

SYMPLECTIC RK METHODS AND SYMPLECTIC PRK METHODS WITH REAL EIGENVALUES ^{*1)}

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Abstract

Properties of symplectic Runge-Kutta (RK) methods and symplectic partitioned Runge-Kutta (PRK) methods with real eigenvalues are discussed in this paper. It is shown that an s stage such method can't reach order more than $s + 1$. Particularly, we prove that no symplectic RK method with real eigenvalues exists in stage s of order $s + 1$ when s is even. But an example constructed by using the \mathbf{W} -transformation shows that PRK method of this type does not necessarily meet this order barrier. Another useful way other than \mathbf{W} -transformation to construct symplectic PRK method with real eigenvalues is then presented. Finally, a class of efficient symplectic methods is recommended.

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Key words: Runge-Kutta method, Partitioned Runge-Kutta method, Symplectic, Real eigenvalues.

1. Introduction

A Hamiltonian system

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad \dot{q}_i = \frac{\partial H}{\partial p_i}, \quad 1 \leq i \leq d, \quad (1)$$

is a particular instance of the general systems of differential equations

$$\frac{dy}{dt} = F(y), \quad \text{with } y = [p, q]^T \in \mathbf{R}^D, \quad D = 2d, \quad \text{and, } F = J^{-1}\nabla H, \quad (2)$$

where, $J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix}$ is the standard symplectic matrix.

When an s stage RK method (A, b, c) , i.e. ,

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

applied to system (2), it advances the numerical solution from time t_n to time $t_{n+1} = t_n + h$ through the relation

$$y^{n+1} = y^n + h \sum_{i=1}^s b_i F(Y_i), \quad (3)$$

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where the stage vectors Y_i are given by

$$Y_i = y^n + h \sum_{j=1}^s a_{ij} F(Y_j), 1 \leq i \leq s. \quad (4)$$

If the method is implicit, (4) provides a coupled system of $s \times \mathcal{D}$ algebraic equations for the $s \times \mathcal{D}$ components of the stage vectors. The computational cost per step of an implicit RK method is then definitely great, especially if s or \mathcal{D} in large scale, and has become an obstacle to the application of those methods in practice. But a technique due to Butcher and Bickart can remarkably reduce the computation. We simply explain their idea as follows.

First, we introduce the increments

$$Z_i = Y_i - y^n,$$

then (4) can be rewritten as

$$\begin{bmatrix} Z_1 \\ \vdots \\ Z_s \end{bmatrix} = h(A \otimes I) \begin{bmatrix} F(y^n + Z_1) \\ \vdots \\ F(y^n + Z_s) \end{bmatrix}, \quad (5)$$

where the symbol \otimes denotes the Kronecker product.

The simplified Newton iteration for (5) reads

$$(I - hA \otimes J_F) \Delta \mathbf{Z}^{(k)} = -\mathbf{Z}^{(k)} + h(A \otimes I) \mathbf{F}(\mathbf{Z}^{(k)}), \quad \mathbf{Z}^{(k+1)} = \mathbf{Z}^{(k)} + \Delta \mathbf{Z}^{(k)}. \quad (6)$$

Here, $\mathbf{Z} = [Z_1, \dots, Z_s]$, $\mathbf{F}(\mathbf{Z}) = [F(y^n + Z_1)^T, \dots, F(y^n + Z_s)^T]^T$, $J_F = \frac{\partial \mathbf{F}}{\partial \mathbf{Y}}(y^n)$. If A is invertible, then the technique mentioned above is to premultiply (6) by $(hA)^{-1} \otimes I$ and transform A^{-1} into a matrix D with a simpler structure (for instance diagonal, block diagonal, triangular)

$$T^{-1} A^{-1} T = D.$$

In the transformed variables

$$\mathbf{W} = (T^{-1} \otimes I) \mathbf{Z},$$

the iteration (6) reads

$$\begin{cases} (h^{-1} D \otimes I - I \otimes J_F) \Delta \mathbf{W}^{(k)} = -h^{-1} (D \otimes I) \mathbf{W}^{(k)} + (T^{-1} \otimes I) \mathbf{F}((T \otimes I) \mathbf{W}^{(k)}), \\ \mathbf{W}^{(k+1)} = \mathbf{W}^{(k)} + \Delta \mathbf{W}^{(k)}. \end{cases} \quad (7)$$

