\phi_0(\nu), \\ \bar{a}_{ij}^* = \bar{a}_{s+1-i,s+1-j}, \\ \bar{b}_j^*(\nu) = c_{s+1-i}b_j^*(\nu). \end{cases} \tag{2.46}$$

Since c_i $(i = 1, \dots, s)$ are constants, the third condition in (2.46) cannot be valid. The proof is complete. □

2.2.5 Numerical Experiments

In this subsection, the effectiveness of the one-stage explicit symplectic ARKN method SARKN1s2 is shown for three Hamiltonian systems, compared with a symplectic exponentially fitted modified RKN method, a symplectic RKN scheme and the Störmer–Verlet method (2.39) as listed below:

- S-V: the symplectic Störmer–Verlet method (2.39) of order two.
- SRKN3s4: the symplectic three-stage RKN scheme of order four given in [9].
- SEFRKN2s2: the symplectic exponentially fitted modified two-stage RKN method of order two with the FSAL technique developed in [15].
- SARKN1s2: the one-stage explicit SARKN method (2.38) of order two proposed in this chapter.

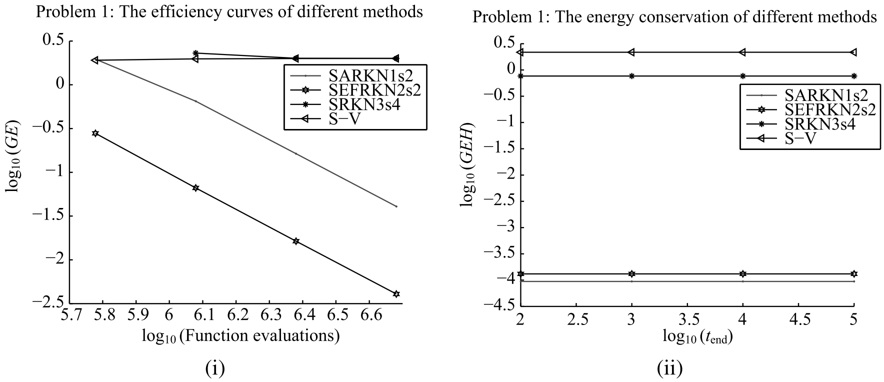

Fig. 2.2 Problem 2.1. (**i**) The logarithm of the maximum global error (GE) over the integration interval against the logarithm of the number of function evaluations. (**ii**) The logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t_{\text{end}})$. Reprinted from Ref. [14], Copyright 2012, with permission from Elsevier

Problem 2.1 Consider the Duffing equation

$$\ddot{q} + \omega^2 q = 2k^2 q^3 - k^2 q$$

with the parameters $\omega = 5$ and $k = 0.03$.

This is a Hamiltonian system with the Hamiltonian

$$H(p, q) = \frac{1}{2} p^2 + \frac{1}{2}\left(\omega^2 + k^2\right) q^2 - \frac{k^2}{2} q^4.$$

Given the initial values $q(0) = 0$, $\dot{q}(0) = \omega$, the exact solution is the Jacobian elliptic function $q(t) = sn(\omega t; k/\omega)$.

We first integrate the problem on the interval [0, 10^5] with the stepsizes $h = \frac{1}{3 \cdot 2^i}$, $i = 1, 2, 3, 4$ for the one-stage methods SARKN1s2, S-V and the two-stage method SEFRKN2s2 of FSAL-type, and stepsizes $3h$ for the three-stage method SRKN3s4. The efficiency curves are presented in Fig. 2.2(i). Then we integrate the problem with the stepsize $h = 1/6$ on different intervals $[0, t_{\text{end}}]$, $t_{\text{end}} = 10^i$, $i = 2, 3, 4, 5$. The errors of the Hamiltonian are shown in Fig. 2.2(ii).

Problem 2.2 Consider the Fermi–Pasta–Ulam (FPU [2]) problem in [8, 9] by Hairer et al.

The problem is a well-known model in statistical mechanics which reveals highly unexpected dynamical behavior. By a transformation of variables, the model can be cast into a Hamiltonian system with the Hamiltonian

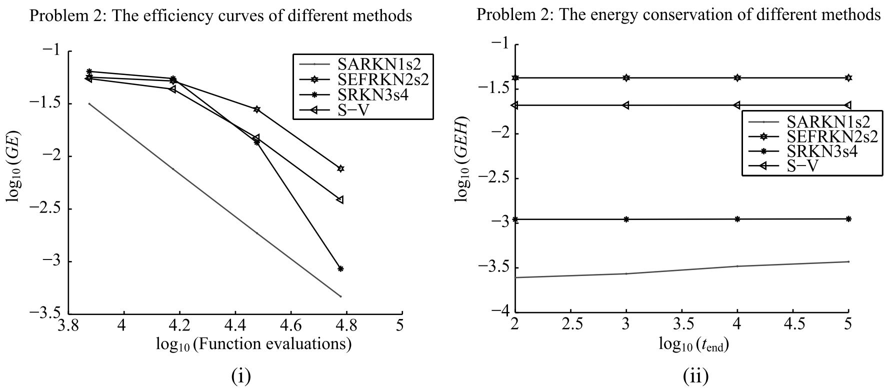

Fig. 2.3 Problem 2.2. (**i**) The logarithm of the maximum global error (GE) over the integration interval against the logarithm of the number of function evaluations. (**ii**) The logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t_{\text{end}})$. Reprinted from Ref. [14], Copyright 2012, with permission from Elsevier

$$H(y,x) = \frac{1}{2}\sum_{i=1}^{2m} y_i^2 + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{m+i}^2 + \frac{1}{4}\Bigg((x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4\Bigg),$$

where ω is assumed to be large, x_i represents a scaled displacement of the ith stiff spring, x_{m+i} is a scaled expansion (or compression) of the ith stiff spring, and y_i, y_{m+i} are their velocities (or momenta). The system is equivalent to the second-order oscillatory system

$$\ddot{x} + Kx = -\nabla U(x),$$

where

$$K = \begin{pmatrix} \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathbf{0}_{m\times m} & \omega^2 I_{m\times m} \end{pmatrix}$$

and

$$U(x) = \frac{1}{4}\Bigg((x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4\Bigg).$$

In the experiment, we choose $m = 3$, $\omega = 50$, $x_1(0) = 1$, $y_1(0) = 1$, $x_4(0) = \frac{1}{\omega}$, $y_4(0) = 1$, and zero for the remaining initial values.

