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REDUCIBILITY AND CHARACTERIZATION OF SYMPLECTIC RUNGE–KUTTA METHODS *

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Dedicated to Professor Wilhelm Niethammer on the occasion of his 60th birthday.

Abstract. Hamiltonian systems arise in many areas of physics, mechanics, and engineering sciences as well as in pure and applied mathematics. To their symplectic integration certain Runge–Kutta–type methods are profitably applied (see Sanz–Serna and Calvo [10]). In this paper Runge–Kutta and partitioned Runge–Kutta methods are considered. Different features of symmetry are distinguished using reflected and transposed methods. The property of DJ–irreducibility ensures symplectic methods having nonvanishing weights. A characterization of symplectic methods is deduced, from which many attributes of such methods and hints for their construction follow. Order conditions up to order four can be checked easily by simplifying assumptions. For symplectic singly–implicit Runge–Kutta methods the order barrier is shown to be two.

Key words. Hamiltonian system, symplectic method, Runge–Kutta and partitioned Runge–Kutta method, DJ–reducibility.

AMS subject classification. 65L06.

1. Introduction.

Consider the partitioned system of differential equations

$$\dot{p} = f(p,q,t), \quad \dot{q} = g(p,q,t), \tag{1.1}$$

where the points $(p,q) = (p_1,...,p_n,q_1,...,q_n)^T$ are elements of the domain $\mathcal{M}$ in the space $\mathbb{R}^{2n}$ and $t \in I$, where I is an open interval of the real line $\mathbb{R}$.

Suppose f and g are given as

$$f = (f_1,\dots,f_n)^T = \left(-\frac{\partial H}{\partial q_1},\dots,-\frac{\partial H}{\partial q_n}\right)^T, \quad g = (g_1,\dots,g_n)^T = \left(\frac{\partial H}{\partial p_1},\dots,\frac{\partial H}{\partial p_n}\right)^T,$$

where $H = H(p,q,t)$ is a sufficiently smooth real function on $\mathcal{M} \times I$, i.e., $H \in C^{(2)}(\mathcal{M} \times I)$. Then (1.1) is called a nonautonomous *Hamiltonian system*, H *Hamiltonian* and $\mathcal{M}$ *phase space*. In many applications the Hamiltonian H does not explicitly depend on t, and one has an autonomous Hamiltonian system. Every nonautonomous Hamiltonian system can be written as an autonomous Hamiltonian system (see Sanz–Serna and Calvo [10, p. 44]). First, we consider partitioned systems, and then Hamiltonian systems.

Let the initial values $(p(t_0), q(t_0)) = (p_0, q_0) \in \mathcal{M}$ be given. Then the initial value problem for a system of ordinary differential equations can be treated by Runge–Kutta methods. An s–stage Runge–Kutta method β is uniquely determined by a generating matrix $\mathcal{A} = (c, A, b)$ consisting of the node vector $c = (c_1,\dots,c_s)^T$, the coefficient matrix $A = (a_{ij})$ with $i,j = 1(1)s$, and the weight vector $b = (b_1,\dots,b_s)^T$. Further, we use the shifted coefficient matrix $C = A - \frac{1}{2}eb^T$ and the abbreviations $B = \mathrm{diag}(b_1,\dots,b_s) and\ e = (1,\dots,1)^T$. A Runge–Kutta method $\beta(\mathcal{A})$ is said to be of (p,k,ℓ)–type if it satisfies exactly the simplifying assumptions $B(p), C(k)$ and $D(\ell)$ with $\max\{k,\ell\} \le p$ (Butcher [2], see Dekker and Verwer [5, p. 57]). Corresponding assumptions are defined for partitioned Runge–Kutta methods.

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The stability functions relative to the concept of A–stability and AN–stability are given by

$$W(z) = 1 + zb^T(I - zA)^{-1}e \quad \text{and} \quad K(Z) = 1 + b^T Z(I - AZ)^{-1}e,$$

respectively, where I is the unit matrix, and $Z = \mathrm{diag}(z_1, ..., z_s)$ with $z_j = z_k$ whenever $c_j = c_k$. We also need the representations

$$W(z) = \frac{\det(I + z(eb^T - A))}{\det(I - zA)} \quad \text{and} \quad K(Z) = \frac{\det(I + (eb^T - A)Z)}{\det(I - AZ)}. \tag{1.2}$$

The stability matrix relative to the concept of B–stability is defined by

$$M = BC + C^T B.$$

Further, we consider the *reflected* and, in case of $\det(B) \neq 0$, the *transposed* Runge–Kutta methods β^* and β^τ generated by

$$\begin{array}{rclcl} \mathcal{A}^* &=& (c^*, A^*, b^*) &=& \left(e - \mathcal{P}c, \mathcal{P}(eb^T - A)\mathcal{P}, \mathcal{P}b\right), \\ \mathcal{A}^\tau &=& (c^\tau, A^\tau, b^\tau) &=& \left(e - \mathcal{P}c, \mathcal{P}(BAB^{-1})^T\mathcal{P}, \mathcal{P}b\right) \end{array}$$

(Scherer and Türke [12]), where the permutation matrix $\mathcal{P}$ is defined by $\mathcal{P}b = (b_s, ..., b_1)^T$. A method β is of (p, k, ℓ)–type if and only if β^* is of (p, k, ℓ)–type, and likewise if and only if β^τ is of (p, ℓ, k)–type. This provides interesting connections to the well–known methods of Gauss–, Radau– and Lobatto–type. Reflected Runge–Kutta methods were first studied in [11] (see Butcher [3, p. 221]); sometimes they are called adjoint methods. One easily deduces the relations

$$C^* = -\mathcal{P}C\mathcal{P}, \quad M^* = -\mathcal{P}M\mathcal{P} \quad \text{and} \quad C^\tau = \mathcal{P}(BCB^{-1})^T\mathcal{P}, \quad M^\tau = \mathcal{P}M\mathcal{P}.$$

It is very instructive to study different symmetry features of Runge–Kutta methods. We distinguish the cases $\beta = \beta^*$ (usual symmetry), $\beta = \beta^\tau$, $\beta^* = \beta^\tau$, and $\beta = \beta^* = \beta^\tau$ (total symmetry; e.g., the Gauss–Runge–Kutta methods are totally symmetric). A method with $\beta = \beta^*$ satisfies $W(z) = (W(-z))^{-1}$. A method with $\beta^* = \beta^\tau$ satisfies $K(Z) = (K(-Z))^{-1}$ and $M = 0$, and further, it is of (p, ℓ, ℓ)–type for some $\ell \leq p$. For Hamiltonian systems such methods are profitably used.