In the case where D is a diagonal matrix with diagonal entries λ_i , the eigenvalues of A^{-1} , the matrix $(h^{-1} D \otimes I - I \otimes J_F)$ to be factorized is now block diagonal with s blocks $h^{-1} \lambda_i I - J_F$. Hence now it is only necessary to factorize $s \mathcal{D} \times \mathcal{D}$ matrices with an operation count $sO(\mathcal{D}^3)$. This is to be compared with the factorization of an $s\mathcal{D}$ -dimensional matrix in (5) with a count $O((s\mathcal{D})^3)$. So it is much computationally efficient if λ_i are all real, i.e., A has real eigenvalues only. Two particular cases of implicit methods, called SIRK (Singly Implicit Runge-Kutta method) and DIRK (Diagonally Implicit Runge-Kutta method), occur, respectively, when A has a unique non-zero real eigenvalue λ , i.e., $\sigma(A) = \lambda$ and $a_{ij} = 0$ for $i < j$, and they have almost the same efficiency as the multi-step methods. As is known, symplectic RK methods and symplectic PRK methods for non-separable Hamiltonian systems must be implicit. In this paper, we mainly focus on the symplectic RK methods and symplectic PRK methods with real eigenvalues for Hamiltonian system(1). Firstly, we show that an s stage RK&PRK method with real eigenvalues can not reach order more than $s + 1$. It is then proved that no symplectic RK method with real eigenvalues exists in stage s of order $s + 1$ when s is even. But symplectic PRK methods of this type don't necessarily meet this order barrier, and this is shown by an example constructed by using \mathbf{W} -transformation. An useful way other than \mathbf{W} -transformation to construct symplectic PRK methods with real eigenvalues is then presented. The conclusion we make is that, in high order level, composition methods due to Yoshida (see[5]) are of our advantage in consideration of the efficiency for these algorithms. Finally, a class of symplectic efficient methods of low order is recommended.

2. Properties and Construction of Symplectic RK&PRK Methods With Real Eigenvalues

In order to give the properties of RK methods with real eigenvalues here we quote a result in [4],

Theorem 2.1. *Let $R(z)$ be the stability function of an s stage RK method with coefficient (A, b, c) and suppose that it be an approximation to e^z of order p with real poles only. Then $p \leq k + 1 \leq s + 1$, where k is the degree of $R(z)$'s numerator.*

Now, we can obtain

Corollary 2.1. *Let (A, b, c) be an s stage RK method of order p with real eigenvalues only, then $p \leq k + 1 \leq s + 1$.*

Proof. Notice that $R(z) = \frac{P(z)}{Q(z)} = \frac{\det(I - zA + zeb^T)}{\det(I - zA)}$ and the reciprocals of the poles of $R(z)$ are the non-zero eigenvalues of A , and vice versa, it is a straightforward deduction from theorem 2.1.

Corollary 2.2. *Only one stage Gauss method, i.e., midpoint method has real eigenvalues only. Radau IB, Radau IIB methods(see [10]) can't have real eigenvalues only, if $s \geq 2$. Meanwhile, the stage of Lobatto IIIA, IIIB and IIIS methods with real eigenvalues can only be $s = 2$.*

Proof. For Gauss methods, $p = 2s$, by $p \leq s + 1$, we have $s \leq 1$. For Radau IB and Radau IIB methods, $p = 2s - 1$, by $2s - 1 \leq s + 1$, we have $s \leq 2$. Further, we can see from theorem 2.2 below, 2-stage Radau IB and Radau IIB methods, which are of order 3 can't have real eigenvalues only. In the case of Lobatto IIIA, IIIB, and IIIS, $R(z)$ are all Padé(s-1,s-1)-approximation and $p = 2s - 2$, hence by $2s - 2 \leq s - 1 + 1$, we have $s \leq 2$, i.e., $s = 2$ since there doesn't exist 1 stage method in Lobatto family.

Corollary 2.2 shows that most of higher order symplectic RK methods based on quadrature formula are not of this type in discussion. In fact, we have the following order barrier for symplectic RK methods with real eigenvalues.

