## CHARACTERIZATION AND CONSTRUCTION OF LINEAR SYMPLECTIC RK-METHODS\*1)

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#### Abstract

A characterization of linear symplectic Runge-Kutta methods, which is based on the W-transformation of Hairer and Wanner, is presented. Using this characterization three classes of high order linear symplectic Runge-Kutta methods are constructed. They include and extend known classes of high order linear symplectic Runge-Kutta methods.

### 1. Introduction

The present paper is a continuation of [13] where characterizations of symmetric and symplectic Runge-Kutta methods, based on the W-transformation of Hairer and Wanner, were presented. Using the characterization of symplectic Runge-Kutta methods, two classes of high order symplectic Runge-Kutta methods were constructed there. In the present paper we shall discuss a characterization of linear symplectic Runge-Kutta methods, which is based on the W-transformation of Hairer and Wanner. Up to now only symmetric one-step methods are found to be linear symplectic in the class of high order one-step methods. We shall construct three classes of high order linear symplectic Runge-Kutta methods, which include and extend known classes of high order linear symplectic Runge-Kutta methods. In this paper we shall continue to use the notation in [13].

It is well known that the stability function of implicit Runge-Kutta methods may

be written as

$$R(z) = \frac{\det(I - zA + zeb^T)}{\det(I - zA)},$$
(1.1)

or 
$$R(z) = 1 + zb^{T}(I - zA)^{-1}e. (1.1)$$

In [6] Feng has proved that the necessary and sufficient condition of linear symplectic schemes is

$$R(z)R(-z)=1. (1.2)$$

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From [6] we can easily obtain that symmetric Runge-Kutta methods are linear symplectic. In [13] we have proved

Theorem 1.1. An s-stage RK-method with distinct nodes  $c_i$  and  $b_i \neq 0$  satisfying  $B(p), C(\eta)$  and  $D(\xi)$  with  $p \geq s + \zeta$  is symmetric if and only if

a)  $\tilde{P}c = e - c$  for the permutation matrix  $\tilde{P}$ ,

b) the transformation matrix X of the method takes the following form

$$X = W^T B A W = \begin{pmatrix} 1/2 & -\xi_1 \\ \xi_1 & \ddots & \ddots \\ & \ddots & 0 & -\xi_{\nu} \\ & & \xi_{\nu} & R_{\nu} \end{pmatrix}, where \ \nu = \min(\eta, \zeta) \tag{1.3}$$

having the residue matrix  $R_{\nu}$  whose (k,l)-th element  $r_{kl}=0$  if k+l is even, where the (i,j)-th element of permutation matrix  $\widetilde{P}$  is the Kronecker  $\delta_{i,s+1-j}$ .

In [9] Hairer and Wanner have found that the stability function in terms of the transformed RK-matrix  $X = W^{-1}AW$  can be expressed as

$$R(z) = \frac{\det(I - zX + ze_1e_1^T)}{\det(I - zX)},$$
(1.4)

or

$$R(z) = 1 + ze_1^T (I - zX)^{-1}e_1, (1.4)'$$

that is, R(z) depends only on X and not on the underlying quadrature formula. Thus, Theorem 1.1 condition b) should be a characterization of linear symplectic Runge-Kutta methods, which is based on the W-transformation of Hairer and Wanner. Note that there exists a difference between the definition of transformation matrices

$$X^* = W^{-1}AW$$

and

$$X = W^T B A W,$$

but it is not essential. The two matrices are related by

$$X = W^T B W X^*. (1.5)$$

In general, X and  $X^*$  should possess identical properties. We can obtain at least the following result:

Lemma 1.2. For the transformation matrices specified by  $X^* = W^{-1}AW$  and  $X = W^TBAW$  respectively, if one of  $(X - \frac{1}{2}e_1e_1^T)$  and  $(X^* - \frac{1}{2}e_1e_1^T)$  satisfies condition b) in Theorem 1.1, then the other does also if and only if the (k, l)-th element of matrix  $W^TBW$  vanishes if k+l is odd.