2. Partitioned Runge–Kutta methods.

Consider the separable not–necessarily Hamiltonian system

$$\dot{p} = f(q, t), \quad \dot{q} = g(p, t), \tag{2.1}$$

with the initial values $(p(t_0), q(t_0)) = (p_0, q_0)$ and apply two s–stage Runge–Kutta methods $\beta^{(1)}(\mathcal{A}^{(1)})$ and $\beta^{(2)}(\mathcal{A}^{(2)})$ in the following way

$$\begin{array}{rcll} P_i &=& p_m + h\displaystyle\sum_{j=1}^{s} a_{ij}^{(1)} f(Q_j, t_m + c_j^{(2)}h), & i = 1(1)s, \\ Q_i &=& q_m + h\displaystyle\sum_{j=1}^{s} a_{ij}^{(2)} g(P_j, t_m + c_j^{(1)}h), & i = 1(1)s, \\ p_{m+1} &=& p_m + h\displaystyle\sum_{i=1}^{s} b_i^{(1)} f(Q_i, t_m + c_i^{(2)}h), & \\ q_{m+1} &=& q_m + h\displaystyle\sum_{i=1}^{s} b_i^{(2)} g(P_i, t_m + c_i^{(1)}h). & \end{array}$$

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Then, this method generated by $\mathcal{A}^{(1,2)} = (\mathcal{A}^{(1)}; \mathcal{A}^{(2)})$ is called s–stage partitioned Runge–Kutta method $\beta^{(1,2)}$. Changing the sequence yields the method $\beta^{(2,1)}(\mathcal{A}^{(2,1)})$. A partitioned Runge–Kutta method is called explicit if P_i and Q_j are recursively computable when applied to (2.1), and implicit otherwise. In the explicit case, after certain permutations, P_i and Q_j are computable with increasing indices. So, the partitioned Runge–Kutta method $\beta^{(1,2)}$ $(\mathcal{A}^{(1,2)})$ is explicit if and only if the elements of $A^{(1)}$ and $A^{(2)}$ satisfy

$$a_{ij}^{(1)} = a_{ij}^{(2)} = 0 \quad (i < j) \qquad \text{and} \qquad a_{ii}^{(1)} a_{ii}^{(2)} = 0 \quad \text{for} \quad i, j = 1(1)s.$$

Further, we refer to the matrices

$$B^{(\nu)} = \operatorname{diag}(b_1^{(\nu)}, \ldots, b_s^{(\nu)}) \quad \text{and} \quad C^{(\nu)} = A^{(\nu)} - \frac{1}{2} e b^{(\nu)^T}$$

with $\nu = 1, 2$, and

$$M^{(1,2)} = B^{(1)} C^{(2)} + C^{(1)^T} B^{(2)}.$$

In a similar way as for Runge–Kutta methods, *reflected* and *transposed* partitioned methods $\beta^{(1,2)^*}$ and $\beta^{(1,2)^\tau}$ are defined by the generating matrices

$$\begin{aligned} \mathcal{A}^{(1,2)^*} &= (\mathcal{A}^{(1)^*}; \mathcal{A}^{(2)^*}) \\ \mathcal{A}^{(1,2)^\tau} &= \Big(e - \mathcal{P}c^{(1)}, \mathcal{P}\left(B^{(1)} A^{(2)} B^{(2)^{-1}}\right)^T \mathcal{P}, \mathcal{P}b^{(1)}\, ; \\ &\qquad e - \mathcal{P}c^{(2)}, \mathcal{P}\left(B^{(2)} A^{(1)} B^{(1)^{-1}}\right)^T \mathcal{P}, \mathcal{P}b^{(2)} \Big) \end{aligned}$$

$(\det(B^{(\nu)}) \neq 0$ for $\nu = 1, 2)$. One easily deduces the properties

$$\beta^{(1,2)^{**}} = \beta^{(1,2)}, \quad \beta^{(1,2)^{\tau\tau}} = \beta^{(1,2)},$$

and the relations

$$C^{(\nu)^*} = -\mathcal{P}C^{(\nu)}\mathcal{P}, \quad C^{(\nu)^\tau} = \mathcal{P}\left(B^{(\nu)} C^{(3-\nu)} B^{(3-\nu)^{-1}}\right)^T \mathcal{P}, \qquad \text{for } \nu = 1, 2,$$

and

$$M^{(1,2)^*} = -\mathcal{P}M^{(1,2)}\mathcal{P}, \quad M^{(1,2)^\tau} = \mathcal{P}M^{(1,2)}\mathcal{P}.$$

Further, we consider the symmetry features of partitioned Runge–Kutta methods $\beta^{(1,2)} = \beta^{(1,2)^*}$ (i.e., $\beta^{(1,2)}$ is symmetric in the usual sense), $\beta^{(1,2)} = \beta^{(1,2)^\tau}$, $\beta^{(1,2)^*} = \beta^{(1,2)^\tau}$, and $\beta^{(1,2)} = \beta^{(1,2)^*} = \beta^{(1,2)^\tau}$ (i.e., $\beta^{(1,2)}$ is totally symmetric).

