



# Order Properties of Symplectic Runge-Kutta-Nyström Methods

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**Abstract**—In this paper, some characteristics and order properties of symplectic Runge-Kutta-Nyström (RKN) methods are given. By using a transformation technique, a family of high-order implicit symplectic RKN methods of order  $2s - 1$  or order  $2s$  is constructed, and some available symplectic RKN methods including singly-implicit, multiply-implicit, and diagonally-implicit symplectic RKN methods are investigated. As examples, two-stage and three-stage symplectic RKN methods are derived in detail. © 2004 Elsevier Ltd. All rights reserved.

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## 1. INTRODUCTION

For a *Hamiltonian* dynamical system such as

$$\dot{p} = -\frac{\partial V(q)}{\partial q}, \quad \dot{q} = W^{-1}p, \quad p, q \in \mathbb{R}^n, \quad (1.0)$$

with constant diagonal (nondegenerate) matrix  $W$ , function  $V$ , and Hamiltonian  $H(p, q) = (1/2)p^T W^{-1}p + V(q)$ , it has been suggested that the *symplectic* difference schemes should be employed to integrate it (see, for example, [1–3]). It is well known that (1.0) is equivalent to the second-order system

$$\ddot{q} = -W^{-1} \frac{\partial V(q)}{\partial q} = f(q), \quad q \in \mathbb{R}^n.$$

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For integrating the above second-order system with the initial value  $p(t_0) = p_0, q(t_0) = q_0$ , or equivalently,

$$\dot{y} = f(y), \quad y(t_0) = y_0, \quad \dot{y}(t_0) = \dot{y}_0, \tag{1.1}$$

where  $y$  and  $\dot{y}$  correspond to  $q$  and  $p$ , respectively, we consider the  $s$ -stage RKN method

$$\begin{array}{c|c} c & A \\ \hline & b^\top \\ & d^\top \end{array} \tag{1.2}$$

where  $c = (c_1, c_2, \dots, c_s)^\top, b = (b_1, b_2, \dots, b_s)^\top, d = (d_1, d_2, \dots, d_s)^\top, A = [a_{ij}]$  is an  $s \times s$  matrix, and  $c_i (1 \leq i \leq s)$  are distinct. Method (1.2) applied to (1.1) reads

$$Y_i = y_n + hc_i \dot{y}_n + h^2 \sum_{j=1}^s a_{ij} f(Y_j), \quad i = 1, 2, \dots, s, \tag{1.3a}$$

$$\dot{y}_{n+1} = \dot{y}_n + h \sum_{i=1}^s d_i f(Y_i), \tag{1.3b}$$

$$y_{n+1} = y_n + h \dot{y}_n + h^2 \sum_{i=1}^s b_i f(Y_i). \tag{1.3c}$$

Suris [3] proved that method (1.3) is symplectic if

$$b_i = d_i(1 - c_i), \quad i = 1, 2, \dots, s, \tag{1.4a}$$

$$d_i(b_j - a_{ij}) = d_j(b_i - a_{ji}), \quad i, j = 1, 2, \dots, s \tag{1.4b}$$

(see also [4]). Conditions (1.4) are also necessary for methods without redundant stages to be symplectic (see [5]). In the following sections, we use the expression ‘‘symplectic RKN methods’’ to refer to RKN methods that satisfy (1.4). So far, order conditions of symplectic RKN methods have been systematically investigated (see [5–9]) by special Nyström rooted trees, and some available explicit symplectic RKN methods are given in [5,7,9–11]. Okunbor and Skeel [4] showed that an explicit RKN method is symplectic if and only if its adjoint is explicit. For implicit RKN methods, Ramaswami [12] derived a one-parameter family of symplectic RKN methods of order  $2s - 1$  by using the perturbed collocation technique, and Burnton and Scherer [13] discussed Gauss RKN methods and proved that they are always symmetric and that symmetry is equivalent to symplecticity.

In this paper, some characteristics and order properties of symplectic RKN methods are given. By modifying slightly the transformation technique in [14,15], a family of high-order implicit symplectic RKN methods of order  $2s - 1$  or order  $2s$  is constructed, and some available symplectic RKN methods including singly-implicit, multiply-implicit, and diagonally-implicit symplectic RKN methods are investigated. As examples, two-stage and three-stage symplectic RKN methods are derived in detail.

## 2. SOME ORDER PROPERTIES

Let  $D = \text{diag}(d), C = \text{diag}(c)$ , and

$$M = DA - A^\top D + bd^\top - db^\top, \quad c^k = (c_1^k, c_2^k, \dots, c_s^k)^\top, \quad k = 0, 1, 2, \dots,$$

$$g_{k+1} = (k + 1)kb^\top c^{k-1}, \quad \bar{g}_k = kd^\top c^{k-1}, \quad k = 1, 2, \dots,$$

$$\psi_{rm} = rm \sum_{i,j=1}^s d_i c_i^{r-1} a_{ij} c_j^{m-1}, \quad r, m = 1, 2, \dots$$

Obviously,  $g_{k+1} = (k + 1)\bar{g}_k - k\bar{g}_{k+1}$  if (1.4a) holds. Introduce the following simplifying assumptions (see [16,17]):

$$\begin{aligned} B(\eta) : \quad & g_{k+1} = 1, & k = 1, 2, \dots, \eta, \\ BD(\eta) : \quad & \bar{g}_k = 1, & k = 1, 2, \dots, \eta, \\ C(\eta) : \quad & (k + 1)kAc^{k-1} = c^{k+1}, & k = 1, 2, \dots, \eta, \\ D(\eta) : \quad & d^\top C^{k-1}A = \frac{d^\top C^{k+1}}{k(k+1)} - \frac{d^\top C}{k} + \frac{d^\top}{k+1}, & k = 1, 2, \dots, \eta. \end{aligned}$$

Now we present some properties of the above simplifying assumptions.