Figure 2.3(i) shows the efficiency curves on the interval $[0, 50]$ with the stepsizes $h = \frac{1}{75\cdot 2^i}$, $i = 1, 2, 3, 4$ for one-stage methods SARKN1s2, S-V and the two-stage method SEFRKN2s2 of FSAL-type, and stepsizes $3h$ for the three-stage method SRKN3s4. Then the problem is integrated on the interval $[0, t_{\text{end}}]$, $t_{\text{end}} = 10^i$,

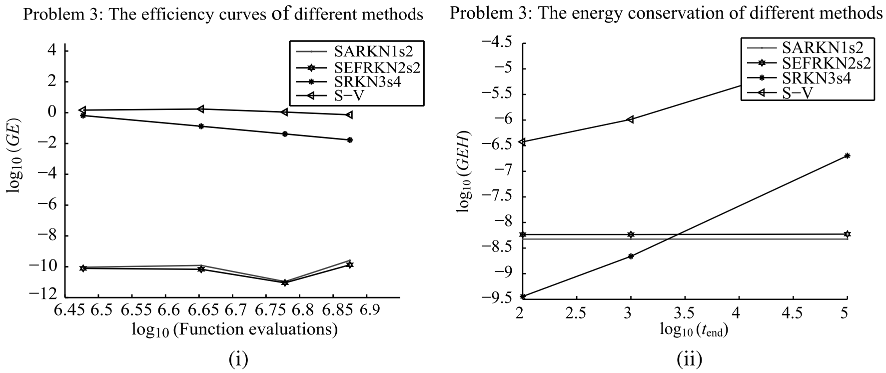

Fig. 2.4 Problem 2.3. (**i**) The logarithm of the maximum global error (GE) over the integration interval against the logarithm of the number of function evaluations. (**ii**) The logarithm of the maximum global error of Hamiltonian $GEH = \max |H_n - H_0|$ against $\log_{10}(t_{\text{end}})$. Reprinted from Ref. [14], Copyright 2012, with permission from Elsevier

$i = 2, 3, 4, 5$ with the stepsize $h = 0.008$. The global errors of the Hamiltonian are presented in Fig. 2.3(ii).

Problem 2.3 Consider the "almost periodic" orbital problem in [6] by Franco and Palacios

$$\ddot{z} + z = \varepsilon e^{i\psi t}, \quad z(0) = 1,\ \dot{z}(0) = i,\ z \in \mathbb{C},$$

or equivalently,

$$\begin{aligned}
\ddot{u} + u &= \varepsilon \cos(\psi t), \quad u(0) = 1,\ \dot{u}(0) = 0, \\
\ddot{v} + v &= \varepsilon \sin(\psi t), \quad v(0) = 0,\ \dot{v}(0) = 1,
\end{aligned}$$

where $\varepsilon = 0.001$, $\psi = 0.01$. The true solution of the problem is

$$z(t) = u(t) + iv(t),$$

where

$$\begin{aligned}
u(t) &= \frac{1 - \varepsilon - \psi^2}{1 - \psi^2}\cos(t) + \frac{\varepsilon}{1 - \psi^2}\cos(\psi t), \\
v(t) &= \frac{1 - \varepsilon\psi - \psi^2}{1 - \psi^2}\sin(t) + \frac{\varepsilon}{1 - \psi^2}\sin(\psi t).
\end{aligned}$$

The Hamiltonian for the system is

$$H = \frac{\dot{u}^2 + \dot{v}^2}{2} + \frac{u^2 + v^2}{2} - \varepsilon\cos(\psi t)u - \varepsilon\sin(\psi t)v.$$

The problem is integrated on the interval $[0, 10^5]$ with the stepsizes $h = 0.2/3i$, $i = 2, 3, 4, 5$ for one-stage methods SARKN1s2, S-V and the two-stage method SEFRKN2s2 of FSAL-type, and stepsizes $3h$ for the three-stage method SRKN3s4. The global errors of solutions are displayed in Fig. 2.4(i). Then the problem is integrated on the intervals $[0, 10^i]$, $i = 2, 3, 4, 5$ with the stepsize $h = \frac{1}{24}$. The errors of the Hamiltonian are presented in Fig. 2.4(ii).

In the above experiments, for Duffing equation, the method SEFRKN2s2 is more efficient than the method SARKN1s2, however, for the FPU problem, SARKN1s2 is more efficient than SEFRKN2s2. For the "almost periodic" orbital problem, the two methods have almost the same efficiency. Concerning the preservation of the Hamiltonian function, the method SARKN1s2 shows better behavior than the other three symplectic methods. The Hamiltonian of Problem 3 is not constant but is time-dependent. The Hamiltonian errors of the methods SARKN1s2 and SEFRKN2s2 are smaller than those of the other two methods.

2.3 Multidimensional ARKN Methods

Many systems of second-order differential equations arising in applications have the general form

$$\begin{cases} y'' + My = f\left(y, y'\right), \\ y(x_0) = y_0, \quad y'(x_0) = y_0', \end{cases} \tag{2.47}$$

where $M \in \mathbb{R}^{d\times d}$ is a positive semi-definite matrix (not necessarily diagonal nor symmetric, in general) that implicitly contains the main frequencies of the oscillatory problem, and $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$.

In the particular case where $M \in \mathbb{R}^{d\times d}$ is a symmetric and positive semi-definite matrix, Franco [4] is the first to attempt to extend his ARKN methods in [5] for the scalar equation (2.1) to the system (2.47) with the perturbed function f not depending on the first derivative y'. But his order conditions of the methods are based on the one-dimensional theory.

The purpose of this section is to give a standard form of the multidimensional ARKN integrators for systems of second-order oscillatory equations and to derive the order conditions via the Nyström tree theory.

2.3.1 Formulation of the Scheme

Let

$$u(x) = \left(y(x)^{\mathrm{T}}, y'(x)^{\mathrm{T}}\right)^{\mathrm{T}}, \quad u_0 = \left(y_0^{\mathrm{T}}, y_0'^{\mathrm{T}}\right)^{\mathrm{T}},$$

$$G\big(u(x)\big) = \big(0^{\mathrm{T}}, f\big(u(x)\big)^{\mathrm{T}}\big)^{\mathrm{T}} = \big(0^{\mathrm{T}}, f\big(y(x), y'(x)\big)^{\mathrm{T}}\big)^{\mathrm{T}},$$

and

$$W = \begin{pmatrix} \mathbf{0} & I_d \\ -M & \mathbf{0} \end{pmatrix}.$$

Then the initial value problem (2.47) can be rewritten in a more compact form as

$$\begin{cases} u' = Wu + G(u), \\ u(x_0) = u_0, \end{cases} \tag{2.48}$$

which is a system of first-order nonhomogeneous differential equations, where W is a $2d \times 2d$ constant matrix. From the well-known variation-of-constants formula, the solution at $x \geq x_0$ of the system (2.48) has the form

$$u(x) = \exp\big((x - x_0)W\big)u_0 + \int_{x_0}^{x} \exp\big((x - \xi)W\big)G\big(u(\xi)\big)\,\mathrm{d}\xi. \tag{2.49}$$

Here and hereafter, the integral of a matrix-valued or vector-valued function is understood componentwise.