EXAMPLE 2.1. *Consider the method $\beta^{(1,2)}$ $(\mathcal{A}^{(1,2)})$ with*

$$c^{(1)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \; A^{(1)} = \begin{bmatrix} 0 & 0 \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}, \; b^{(1)} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, \; c^{(2)} = \tfrac{1}{2}e, \; A^{(2)} = A^{(1)^\tau}, \; b^{(2)} = b^{(1)},$$

which is explicit in the following sense:

$$\begin{aligned} &P_1 = p_m, \quad Q_1 = Q_2 = q_m + \tfrac{h}{2} g(P_1, t_m), \quad P_2 = p_m + hf\left(Q_1, t_m + \tfrac{h}{2}\right), \\ &p_{m+1} = P_2, \qquad q_{m+1} = Q_1 + \tfrac{h}{2} g(P_2, t_m + h). \end{aligned} \tag{2.2}$$

Notice that $\beta^{(1)}$ *and* $\beta^{(2)}$ *are symmetric in the usual sense. The partitioned method* $\beta^{(1,2)}$ *is totally symmetric with* $M^{(1,2)} = 0$ *and has second order.*

EXAMPLE 2.2. *Consider the method* $\beta^{(1,2)}$ $(\mathcal{A}^{(1,2)})$ *with weight vectors* $b^{(1)}$, $b^{(2)}$, *the coefficient matrices*

$$A^{(1)} = \begin{bmatrix} b_1^{(1)} & & 0 \\ \vdots & \ddots & \\ b_1^{(1)} & \cdots & b_s^{(1)} \end{bmatrix}, \quad A^{(2)} = \begin{bmatrix} 0 & & & 0 \\ b_1^{(2)} & \ddots & & \\ \vdots & \ddots & \ddots & \\ b_1^{(2)} & \cdots & b_{s-1}^{(2)} & 0 \end{bmatrix},$$

and node vectors $c^{(\nu)} = A^{(\nu)}e$ *with* $\nu = 1, 2$, *which is explicit and satisfies* $M^{(1,2)} = 0$ *(see Sanz–Serna and Calvo [10, Sec. 8.4]). The 1–stage method of order one is generated by*

$$\mathcal{A}^{(1,2)} = ([1], [1], [1]; [0], [0], [1]). \tag{2.3}$$

The 3–stage method of order three with the coefficients

$$b_1^{(1)} = \frac{7}{24}, \quad b_2^{(1)} = \frac{3}{4}, \quad b_3^{(1)} = -\frac{1}{24}, \quad b_1^{(2)} = \frac{2}{3}, \quad b_2^{(2)} = -\frac{2}{3}, \quad b_3^{(2)} = 1$$

is one of the first partitioned Runge–Kutta methods (Ruth [9]). Choosing the coefficients as

$$b_1^{(1)} = 1, \quad b_2^{(1)} = -\frac{2}{3}, \quad b_3^{(1)} = \frac{2}{3}, \quad b_1^{(2)} = -\frac{1}{24}, \quad b_2^{(2)} = \frac{3}{4}, \quad b_3^{(2)} = \frac{7}{24}$$

yields also a third order method with $M^{(1,2)} = 0$.

The reflected method of $\beta^{(1,2)}(\mathcal{A}^{(1,2)})$ with $\mathcal{A}^{(1,2)}$ as in (2.3) is the method $\beta^{(2,1)}$ generated by $\mathcal{A}^{(2,1)} = ([0], [0], [1]; [1], [1], [1])$. Performing one step of $\beta^{(2,1)}$, with steplength $\frac{h}{2}$ followed by one step of $\beta^{(1,2)}$ with steplength $\frac{h}{2}$, yields method (2.2); performing the steps in reverse sequence also yields a totally symmetric explicit partitioned Runge–Kutta method.

3. Reducibility of partitioned methods. A Runge–Kutta method is usually assumed to be irreducible. Stages which are evidently equivalent are excluded from the outset. But, there are finer concepts of reducibility (see Dekker and Verwer [5, p. 107]). Similar considerations are presented for partitioned methods.

EXAMPLE 3.1. *Consider the explicit 2–stage partitioned Runge–Kutta method of order two generated by*

$$\mathcal{A}^{(1,2)} = \left(\begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}; \begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ \frac{1}{2} & 0 \end{bmatrix}, \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \right), \tag{3.1}$$

which consists of four half–stages computing P_1, Q_1, P_2, Q_2, *where* Q_1 *is superfluous. The same numerical result is produced by three half–stages*

$$\begin{aligned} P_1 &= p_m, \\ P_2 &= p_m + hf(Q_1, t_m + \tfrac{h}{2}), \\ p_{m+1} &= P_2. \end{aligned} \qquad \begin{aligned} Q_1 &= q_m + \tfrac{h}{2} g(P_1, t_m), \\ q_{m+1} &= Q_1 + \tfrac{h}{2} g(P_2, t_m + h), \end{aligned} \tag{3.2}$$

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Obviously, this method is generated by

$$\mathcal{A}^{(1,2)} = \left(\begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \end{bmatrix}; \begin{bmatrix} \frac{1}{2} \end{bmatrix}, \begin{bmatrix} \frac{1}{2} & 0 \end{bmatrix}, \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \right).$$

Hence, the method is called a (2,1)–stage partitioned Runge–Kutta method. Method (2.2) produces the same numerical result as method (3.2).