LEMMA 2.1.

(1) If (1.4a) holds, then

$$BD(\eta + 1) \implies B(\eta), \quad B(\eta) \quad \text{and} \quad BD(1) \implies BD(\eta + 1);$$

(2)  $B(s)$  and  $BD(s + 1) \implies (1.4a)$  holds;

(3)  $C(\eta) \iff \psi_{rm} = r\bar{g}_{r+m+1}/(m + 1)(m + r + 1), 1 \leq r \leq s, 1 \leq m \leq \eta$ , if  $d_i \neq 0, 1 \leq i \leq s$ ,

$$D(\eta) \iff \psi_{rm} = \frac{m\bar{g}_{r+m+1}}{(r + 1)(m + r + 1)} - \frac{m\bar{g}_{m+1}}{m + 1} + \frac{r\bar{g}_m}{r + 1}, \quad 1 \leq r \leq \eta, \quad 1 \leq m \leq s;$$

(4)  $C(\eta), D(\xi)$ , and  $BD(1) \implies BD(\xi + \eta + 1), 1 \leq \xi, \eta \leq s, \xi \neq \eta$ ;

(5)  $C(\eta), D(\eta)$ , and  $BD(1) \implies BD(2\eta), 1 \leq \eta \leq s$ .

PROOF. The conclusions in (1) immediately follow from the given conditions and the fact that  $g_{k+1} = (k + 1)\bar{g}_k - k\bar{g}_{k+1}$  ( $k \geq 1$ ) if (1.4a) holds. By means of  $B(s)$  and  $BD(s + 1)$ , we have

$$b^\top c^{k-1} = \frac{1}{(k + 1)k}, \quad d^\top Cc^{k-1} = \frac{1}{k + 1}, \quad d^\top c^{k-1} = \frac{1}{k}, \quad k = 1, 2, \dots, s.$$

Thus,

$$(b^\top - d^\top + d^\top C)c^{k-1} = 0, \quad k = 1, 2, \dots, s.$$

The conclusions in (2) follow from the above formula and the fact that the values  $c_i$  ( $1 \leq i \leq s$ ) are distinct.

The conclusions in (3) can be directly deduced. By use of recursion, (4) and (5) follow from (3). ■

THEOREM 2.2. Let method (1.2) satisfy (1.4a) and  $BD(3)$ .

(1) If  $C(\eta)$  ( $1 \leq \eta \leq s$ ) holds, then this method is symplectic if and only if  $BD(2\eta), D(\eta)$ , and (2.2c) hold.

(2) If  $D(\eta)$  ( $1 \leq \eta \leq s$ ) holds, and  $d_i \neq 0$  for  $1 \leq i \leq s$ , then this method is symplectic if and only if  $BD(2\eta), C(\eta)$ , and (2.2c) hold.

PROOF. Note that the values  $c_i$  ( $1 \leq i \leq s$ ) are distinct. Let  $U = [u_{ij}], u_{ij} = jc_i^{j-1}, 1 \leq i, j \leq s$ , and transform the skew-symmetric matrix  $M$  into

$$U^\top MU = H = [h_{rm}], \tag{2.1}$$

where  $h_{rr} = 0$  and

$$h_{rm} = -h_{mr} = \psi_{rm} - \psi_{mr} + \frac{1}{r + 1}g_{r+1}\bar{g}_m - \frac{1}{m + 1}g_{m+1}\bar{g}_r, \quad r \neq m, \quad 1 \leq r, m \leq s.$$

Obviously, method (1.2) is symplectic iff  $H = 0$  and (1.4a) holds. If  $C(\eta)$  holds, then  $H = 0$  iff

$$\frac{r - m}{(r + 1)(m + 1)} \bar{g}_{r+m+1} + \omega(r, m) = 0, \quad 1 \leq r < m \leq \eta, \tag{2.2a}$$

$$\psi_{rm} - \frac{m}{(r + 1)(r + m + 1)} \bar{g}_{r+m+1} + \omega(r, m) = 0, \quad 1 \leq r \leq \eta, \quad \eta < m \leq s, \tag{2.2b}$$

$$\psi_{rm} - \psi_{mr} + \omega(r, m) = 0, \quad \eta < r < m \leq s, \tag{2.2c}$$

where

$$\omega(r, m) = \frac{m}{m + 1} \bar{g}_{m+1} \bar{g}_r - \frac{r}{r + 1} \bar{g}_{r+1} \bar{g}_m.$$

When  $BD(3)$  holds, it is easy to show that (2.2a) holds iff  $BD(2\eta)$  holds, and (2.2b) holds iff  $D(\eta)$  holds. Thus, Conclusion (1) follows, and Conclusion (2) can be similarly proved. ■