The following matrix-variation-of-constants formula gives a significant insight into the structure of the solution to the system (2.47), which motivates the formulation of multidimensional ARKN scheme.

Theorem 2.9 (Wu et al. [19]) *The exact solution of* (2.47) *and its derivative satisfy*

$$\begin{cases} y(x) = \phi_0\big((x - x_0)^2 M\big)y_0 + (x - x_0)\phi_1\big((x - x_0)^2 M\big)y_0' \\ \qquad\qquad + \displaystyle\int_{x_0}^{x} (x - \xi)\phi_1\big((x - \xi)^2 M\big)\hat{f}(\xi)\,\mathrm{d}\xi, \\ y'(x) = -(x - x_0)M\phi_1\big((x - x_0)^2 M\big)y_0 + \phi_0\big((x - x_0)^2 M\big)y_0' \\ \qquad\qquad + \displaystyle\int_{x_0}^{x} \phi_0\big((x - \xi)^2 M\big)\hat{f}(\xi)\,\mathrm{d}\xi \end{cases} \tag{2.50}$$

for $x_0, x \in (-\infty, +\infty)$, *where* $\hat{f}(\xi) = f(y(\xi), y'(\xi))$ *and the* matrix-valued *functions* $\phi_0(M)$ *and* $\phi_1(M)$ *are defined by*

$$\phi_0(M) = \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k)!}, \qquad \phi_1(M) = \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k+1)!}. \tag{2.51}$$

Proof It is easy to see that

$$W^2 = \begin{pmatrix} -M & \mathbf{0} \\ \mathbf{0} & -M \end{pmatrix}, \qquad W^3 = \begin{pmatrix} \mathbf{0} & -M \\ M^2 & \mathbf{0} \end{pmatrix}.$$

An argument by induction yields the result that, for every nonnegative integer k,

$$W^k = (-1)^{\lfloor k/2\rfloor} \begin{pmatrix} \frac{1+(-1)^k}{2} M^{\lfloor k/2\rfloor} & \frac{1-(-1)^k}{2} M^{\lfloor k/2\rfloor} \\ -M\frac{1-(-1)^k}{2} M^{\lfloor k/2\rfloor} & \frac{1+(-1)^k}{2} M^{\lfloor k/2\rfloor} \end{pmatrix},$$

where $\lfloor k/2\rfloor$ stands for the integer part of $k/2$. Then

$$\begin{aligned}
&\exp\bigl((x-x_0)W\bigr) \\
&= \begin{pmatrix} I_d - \frac{(x-x_0)^2 M}{2!} + \frac{(x-x_0)^4 M^2}{4!} + \cdots & (x-x_0)I_d - \frac{(x-x_0)^3 M}{3!} + \cdots \\ -(x-x_0)M + \frac{(x-x_0)^3 M^2}{3!} + \cdots & I_d - \frac{(x-x_0)^2 M}{2!} + \frac{(x-x_0)^4 M^2}{4!} + \cdots \end{pmatrix} \\
&= \begin{pmatrix} \phi_0((x-x_0)^2 M) & (x-x_0)\phi_1((x-x_0)^2 M) \\ -(x-x_0)M\phi_1((x-x_0)^2 M) & \phi_0((x-x_0)^2 M) \end{pmatrix},
\end{aligned}$$

and (2.49) becomes

$$\begin{aligned}
\begin{pmatrix} y(x) \\ y'(x) \end{pmatrix} &= \begin{pmatrix} \phi_0((x-x_0)^2 M) & (x-x_0)\phi_1((x-x_0)^2 M) \\ -(x-x_0)M\phi_1((x-x_0)^2 M) & \phi_0((x-x_0)^2 M) \end{pmatrix} \begin{pmatrix} y_0 \\ y_0' \end{pmatrix} \\
&\quad + \int_{x_0}^{x} \begin{pmatrix} \phi_0((x-\xi)^2 M) & (x-\xi)\phi_1((x-\xi)^2 M) \\ -(x-\xi)M\phi_1((x-\xi)^2 M) & \phi_0((x-\xi)^2 M) \end{pmatrix} \\
&\quad \times \begin{pmatrix} 0 \\ f(y(\xi), y'(\xi)) \end{pmatrix} \mathrm{d}\xi \\
&= \begin{pmatrix} \phi_0((x-x_0)^2 M)y_0 + (x-x_0)\phi_1((x-x_0)^2 M)y_0' \\ \phi_0((x-x_0)^2 M)y_0' - (x-x_0)M\phi_1((x-x_0)^2 M)y_0 \end{pmatrix} \\
&\quad + \begin{pmatrix} \int_{x_0}^{x} (x-\xi)\phi_1((x-\xi)^2 M)\hat{f}(\xi)\,\mathrm{d}\xi \\ \int_{x_0}^{x} \phi_0((x-\xi)^2 M)\hat{f}(\xi)\,\mathrm{d}\xi \end{pmatrix}.
\end{aligned}$$

This is exactly the vector form of (2.50). The proof is complete. □

The variation-of-constants formula, which is free from the decomposition of M, first appeared in [19] by Wu et al. Clearly, if $y(x_n)$ and $y'(x_n)$ are prescribed, it follows from (2.50) that

$$\begin{cases} y(x_n+h) = \phi_0(V)y(x_n) + h\phi_1(V)y'(x_n) \\ \qquad\qquad + \displaystyle\int_{x_n}^{x_n+h} (x_n+h-\xi)\phi_1\bigl((x_n+h-\xi)^2 M\bigr)\hat{f}(\xi)\,\mathrm{d}\xi, \\ y'(x_n+h) = -hM\phi_1(V)y(x_n) + \phi_0(V)y'(x_n) \\ \qquad\qquad + \displaystyle\int_{x_n}^{x_n+h} \phi_0\bigl((x_n+h-\xi)^2 M\bigr)\hat{f}(\xi)\,\mathrm{d}\xi, \end{cases} \tag{2.52}$$

where $V = h^2 M$. With the change of variable $\xi = x_n + hz$, the formula (2.52) can be written as

$$\begin{cases} y(x_n+h) = \phi_0(V)y(x_n) + h\phi_1(V)y'(x_n) \\ \qquad\qquad + h^2 \int_0^1 (1-z)\phi_1\big((1-z)^2 V\big)\hat{f}(x_n+hz)\,\mathrm{d}z, \\ y'(x_n+h) = -hM\phi_1(V)y(x_n) + \phi_0(V)y'(x_n) \\ \qquad\qquad + h\int_0^1 \phi_0\big((1-z)^2 V\big)\hat{f}(x_n+hz)\,\mathrm{d}z. \end{cases} \tag{2.53}$$