Definition 3.2. *The method, generated by* $\mathcal{A}^{(1,2)} = (c^{(1)}, A^{(1)}, b^{(1)}; c^{(2)}, A^{(2)}, b^{(2)})$ *with* $c^{(1)}, b^{(2)} \in \mathbb{R}^{s_1}$*,* $A^{(1)} \in \mathbb{R}^{s_1 \times s_2}$*,* $A^{(2)} \in \mathbb{R}^{s_2 \times s_1}$*,* $c^{(2)}, b^{(1)} \in \mathbb{R}^{s_2}$ *in the following way*

$$\begin{aligned}
P_i &= p_m + h \sum_{j=1}^{s_2} a_{ij}^{(1)} f(Q_j, t_m + c_j^{(2)} h), \quad i = 1(1)s_1, \\
Q_i &= q_m + h \sum_{j=1}^{s_1} a_{ij}^{(2)} g(P_j, t_m + c_j^{(1)} h), \quad i = 1(1)s_2, \\
p_{m+1} &= p_m + h \sum_{i=1}^{s_2} b_i^{(1)} f(Q_i, t_m + c_i^{(2)} h), \\
q_{m+1} &= q_m + h \sum_{i=1}^{s_1} b_i^{(2)} g(P_i, t_m + c_i^{(1)} h),
\end{aligned}$$

is called an (s_1, s_2)*–stage partitioned Runge–Kutta method* $\beta^{(1,2)}(\mathcal{A}^{(1,2)})$*. Moreover, for* $s_1 = s_2 = s$ *it is called s–stage method. An* (s_1, s_2)*–stage partitioned Runge–Kutta method is said to be explicit if* P_i *and* Q_j *are recursively computable, and implicit otherwise.*

In the explicit case we assume that P_i and Q_j are computable with increasing indices. In view of symmetry features we are interested in methods with nonvanishing weights. We next generalize the definition of DJ–reducibility for partitioned Runge–Kutta methods from the DJ–reducibility of Runge–Kutta methods of Dahlquist and Jeltsch [4]. The concept of S–reducibility is not discussed here.

Definition 3.3. *A* (s_1, s_2)*–stage partitioned Runge–Kutta method* $\beta^{(1,2)}(\mathcal{A}^{(1,2)})$ *is said to be DJ–reducible if there exist sets* $S_1, T_1, S_2,$ *and* T_2 *such that* $S_1 \cap T_1 = \emptyset$*,* $S_2 \cap T_2 = \emptyset$*,* $S_1 \neq \emptyset$ *or* $S_2 \neq \emptyset$*,* $S_1 \cup T_1 = \{1, \ldots, s_2\}$*,* $S_2 \cup T_2 = \{1, \ldots, s_1\}$ *and*

$$\begin{aligned}
b_j^{(1)} &= 0 \quad (j \in S_1), & b_j^{(2)} &= 0 \quad (j \in S_2), \\
a_{ij}^{(1)} &= 0 \quad (i \in T_2, j \in S_1), & a_{ij}^{(2)} &= 0 \quad (i \in T_1, j \in S_2).
\end{aligned} \tag{3.3}$$

The method is said to be DJ–irreducible if it is not DJ–reducible.

Remark 3.4. *Assume the existence of* $S_1, T_1, S_2,$ *and* T_2 *as in Definition 3.3. Then* Q_j *with* $j \in S_1$ *does not influence* P_i *with* $i \in T_2$ *nor* p_{m+1}*, and* P_j *with* $j \in S_2$ *does not influence* Q_i *with* $i \in T_1$ *nor* q_{m+1}*, and the following rule for DJ–reduction holds:*
If $S_1 \neq \emptyset$*, then cancel the j–th element of* $b^{(1)}$ *and of* $c^{(2)}$*, the j–th row of* $A^{(2)}$*, and the j–th column of* $A^{(1)}$ *with* $j \in S_1$*.*
If $S_2 \neq \emptyset$*, then cancel the j–th element of* $b^{(2)}$ *and of* $c^{(1)}$*, the j–th row of* $A^{(1)}$*, and the j–th column of* $A^{(2)}$ *with* $j \in S_2$*.*
For example, the method generated by (3.1) is DJ–reducible to (3.2) with $S_1 = \{1\}, T_1 = \{2\}, S_2 = \emptyset, T_2 = \{1, 2\}$*.*

Further, we refer to the matrices

$$B^{(\nu)} = \mathrm{diag}(b_1^{(\nu)}, \ldots, b_{s_{3-\nu}}^{(\nu)}) \quad \text{and} \quad C^{(\nu)} = A^{(\nu)} - \tfrac{1}{2} e_{s_\nu} b^{(\nu)^T},$$

where $e_{s_\nu} \in \mathbb{R}^{s_\nu}$ with $\nu = 1, 2$, and

$$M^{(1,2)} = B^{(1)} C^{(2)} + C^{(1)^T} B^{(2)}.$$

Reflected and transposed (s_1, s_2)–stage partitioned Runge–Kutta methods $\beta^{(1,2)^*}$ and $\beta^{(1,2)^\tau}$ are defined by the generating matrices

$$\begin{aligned}
\mathcal{A}^{(1,2)^*} &= \Big(e_{s_1} - \mathcal{P}_{s_1} c^{(1)}, \mathcal{P}_{s_1} \left(e_{s_1} b^{(1)^T} - A^{(1)}\right) \mathcal{P}_{s_2}, \mathcal{P}_{s_2} b^{(1)} \; ; \\
&\qquad e_{s_2} - \mathcal{P}_{s_2} c^{(2)}, \mathcal{P}_{s_2} \left(e_{s_2} b^{(2)^T} - A^{(2)}\right) \mathcal{P}_{s_1}, \mathcal{P}_{s_1} b^{(2)} \Big), \\
\mathcal{A}^{(1,2)^\tau} &= \Big(e_{s_1} - \mathcal{P}_{s_1} c^{(1)}, \mathcal{P}_{s_1} \left(B^{(1)} A^{(2)} B^{(2)^{-1}}\right)^T \mathcal{P}_{s_2}, \mathcal{P}_{s_2} b^{(1)} \; ; \\
&\qquad e_{s_2} - \mathcal{P}_{s_2} c^{(2)}, \mathcal{P}_{s_2} \left(B^{(2)} A^{(1)} B^{(1)^{-1}}\right)^T \mathcal{P}_{s_1}, \mathcal{P}_{s_1} b^{(2)} \Big)
\end{aligned}$$