Lemma 2.1. *Let (A, b, c) be an s stage Runge-Kutta method with coefficients a_{ij}, b_j, c_i ($i, j = 1, \dots, s$) and (A^*, b^*, c^*) be its adjoint method. If (A, b, c) is symplectic, then (A^*, b^*, c^*) is also symplectic and the two methods have the same stability function.*

Proof. The coefficients of the adjoint method (A^*, b^*, c^*) is (see[3], II.8, theorem 8.3)

$$\begin{aligned} c_i^* &= 1 - c_{s+1-i} \\ a_{ij}^* &= b_{s+1-j} - a_{s+1-i, s+1-j} \\ b_j^* &= b_{s+1-j}. \end{aligned}$$

Now, the symplecticity of (A^*, b^*, c^*) can be seen by verifying the symplecticity criterion for RK methods (see [3], II.16, theorem 16.6),

$$\begin{aligned} b_i^* a_{ij}^* + b_j^* a_{ji}^* - b_i^* b_j^* &= b_{s+1-i}(b_{s+1-j} - a_{s+1-i, s+1-j}) + b_{s+1-j}(b_{s+1-i} - a_{s+1-j, s+1-i}) - b_{s+1-j} b_{s+1-i} \\ &= b_{s+1-i} b_{s+1-j} - b_{s+1-i} a_{s+1-i, s+1-j} - b_{s+1-j} a_{s+1-j, s+1-i} = 0. \end{aligned}$$

Let $R(z)$ and $R^*(z)$ be the stability function of the methods (A, b, c) and (A^*, b^*, c^*) , respectively. In order to prove $R(z) = R^*(z)$, we firstly prove that $R^*(z) = (R(-z))^{-1}$. In fact, applying (A, b, c) to the linear system $y' = \lambda y$ yields

$$y_h(x + h) = R(z)y_h(x), \quad z = \lambda h, \tag{8}$$

and $R^*(z) = (R(-z))^{-1}$ can be seen by replacing $h \rightarrow -h$ and then $x \rightarrow x + h$ in (8).

Next, applying the method to the linear Hamiltonian system

$$\dot{p} = \lambda p, \quad \dot{q} = -\lambda q \tag{9}$$

yields

$$p_1 = R(z)p_0, \quad q_1 = R(-z)q_0.$$

By the symplecticity, we have

$$dp_0 \wedge dq_0 = dp_1 \wedge dq_1 = R(z)R(-z)dp_0 \wedge dq_0.$$

Hence $R(z)R(-z) = 1$ and therefore $R(z) = (R(-z))^{-1} = R^*(z)$. The proof is completed.

Lemma 2.2. *Let φ_t be the exact flow of $y' = f(y), y(t_0) = y_0$ and let Φ_h be a one-step method of order p satisfying*

$$\Phi_h(y_0) = \varphi_h(y_0) + C(y_0)h^{p+1} + O(h^{p+2}).$$

The adjoint method Φ_h^* then has the same order p and we have

$$\Phi_h^*(y_0) = \varphi_h(y_0) + (-1)^p C(y_0)h^{p+1} + O(h^{p+2}).$$

Proof. Put $\mathbf{y}_1 = \Phi_h^*(\mathbf{y}_0)$ and let \mathbf{e}^* denote the local error of Φ_h^* , i.e.,

$$\mathbf{e}^* = \mathbf{y}_1 - \varphi_h(\mathbf{y}_0) = \Phi_h^*(\mathbf{y}_0) - \varphi_h(\mathbf{y}_0),$$

Let \mathbf{e} denote the local error of Φ_{-h} , i.e.,

$$\mathbf{e} = \Phi_{-h}(\mathbf{y}_1) - \mathbf{y}_0,$$

then from the first equation of the lemma, we have

$$\mathbf{e} = (-1)^{p+1} \mathbf{C}(\varphi_h(\mathbf{y}_0)) \mathbf{h}^{p+1} + O(\mathbf{h}^{p+2}).$$

Because

$$\mathbf{y}_0 = \Phi_{-h}(\mathbf{y}_1) = \Phi_{-h}(\varphi_h(\mathbf{y}_0)) + (\mathbf{I} + O(\mathbf{h}))\mathbf{e}^*,$$

hence,

$$\mathbf{e} = -(\mathbf{I} + O(\mathbf{h}))\mathbf{e}^*.$$

Notice that $\varphi_h(\mathbf{y}_0) = \mathbf{y}_0 + O(\mathbf{h})$, so

$$\mathbf{e}^* = (-1)^p \mathbf{C}(\mathbf{y}_0) \mathbf{h}^{p+1} + O(\mathbf{h}^{p+2}).$$

The proof is completed.