**THEOREM 2.3.** *For an RKN method of order  $\eta (\geq 5)$ , we assume that  $d_i > 0$  for  $1 \leq i \leq s$ . Then  $C(\lceil(\eta - 3)/2\rceil)$  holds.*

**PROOF.** This proof is similar to that of the lemma in [18]. The order conditions

$$\begin{aligned} \sum_{i,j,l} d_i a_{ij} c_j^{k-1} a_{il} c_l^{k-1} &= \frac{1}{(2k + 3)k^2(k + 1)^2}, \\ \sum_{i,j} d_i c_i^{k+1} a_{ij} c_j^{k-1} &= \frac{1}{(2k + 3)k(k + 1)}, \\ \sum_i d_i c_i^{2k+2} &= \frac{1}{2k + 3} \end{aligned}$$

for the SN-trees (see [9,16,17]) of order  $2k + 3$  sketched in Figure 1 imply that

$$\sum_i d_i \left( \sum_j a_{ij} c_j^{k-1} - \frac{c_i^{k+1}}{k(k + 1)} \right)^2 = 0$$

for  $2k + 3 \leq \eta$ . Since the  $d_i$  are positive, the individual terms must be zero. ■

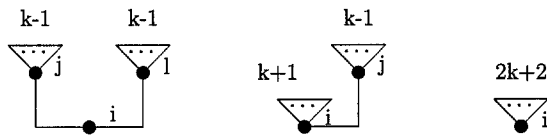


Figure 1.

From Theorems 2.2 and 2.3, we get the following.

**THEOREM 2.4.** *If an RKN method of order  $\eta (\geq 5)$  is symplectic with  $d_i > 0$  for  $i = 1, 2, \dots, s$ , then  $C(\lceil(\eta - 3)/2\rceil)$ ,  $BD(\eta)$ , and  $D(\lceil(\eta - 3)/2\rceil)$  must hold.*

**THEOREM 2.5.** *If method (1.2) is symplectic, and satisfies  $C(\eta)$  (or  $D(\eta)$  with  $d_i \neq 0, i = 1, 2, \dots, s$ ) and  $BD(2\eta + 2)$ , where  $1 \leq \eta \leq s - 1$ , then this method is of order at least  $2\eta + 2$ .*

**PROOF.** The proof is similar to that of Theorem 2.5 in [19]. By means of Theorem 2.2, the assumptions of Theorem 2.5 mean that the conditions  $C(\eta)$ ,  $D(\eta)$ , and  $BD(2\eta + 2)$  all hold. Following the notation in [16], let  $SNT_{2\eta+2}$  denote the set of all special Nyström rooted trees with no more than  $2\eta + 2$  nodes. For each tree  $u \in SNT_{2\eta+2}$ , we associate two numbers  $\rho(u)$ ,  $\gamma(u)$ , and a  $\rho(u)^{\text{th}}$  polynomial  $\Phi(u)$  in the coefficients  $a_{ij}$ ,  $d_j$ , and  $c_j$ . Here  $\rho(u)$  denotes the number of nodes in  $u$ ,  $\gamma(u)$  denotes the density of the tree  $u$  (i.e., the product of  $\rho(v)$  over  $v$  where for each node

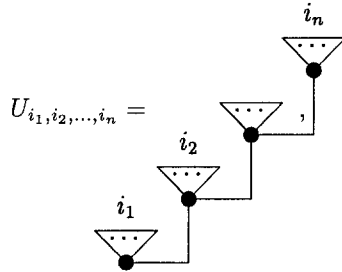
of  $u$ ,  $v$  is the subtree formed from that node and all nodes that can be reached from it by following upward growing branches). To show that the RKN method (1.2) satisfying the conditions assumed in Theorem 2.5 is of order at least  $2\eta+2$ , we need to prove that  $\Phi(u) = 1/\gamma(u)$  for all  $u \in \text{SNT}_{2\eta+2}$  (see [16,17]). Since  $C(1)$  holds, we can always use the abbreviation  $\sum_k a_{jk} = c_j^2/2$  in writing the formula for  $\Phi(u)$ .

Suppose a tree  $u \in \text{SNT}_{2\eta+2}$  has a fat node “ $l$ ”, other than the root, which is connected via a meagre son with the other fat node “ $m$ ” connected with  $k$  meagre end-nodes, where  $k < \eta$ . Then, when  $C(\eta)$  holds, as shown in Proposition 16 of [17] and Lemma 4.1 of [13], we have

$$\Phi(u) = \sum_{l=1}^s \Phi_l(u) \sum_{m=1}^s a_{lm} c_m^k = \frac{1}{(k+1)(k+2)} \sum_{l=1}^s \Phi_l(u) c_l^{k+2} = \frac{1}{(k+2)(k+1)} \Phi(\bar{u}),$$

$$\rho(u) = \rho(\bar{u}), \quad \gamma(u) = (k+2)(k+1)\gamma(\bar{u}),$$

where  $\Phi_l(u)$  are some polynomials, the SN rooted tree  $\bar{u}$  is the same as  $u$  except that the  $k$  nodes referred to above are all moved one step closer to the root. This means that  $\Phi(u) = 1/\gamma(u)$  is equivalent to  $\Phi(\bar{u}) = 1/\gamma(\bar{u})$ . Thus, all SN rooted trees with this property that characterised  $u$  can be removed from consideration. With all the SN rooted trees removed in the aforementioned way, there remain only SN rooted trees of the form