Approximating the two integrals in (2.53) by suitable quadrature formulae results in the following scheme for multidimensional problems (2.47).

Definition 2.5 An s-stage *multidimensional ARKN method* for solving the oscillatory system (2.47) is defined as

$$\begin{cases} Y_i = y_n + hc_i y_n' + h^2 \sum_{j=1}^{s} \bar{a}_{ij}\big(f\big(Y_j, Y_j'\big) - MY_j\big), \quad i = 1, \ldots, s, \\ Y_i' = y_n' + h\sum_{j=1}^{s} a_{ij}\big(f\big(Y_j, Y_j'\big) - MY_j\big), \quad i = 1, \ldots, s, \\ y_{n+1} = \phi_0(V)y_n + h\phi_1(V)y_n' + h^2 \sum_{i=1}^{s} \bar{b}_i(V) f\big(Y_i, Y_i'\big), \\ y_{n+1}' = -hM\phi_1(V)y_n + \phi_0(V)y_n' + h\sum_{i=1}^{s} b_i(V) f\big(Y_i, Y_i'\big), \end{cases} \tag{2.54}$$

where c_i, $\bar{a}_{ij}$, a_{ij}, $i, j = 1, \ldots, s$ are constants and the weights $\bar{b}_i(V)$, $b_i(V)$, $i = 1, \ldots, s$ in the updates are real matrix-valued functions of V.

Undoubtedly, the multidimensional ARKN methods are an important improvement on the classical RKN methods since they have the favorable property that they integrate exactly the linear system $y'' + My = \mathbf{0}$.

In the block-matrix notation with Kronecker products, (2.54) can be expressed as

$$\begin{cases} Y = e \otimes y_n + hc \otimes y_n' + h^2(\bar{A} \otimes I_d)\big(f\big(Y, Y'\big) - (I_s \otimes M)Y\big), \\ Y' = e \otimes y_n' + h(A \otimes I_d)\big(f\big(Y, Y'\big) - (I_s \otimes M)Y\big), \\ y_{n+1} = \phi_0(V)y_n + h\phi_1(V)y_n' + h^2\bar{b}^{\mathrm{T}}(V) f\big(Y, Y'\big), \\ y_{n+1}' = -hM\phi_1(V)y_n + \phi_0(V)y_n' + hb^{\mathrm{T}}(V) f\big(Y, Y'\big), \end{cases} \tag{2.55}$$

where e is an $s \times 1$ vector of units, and the block vectors involved are defined by

$$Y = \left(Y_1^{\mathrm{T}}, \ldots, Y_s^{\mathrm{T}}\right)^{\mathrm{T}}, \quad Y' = \left(Y_1'^{\mathrm{T}}, \ldots, Y_s'^{\mathrm{T}}\right)^{\mathrm{T}},$$
$$f\left(Y, Y'\right) = \left(f\left(Y_1, Y_1'\right)^{\mathrm{T}}, \ldots, f\left(Y_s, Y_s'\right)^{\mathrm{T}}\right)^{\mathrm{T}}.$$

2.3.2 Order Conditions

Apart from the functions $\phi_0(M)$ and $\phi_1(M)$ given in (2.51), we define a series of matrix-valued ϕ-functions as follows:

$$\phi_l(M) = \sum_{j=0}^{\infty} \frac{(-1)^j M^j}{(2j+l)!}, \quad l = 2, 3, \ldots. \tag{2.56}$$

This definition was first introduced in [19] by Wu et al. The following interesting properties of these functions are immediate.

Proposition 2.1 *For $l = 0, 1, \ldots,$ the ϕ-functions defined by* (2.51) *and* (2.56) *satisfy the following.*

(i) $\lim_{M \to \mathbf{0}} \phi_l(M) = \frac{1}{l!} I_d$.
(ii) *For any real number α,*

$$\begin{aligned} &\int_0^1 \frac{(1-\xi)\phi_1(\alpha^2(1-\xi)^2 M)\xi^j}{j!}\,\mathrm{d}\xi = \phi_{j+2}\left(\alpha^2 M\right), \\ &\int_0^1 \frac{\phi_0(\alpha^2(1-\xi)^2 M)\xi^j}{j!}\,\mathrm{d}\xi = \phi_{j+1}\left(\alpha^2 M\right). \end{aligned} \tag{2.57}$$

Now we are ready to give the asymptotic expansions of the true solution of the problem (2.47) and its derivative in powers of h as follows:

$$\begin{aligned} y(x_n + h) &= \phi_0(V) y_n + h\phi_1(V) y_n' + \sum_{j=0}^{\infty} h^{j+2} \phi_{j+2}(V) \hat{f}_n^{(j)}, \\ y'(x_n + h) &= -hM\phi_1(V) y_n + \phi_0(V) y_n' + \sum_{j=0}^{\infty} h^{j+1} \phi_{j+1}(V) \hat{f}_n^{(j)}, \end{aligned} \tag{2.58}$$

where $\hat{f}_n^{(j)} = \frac{\mathrm{d}^j}{\mathrm{d}z^j} \hat{f}(z)|_{z=x_n}$ is the jth derivative of $\hat{f}(z)$ at $z = x_n$. In order to prove the first expansion in (2.58), we utilize the series expansion of $\hat{f}(\xi)$ in the integrand of (2.52) to get

$$y(x_n + h) = \phi_0(V) y_n + h\phi_1(V) y_n' + h^2 \int_0^1 (1-z)\phi_1\left((1-z)^2 V\right) \hat{f}(x_n + zh)\,\mathrm{d}z$$

$$
\begin{aligned}
&= \phi_0(V)y_n + h\phi_1(V)y_n' + h^2\int_0^1 (1-z)\phi_1\big((1-z)^2V\big)\sum_{j=0}^{\infty}\frac{h^j}{j!}z^j \hat{f}_n^{(j)}\,\mathrm{d}z \\
&= \phi_0(V)y_n + h\phi_1(V)y_n' \\
&\quad + \sum_{j=0}^{\infty} h^{j+2}\bigg(\int_0^1 (1-z)\phi_1\big((1-z)^2V\big)\frac{z^j}{j!}\,\mathrm{d}z\bigg)\hat{f}_n^{(j)} \\
&= \phi_0(V)y_n + h\phi_1(V)y_n' + \sum_{j=0}^{\infty} h^{j+2}\phi_{j+2}(V)\hat{f}_n^{(j)}.
\end{aligned}
$$