Theorem 2.2. *No symplectic RK method with real eigenvalues exists in stage s of order $p = s + 1$ when s is even.*

Proof. Let the method be (A, b, c) and $R(z), R^*(z)$ have the same meaning as above. We take $f(y) = \lambda y, y_0 = 1$ in lemma 2.2 and can have

$$R(z) = e^z + C(1)h^{p+1} + O(h^{p+2}), \quad R^*(z) = e^z + (-1)^p C(1)h^{p+1} + O(h^{p+2}).$$

Because $R(z) = R^*(z)$ by lemma 2.1 implies $C(1) = (-1)^p C(1)$, and therefore $C(1) = 0$ since $p = s + 1$ and s is an even number. So, $R(z)$ must be an approximation to e^z at least of order $s + 2$. A contradiction to theorem 2.1, which complete the proof.

In theorem 2.2, we in fact proved that the stability function $R(z)$ of a symplectic RK method must be an approximation to e^z of even order.

Iserles[6] constructed symplectic RK methods with the help of perturbed collocation and Hairer and Wanner[2] constructed a family of stage 3, order 4, symplectic RK method based on \mathbf{W} -transformation(see[4]). By theorem 2.2, no symplectic RK method with real eigenvalues exists of stage 4, order 5, but the PRK methods of this type do exist. Now, based on \mathbf{W} -transformation, we construct a family of symplectic PRK method with real eigenvalues of order 5 in stage 4.

Theorem 2.3. *Let $c_i (i = 1, 2, 3, 4)$ be the (real) zeros of*

$$M(x) = P_4(x) + \theta P_2(x), \text{ where } \theta \leq \frac{9}{4\sqrt{5}}, P_k(x) = \sum_{j=0}^k (-1)^{j+k} \begin{bmatrix} k \\ j \end{bmatrix} \begin{bmatrix} j+k \\ j \end{bmatrix} x_j, \quad (10)$$

and $b_i \neq 0 (i = 1, 2, 3, 4)$, the weights of the corresponding quadrature formula. Further, let $\alpha, \beta, \gamma, \eta$ be four numbers satisfying

$$70\alpha + 71\eta = 0, \quad (11)$$

$$70(\alpha - t) + 71 = 0, \text{ where } t = u\beta\gamma, u = \sum_{i=1}^4 b_3 P_3^2(x_i). \quad (12)$$

$$|\eta| \geq 117.3, \quad (13)$$

where 117.3 is the largest root of $\frac{1}{4}q^2 + \frac{1}{27}p^3 = 0, p = -\frac{1}{3} \times (\frac{\eta+35}{70})^2 + \frac{\eta+35}{140}, q = \frac{2}{27}(\frac{\eta+35}{70})^3(\frac{\eta-58}{140}) + \frac{71-7\eta}{840}$. Then a symplectic PRK method with coefficient (A, \bar{A}, b, c) of order 5 with real eigenvalues is obtained by,

$$W^T B A W = \begin{bmatrix} \frac{1}{2} & -\xi_1 & 0 & 0 \\ \xi_1 & 0 & -\xi_2 & 0 \\ 0 & \xi_2 & \alpha & u\beta \\ 0 & 0 & u\gamma & u\eta \end{bmatrix}, \tag{14}$$

$$W^T B \bar{A} W = \begin{bmatrix} \frac{1}{2} & -\xi_1 & 0 & 0 \\ \xi_1 & 0 & -\xi_2 & 0 \\ 0 & \xi_2 & -\alpha & -u\gamma \\ 0 & 0 & -u\beta & -u\eta \end{bmatrix}, \tag{15}$$

where $\xi_1 = \frac{1}{2\sqrt{3}}, \xi_2 = \frac{1}{2\sqrt{15}}, w_{ij} = P_{j-1}(c_i) (i, j = 1, 2, 3, 4)$, and $B = \text{diag}(b_1, b_2, b_3, b_4)$.