($\det(B^{(\nu)}) \neq 0$ for $\nu = 1, 2$), where the permutation matrices $\mathcal{P}_{s_\nu} \in \mathbb{R}^{s_\nu \times s_\nu}$ are defined by $\mathcal{P}_{s_\nu} b^{(3-\nu)} = (b_{s_\nu}^{(3-\nu)}, \ldots, b_1^{(3-\nu)})^T$ for $\nu = 1, 2$. The properties

$$\beta^{(1,2)^{**}} = \beta^{(1,2)}, \qquad \beta^{(1,2)^{\tau\tau}} = \beta^{(1,2)},$$

and the relations

$$C^{(\nu)^*} = -\mathcal{P}_{s_\nu} C^{(\nu)} \mathcal{P}_{s_{3-\nu}}, \quad C^{(\nu)^\tau} = \mathcal{P}_{s_\nu} \left(B^{(\nu)} C^{(3-\nu)} B^{(3-\nu)^{-1}}\right)^T \mathcal{P}_{s_{3-\nu}}$$

for $\nu = 1, 2$, and

$$M^{(1,2)^*} = -\mathcal{P}_{s_2} M^{(1,2)} \mathcal{P}_{s_1}, \qquad M^{(1,2)^\tau} = \mathcal{P}_{s_2} M^{(1,2)} \mathcal{P}_{s_1}$$

are easily deduced.

With regard to s–stage Runge–Kutta methods, the following simplifying assumptions are useful:

$$\begin{aligned}
\hat{B}(p): \quad & \sum_{i=1}^{s_2} b_i^{(1)} (c_i^{(2)})^{\nu-1} = \sum_{i=1}^{s_1} b_i^{(2)} (c_i^{(1)})^{\nu-1} = \frac{1}{\nu}, \; \nu = 1(1)p; \\
\hat{C}(k): \quad & \sum_{j=1}^{s_2} a_{ij}^{(1)} (c_j^{(2)})^{\nu-1} = \frac{1}{\nu} (c_i^{(1)})^\nu, \; i = 1(1)s_1, \nu = 1(1)k, \\
& \sum_{j=1}^{s_1} a_{ij}^{(2)} (c_j^{(1)})^{\nu-1} = \frac{1}{\nu} (c_i^{(2)})^\nu, \; i = 1(1)s_2, \nu = 1(1)k; \\
\hat{D}(\ell): \quad & \sum_{i=1}^{s_2} b_i^{(1)} (c_i^{(2)})^{\nu-1} a_{ij}^{(2)} = \frac{1}{\nu} b_j^{(2)} \big(1 - (c_j^{(1)})^\nu\big), \; j = 1(1)s_1, \nu = 1(1)\ell, \\
& \sum_{i=1}^{s_1} b_i^{(2)} (c_i^{(1)})^{\nu-1} a_{ij}^{(1)} = \frac{1}{\nu} b_j^{(1)} \big(1 - (c_j^{(2)})^\nu\big), \; j = 1(1)s_2, \nu = 1(1)\ell.
\end{aligned}$$

A partitioned Runge–Kutta method is said to be of (p,k,ℓ)–type if it satisfies exactly $\hat{B}(p), \hat{C}(k)$ and $\hat{D}(\ell)$ with $\max\{k,\ell\} \leq p$.

The definitions of usual symmetry and total symmetry are analogous to the definitions for s–stage methods.

EXAMPLE 3.5. *The 4–stage method generated by*

$$\begin{array}{llllllll} b_1^{(1)} &=& 0, & b_2^{(1)} &=& \frac{1}{3}(2+\alpha), & b_3^{(1)} &=& -\frac{1}{3}(1+2\alpha), & b_4^{(1)} &=& b_2^{(1)}, \\ b_1^{(2)} &=& \frac{1}{6}(2+\alpha), & b_2^{(2)} &=& \frac{1}{6}(1-\alpha), & b_3^{(2)} &=& b_2^{(2)}, & b_4^{(2)} &=& b_1^{(2)}, \end{array}$$

where $\alpha = \sqrt[3]{2} + \frac{1}{\sqrt[3]{2}}$, *and* $A^{(1)}$, $A^{(2)}$, $c^{(1)}$, $c^{(2)}$ *as in Example 2.2, is of order four (Qin [7]) and DJ–reducible to the* $(4,3)$*–stage method generated by* $\mathcal{A}^{(1,2)} =$

$$\left(\begin{bmatrix} 0 \\ c_2^{(1)} \\ c_3^{(1)} \\ c_4^{(1)} \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ b_2^{(1)} & 0 & 0 \\ b_2^{(1)} & b_3^{(1)} & 0 \\ b_2^{(1)} & b_3^{(1)} & b_4^{(1)} \end{bmatrix}, \begin{bmatrix} b_2^{(1)} \\ b_3^{(1)} \\ b_4^{(1)} \end{bmatrix}; \begin{bmatrix} c_2^{(2)} \\ c_3^{(2)} \\ c_4^{(2)} \end{bmatrix}, \begin{bmatrix} b_1^{(2)} & 0 & 0 & 0 \\ b_1^{(2)} & b_2^{(2)} & 0 & 0 \\ b_1^{(2)} & b_2^{(2)} & b_3^{(2)} & 0 \end{bmatrix}, \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \\ b_3^{(3)} \\ b_4^{(3)} \end{bmatrix} \right).$$

The relevant sets of Definition 3.3 are $S_1 = \{1\}$, $T_1 = \{2,3,4\}$, $S_2 = \emptyset$, $T_2 = \{1,2,3,4\}$.