where  $i_1, i_2, \dots, i_n$  are nonnegative integers, and  $i_n \geq \eta$  when  $n > 1$ . It is easy to identify that

$$\rho(u_{i_1, i_2, \dots, i_n}) = \sum_{l=1}^{n-1} (i_l + 2) + i_n + 1 \leq 2\eta + 2, \tag{2.3a}$$

$$\gamma(u_{i_1, i_2, \dots, i_n}) = \prod_{j=1}^{n-1} \left( \sum_{l=j}^{n-1} (i_l + 2) + i_n + 1 \right) \prod_{j=2}^n \left( \sum_{l=j}^n (i_l + 2) \right) (i_n + 1), \tag{2.3b}$$

$$\Phi(u_{i_1, i_2, \dots, i_n}) = d^T \prod_{l=1}^{n-1} (C^{i_l} A) c^{i_n}. \tag{2.3c}$$

We thus only need to prove that

$$\Phi(u_{i_1, i_2, \dots, i_n}) = \frac{1}{\gamma(u_{i_1, i_2, \dots, i_n})}, \quad \text{for } \sum_{l=1}^{n-1} (i_l + 2) + i_n + 1 \leq 2\eta + 2, \tag{2.4}$$

where  $i_n \geq \eta$  when  $n > 1$ . When  $n = 1$ , (2.4) is a direct consequence of  $BD(2\eta + 2)$ , and it is also easy to show that (2.4) holds for  $n = 2$ , i.e.,

$$d^T C^{i_1} A c^{i_2} = \frac{1}{(i_2 + 1)(i_2 + 2)(i_1 + i_2 + 3)}, \quad \text{for } i_1 + i_2 \leq 2\eta - 1, \quad i_2 \geq \eta. \tag{2.5}$$

In fact, since  $i_1 + i_2 \leq 2\eta - 1$ ,  $i_2 \geq \eta$ , we have  $i_1 < \eta - 1$ . Equation (2.5) with  $i_1 < \eta$  follows directly from  $D(\eta)$  and  $BD(2\eta + 2)$ . Now we only need to prove that

$$\Phi(u_{i_1, i_2, \dots, i_n}) = \frac{1}{\gamma(u_{i_1, i_2, \dots, i_n})}, \quad \text{for } \sum_{l=1}^m (i_l + 2) + i_{m+1} + 1 \leq 2\eta + 2$$

under the inductive assumption that (2.4) holds when  $n = m$ , where  $2 \leq m < 2\eta + 2$ ,  $i_{m+1} \geq \eta$ . Because

$$i_{m+1} \geq \eta, \quad i_1 + i_{m+1} + 3 < \sum_{l=1}^m (i_l + 2) + i_{m+1} + 1 \leq 2\eta + 2,$$

we have  $i_1 < \eta$ , and therefore, according to  $D(\eta)$  and the inductive assumption,

$$\begin{aligned} \Phi(u_{i_1, \dots, i_{m+1}}) &= (d^\top C^{i_1} A) \prod_{l=2}^m (C^{i_l} A) c^{i_{m+1}} \\ &= \left( \frac{Dc^{i_1+2}}{(i_1+1)(i_1+2)} - \frac{Dc}{i_1+1} + \frac{d}{i_1+2} \right)^\top \prod_{l=2}^m (C^{i_l} A) c^{i_{m+1}} \\ &= \frac{1}{i_1+2} d^\top \prod_{l=2}^m (C^{i_l} A) c^{i_{m+1}} - \frac{1}{i_1+1} d^\top C^{i_2+1} A \prod_{l=3}^m (C^{i_l} A) c^{i_{m+1}} \\ &\quad + \frac{1}{(i_1+1)(i_1+2)} d^\top C^{i_1+i_2+2} A \prod_{l=3}^m (C^{i_l} A) c^{i_{m+1}} \\ &= \left( \frac{1}{(i_1+2)\kappa(2, m)} - \frac{1}{(i_1+1)(\kappa(2, m)+1)} + \frac{1}{(i_1+1)(i_1+2)(\kappa(2, m)+i_1+2)} \right) \\ &\quad \times \left( \prod_{j=3}^m \kappa(j, m) \prod_{j=3}^{m+1} \left( \sum_{l=j}^{m+1} (i_l + 2) \right) (i_{m+1} + 1) \right)^{-1} \\ &= \left( \kappa(1, m)\kappa(2, m) \sum_{l=2}^{m+1} (i_l + 2) \prod_{j=3}^m \kappa(j, m) \prod_{j=3}^{m+1} \left( \sum_{l=j}^{m+1} (i_l + 2) \right) (i_{m+1} + 1) \right)^{-1} \\ &= \frac{1}{\gamma(u_{i_1, \dots, i_{m+1}})}, \end{aligned}$$

where  $\kappa(j, m) = \sum_{l=j}^m (i_l + 2) + i_{m+1} + 1$ . This completes the proof of Theorem 2.5. ■

Using Theorems 2.2 and 2.5, we have the following.

**COROLLARY 2.6.** *If method (1.2) is symplectic, and the conditions  $BD(2\eta + i)$  ( $i = 0, 1, 2$ ) and  $C(\eta)$  (or  $D(\eta)$  with  $d_i \neq 0$ ,  $1 \leq i \leq s$ ) hold, then its order is at least  $2\eta + i$ ,  $i = 0, 1, 2$ .*

For the special cases  $\eta = s, s-1, s-2$ , Lemma 2.1 and Theorems 2.2 and 2.5 yield the following.