Proof. Formulas (10), (14), (15) imply conditions $B(6), C(2), D(2)$ of Butcher (see[4], Lemma 5.15 and Theorem 5.11), which mean order 5 for the PRK method, and they also conform to the criteria for symplecticity of the PRK method (see[9]),

$$X + \bar{X}^T - e_1 e_1^T = 0, \text{ where } X = W^T B A W, \bar{X} = W^T B \bar{A} W, e_1 = W^T b.$$

If we put $J = W^T B W = \text{diag}(1, 1, 1, u)$, then the eigenvalues of A and \bar{A} are those of

$$Y = W^{-1} A W = J^{-1} W^T B A W = \begin{bmatrix} \frac{1}{2} & -\xi_1 & 0 & 0 \\ \xi_1 & 0 & -\xi_2 & 0 \\ 0 & \xi_2 & \alpha & u\beta \\ 0 & 0 & u\gamma & u\eta \end{bmatrix}, \tag{16}$$

$$\text{and } \bar{Y} = W^{-1} \bar{A} W = J^{-1} W^T B \bar{A} W = \begin{bmatrix} \frac{1}{2} & -\xi_1 & 0 & 0 \\ \xi_1 & 0 & -\xi_2 & 0 \\ 0 & \xi_2 & -\alpha & -u\gamma \\ 0 & 0 & -u\beta & -u\eta \end{bmatrix}. \tag{17}$$

We pre-require that $P(\lambda) = |\lambda I - A|$ and $Q(\lambda) = |\lambda I - \bar{Y}|$ have a same root $\lambda_1 = 1$ which leads to (11) and (12). Then the roots of the cubic polynomial $P_1(\lambda) = \frac{P(\lambda)}{\lambda-1}$ are all real iff

$$D = \frac{1}{4}q^3 + \frac{1}{27}p^3 \leq 0, p = -\frac{1}{3} \times (\frac{\eta + 35}{70})^2 + \frac{\eta + 35}{140}, q = \frac{2}{27}(\frac{\eta + 35}{70})^3(\frac{\eta - 58}{140}) + \frac{71 - 7\eta}{840},$$

where D denotes the roots discriminant for the cubic equation $P_1(\lambda) = 0$. A straightforward computation leads to:

$$\eta \leq -87.459 \text{ or } 4.644 \leq \eta \leq 45.666 \text{ or } \eta \geq 111.73.$$

An analogous procedure applied to $Q_1(\lambda) = \frac{Q(\lambda)}{\lambda-1} = 0$ leads to :

$$\eta \geq 87.459 \text{ or } -45.666 \leq \eta \leq -4.644 \text{ or } \eta \leq -111.73.$$

Combining all these restrictions on η leads to (13). The proof is completed.

Next, we will give an example constructed as theorem 2.3.

Example 2.1. Taking $\theta = -\frac{9}{\sqrt{5}}, \alpha = -\frac{5538}{35}, \beta = -\frac{71\sqrt{35}}{49}, \gamma = \frac{93\sqrt{35}}{70}, \eta = 156$, then we can obtain an 4 stage 5th order symplectic PRK method with real eigenvalues

0	$\frac{713}{28}$	$\frac{5860-7999\sqrt{5}}{84}$	$\frac{5860+7999\sqrt{5}}{84}$	$-\frac{13859}{84}$
$\frac{5-\sqrt{5}}{10}$	$\frac{3481-4879\sqrt{5}}{280}$	$\frac{65539+59\sqrt{5}}{840}$	$\frac{-87341-1445\sqrt{5}}{840}$	$\frac{11779-14637\sqrt{5}}{840}$
$\frac{5+\sqrt{5}}{10}$	$\frac{3481+4879\sqrt{5}}{280}$	$\frac{-87341+1445\sqrt{5}}{840}$	$\frac{65539-59\sqrt{5}}{840}$	$\frac{11779-15938\sqrt{5}}{840}$
1	$-\frac{2803}{14}$	$\frac{5251+7289\sqrt{5}}{84}$	$\frac{5251-7289\sqrt{5}}{84}$	$\frac{520}{21}$
	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$

0	$-\frac{533}{21}$	$\frac{-10373+14637\sqrt{5}}{168}$	$\frac{-10373-14637\sqrt{5}}{168}$	$\frac{12505}{84}$
$\frac{5-\sqrt{5}}{10}$	$\frac{-5285+7999\sqrt{5}}{420}$	$\frac{-65189-59\sqrt{5}}{840}$	$\frac{-87691-1445\sqrt{5}}{840}$	$\frac{-5216-7289\sqrt{5}}{420}$
$\frac{5+\sqrt{5}}{10}$	$\frac{-5285-7999\sqrt{5}}{420}$	$\frac{-87691+1445\sqrt{5}}{840}$	$\frac{-65189+59\sqrt{5}}{840}$	$\frac{-5216-7289\sqrt{5}}{420}$
1	$\frac{2311}{14}$	$\frac{-3903-5313\sqrt{5}}{56}$	$\frac{-3903+5313\sqrt{5}}{56}$	$-\frac{691}{28}$
	$\frac{1}{12}$	$\frac{5}{12}$	$\frac{5}{12}$	$\frac{1}{12}$

A simple analysis can show that it more efficient than 3-stage Radau *IB* and Radau *ITB* methods, which are also of order 5(see[10]).