The second expansion in (2.58) can be obtained in a similar way. For $j \geq 2$, $\hat{f}_n^{(j)}$ can be expressed by the series

$$
\begin{aligned}
\hat{f}_n^{(j)} &= \big(\tilde{f}\big(y, y'\big) + My\big)^{(j)}\big|_{x=x_n} \\
&= \sum_{t\in NT_{j+2}} \alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big) + M\sum_{t\in NT_j}\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big),
\end{aligned}
$$

where t is the Nyström tree associated with an elementary differential $\mathscr{F}(t)(y_n, y_n')$ of the function $\tilde{f}(y, y') = f(y, y') - My$ at (y_n, y_n'). Then we have

$$
\begin{aligned}
y(x_n + h) &= \phi_0(V)y_n + h\phi_1(V)y_n' + \sum_{j=0}^{\infty} h^{j+2}\phi_{j+2}(V)\hat{f}_n^{(j)} \\
&= \phi_0(V)y_n + h\phi_1(V)y_n' + \sum_{j=0}^{\infty} h^{j+2}\phi_{j+2}(V)\sum_{t\in NT_{j+2}}\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big) \\
&\quad + h^2M\phi_2(V)y_n + h^3M\phi_3(V)y_n' \\
&\quad + M\sum_{j=2}^{\infty} h^{j+2}\phi_{j+2}(V)\sum_{t\in NT_j}\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big).
\end{aligned}
$$

On the other hand, from II.14 of [10], we have (in the notation of this book)

$$
(Y_i)^{(q+1)}\big|_{h=0} = \sum_{t\in NT_{q+1}} \alpha(t)\gamma(t)\sum_{j=1}^{s}\bar{a}_{ij}\Phi_j(t)\mathscr{F}(t)\big(y_n, y_n'\big),
$$

where $\gamma(t)$ is the density of the Nyström tree t and $\Phi_j(t)$, $j = 1, \ldots, s$ are the elementary weight vectors as defined in Chap. 1. Then we expand the numerical solution as

$$
\begin{aligned}
y_{n+1} &= \phi_0(V)y_n + h\phi_1(V)y_n' + h^2\sum_{i=1}^{s}\bar{b}_i(V)\big(f\big(Y_i, Y_i'\big) - MY_i\big) \\
&\quad + h^2\sum_{i=1}^{s}\bar{b}_i(V)MY_i \\
&= \phi_0(V)y_n + h\phi_1(V)y_n' \\
&\quad + \sum_{j=0}^{\infty}\frac{h^{j+2}}{(j+2)!}\sum_{t\in NT_{j+2}}\gamma(t)\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big) \\
&\quad + h^2M\big(e^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)y_n + h^3M\big(c^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)y_n' \\
&\quad + M\sum_{j=2}^{\infty}\frac{h^{j+2}}{j!}\sum_{t\in NT_j}\gamma(t)\big(\big(\bar{A}\Phi(t)\big)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big).
\end{aligned}
$$

Consequently, the local error of y_{n+1} can be expressed by

$$
\begin{aligned}
e_{n+1} &= y_{n+1} - y(x_n + h) \\
&= \sum_{j=0}^{\infty}h^{j+2}\sum_{t\in NT_{j+2}}\left(\frac{\gamma(t)}{\rho(t)!}\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V) - \phi_{\rho(t)}(V)\right)\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big) \\
&\quad + h^2M\big(\big(e^{\mathrm{T}}\otimes I_d\big)\bar{b}(V) - \phi_2(V)\big)y_n + h^3M\big(\big(c^{\mathrm{T}}\otimes I_d\big)\bar{b}(V) - \phi_3(V)\big)y_n' \\
&\quad + M\sum_{j=2}^{\infty}h^{j+2}\sum_{t\in NT_j}\left(\frac{\gamma(t)}{\rho(t)!}\big(\big(\bar{A}\Phi(t)\big)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V) - \phi_{\rho(t)+2}(V)\right) \\
&\quad \times \alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big).
\end{aligned}
$$

Similarly, we have

$$
\begin{aligned}
y'(x_n + h) &= -hM\phi_1(V)y_n + \phi_0(V)y_n' \\
&\quad + \sum_{j=0}^{\infty}h^{j+1}\phi_{j+1}(V)\sum_{t\in NT_{j+2}}\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big) \\
&\quad + hM\phi_1(V)y_n + h^2M\phi_2(V)y_n' \\
&\quad + M\sum_{j=2}^{\infty}h^{j+1}\phi_{j+1}(V)\sum_{t\in NT_j}\alpha(t)\mathscr{F}(t)\big(y_n, y_n'\big),
\end{aligned}
$$

and

$$
\begin{aligned}
y'_{n+1} &= -hM\phi_1(V)y_n + \phi_0(V)y'_n \\
&\quad + h\sum_{i=1}^{s} b_i(V)\big(f\big(Y_i, Y'_i\big) - MY_i\big) + h\sum_{i=1}^{s} b_i(V)MY_i \\
&= -hM\phi_1(V)y_n + \phi_0(V)y'_n \\
&\quad + \sum_{j=0}^{\infty}\frac{h^{j+1}}{(j+2)!}\sum_{t\in NT_{j+2}}\gamma(t)\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)b(V)\alpha(t)\mathscr{F}(t)\big(y_n, y'_n\big) \\
&\quad + hM\big(e^{\mathrm{T}}\otimes I_d\big)b(V)y_n + h^2M\big(c^{\mathrm{T}}\otimes I_d\big)b(V)y'_n \\
&\quad + M\sum_{j=2}^{\infty}\frac{h^{j+1}}{j!}\sum_{t\in NT_j}\gamma(t)\big(\big(\bar{A}\Phi(t)\big)^{\mathrm{T}}\otimes I_d\big)b(V)\alpha(t)\mathscr{F}(t)\big(y_n, y'_n\big).
\end{aligned}
$$