The method with

$$\begin{array}{llllllll} b_1^{(1)} &=& \frac{1}{6}(2+\alpha), & b_2^{(1)} &=& \frac{1}{6}(1-\alpha), & b_3^{(1)} &=& b_2^{(1)}, & b_4^{(1)} &=& b_1^{(1)}, \\ b_1^{(2)} &=& \frac{1}{3}(2+\alpha), & b_2^{(2)} &=& -\frac{1}{3}(1+2\alpha), & b_3^{(2)} &=& b_1^{(2)}, & b_4^{(2)} &=& 0 \end{array}$$

is also of fourth order and DJ–reducible to a $(3,4)$*–stage method. The relevant sets are* $S_1 = \emptyset$, $T_1 = \{1,2,3,4\}$, $S_2 = \{4\}$, $T_2 = \{1,2,3\}$.

The symmetry feature $\beta^{(1,2)^*} = \beta^{(1,2)}$ *of these methods is easily checked by verfying* $\mathcal{A}^{(1,2)^*} = \mathcal{A}^{(1,2)}$ *in the DJ–irreducible form.*

4. Symplectic Runge–Kutta methods. Now consider the autonomous Hamiltonian system

$$\dot{p} = f(p,q), \quad \dot{q} = g(p,q) \tag{4.1}$$

with the Hamiltonian H. The important property is that all elements $\mathcal{F}_t$ of the *Hamiltonian phase flow* $\{\mathcal{F}_t\}$ are symplectic, i.e., they preserve the symplectic structure $dp \wedge dq$ of the phase space $\mathcal{M}$ (see Arnol'd [1]). Recall that $\mathcal{F}_t$ is the mapping

$$\mathcal{F}_t : (p_0, q_0) \;\rightarrow\; (p(t), q(t)),$$

where $(p(t), q(t))$ is the solution of (4.1) with initial values (p_0, q_0) at time $t = 0$. For given $t \in \mathbb{R}$ it is possible that $\mathcal{F}_t$ is not defined or defined only on a subset of $\mathcal{M}$. An appropriate one–step method must meet this symplectic property, too, i.e., the mapping $(p_m, q_m) \;\rightarrow\; (p_{m+1}, q_{m+1})$ must be symplectic. Methods with this property when applied to Hamiltonian systems are called *a–symplectic*; methods with this property when applied to separable Hamiltonian systems are called *s–symplectic*; and methods with this property when applied to linear Hamiltonian systems are called *l–symplectic*.

First, we refer to the well–known results on symplectic methods of Lasagni, Sanz–Serna and Suris (see Sanz–Serna and Calvo [10, Sec. 6.2 and 6.3]).

THEOREM 4.1. *A Runge–Kutta method β with $M = 0$ is a–symplectic. A partitioned Runge–Kutta method with $M^{(1,2)} = 0$ is s–symplectic.*

For Runge–Kutta methods and partitioned Runge–Kutta methods without equivalent stages, the conditions $M = 0$ and $M^{(1,2)} = 0$ are also necessary (see Sanz–Serna and Calvo [10, Sec. 6.5]).

By simple modifications of the proof of the second statement in Theorem 4.1 the following result is given.

COROLLARY 4.2. *An (s_1, s_2)–stage partitioned Runge–Kutta method with $M^{(1,2)} = 0$ is s–symplectic.*

The following results are important for the characterization of symplectic methods.

THEOREM 4.3. *A DJ–irreducible Runge–Kutta method $\beta(\mathcal{A})$ with $M = 0$ satisfies $b_i \neq 0$ for $i = 1(1)s$. A DJ–irreducible (s_1, s_2)–stage Runge–Kutta method $\beta^{(1,2)}(\mathcal{A}^{(1,2)})$ with $M^{(1,2)} = 0$ satifies $b_i^{(1)} \neq 0$ for $i = 1(1)s_2$, and $b_i^{(2)} \neq 0$ for $i = 1(1)s_1$.*

Proof. We show the second statement. The first is known from similar considerations (Dahlquist and Jeltsch [4]). Suppose $b_\nu^{(1)} = 0$ for some index ν. Then all elements in the ν–th row of $B^{(1)}A^{(2)}$ and of $b^{(1)}b^{(2)^T}$ are zero. Since $M^{(1,2)} = 0$, all elements in the ν–th row of $A^{(1)^T}B^{(2)}$ must also be zero, i.e., $b_i^{(2)}a_{i\nu}^{(1)} = 0$ for all i. Now, suppose $b_\mu^{(2)} = 0$ for some index μ. Then all elements in the μ–th column of $A^{(1)^T}B^{(2)}$ and of $b^{(1)}b^{(2)^T}$ are zero. Since $M^{(1,2)} = 0$, all elements in the μ–th column of $B^{(1)}A^{(2)}$ must also be zero, i.e., $b_i^{(1)}a_{i\mu}^{(2)} = 0$ for all i. All of this implies (3.3) for the sets

$$S_1 = \{\nu \mid b_\nu^{(1)} = 0\}, T_1 = \{1, ..., s_2\}\backslash S_1, S_2 = \{\mu \mid b_\mu^{(2)} = 0\}, T_2 = \{1, ..., s_1\}\backslash S_2,$$

a contradiction to DJ–irreducibility. □

Now, we present characterizations of DJ–irreducible methods satisfying $M = 0$ and $M^{(1,2)} = 0$, respectively.