Proof. Let

By the assumption and  $X = W^T B W X^*$  we have

$$\widetilde{I}\left(X-\frac{1}{2}e_1e_1^T\right)\widetilde{I}^T=-\left(X-\frac{1}{2}e_1e_1^T\right)=-W^TBW\left(X^*-\frac{1}{2}e_1e_1^T\right).$$

On the other hand, there is

$$\begin{split} \widetilde{I}\Big(X - &\frac{1}{2}e_1e_1^T\Big)\widetilde{I}^T = \widetilde{I}W^TBW\Big(X^* - \frac{1}{2}e_1e_1^T\Big)\widetilde{I}^T \\ &= \widetilde{I}W^TBW\widetilde{I}^T\widetilde{I}\Big(X^* - \frac{1}{2}e_1e_1^T\Big)\widetilde{I}^T \\ &= W^TBW\widetilde{I}\Big(X^* - \frac{1}{2}e_1e_1^T\Big)\widetilde{I}^T. \end{split}$$

Thus we obtain

Thus we obtain 
$$\widetilde{I}\left(X^*-\frac{1}{2}e_1e_1^T\right)\widetilde{I}^T+\left(X^*-\frac{1}{2}e_1e_1^T\right)=0.$$

The reverse is also obvious.

In Section 2, we shall give a characterization of linear symplectic Runge-Kutta methods, which is based on the W-transformation of Hairer and Wanner and other results. Using these results the existing linear symplectic Runge-Kutta methods (including block implicit one-step methods and composite multistep methods) are verified. In Section 3, we construct three classes of linear symplectic Runge-Kutta methods using the characterization of linear sympletic Runge-Kutta methods. Finally, examples of new methods for two and three stages are given .

## 2. Characterization of linear symplectic RK-methods

Let  $\Omega$  be a domain (i.e. a non-empty, open, connected set) in the oriented Euclidean space  $\mathbb{R}^{2d}$  of the point  $(p,q)=(p_1,\cdots,p_d;q_1,\cdots,q_d)$ . If H is a sufficiently smooth real function defined in  $\Omega$ , then the Hamiltonian system of differential equations with Hamiltonian H is given by

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} =: f_i(p,q), \qquad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} =: g_i(p,q), \qquad 1 \le i \le d. \tag{2.1}$$

The integer d is called the number of degrees of freedom and  $\Omega$  is the phase space.

A smooth transformation  $(p,q)=\psi(p^*,q^*)$  defined in  $\Omega$  is said to be symplectic (with respect to symplectic matrix J) if the Jacobian  $\psi' = \frac{\sigma(p,q)}{R(n^*,q^*)}$  satisfies

$$\psi'^T J \psi' = \frac{\partial (p,q)^T}{\partial (p^*,q^*)} J \frac{\partial (p,q)}{\partial (p^*,q^*)} = J, \quad \forall (p^*,q^*) \in \Omega,$$

where  $J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}$  is the so-called standard symplectic matrix.

This property is the hallmark of Hamiltonian systems.

In this paper, we restrict our interest to one step methods. If h denotes the steplength and  $(p^n, q^n)$  denotes the numerical approximations at time  $t_n = nh$  to the value  $(p(t_n), q(t_n))$  of a solution of (2.1), the one-step method is specified by a smooth mapping

 $(p^{n+1},q^{n+1})=\psi_{h,H}(p^n,q^n)$ 

and  $\psi_{h,H}$  is assumed to depend only smoothly on h and H. In numerically solving the Hamiltonian systems of differential equations (2.1), it is natural to require that numerical solutions should preserve the property of symplecticity. Then the numerical method

$$(p^{n+1},q^{n+1})=\psi_{h,H}(p^n,q^n)$$

should be a symplectic transformation. To sum up, we give the following definitions.

Definition 2.1. A one-step method is called symplectic if, as applied to Hamiltonian systems (2.1), the underlying formula of generating numerical solutions  $(p^{n+1}, q^{n+1})$ ,  $(p^{n+1}, q^{n+1}) = \psi_{h,H}(p^n, q^n)$ , is a symplectic transformation, that is,

$$\psi_{h,H}^{'T}J\psi_{h,H}^{'} = \frac{\partial(p^{n+1},q^{n+1})^{T}}{\partial(p^{n},q^{n})}J\frac{\partial(p^{n+1},q^{n+1})}{\partial(p^{n},q^{n})} = J, \qquad \forall (p^{n},q^{n}) \in \Omega$$
 (2.2)

holds, where  $\psi'_{h,H} = \frac{\partial (p^{n+1}, q^{n+1})^T}{\partial (p^n, q^n)}$  is the Jacobian matrix of the transformation.