Theorem 2.3 shows that symplectic PRK method with real eigenvalues doesn't necessarily meet the order barrier in theorem 2.2. The following property of symplectic PRK methods with real eigenvalues may provide another way other than **W**-transformation as used in theorem 2.3 to construct such PRK methods.

Theorem 2.4. *Suppose (A, b, c) is a symmetric RK method with distinct nodes c_i and $b_i \neq 0$ ($i = 1, \dots, s$), then $(\bar{A}, \bar{b}, \bar{c})$ ($\bar{a}_{ij} = b_j(1 - \frac{a_{ji}}{b_i}), \bar{c}_i = \sum_{j=1}^s \bar{a}_{ij}, i, j = 1, 2, \dots, s$) is also a symmetric one, and they have the same stability function, i.e.*

$$R(z) = \frac{\det(I + zA)}{\det(I - zA)} = \frac{\det(I + z\bar{A})}{\det(I - z\bar{A})}. \tag{18}$$

Further, A and \bar{A} have the same eigenvalues.

Proof. By the symmetry of (A, b, c) , we have $a_{ij} + a_{s+1-i, s+1-j} = b_j = b_{s+1-j}$. So,

$$\bar{a}_{ij} + \bar{a}_{s+1-i, s+1-j} = b_j(1 - \frac{a_{ji}}{b_i}) + b_{s+1-j}(1 - \frac{a_{s+1-j, s+1-i}}{b_{s+1-i}}) \tag{19}$$

$$= b_j + b_{s+1-j} - (\frac{b_j}{b_i}a_{ji} + \frac{b_{s+1-j}}{b_{s+1-i}}a_{s+1-j, s+1-i}) \tag{20}$$

$$= 2b_j - \frac{b_j}{b_i}(a_{ji} + a_{s+1-j, s+1-i}) = 2b_j - \frac{b_j}{b_i} \times b_i = b_j = b_{s+1-j}, \tag{21}$$

holds for $j = 1, 2, \dots, s$, which means that (\bar{A}, \bar{b}, c) is also symmetric.

Obviously, (A, \bar{A}, b, c) is a symplectic PRK method according to the symplecticity criterion for PRK methods (see[9]), and when it is applied to the linear Hamiltonian system (9), it leads to

$$p_1 = R(z)p_0, R(z) = \frac{\det(I+zA)}{\det(I-zA)},$$

$$q_1 = \bar{R}(-z)q_0, \bar{R}(-z) = \frac{\det(I-z\bar{A})}{\det(I+zA)}, z = \lambda h.$$

By the symplecticity,

$$dp_0 \wedge dq_0 = dp_1 \wedge dq_1 = R(z)\bar{R}(-z)dp_0 \wedge dq_0,$$

thus $R(z)\bar{R}(-z) = 1$, which implies (18), i.e., $R(z) = \bar{R}(z)$. Since the reciprocals of the poles of $R(z)$ and $\bar{R}(z)$ are the non-zero eigenvalues of A and \bar{A} , respectively, and vice versa, so A and \bar{A} have the same eigenvalues.

Remark 2.1. Theorem 2.4 provides a way to construct symplectic PRK methods with real eigenvalues. For any given symmetric RK method (A, b, c) with distinct nodes c_i and non-zero b_i , we can obtain a symplectic PRK method $(A, \bar{A}, b, c, \bar{c})$ as we did in the theorem, and if A has real eigenvalues only, then $(A, \bar{A}, b, c, \bar{c})$ also has real eigenvalues only.

The construction of the symmetric method (A, b, c) can see [1]. About the order of the obtained PRK methods, we refer to [10] theorem 2.2 in high order level and in lower order level, this can be verified easily.