THEOREM 4.4. *A DJ–irreducible Runge–Kutta method $\beta(\mathcal{A})$ satisfies*

$$M = 0 \quad \text{if and only if} \quad \beta^* = \beta^\tau.$$

A DJ–irreducible (s_1, s_2)–stage partitioned Runge–Kutta method $\beta^{(1,2)}(\mathcal{A}^{(1,2)})$ satisfies

$$M^{(1,2)} = 0 \quad \text{if and only if} \quad \beta^{(1,2)^*} = \beta^{(1,2)^\tau}.$$

Proof. Since the method is DJ–irreducible, $M = 0$ and $M^{(1,2)} = 0$ imply nonvanishing weights. Hence, $M = 0$ is equivalent to

$$eb^T - A = B^{-1}A^TB, \tag{4.2}$$

and to

$$\mathcal{P}\left(eb^T - A\right)\mathcal{P} = \mathcal{P}\left(BAB^{-1}\right)^T\mathcal{P}.$$

In a similar way $M^{(1,2)} = 0$ is equivalent to

$$e_{s_2}b^{(2)^T} - A^{(2)} = B^{(1)^{-1}}A^{(1)^T}B^{(2)},$$

and to

$$\mathcal{P}_{s_2}\left(e_{s_2}b^{(2)^T}-A^{(2)}\right)\mathcal{P}_{s_1}=\mathcal{P}_{s_2}\left(B^{(2)}A^{(1)}B^{(1)^{-1}}\right)^T\mathcal{P}_{s_1}.$$

Also, $M^{(1,2)^T}=0$ is equivalent to

$$e_{s_1}b^{(1)^T}-A^{(1)}=B^{(2)^{-1}}A^{(2)^T}B^{(1)},$$

and to

$$\mathcal{P}_{s_1}\left(e_{s_1}b^{(1)^T}-A^{(1)}\right)\mathcal{P}_{s_2}=\mathcal{P}_{s_1}\left(B^{(1)}A^{(2)}B^{(2)^{-1}}\right)^T\mathcal{P}_{s_2}.$$

Hence, the statements follow. □

From these characterizations many attributes of such methods and hints for their construction follow.

COROLLARY 4.5. *A Runge–Kutta method $\beta(\mathcal{A})$ with nonvanishing weights satisfies* $\mathrm{diag}(M)=0$ *if and only if $a_{ii}=\frac{1}{2}b_i$ for $i=1(1)s$. A Runge–Kutta method $\beta(\mathcal{A})$ satisfies $M=0$ if and only if the reflected method, and likewise the transposed method, satisfies this condition. An (s_1,s_2)–stage partitioned method $\beta^{(1,2)}(\mathcal{A}^{(1,2)})$ satisfies $M^{(1,2)}=0$ if and only if the reflected method, and likewise the transposed method, satisfies this condition.*

Further, symplectic Runge–Kutta methods are derived by composition of two or more methods (Qin [8]) and by a subsequent reduction. With respect to partitioned methods consider a method $\beta(\mathcal{A})$, then the partitioned methods $\beta^{(1,2)}(\mathcal{A};\mathcal{A}^*)$ and $\beta^{(1,2)}(\mathcal{A};\mathcal{A}^\tau)$ satisfy $M^{(1,2)}=0$.

COROLLARY 4.6. *A DJ–irreducible Runge–Kutta method with $M=0$ and a DJ–irreducible (s_1,s_2)–stage partitioned Runge–Kutta method with $M^{(1,2)}=0$ are of (p,ℓ,ℓ)–type for some $\ell\le p$.*

For the proof one has to study the symplifying assumptions under reflection and transposition. Using $\beta^*=\beta^\tau$ and $\beta^{(1,2)^*}=\beta^{(1,2)^\tau}$ yield the statement.

A Runge–Kutta method is l–symplectic if and only if the stability function W satisfies $W(z)=(W(-z))^{-1}$ (see Sanz–Serna and Calvo [10, p. 76]). Similar considerations are possible in the nonlinear case.

THEOREM 4.7. *A DJ–irreducible Runge–Kutta method β without equivalent stages is a–symplectic if and only if the stability function K satisfies*

$$K(Z)=(K(-Z))^{-1}. \tag{4.3}$$

Proof. We use the fact that the method is a–symplectic if and only if $M=0$. First, we show the necessity of (4.3). Let $X\in\mathbb{R}^{s\times s}$. Then the equation of Schur (see Gantmacher [6, p. 71]) yields

$$\det(I+ZX)=\det(I+XZ). \tag{4.4}$$

Since $M=0$ and $BZ=ZB$, from (4.2) and (4.4) it follows that

$$\det(I+(eb^T-A)Z)=\det(I+B^{-1}A^TBZ)=\det(I+A^TZ)=\det(I+AZ)$$

and that

$$\begin{aligned}\det(I-AZ)&=\det(I-(eb^T-B^{-1}A^TB)Z)=\det(I-(eb^T-A)^TZ)\\&=\det(I-(eb^T-A)Z).\end{aligned}$$

With the representation (1.2) of $K(Z)$ the necessity of (4.3) is shown.

The sufficiency of (4.3) follows from the relation

$$|K(iY)|^2 - 1 = K(iY)K(-iY) - 1 = 0,$$

where $Y = \mathrm{diag}(y_1, \ldots, y_s)$ with $y_j \in \mathbb{R}$ for $j = 1(1)s$, and from the representation of the expression $|K(Z)|^2 - 1$ (see Dekker and Verwer [5, p. 105]). ◻

Since the condition $M = 0$ implies a (p, ℓ, ℓ)–type method with $\ell \leq p$, and since assumptions $B(p)$, $C(\ell)$ and $D(\ell)$ establish that order $p = 2\ell + 1$ (see Dekker and Verwer [5, p. 59]), it is very easy to check the order of such Runge–Kutta methods. In the case of autonomous systems, $C(1)$ imports the definition of the nodes c_i with $i = 1(1)s$. At a glance, we recognize that $B(1)$and $C(1)$ imply $B(2)$, and hence, the well–known result that a consistent Runge–Kutta method (i.e. $B(1)$ holds) with $M = 0$ has order two (see Sanz–Serna and Calvo [10, p. 90]) is obvious. Further, we recognize that a method with $M = 0$ has order three if $B(3)$ and $C(1)$ are satisfied, and order four if order three and the usual symmetry are satisfied.