Definition 2.2. A gne-step method is called linear symplectic if it is symplectic for linear Hamiltonian systems.

For Hamiltonian systems there exists the relation

$$\frac{\partial (f,g)^T}{\partial (p,q)}J + J\frac{\partial (f,g)}{\partial (p,g)} = 0.$$
 (2.3)

For notational simplicity, we assume d = 1 in the following. The Runge-Kutta methods with tableau

applied to the Hamiltonian systems (2.1), by virtue of the relation (2.3), we may obtain

$$\frac{\partial (p^{n+1}, q^{n+1})^{T}}{\partial (p^{n}, q^{n})} J \frac{\partial (p^{n+1}, q^{n+1})}{\partial (p^{n}, q^{n})} \\
= J - h^{2} \sum_{i,j=1}^{s} m_{i,j} \frac{\partial (f(p_{i}, q_{i}), g(p_{i}, q_{i}))^{T}}{\partial (p^{n}, q^{n})} J \frac{\partial (f(p_{j}, q_{j}), g(p_{j}, q_{j}))}{\partial (p^{n}, q^{n})}, \qquad (2.5)$$

where

$$m_{i,j} = b_i a_{i,j} + b_j a_{j,i} - b_i b_j, \qquad 1 \leq i, j \leq s,$$

that is, the so-called M matrix introduced in [2] where it is used to define algebraic stability in the study of stability criteria of implicit RK-methods. Obviously, if the coefficients of the method (2.4) satisfy

$$m_{i,j} = 0$$
,  $1 \le i, j \le s$ , or  $M = BA + A^TB - bb^T = 0$ ,

then the method is symplectic. The result was discovered independently by Lasagni<sup>[10]</sup>, Sanz-Serna<sup>[12]</sup> and<sup>[14]</sup>.

For linear Hamiltonian systems, in fact  $\frac{\partial (f,g)^T}{\partial (p,q)} = C$  is a constant matrix, and then the second term on the right-hand side of (2.5) may be expanded as a series about  $h^2C^TJC$ . Finally, (2.5) becomes

$$\frac{\partial (p^{n+1}, q^{n+1})^T}{\partial (p^n, q^n)} J \frac{\partial (p^{n+1}, q^{n+1})}{\partial (p^n, q^n)} = J - \sum_{k \ge 1} m_{i,j}^{(k-1)} h^{2k} (C^T)^k J C^k, \tag{2.6}$$

where  $m_{i,j}^{(0)} = m_{i,j}$ .

A question follows immediately; for linear symplectic methods, what is the characterization of  $M^{(k)}(k=0,1,2,\cdots)$  matrix?

Using (1.1)', expanding  $(I - Az)^{-1}$  and  $(I + zA)^{-1}$  in origin Taylor series about z and inserting them into (1.2) give the following result:

Theorem 2.1. An s-stage implicit RK-method is linear symplectic if and only if

$$e^{T}\left(\sum_{l=0}^{2k}(-1)^{l}(A^{T})^{2k-l}MA^{l}\right)e=0, \quad k=0,1,2,\cdots,$$
 (2.7)

and there is

$$M^{(k)} = \left(\sum_{l=0}^{2k} (-1)^l (A^T)^{2k-l} M A^l\right), \quad k = 0, 1, 2, \cdots.$$

Corollary 1. For linear symplectic RK-methods,

$$e^T M e = 0$$

is necessary but not sufficient.

For example, a 2-stage one-step method with order 2

$$egin{array}{c|ccccc} 0 & 0 & 0 \\ \hline 1 & 0 & 1 \\ \hline & 1 & 1 \\ \hline \hline 2 & 2 \\ \hline \end{array}$$

satisfies  $e^T M e = 0$  but is not linear symplectic.