Example 2.2. In [7], a family of singly implicit collocation method with one parameter λ is given by

$\lambda(2 - \sqrt{2})$	$\lambda(1 - \frac{\sqrt{2}}{4})$	$\lambda(1 - \frac{3\sqrt{2}}{4})$	(22)
$\lambda(2 + \sqrt{2})$	$\lambda(1 + \frac{3\sqrt{2}}{4})$	$\lambda(1 + \frac{\sqrt{2}}{4})$	
	$\frac{1}{2}(1 + \sqrt{2} - \frac{1}{2\lambda\sqrt{2}})$	$\frac{1}{2}(1 - \sqrt{2} + \frac{1}{2\lambda\sqrt{2}})$	

Here λ is the unique eigenvalues of A , i.e., $\sigma(A) = \lambda$. It is easy to know that a collocation method is symmetric iff the collocation nodes are symmetric, i.e., $c_i + c_{s+1-i} = 1$. So, taking $\lambda = \frac{1}{4}$ such that $\lambda(2 - \sqrt{2}) + \lambda(2 + \sqrt{2}) = 1$, i.e., the above method is symmetric and compute \bar{A} , then we can get a symplectic PRK method,

$$\begin{array}{c|cc}
 \frac{2-\sqrt{2}}{4} & \frac{4-\sqrt{2}}{16} & \frac{4-3\sqrt{2}}{16} \\
 \frac{2+\sqrt{2}}{4} & \frac{4+3\sqrt{2}}{16} & \frac{4+\sqrt{2}}{16} \\
 \hline
 & \frac{1}{2} & \frac{1}{2}
 \end{array}
 \quad
 \begin{array}{c|cc}
 \frac{4+\sqrt{2}}{8} & \frac{4-\sqrt{2}}{16} & \frac{4+3\sqrt{2}}{16} \\
 \frac{4-\sqrt{2}}{8} & \frac{4-3\sqrt{2}}{16} & \frac{4+\sqrt{2}}{16} \\
 \hline
 & \frac{1}{2} & \frac{1}{2}
 \end{array}
 \tag{23}$$

Obviously, this is a method of order 2 due to its symmetry. But here we would like to point out that the 2 stage 2nd order Lobatto *IIIS* method (see[1])

$$\begin{array}{c|cc}
 0 & \frac{1}{4} & 0 \\
 1 & \frac{1}{2} & \frac{1}{4} \\
 \hline
 & \frac{1}{2} & \frac{1}{2}
 \end{array}
 \tag{24}$$

is superior to method(23) when applied in practice.

As is shown in this section, no symplectic RK method with real eigenvalues exists of order $s + 1$ in stage s when s is even, and though we can resort to PRK methods in this case, the complexity of such methods in high order level can be partially seen in example 2.1. When the stage s is odd, the most often used methods include the 1 stage 2nd order midpoint formula (see Table 3.2(2), Sect. 3) and the 3 stage 4th order symmetric composition of midpoint formula (see Table 3.4, Sect. 3), but in higher order level, even we can find such RK method of order $s + 1$, e.g., 5 stages 6th order symplectic RK method with real eigenvalues, its computational efficiency can not be comparable to that of the 7 stages 6th order symmetric composition of midpoint formula(see [5], V.3.2). So, for efficient symplectic methods of high order for system (1), we recommend composition methods(ref. [5,8,11]).

3. A Class of Efficient Symplectic Method

In this section, we will recommend some symplectic RK and PRK methods with real eigenvalues from order 1 to order 4. We also give some analysis for some of these methods when they applied to system (1) in practice. In higher order level, as has discussed in the final part of section 2, we recommend composition methods (ref.[5,8,11]).

Table 3.1 **Order 1**

$$\begin{array}{c|c}
 0 & 0 \\
 \hline
 & 1
 \end{array}
 \quad
 \begin{array}{c|c}
 1 & 1 \\
 \hline
 & 1
 \end{array}$$

Symplectic Euler method

Only one d -dimensional equation is needed to solve when applied to system (1).

Table 3.2 **Order 2**

$$\begin{array}{c|cc}
 0 & 0 & 0 \\
 1 & \frac{1}{2} & \frac{1}{2} \\
 \hline
 & \frac{1}{2} & \frac{1}{2}
 \end{array}
 \quad
 \begin{array}{c|cc}
 0 & \frac{1}{2} & 0 \\
 1 & \frac{1}{2} & 0 \\
 \hline
 & \frac{1}{2} & \frac{1}{2}
 \end{array}$$

1). Lobatto *IIIA*-Lobatto *IIIB* method (see [9])

Two d dimensional equations are needed to solve. It's one of the most efficient methods among methods of order 2.