**COROLLARY 2.7.**

- (1) *If conditions  $BD(3)$ ,  $C(s)$  (or  $D(s)$ ) hold, then method (1.2) is symplectic iff (1.4a),  $BD(2s)$ , and  $D(s)$  (or  $C(s)$ ) hold.*
- (2) *If conditions  $BD(3)$ ,  $C(s-1)$  (or  $D(s-1)$ ) with  $d_i \neq 0$ ,  $1 \leq i \leq s$  hold, then method (1.2) is symplectic iff (1.4a),  $BD(2s-2)$ , and  $D(s-1)$  (or  $C(s-1)$ ) hold.*
- (3) *If conditions  $BD(3)$ ,  $C(s-2)$  (or  $D(s-2)$ ) with  $d_i \neq 0$ ,  $1 \leq i \leq s$  hold, then method (1.2) is symplectic iff (1.4a),  $BD(2s-4)$  and  $D(s-2)$  (or  $C(s-2)$ ) hold and*

$$\psi_{s-1, s} - \psi_{s, s-1} - \frac{s-1}{s} + \frac{s}{s+1} \bar{g}_{s+1} = 0. \tag{2.6}$$

By means of the above results, in Table 1, we list the order conditions of five types of higher-order symplectic RKN methods.

In Table 1, the type I–V methods are Gauss, Gauss, Radau, Lobatto, Lobatto RKN methods when  $c_i$  ( $1 \leq i \leq s$ ) are chosen as the abscissas of the corresponding quadrature formulas, respectively. Symplecticity of the type-II methods (i.e., Gauss RKN methods of order  $2s$ ) has been discussed in [13].

Table 1.

Type	Order	Symplectic Order Conditions
I	2s	$BD(2s), C(s), D(s), (1.4a), s \geq 2$
II	2s	$BD(2s), C(s-1), D(s-1), (1.4a), s \geq 2$
III	2s-1	$BD(2s-1), C(s-1), D(s-1), (1.4a), s \geq 2$
IV	2s-2	$BD(2s-2), C(s-1), D(s-1), (1.4a), s \geq 3$
V	2s-2	$BD(2s-2), C(s-2), D(s-2), (1.4a), (2.6), s \geq 3$

When  $s = 1$ , it is easy to show that the one-stage RKN method satisfying the conditions  $BD(2), C(1), D(1)$  is as follows.

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{8} \\ \hline & \frac{1}{2} \\ & 1 \end{array}$$

It is symplectic and of order 2.

When  $s \geq 2$ , the type-I methods can be given by

$$d^\top = \left(1, \frac{1}{2}, \dots, \frac{1}{s}\right) V_s^{-1}, \quad b = d - Dc, \quad A = \bar{V}_s V_s^{-1},$$

where  $V_s = [c_i^{j-1}]$  and

$$\bar{V}_s = \left[ \frac{c_i^{j+1}}{(j(j+1))} \right] \in R^{s \times s}, \quad kd^\top c^{k-1} = 1, \quad s+1 \leq k \leq 2s.$$

For example, the two-stage four-order symplectic RKN methods satisfying  $BD(4), C(2), D(2)$ , and (1.4a) are given by

$$c^\top = \left(\frac{1}{2} - \frac{\sqrt{3}}{6}, \frac{1}{2} + \frac{\sqrt{3}}{6}\right), \quad d^\top = \left(\frac{1}{2}, \frac{1}{2}\right), \quad b = d - Dc, \quad A = \bar{V}_2 V_2^{-1}.$$

The three-stage six-order symplectic RKN methods satisfying  $BD(6), C(3), D(3)$ , and (1.4a) are given by

$$c^\top = \left(\frac{1}{2} - \frac{\sqrt{15}}{10}, \frac{1}{2}, \frac{1}{2} + \frac{\sqrt{15}}{10}\right), \quad d^\top = \left(\frac{5}{18}, \frac{4}{9}, \frac{5}{18}\right), \quad b = d - Dc, \quad A = \bar{V}_3 V_3^{-1}.$$

### 3. A FAMILY OF HIGH-ORDER SYMPLECTIC RKN METHODS

We consider the type-III symplectic RKN methods, i.e., the RKN methods satisfying (1.4a),  $BD(2s-1), C(s-1), D(s-1), s \geq 2$  by modifying slightly the transformation technique in [14,15]. Let  $c_i \neq 0 (i = 1, 2, \dots, s), V_s = [c_i^{j-1}]$ , and

$$\begin{aligned} \bar{A} = [\bar{a}_{ij}] &= C^{-1}A, & \text{i.e., } \bar{a}_{ij} &= \frac{a_{ij}}{c_i}, \quad i, j = 1, 2, \dots, s, \\ \bar{A}_s = [\alpha_{ij}] &= V_s^{-1} \bar{A} V_s, & \text{i.e., } \bar{A} &= V_s \bar{A}_s V_s^{-1}. \end{aligned}$$

$BD(2s-1)$  means

$$d^\top = \left(1, \frac{1}{2}, \dots, \frac{1}{s}\right) V_s^{-1}, \quad (s+i)d^\top c^{s+i-1} = 1, \quad i = 1, 2, \dots, s-1. \tag{3.1}$$