It might be conjectured that the RK-method which satisfies the conditions

$$e^T M e = 0$$

and

$$e^{T} \left( \sum_{l=0}^{2} (-1)^{l} (A^{T})^{2-l} M A^{l} \right) e = 0$$

is linear symplectic. The following example gives a negative answer. A 3-stage Lobatto-.

where  $\forall \beta \in I\!\!R$ , satisfies  $e^T M e = 0$  and  $e^T \Big( \sum_{l=0}^2 (-1)^l (A^T)^{2-l} M A^l \Big) e = 0$ , but is not linear symplectic.

Motivated by the above examples, we may conjecture that an s-stage implicit RK-method with order  $p \ge s$  is linear symplectic, if

$$e^{T}\left(\sum_{l=0}^{2k}(-1)^{l}(A^{T})^{2k-l}MA^{l}\right)e=0, \quad k=0,1,2,\cdots,s-1.$$
 (2.8)

Obviously, even if the answer is affirmative, it is inconvenient to use the relation (2.8) to check whether a one-step method is linear symplectic.

For a special class of implicit RK-methods, namely symmetric methods, we shall give a set of conditions for checking linear symplectic methods, which is based on M matrix, later in this section. Now we discuss symmetric methods from another angle. In [13] it was shown that an s-stage RK-method is symmetric if and only if for the permutation matrix  $\tilde{P}$  whose (i,j)-th element is the Kronecker  $\delta_{i,s+1-j}$ ,

$$A + \widetilde{P}A\widetilde{P}^T = eb^T \tag{2.9}$$

and

$$\tilde{P}b = b \tag{2.10}$$

hold. From this, we can obtain easily the following result:

Theorem 2.2. Symmetric Runge-Kutta methods are linear symplectic.

Proof. By (2.9) there is

$$\det(I-zA+zeb^T)=\det(I+z\widetilde{P}A\widetilde{P}^T)=\det(I+zA).$$

According to (1.1), R(z)R(-z) = 1 holds.

Recalling Theorem 1.1 and in combination with the result [9], that the stability function in terms of the transformed RK-matrix  $X = W^{-1}AW$  depends only on X and not on the underlying quadrature formula, we can obtain

Theorem 2.3. An s-stage high-order IRK-method with distinct nodes  $c_i$  and  $b_i \neq 0$  satisfying B(p),  $C(\eta)$  and  $D(\zeta)$  with  $p \geq s+\zeta$  is linear symplectic, if the (k,l)-th element of the residue matrix  $R_{\nu}$  in the transformation matrix X satisfies  $r_{kl} = 0$  as k+l is even.

Proof. By 
$$W^TBe = W^Tb = e_1$$
 and  $X = W^TBWX^*$  there is 
$$W^TB(I - zA + zeb^T)W = W^TBW - zX + ze_1e_1^T$$
$$= W^TBW(I - zX^* + ze_1e_1^T).$$

Hence formula (1.1) becomes

$$R(z) = \frac{\det(I - zX^* + ze_1e_1^T)}{\det(I - zX^*)}.$$

Furthmore, by Lemma 1.2 and the property of the residue matrix  $R_{\nu}$  we obtain

$$R(z) = \frac{\det\left(\widetilde{I}(I - zX^* + ze_1e_1^T)\widetilde{I}^T\right)}{\det(I - zX^*)} = \frac{\det(I + zX^*)}{\det(I - zX^*)}.$$

For symmetric RK-methods conditions (2.9) and (2.10) imply

$$\tilde{P}c = e - c \tag{2.11}$$

and

$$M = -\tilde{P}M\tilde{P}^T. (2.12)$$

For example, for (2.12), by (2.9) and (2.10) there is

$$BA + \tilde{P}BA\tilde{P}^T - bb^T = 0.$$

Then, adding

$$(BA + \tilde{P}BA\tilde{P}^T - bb^T)^T = 0$$

to the formula above we may obtain (2.12). But, under conditions (2.10) and (2.11), we cannot obtain (2.9) from (2.12). Then, for arbitrary s (stage of RK-method) there is the following result:

Theorem 2.4. An s-stage RK-method is linear symplectic if (2.10)-(2.12) and

$$C(\eta), \eta \ge s-2$$
 or  $D(\zeta), \zeta \ge s-2$  (2.13)

hold.