Then we get the local error of y'_{n+1} as

$$
\begin{aligned}
e'_{n+1} &= y'_{n+1} - y'(x_n + h) \\
&= \sum_{j=0}^{\infty} h^{j+1}\sum_{t\in NT_{j+2}}\left(\frac{\gamma(t)}{\rho(t)!}\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)b(V) - \phi_{\rho(t)-1}(V)\right)\alpha(t)\mathscr{F}(t)\big(y_n, y'_n\big) \\
&\quad + hM\big(\big(e^{\mathrm{T}}\otimes I_d\big)b(V) - \phi_1(V)\big)y_n + V\big(\big(c^{\mathrm{T}}\otimes I_d\big)b(V) - \phi_2(V)\big)y'_n \\
&\quad + M\sum_{j=2}^{\infty} h^{j+1}\sum_{t\in NT_j}\left(\frac{\gamma(t)}{\rho(t)!}\big(\big(\bar{A}\Phi(t)\big)^{\mathrm{T}}\otimes I_d\big)b(V) - \phi_{\rho(t)+1}(V)\right) \\
&\quad \times \alpha(t)\mathscr{F}(t)\big(y_n, y'_n\big).
\end{aligned}
$$

The above analysis proves the following theorem.

Theorem 2.10 *A multidimensional ARKN method* (2.54) *has order p if and only if the following conditions are satisfied*:

$$
\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)}(V) = \mathscr{O}\big(h^{p-\rho(t)+1}\big), \quad \textit{for } t\in\bigcup_{q=2}^{p} NT_q, \tag{2.59}
$$

$$
\big(\big(\bar{A}\Phi(t)\big)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)+2}(V) = \mathscr{O}\big(h^{p-\rho(t)-1}\big), \quad \textit{for } t\in\bigcup_{q=2}^{p-2} NT_q, \tag{2.60}
$$

$$
\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)b(V) - \frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)-1}(V) = \mathscr{O}\big(h^{p-\rho(t)+2}\big), \quad \textit{for } t\in\bigcup_{q=2}^{p+1} NT_q, \tag{2.61}
$$

$$\big((\bar{A}\Phi(t))^{\mathrm{T}}\otimes I_d\big)b(V)-\frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)+1}(V)=\mathscr{O}\big(h^{p-\rho(t)}\big),\quad \textit{for } t\in\bigcup_{q=2}^{p-1}NT_q,\tag{2.62}$$

where t is the Nyström tree associated with an elementary differential $\mathscr{F}(t)(y_n,y_n')$ of the function $\tilde{f}(y,y')=f(y,y')-My$ at (y_n,y_n').

Theorem 2.11 *The condition* (2.59) *in Theorem* 2.10 *implies the condition* (2.60) *and the condition* (2.61) *implies the condition* (2.62).

Proof Let $\hat{t}$ be a Nyström tree of order $\rho(\hat{t})\le p-2$ and denote by t the Nyström tree of order $\rho(t)=\rho(\hat{t})+2$ obtained by connecting the root of $\hat{t}$ downward to a white vertex and then to a new black root. From the definitions of functions ρ, γ and Φ (see Chap. 1), it follows that

$$\gamma(t)=\big(\rho(\hat{t})+2\big)\big(\rho(\hat{t})+1\big)\gamma(\hat{t})\quad\text{and}\quad \Phi(t)=\bar{A}\Phi(\hat{t}).$$

The condition (2.59) ensures that

$$\begin{aligned}
&\big((\bar{A}\Phi(\hat{t}))^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)-\frac{\rho(\hat{t})!}{\gamma(\hat{t})}\phi_{\rho(\hat{t})+2}(V)\\
&=\big((\bar{A}\Phi(\hat{t}))^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)-\frac{\rho(\hat{t})+2}{\rho(\hat{t})+2}\cdot\frac{\rho(\hat{t})+1}{\rho(\hat{t})+1}\cdot\frac{\rho(\hat{t})!}{\gamma(\hat{t})}\phi_{\rho(\hat{t})+2}(V)\\
&=\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)-\frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)}(V)\\
&=\mathscr{O}\big(h^{p-\rho(t)+1}\big)\\
&=\mathscr{O}\big(h^{p-\rho(\hat{t})-1}\big),\quad \rho(\hat{t})=2,\dots,p-2.
\end{aligned}$$

Similarly, the condition (2.61) can be used to deduce the condition (2.62). The proof is complete. □

From Theorem 2.10 and Theorem 2.11, we arrive at the main conclusion of this section.

Theorem 2.12 *A multidimensional ARKN method* (2.54) *has order p if and only if the following conditions are satisfied*:

$$\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)\bar{b}(V)-\frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)}(V)=\mathscr{O}\big(h^{p-\rho(t)+1}\big),\quad t\in\bigcup_{q=2}^{p}NT_q,$$

$$\big(\Phi(t)^{\mathrm{T}}\otimes I_d\big)b(V)-\frac{\rho(t)!}{\gamma(t)}\phi_{\rho(t)-1}(V)=\mathscr{O}\big(h^{p-\rho(t)+2}\big),\quad t\in\bigcup_{q=2}^{p+1}NT_q.$$

2.3.3 Practical Multidimensional ARKN Methods

In this subsection, we derive three effective multidimensional ARKN methods of orders three, four and five, respectively, for the system (2.47) in the special case that the derivative $y'(x)$ is absent in the function f (see [17]).

First, we consider two-stage explicit ARKN methods with the following Butcher tableau:

$$\begin{array}{c|c} c & \bar{A} \\ \hline & \bar{b}^{\mathrm{T}}(V) \\ \hline & b^{\mathrm{T}}(V) \end{array} \quad = \quad \begin{array}{c|cc} c_1 & 0 & 0 \\ c_2 & \bar{a}_{21} & 0 \\ \hline & \bar{b}_1(V) & \bar{b}_2(V) \\ \hline & b_1(V) & b_2(V) \end{array}$$

From Theorem 2.12, a two-stage ARKN method has order three if and only if

$$\begin{aligned} &\big(e^{\mathrm{T}} \otimes I\big)b(V) = \phi_1(V) + \mathscr{O}\big(h^3\big), && \big(c^{\mathrm{T}} \otimes I\big)b(V) = \phi_2(V) + \mathscr{O}\big(h^2\big), \\ &\big(\big(c^2\big)^{\mathrm{T}} \otimes I\big)b(V) = 2\phi_3(V) + \mathscr{O}(h), && \big((\bar{A}e)^{\mathrm{T}} \otimes I\big)b(V) = \phi_3(V) + \mathscr{O}(h), \\ &\big(e^{\mathrm{T}} \otimes I\big)\bar{b}(V) = \phi_2(V) + \mathscr{O}\big(h^2\big), && \big(c^{\mathrm{T}} \otimes I\big)\bar{b}(V) = \phi_3(V) + \mathscr{O}(h), \end{aligned} \tag{2.63}$$

where I is the 2×2 identity matrix and $e = (1, 1)^{\mathrm{T}}$.