With respect to an efficient implementation singly–implicit Runge–Kutta methods, i. e., methods with a single eigenvalue γ, were introduced and studied in detail (see Dekker and Verwer [5, p. 76], Türke [13]). Now we are interested in such methods with $M = 0$, but there exists a strong order barrier.

THEOREM 4.8. *A singly–implicit Runge–Kutta method with $M = 0$ has at most order two.*

Proof. Without loss of generality we assume nonvanishing weights (see Theorem 4.3) and show that the order of approximation of $W(z)$ to $\exp(z)$ is at most two. The condition $M = 0$ implies that A^* and A^τ are equal and similar to A^T; hence,

$$W(z) = \frac{\det(I + z\mathcal{P}A^*\mathcal{P})}{\det(I - zA)} = \frac{\det(I + zA)}{\det(I - zA)} = \left(\frac{1 + \gamma z}{1 - \gamma z}\right)^s.$$

Observing that $\mathrm{trace}(A) = \frac{1}{2}$, we find that $s\gamma = \frac{1}{2}$. With $|z| < \frac{1}{\gamma}$, consider the power series

$$W(z) = 1 + 2s\gamma z + 2s^2\gamma^2 z^2 + \tfrac{2}{3}s(2s^2 + 1)\gamma^3 z^3 + O(z^4)(z \to 0).$$

Then $2s\gamma = 1$, $2s^2\gamma^2 = \frac{1}{2}$, and $\frac{2}{3}s(2s^2 + 1)\gamma^3 \neq \frac{1}{6}$ holds for all s. ◻

EXAMPLE 4.9. *All DJ–irreducible a–symplectic semi–implicit Runge–Kutta methods are generated by*

$$A = \begin{bmatrix} \frac{b_1}{2} & & & 0 \\ b_1 & \ddots & & \\ \vdots & \ddots & \ddots & \\ b_1 & \ldots & b_{s-1} & \frac{b_s}{2} \end{bmatrix}, \; b = \begin{bmatrix} b_1 \\ \vdots \\ b_s \end{bmatrix} \quad \textit{with} \;\; b_i \neq 0, \;\; i = 1(1)s.$$

As mentioned earlier we assume that there are no equivalent half–stages in partitioned Runge–Kutta methods. A detailed study of the generating matrix of explicit partitioned methods yields the following result.

COROLLARY 4.10. *All DJ–irreducible explicit (s_1, s_2)–stage partitioned Runge–Kutta methods $\beta^{(1,2)}$ with $M^{(1,2)} = 0$ are generated by $\mathcal{A}^{(1,2)}$ where $|s_1 - s_2| \leq 1$ and*

$$
\begin{aligned}
&a_{ij}^{(1)} = 0 && \textit{for } i < j,\ i = 1(1)s_1 \textit{ and } j = 1(1)s_2,\\
&a_{ij}^{(2)} = 0 && \textit{for } i < j,\ i = 1(1)s_2 \textit{ and } j = 1(1)s_1,\\
&a_{ij}^{(1)} = b_j^{(1)} && \textit{for } i > j,\ i = 1(1)s_1 \textit{ and } j = 1(1)s_2,\\
&a_{ij}^{(2)} = b_j^{(2)} && \textit{for } i > j,\ i = 1(1)s_2 \textit{ and } j = 1(1)s_1,\\
&a_{ii}^{(1)} = 0 && \textit{and } a_{ii}^{(2)} = b_i^{(2)} \textit{ for } i = 1(1)s_2 \textit{ if } s_1 = s_2 + 1,\\
&a_{ii}^{(1)} = b_i^{(1)} && \textit{and } a_{ii}^{(2)} = 0 \quad \textit{for } i = 1(1)s_1 \textit{ if } s_1 = s_2 - 1,\\
&a_{ii}^{(1)} = 0 && \textit{and } a_{ii}^{(2)} = b_i^{(2)} \textit{ for } i = 1(1)s \quad \textit{or}\\
&a_{ii}^{(1)} = b_i^{(1)} && \textit{and } a_{ii}^{(2)} = 0 \quad \textit{for } i = 1(1)s \quad \textit{if } s_1 = s_2 = s.
\end{aligned}
$$

For Runge–Kutta methods, it is easy to check the order of (s_1, s_2)–stage partitioned Runge–Kutta methods by using the simplifying assumptions. In the case of autonomous systems $\hat{C}(1)$ imports the definition of the nodes $c_i^{(1)}$ and $c_i^{(2)}$ for $i = 1(1)s_1$ and $i = 1(1)s_2$, respectively. We consider methods up to order four. If $M^{(1,2)} = 0$, and if $\hat{B}(1)$ and $\hat{C}(1)$ are given, then in $\hat{B}(2)$ the two conditions for $\nu = 2$ are equivalent. Further, a (s_1, s_2)–stage partitioned Runge–Kutta method with $M^{(1,2)} = 0$ has order two if $\hat{C}(1)$ and $\hat{B}(2)$ hold, order three if $\hat{C}(1)$ and $\hat{B}(3)$ hold, and order four if it is order three and the symmetry condition in the usual sense is satisfied. Order conditions of s–stage partitioned Runge–Kutta methods with $M^{(1,2)} = 0$ are known (see Sanz–Serna and Calvo [10, Chap. 7]). These conditions are easily modified for (s_1, s_2)–stage methods.

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