$C(s - 1)$  yields

$$\bar{A}_s = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & \alpha_{1s} \\ \frac{1}{1 \times 2} & 0 & 0 & \cdots & 0 & \alpha_{2s} \\ 0 & \frac{1}{2 \times 3} & 0 & \cdots & 0 & \alpha_{3s} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & \frac{1}{(s-1) \times s} & \alpha_{ss} \end{pmatrix}. \tag{3.2}$$

$D(s - 1)$  means

$$\sum_{j=1}^s \frac{\alpha_{js}}{k+j} = \frac{1}{s(s+1)(s+1+k)}, \quad k = 1, 2, \dots, s-2, \tag{3.3a}$$

$$\sum_{j=1}^s \frac{\alpha_{js}}{s-1+j} = \frac{1}{s(s-1)} \left( \frac{\bar{g}_{2s}}{2s} - \frac{1}{s(s+1)} \right). \tag{3.3b}$$

Therefore, by means of (3.1)–(3.3) and the equalities

$$A = CV_s \bar{A}_s V_s^{-1}, \quad b = d - Dc,$$

we can obtain a two-parameter family of symplectic RKN methods of order  $2s - 1$ . For example,  $c_s$  and  $\alpha_{ss}$  can be chosen as two free parameters. Further, letting  $\bar{g}_{2s} = 1$ , this family belongs to the type-II methods, and is of order  $2s$  and only one free parameter (such as  $\alpha_{ss}$ ). The examples of two-stage and three-stage symplectic RKN methods will be given in Section 5.

#### 4. A FAMILY OF SYMPLECTIC RKN METHODS WITH REAL EIGENVALUES

By using the  $W$ -transformation, Hairer and Wanner [20] obtained some symplectic Runge-Kutta methods with real eigenvalues which were constructed by Iserles [10] with the help of perturbed collocation. In this section, based on the results given in Section 3, we construct some symplectic RKN methods with real eigenvalues and orders  $2s - 1, 2s$ , i.e., singly-implicit and multiply-implicit symplectic RKN methods. An RKN method is said to be singly-implicit if the matrix  $\bar{A}$  has a single real eigenvalue. An RKN method is said to be multiply-implicit if the matrix  $\bar{A}$  has  $s$  real distinct eigenvalues. Singly-implicit RKN methods are very efficiently implementable on a sequential machine, and multiply-implicit RKN methods are very efficiently implementable on an  $s$ -processor machine (see [21]). Let

$$\bar{Y}_i = \frac{Y_i}{c_i}, \quad \bar{f}(\bar{Y}_i) = f(c_i \bar{Y}_i), \quad i = 1, 2, \dots, s.$$

Equation (1.3a) becomes

$$\bar{Y}_i = \frac{y_n}{c_i} + h y_n + h^2 \sum_{j=1}^s \bar{a}_{ij} \bar{f}(\bar{Y}_j), \quad i = 1, 2, \dots, s.$$

Therefore, in essence, the approach to implementing singly-implicit RKN methods and multiply-implicit RKN methods are the same as those to singly-implicit RK methods and multiply-implicit RK methods, respectively.

For singly-implicit RKN methods, let  $\lambda$  denote the single real eigenvalue of  $\bar{A}$  (i.e.,  $\bar{A}_s$ ). We can easily prove that

$$\alpha_{ks} = (-1)^{s-k} \binom{s}{k-1} \frac{(s-1)!s!}{(k-1)!k!} \lambda^{s-k+1}, \quad k = 1, 2, \dots, s. \tag{4.1}$$



Insert (4.1) into (3.3) such that (3.3b) yields

$$\bar{g}_{2s} = 2s \left( (s-1)s \sum_{j=1}^s \frac{\alpha_{js}}{s-1+j} + \frac{1}{s(s+1)} \right), \tag{4.2}$$

and such that (3.3a) includes  $s - 2$  equations with only one unknown number  $\lambda$ . (In general, we cannot find such  $\lambda$  that the  $s - 2$  equations hold.) In general, this would seem to imply that the singly-implicit RKN methods satisfying  $BD(2s - 1)$ ,  $C(s - 1)$ ,  $D(s - 1)$ , and  $s > 3$  are not symplectic. Therefore, usually,  $s \leq 3$ . Further, if  $\bar{g}_{2s} = 1$  (i.e.,  $BD(2s)$  holds), then there exist  $s - 1$  equations and only a free parameter  $\lambda$  in (3.3). This usually means  $s = 2$ . Thus, in Section 5, we only discuss two-stage, three-stage symplectic singly-implicit RKN methods in detail.