Choosing $c_1 = \frac{3}{16}$, $c_2 = \frac{23}{30}$, $\bar{a}_{21} = \frac{139}{450}$ and solving the equations in (2.63) yields

$$\begin{aligned} b_1(V) &= \frac{-c_2\phi_1(V) + \phi_2(V)}{c_1 - c_2}, & b_2(V) &= \frac{c_1\phi_1(V) - \phi_2(V)}{c_1 - c_2}, \\ \bar{b}_1(V) &= \frac{-c_2\phi_2(V) + \phi_3(V)}{c_1 - c_2}, & \bar{b}_2(V) &= \frac{c_1\phi_2(V) - \phi_3(V)}{c_1 - c_2}. \end{aligned} \tag{2.64}$$

This gives a two-stage ARKN method of order three. We denote this method by ARKN2s3.

Next, we construct three-stage explicit ARKN methods of order four with the following Butcher tableau:

$$\begin{array}{c|c} c & \bar{A} \\ \hline & \bar{b}^{\mathrm{T}}(V) \\ \hline & b^{\mathrm{T}}(V) \end{array} \quad = \quad \begin{array}{c|ccc} c_1 & 0 & 0 & 0 \\ c_2 & \bar{a}_{21} & 0 & 0 \\ c_3 & \bar{a}_{31} & \bar{a}_{32} & 0 \\ \hline & \bar{b}_1(V) & \bar{b}_2(V) & \bar{b}_3(V) \\ \hline & b_1(V) & b_2(V) & b_3(V) \end{array}$$

From Theorem 2.12, a three-stage ARKN method is of order four if its coefficients satisfy

$$
\begin{aligned}
&(e^{\mathrm{T}} \otimes I)b(V) = \phi_1(V) + \mathscr{O}(h^4), \qquad (c^{\mathrm{T}} \otimes I)b(V) = \phi_2(V) + \mathscr{O}(h^3),\\
&\bigl((c^2)^{\mathrm{T}} \otimes I\bigr)b(V) = 2\phi_3(V) + \mathscr{O}(h^2), \qquad \bigl((c^3)^{\mathrm{T}} \otimes I\bigr)b(V) = 6\phi_4(V) + \mathscr{O}(h),\\
&\bigl((\bar{A}e)^{\mathrm{T}} \otimes I\bigr)b(V) = \phi_3(V) + \mathscr{O}(h^2), \qquad \bigl((\bar{A}c)^{\mathrm{T}} \otimes I\bigr)b(V) = \phi_4(V) + \mathscr{O}(h),\\
&\bigl((c \cdot \bar{A}e)^{\mathrm{T}} \otimes I\bigr)b(V) = 3\phi_4(V) + \mathscr{O}(h), \qquad (e^{\mathrm{T}} \otimes I)\bar{b}(V) = \phi_2(V) + \mathscr{O}(h^3),\\
&(c^{\mathrm{T}} \otimes I)\bar{b}(V) = \phi_3(V) + \mathscr{O}(h^2), \qquad \bigl((c^2)^{\mathrm{T}} \otimes I\bigr)\bar{b}(V) = 2\phi_4(V) + \mathscr{O}(h),\\
&\bigl((\bar{A}e)^{\mathrm{T}} \otimes I\bigr)\bar{b}(V) = \phi_4(V) + \mathscr{O}(h),
\end{aligned}
\tag{2.65}
$$

where I is the 3×3 identity matrix and $e = (1, 1, 1)^{\mathrm{T}}$. Choosing $c_1 = \frac{1}{8}$, $c_2 = \frac{23}{42}$, $c_3 = \frac{11}{12}$, $\bar{a}_{21} = \frac{71}{441}4$, $\bar{a}_{31} = \frac{2641}{14058}$, $\bar{a}_{32} = \frac{4123}{18744}$ and solving all the equations in (2.65) gives

$$
\begin{aligned}
b_1(V) &= \frac{c_2c_3\phi_1(V) - (c_2 + c_3)\phi_2(V) + 2\phi_3(V)}{(c_1 - c_2)(c_1 - c_3)},\\
b_2(V) &= \frac{-c_1c_3\phi_1(V) + (c_1 + c_3)\phi_2(V) - 2\phi_3(V)}{(c_1 - c_2)(c_2 - c_3)},\\
b_3(V) &= \frac{c_1c_2\phi_1(V) - (c_1 + c_2)\phi_2(V) + 2\phi_3(V)}{(c_1 - c_3)(c_2 - c_3)},\\
\bar{b}_1(V) &= \frac{c_2c_3\phi_2(V) - (c_2 + c_3)\phi_3(V) + 2\phi_4(V)}{(c_1 - c_2)(c_1 - c_3)},\\
\bar{b}_2(V) &= \frac{-c_1c_3\phi_2(V) + (c_1 + c_3)\phi_3(V) - 2\phi_4(V)}{(c_1 - c_2)(c_2 - c_3)},\\
\bar{b}_3(V) &= \frac{c_1c_2\phi_2(V) - (c_1 + c_2)\phi_3(V) + 2\phi_4(V)}{(c_1 - c_3)(c_2 - c_3)}.
\end{aligned}
\tag{2.66}
$$

This gives a three-stage ARKN method of order four. It is denoted by ARKN3s4.