*Proof.* Let  $\tilde{X} = (\tilde{P}W)^T BA(\tilde{P}W)$ . Since  $\tilde{P}c = e - c$ , by the symmetry of Legendre polynomials we have  $\tilde{P}P_k(c) = (-1)^k P_k(c)$  for k = 0(1)s - 1. It then follows that

$$\tilde{X}_{kl} = (-1)^{k+l} X_{kl}. \tag{2.14}$$

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Condition (2.12) may be rewritten as

$$BA + \tilde{P}BA\tilde{P}^T - bb^T = -(BA + \tilde{P}BA\tilde{P}^T - bb^T)^T.$$

We have

$$W^T(BA + \widetilde{P}BA\widetilde{P}^T - bb^T)W = -(W^T(BA + \widetilde{P}BA\widetilde{P}^T - bb^T)W)^T$$

$$\Longrightarrow X + \widetilde{X} = e_1e_1^T = -(X + \widetilde{X} - e_1e_1^T)^T$$

(for more details see [13]), that is, the matrix  $X + \tilde{X} - e_1 e_1^T$  is skew symmetric. Furthermore, according to conditions (2.13) and (2.14), there is

$$X + \widetilde{X} - e_1 e_1^T = 0$$

and the transformation matrix X must satisfy the condition b) in Theorem 1.1. Therefore, the method is linear symplectic.

It may be seen from the proof above that the matrix  $(BA + \tilde{P}BA\tilde{P}^T - bb^T)$  is skew symmetric and  $(BA + \tilde{P}BA\tilde{P}^T - bb^T)e = 0$  if the condition  $s \leq 3$  is used in place of (2.13) in Theorem 2.4 such conclusion holds still.

Up to now Lobatto III A and III B methods are found to be linear symplectic in the class of high order RK-methods (besides symplectic RK-methods). Their linear symplecticness can be verified easily by one of Theorems 2.2–2.4 because the methods are symmetric. In addition, for example, A-stable block implicit one-step methods [15] and A-stable composite multistep methods [1] with the form

$$\bar{y}_m = ey_n + h\bar{d}f_n + h\bar{B}F(\bar{y}_m), \quad n = mr, \quad m = 0, 1, 2, \cdots,$$

where  $\bar{d} = (d_1, d_2, \dots, d_r)^T$ ,  $\bar{y}_m = (y_{n+1}, y_{n+2}, \dots, y_{n+r})^T$ ,  $F(\bar{y}_m) = (f_{n+1}, f_{n+2}, \dots, f_{n+r})^T$  and  $\bar{B} = (b_{ij})_{r+r}$ , are also linear symplectic. In fact, A-stable r-block one-step methods or A-stable r-step composite multistep methods above may be converted into an (r+1)-stage symmetric RK-method which possesses a special Runge-Kutta tableau

By (2.15) and the property of the transformation matrix X of linear symplectic methods, such linear symplectic r-block one-step methods or r-step composite multistep methods can reach at most 2r-th order.

# 3. The Construction of linear symplectic RK-methods

We construct a family of s-stage IRK-methods satisfying at least B(2s-2), C(s-2) and D(s-2), based on the combination

$$M(x) = P_s(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-1}} \alpha P_{s-1}(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-3}} \beta P_{s-2}(x), \tag{3.1}$$

which is linear symplectic, where  $P_{s-i}(x)$ , i=0,1,2, are Legendre polynomials of degree s-i, i=0,1,2, respectively. Here we assume that the roots of M(x), c, are real and distinct, the weights are determined by B(2s-2). Furthermore, by the definition

of W, we compute a matrix W and then choose the transformation matrix as

$$X = \begin{pmatrix} 1/2 & -\xi_1 & & & & & \\ \xi_1 & 0 & \ddots & & & & \\ & \ddots & \ddots & -\xi_{s-2} & & & \\ & & \xi_{s-2} & 0 & -\xi_{s-1}\sigma_1 \\ & & & \xi_{s-1}\sigma_2 & 0 \end{pmatrix}$$
(3.2)

where  $\xi_k = \frac{1}{2\sqrt{4k^2-1}}$  and  $\sigma_1, \sigma_2 \in \mathbb{R}$ .