For multiply-implicit RKN methods, let  $\lambda_1, \lambda_2, \dots, \lambda_s$  denote the real distinct eigenvalues of  $\bar{A}$  (i.e.,  $\bar{A}_s$ ) and let  $\Psi_s(x, \lambda) = \prod_{j=1}^s (x - \lambda_j)$ . Then

$$\Psi_s(x, \lambda) = x^s + \sum_{i=0}^{s-1} (-1)^{s-i} \phi_{s-i}(\lambda) x^i, \tag{4.3}$$

where the  $\phi_i(\lambda)$  are the elementary symmetric functions associated with  $\Psi_s$ . Hence,

$$\phi_1(\lambda) = \sum \lambda_i, \quad \phi_2(\lambda) = \sum_{i < j} \lambda_i \lambda_j, \quad \dots, \quad \phi_s(\lambda) = \prod_{j=1}^s \lambda_j.$$

On the other hand,

$$|xI - \bar{A}_s| = x^s - \sum_{k=0}^{s-1} x^k \alpha_{k+1,s} \frac{k!(k+1)!}{s!(s-1)!}. \tag{4.4}$$

Thus, (4.3) and (4.4) yield

$$\alpha_{ks} = (-1)^{s-k} \frac{s!(s-1)!}{k!(k-1)!} \phi_{s-k+1}(\lambda), \quad k = 1, 2, \dots, s. \tag{4.5}$$

In (3.3) and (4.5), there exist  $s - 1$  algebraic equations and  $s + 1$  parameters  $\lambda_i$  ( $1 \leq i \leq s$ ) and one of  $c_i$  ( $1 \leq i \leq s$ ). Therefore, we can construct a two-parameter family of symplectic multiply-implicit RKN methods of order  $2s - 1$ .

### 5. TWO-STAGE AND THREE-STAGE SYMPLECTIC RKN METHODS

In this section, we will construct two-stage and three-stage symplectic RKN methods with high order and real eigenvalues based on the results given in Sections 3 and 4.

#### 5.1. Two-Stage Symplectic RKN Methods

Consider two-stage RKN methods satisfying  $BD(3)$ ,  $C(1)$ , and  $D(1)$

$$\begin{array}{c|c} \begin{matrix} c_1 \\ c_2 \end{matrix} & \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix} \begin{pmatrix} 1 & c_1 \\ 1 & c_2 \end{pmatrix} \begin{pmatrix} 0 & \alpha_{12} \\ \frac{1}{2} & \alpha_{22} \end{pmatrix} \begin{pmatrix} 1 & c_1 \\ 1 & c_2 \end{pmatrix}^{-1} \\ \hline & \begin{matrix} b_1 & b_2 \\ d_1 & d_2 \end{matrix} \end{array} \tag{5.1}$$

where

$$d_1 = \frac{2c_2 - 1}{2(c_2 - c_1)}, \quad d_2 = 1 - d_1, \quad b_1 = d_1(1 - c_1), \quad b_2 = d_2(1 - c_2),$$

$$\alpha_{12} = \frac{\bar{g}_4}{4} - \frac{2\alpha_{22}}{3} - \frac{1}{6}, \quad (c_1 + c_2) - 2c_1c_2 = \frac{2}{3}.$$

In Sections 2 and 3, we have shown method (5.1) is symplectic and of order at least 3. Thus, we obtain a two-parameter family of two-stage symplectic RKN methods. Further, letting  $\bar{g}_4 = 1$ , we have  $\alpha_{12} = (1/12) - 2\alpha_{22}/3$  and obtain a one-parameter family with order 4 (the parameter is  $\alpha_{22}$ ).

From Section 4, we easily show that method (5.1) is singly-implicit iff

$$\alpha_{12} = -2\lambda^2, \quad \alpha_{22} = 2\lambda, \quad \lambda^2 - \frac{2}{3}\lambda + \frac{1}{8}\left(\bar{g}_4 - \frac{2}{3}\right) = 0, \quad \bar{g}_4 \leq \frac{14}{9}.$$

This means that the symplectic singly-implicit RKN method (5.1) is a one-parameter family of two-stage symplectic RKN methods. Now we give two examples with orders 3 and 4, respectively.

EXAMPLE 5.1.  $c^\top = (1/3, 1)$ ,  $d^\top = (3/4, 1/4)$ ,  $b^\top = (1/2, 0)$ ,  $\alpha_{12} = -2\lambda^2$ ,  $\alpha_{22} = 2\lambda$ ,  $\lambda = (2 \pm \sqrt{2})/6$ .

EXAMPLE 5.2.  $c^\top = ((3 - \sqrt{3})/6, (3 + \sqrt{3})/6)$ ,  $d^\top = (1/2, 1/2)$ ,  $b^\top = ((3 + \sqrt{3})/12, (3 - \sqrt{3})/12)$ ,  $\alpha_{12} = -2\lambda^2$ ,  $\alpha_{22} = 2\lambda$ ,  $\lambda = (4 \pm \sqrt{10})/12$ .

From Section 4, we also easily show that method (5.1) is multiply implicit iff

$$\alpha_{22}^2 - \frac{4}{3}\alpha_{22} + \frac{1}{2}\left(\bar{g}_4 - \frac{2}{3}\right) > 0. \tag{5.2}$$

Inequality (5.2) means  $\bar{g}_4 > 14/9$ ,  $\alpha_{22} \in R$ , or

$$\bar{g}_4 \leq \frac{14}{9}, \quad \alpha_{22} < \frac{4 - \sqrt{28 - 18\bar{g}_4}}{6},$$

or

$$\bar{g}_4 \leq \frac{14}{9}, \quad \alpha_{22} > \frac{4 + \sqrt{28 - 18\bar{g}_4}}{6}.$$

If  $\bar{g}_4 = 1$ , then  $c^\top = ((3 - \sqrt{3})/6, (3 + \sqrt{3})/6)$ ,  $d^\top = (1/2, 1/2)$ ,  $b^\top = ((3 + \sqrt{3})/12, (3 - \sqrt{3})/12)$ ,  $\alpha_{12} = 1/12 - (2/3)\alpha_{22}$ ,  $\alpha_{22} < (4 - \sqrt{10})/6$ , or  $\alpha_{22} > (4 + \sqrt{10})/6$ . For example, we can choose  $\alpha_{22} = 1/12, 4/3$ .