We continue to consider four-stage explicit ARKN methods of order five with the following Butcher tableau:

$$
\begin{array}{c|c}
c & \bar{A}\\
\hline
 & \bar{b}^{\mathrm{T}}(V)\\
\hline
 & b^{\mathrm{T}}(V)
\end{array}
=
\begin{array}{c|cccc}
c_1 & 0 & 0 & 0 & 0\\
c_2 & \bar{a}_{21} & 0 & 0 & 0\\
c_3 & \bar{a}_{31} & \bar{a}_{32} & 0 & 0\\
c_4 & \bar{a}_{41} & \bar{a}_{42} & \bar{a}_{43} & 0\\
\hline
 & \bar{b}_1(V) & \bar{b}_2(V) & \bar{b}_3(V) & \bar{b}_4(V)\\
\hline
 & b_1(V) & b_2(V) & b_3(V) & b_4(V)
\end{array}
$$

The order conditions up to order five are

$$
\begin{aligned}
&\big(e^{\mathrm{T}} \otimes I\big) b(V) = \phi_1(V) + \mathscr{O}\big(h^5\big),\\
&\big(c^{\mathrm{T}} \otimes I\big) b(V) = \phi_2(V) + \mathscr{O}\big(h^4\big),\\
&\big(\big(c^2\big)^{\mathrm{T}} \otimes I\big) b(V) = 2\phi_3(V) + \mathscr{O}\big(h^3\big),\\
&\big((\bar{A}e)^{\mathrm{T}} \otimes I\big) b(V) = \phi_3(V) + \mathscr{O}\big(h^3\big),\\
&\big(\big(c^3\big)^{\mathrm{T}} \otimes I\big) b(V) = 6\phi_4(V) + \mathscr{O}\big(h^2\big),\\
&\big((\bar{A}c)^{\mathrm{T}} \otimes I\big) b(V) = \phi_4(V) + \mathscr{O}\big(h^2\big),\\
&\big((c \cdot \bar{A}e)^{\mathrm{T}} \otimes I\big) b(V) = 3\phi_4(V) + \mathscr{O}\big(h^2\big),\\
&\big(\big(c^4\big)^{\mathrm{T}} \otimes I\big) b(V) = 24\phi_5(V) + \mathscr{O}(h),\\
&\big(\big(c^2 \cdot \bar{A}e\big)^{\mathrm{T}} \otimes I\big) b(V) = 12\phi_5(V) + \mathscr{O}(h),\\
&\big((\bar{A}e \cdot \bar{A}e)^{\mathrm{T}} \otimes I\big) b(V) = 6\phi_5(V) + \mathscr{O}(h),\\
&\big((c \cdot \bar{A}c)^{\mathrm{T}} \otimes I\big) b(V) = 4\phi_5(V) + \mathscr{O}(h),\\
&\big(\big(\bar{A}c^2\big)^{\mathrm{T}} \otimes I\big) b(V) = 2\phi_5(V) + \mathscr{O}(h),\\
&\big(\big(\bar{A}^2 e\big)^{\mathrm{T}} \otimes I\big) b(V) = \phi_5(V) + \mathscr{O}(h),
\end{aligned}
\tag{2.67}
$$

and

$$
\begin{aligned}
&\big(e^{\mathrm{T}} \otimes I\big) \bar{b}(V) = \phi_2(V) + \mathscr{O}\big(h^4\big), && \big(c^{\mathrm{T}} \otimes I\big) \bar{b}(V) = \phi_3(V) + \mathscr{O}\big(h^3\big),\\
&\big(\big(c^2\big)^{\mathrm{T}} \otimes I\big) \bar{b}(V) = 2\phi_4(V) + \mathscr{O}\big(h^2\big), && \big((\bar{A}e)^{\mathrm{T}} \otimes I\big) \bar{b}(V) = \phi_4(V) + \mathscr{O}\big(h^2\big),\\
&\big(\big(c^3\big)^{\mathrm{T}} \otimes I\big) \bar{b}(V) = 6\phi_5(V) + \mathscr{O}(h), && \big((c \cdot \bar{A}e)^{\mathrm{T}} \otimes I\big) \bar{b}(V) = 3\phi_5(V) + \mathscr{O}(h),\\
&\big((\bar{A}c)^{\mathrm{T}} \otimes I\big) \bar{b}(V) = \phi_5(V) + \mathscr{O}(h),
\end{aligned}
\tag{2.68}
$$

where I is the 4×4 identity matrix and $e = (1, 1, 1, 1)^{\mathrm{T}}$.

Under the simplifying assumption $\bar{A}e = \frac{1}{2}c^2$ together with $c = (0, \frac{1}{4}, \frac{7}{10}, 1)^{\mathrm{T}}$, we solve the above equations and obtain

$$
\begin{aligned}
&\bar{a}_{21} = \frac{1}{32}, \qquad \bar{a}_{31} = -\frac{7}{100}, \qquad \bar{a}_{32} = \frac{63}{250},\\
&\bar{a}_{41} = \frac{2}{7}, \qquad \bar{a}_{42} = 0, \qquad \bar{a}_{43} = \frac{3}{14},
\end{aligned}
\tag{2.69}
$$

and

$$
\begin{aligned}
b_1(V) &= \frac{1}{7}\big(7\phi_1(V) - 45\phi_2(V) + 156\phi_3(V) - 240\phi_4(V)\big),\\
b_2(V) &= \frac{32}{27}\big(7\phi_2(V) - 34\phi_3(V) + 60\phi_4(V)\big),\\
b_3(V) &= -\frac{500}{189}\big(\phi_2(V) - 10\phi_3(V) + 24\phi_4(V)\big),\\
b_4(V) &= \frac{1}{9}\big(7\phi_2(V) - 76\phi_3(V) + 240\phi_4(V)\big),\\
\bar{b}_1(V) &= \frac{1}{7}\big(7\phi_2(V) - 45\phi_3(V) + 156\phi_4(V) - 240\phi_5(V)\big),\\
\bar{b}_2(V) &= \frac{32}{27}\big(7\phi_3(V) - 34\phi_4(V) + 60\phi_5(V)\big),\\
\bar{b}_3(V) &= -\frac{500}{189}\big(\phi_3(V) - 10\phi_4(V) + 24\phi_5(V)\big),\\
\bar{b}_4(V) &= \frac{1}{9}\big(7\phi_3(V) - 76\phi_4(V) + 240\phi_5(V)\big).
\end{aligned}
\tag{2.70}
$$

This gives a four-stage ARKN method of order five. It is denoted by ARKN4s5.

Numerical experiments in [17] by Wu et al. show excellent performance of the multidimensional ARKN methods when applied to the oscillatory problems in comparison with the classical RKN methods in the scientific literature.

In [16], the numerical stability for multidimensional ARKN methods is analyzed based on the second-order homogeneous linear test model $y''(x) + \omega^2 y(x) = -\varepsilon y(x)$ with $\omega^2 + \varepsilon > 0$. The analysis of phase properties for multidimensional ARKN methods is also given in [16].

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