According to Theorem 2.3 and Butcher's fundamental theorem [3], the four-parameter family of IRK-methods with coefficients  $A = WXW^TB$ , which is linear symplectic and of order at least 2s - 2, is constructed (see [9] IV.5. for details). Besides such results with the special choice of parameters  $(\alpha, \beta, \sigma_1 \text{ and } \sigma_2)$  we can obtain:

- a)  $\alpha = \beta = 0$  corresponding to s-stage Gauss-type method:
  - 1) order 2s if  $\sigma_1 = \sigma_2 = 1[3]$ ;
  - 2) order 2s-2 with B(2s), C(s-2) and D(s-2), if  $\sigma_1, \sigma_2 \neq 1$ ;
  - 3) order 2s-2 with B(2s), C(s-1) and D(s-2), if  $\sigma_1 \neq 1$  and  $\sigma_2 = 1$ ;
  - 4) order 2s-2 with B(2s), C(s-2) and D(s-1), if  $\sigma_1=1$  and  $\sigma_2\neq 1$ ;
- b)  $\alpha = 0$  and  $\beta = -1$  corresponding to s-stage Lobatto-type methods with order 2s 2:
  - 1) Lobatto III A method if  $\sigma_1 = 0$  and  $\sigma_2 = \frac{1}{b^T P_{s-1}^2(c)}$  [5];
  - 2) Lobatto III B method if  $\sigma_1 = \frac{1}{b^T P_{s-1}^2(c)}$  and  $\sigma_2 = 0[5]$ ;
  - 3) Lobatto III E method if  $\sigma_1 = \sigma_2 = \frac{1}{b^T P_{s-1}^2(c)}$  [11],[4];
  - 4) Lobatto III S method if  $\sigma_1 = \sigma_2 \neq \frac{1}{b^T P_{s-1}^2(c)}$  and  $s \geq 3[4]$ ;
  - 5) Lobatto III X method if  $\sigma_1 \neq \sigma_2$  and, besides 1) and 2);
  - c)  $\beta = 0$  and  $\alpha = 1$  corresponding to s-stage Radau I type method :
- 1) Radau I B method with order 2s-1 satisfying B(2s-1), C(s-1) and D(s-1) if  $\sigma_1 = \sigma_2 = 1[13]$ ;
  - 2) Called as Radau I C method with order 2s-2 satisfying B(2s-1),

C(s-1) and D(s-2) if  $\sigma_1=0$  and  $\sigma_2=1$ ;

- 3) Called as Radau I D method with order 2s-2 satisfying B(2s-1),
- C(s-2) and D(s-1) if  $\sigma_1 = 1$  and  $\sigma_2 = 0$ ;
  - d)  $\beta = 0$  and  $\alpha = -1$  corresponding to s-stage Radau II type method:
    - 1) Radau II B method with order 2s-1 satisfying B(2s-1),
- C(s-1) and D(s-1) if  $\sigma_1 = \sigma_2 = 1$  [13];
  - 2) Called Radau II C method with order 2s-2 satisfying B(2s-1),
- C(s-1) and D(s-2) if  $\sigma_1=0$  and  $\sigma_2=1$ ;
  - 3) Called Radau II D method with order 2s-2 satisfying B(2s-1),
- C(s-2) and D(s-1) if  $\sigma_1=1$  and  $\sigma_2=0$ .

The examples of new methods of Gauss type and Radau type for two and three stages are given in the following.

The 2-and 3-stage Gauss type methods with order 2 and 4 are

$$\frac{1}{2} = \frac{\sqrt{3}}{2} \left[ \frac{1}{1 + (\sigma_1 - \sigma_2)} \frac{\sqrt{3}}{2} \right] = \frac{1}{2} \left( 1 - (\sigma_1 + \sigma_2) \frac{\sqrt{3}}{2} \right)$$