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

2). Implicit midpoint formula

A $2d$ -dimensional equation is needed to solve.

Table 3.3 **Order 3**

$\frac{3+\sqrt{3}}{6}$	$\frac{3+\sqrt{3}}{6}$	0	$\frac{3+\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{3+2\sqrt{3}}{6}$
$\frac{3-\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{3+\sqrt{3}}{6}$	$\frac{3-\sqrt{3}}{6}$	$\frac{1}{2}$	$-\frac{\sqrt{3}}{6}$
	$\frac{1}{2}$	$\frac{1}{2}$		$\frac{1}{2}$	$\frac{1}{2}$

A PRK method constructed directly

Table 3.4 **Order 4**

$\frac{1}{2} + a$	$\frac{1}{2} + a$	0	0
$\frac{1}{2}$	$1 + 2a$	$-(\frac{1}{2} + 2a)$	0
$\frac{1}{2} - a$	$1 + 2a$	$-(1 + 4a)$	$\frac{1}{2} + a$
	$1 + 2a$	$-(1 + 4a)$	$1 + 2a$

1). Symmetric composition of implicit midpoint formula, where $a = \frac{2^{\frac{1}{3}}+2^{-\frac{1}{3}}-1}{6}$.

0	0	0	0	0	0	a	a	0	0	0	0	0
$2a$	a	a	0	0	0	a	a	0	0	0	0	0
$2a$	a	a	0	0	0	$\frac{1}{2}$	a	a	$\frac{1}{2} - 2a$	0	0	0
$1 - 2a$	a	a	$\frac{1}{2} - 2a$	$\frac{1}{2} - 2a$	0	$\frac{1}{2}$	a	a	$\frac{1}{2} - 2a$	0	0	0
$1 - 2a$	a	a	$\frac{1}{2} - 2a$	$\frac{1}{2} - 2a$	0	$1 - a$	a	a	$\frac{1}{2} - 2a$	$\frac{1}{2} - 2a$	a	0
$1 - 2a$	a	a	$\frac{1}{2} - 2a$	$\frac{1}{2} - 2a$	a	$1 - a$	a	a	$\frac{1}{2} - 2a$	$\frac{1}{2} - 2a$	a	0
	a	a	$\frac{1}{2} - 2a$	$\frac{1}{2} - 2a$	a		a	a	$\frac{1}{2} - 2a$	$\frac{1}{2} - 2a$	a	a

2). Symmetric composition of 2-stage LobattoIIIA-LobattoIIIB method, where $a = \frac{2^{\frac{1}{3}}+2^{-\frac{1}{3}}+2}{6}$.

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References

- [1] R.P.K. Chan, On Symmetric Runge-Kutta Methods of High Order, *Computing* 45, 301-309 (1990).
- [2] E. Hairer, S.P. Nørset and G. Wanner, Symplectic Runge-Kutta methods with real eigenvalues, *BIT*, **34** (1994), 3-20.
- [3] E. Hairer and G. Wanner, Solving Ordinary Differential Equations I, pp. 528, Springer-Verlag, 1991.
- [4] E. Hairer and G. Wanner, Solving Ordinary Differential Equations II, pp. 601, Springer-Verlag, 1991.
- [5] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration, Springer-Verlag, 2001.
- [6] A. Iserles, Efficient Runge-Kutta methods for Hamiltonian equations, *Bull. Greek. Math. Soc.*, **32** (1991), 3-20.
- [7] Nørset, S.P., Runge-Kutta methods with a multiple real eigenvalues only, *BIT*, **16** (1976), 388-393.
- [8] Qing Meng-Zhao and Zhu Wen-Jie, Construction of Higher Order Symplectic Schemes by Composition, *Computing*, **47**, (1992), 309-321.
- [9] Sun Geng, Symplectic partitioned Runge-Kutta methods, *J. Comput. Math.*, **11:4** (1993), 365-372.
- [10] Sun Geng, Construction of high order symplectic Runge-Kutta methods, *J. Comput. Math.*, **11:3** (1993), 250-260.
- [11] H. Yoshida, Construction of high order symplectic integrators, *Phys. Lett.*, **150** (1990), 262-268.