### 5.2. Three-Stage Symplectic RKN Methods

Consider three-stage RKN methods satisfying  $BD(5)$ ,  $C(2)$ , and  $D(2)$

$$\begin{array}{c|c} \begin{array}{c} c_1 \\ c_2 \\ c_3 \end{array} & \begin{array}{c} \left( \begin{array}{ccc} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \end{array} \right) \left( \begin{array}{ccc} 1 & c_1 & c_1^2 \\ 1 & c_2 & c_2^2 \\ 1 & c_3 & c_3^2 \end{array} \right) \left( \begin{array}{ccc} 0 & 0 & \alpha_{13} \\ \frac{1}{2} & 0 & \alpha_{23} \\ 0 & \frac{1}{6} & \alpha_{33} \end{array} \right) \left( \begin{array}{ccc} 1 & c_1 & c_1^2 \\ 1 & c_2 & c_2^2 \\ 1 & c_3 & c_3^2 \end{array} \right)^{-1} \\ \hline & \begin{array}{ccc} b_1 & b_2 & b_3 \\ d_1 & d_2 & d_3 \end{array} \end{array} \tag{5.3}$$

where  $b_i = d_i(1 - c_i)$ ,  $i = 1, 2, 3$ , and

$$d_1 = \frac{6c_2c_3 - 3(c_2 + c_3) + 2}{6(c_1 - c_2)(c_1 - c_3)}, \quad d_2 = \frac{6c_1c_3 - 3(c_1 + c_3) + 2}{6(c_2 - c_1)(c_2 - c_3)}, \quad d_3 = 1 - d_1 - d_2, \tag{5.4a}$$

$$6c_1c_2c_3 + 2(c_1 + c_2 + c_3) - 3(c_1c_2 + c_2c_3 + c_1c_3) = \frac{3}{2}, \tag{5.4b}$$

$$5 \left[ \left( \frac{1}{3} - \frac{c_3}{2} \right) (c_1^2 + c_2^2 + c_3^2 + c_1c_2 + c_2c_3 + c_1c_3) + \left( c_3 - \frac{1}{2} \right) c_1c_2(c_1 + c_2 + c_3) + \frac{1}{2}c_3^2 \right] = 1, \tag{5.4c}$$

$$\alpha_{13} = -\frac{2\bar{g}_6}{3} + \frac{3\alpha_{33}}{10} + \frac{19}{30}, \quad \alpha_{23} = \bar{g}_6 - \frac{6\alpha_{33}}{5} - \frac{9}{10}, \tag{5.4d}$$

where  $\bar{g}_6 = 6 \sum_{i=1}^3 d_i c_i^5$ . In Sections 2 and 3, we have shown method (5.3) is symplectic and of order at least 5. Obviously, method (5.3) is a two-parameter family of three-stage symplectic RKN methods. Further, let  $\bar{g}_6 = 1$ , then this method is of order 6 and there exists only a free parameter (such as  $\alpha_{33}$ ). Now we select  $c_3, \alpha_{33}$  as free parameters. Equations (5.4b) and (5.4c) yield

$$c_{1,2} = \frac{1}{2} \left( \delta_1 \mp \sqrt{\delta_1^2 - 4\delta_2} \right), \tag{5.5}$$

where

$$\delta_1 = \frac{2}{5} \left( \frac{15c_3^2 - 16c_3 + 3}{6c_3^2 - 6c_3 + 1} \right), \quad \text{for } c_3 \neq \frac{3 \pm \sqrt{3}}{6},$$

$$\delta_2 = \begin{cases} \frac{((6c_3 - 4)\delta_1 - 4c_3 + 3)}{(12c_3 - 6)}, & \text{for } c_3 \neq \frac{1}{2}, \\ \frac{1}{10}, & \text{for } c_3 = \frac{1}{2}. \end{cases}$$

Insert  $c_1, c_2, c_3$  into (5.4a) and (5.4d) so that  $d, b, \alpha_{13}$ , and  $\alpha_{23}$  can be solved, but  $c_3$  must satisfy

$$\delta_1^2 - 4\delta_2 > 0, \quad \delta_1 \pm \sqrt{\delta_1^2 - 4\delta_2} \neq 2c_3, \quad c_3 \neq \frac{3 \pm \sqrt{3}}{6}.$$

In particular, let  $c_3 = 1/2, \alpha_{33} = 1/2$ , the method is of order 6 and given by

$$c^\top = \left( \frac{5 - \sqrt{15}}{10}, \frac{5 + \sqrt{15}}{10}, \frac{1}{2} \right), \quad b^\top = \left( \frac{5 + \sqrt{15}}{36}, \frac{5 - \sqrt{15}}{36}, \frac{2}{9} \right), \quad d^\top = \left( \frac{5}{18}, \frac{5}{18}, \frac{4}{9} \right), \tag{5.6}$$

$$\alpha_{13} = \frac{7}{60}, \quad \alpha_{23} = -\frac{1}{2}.$$

Letting  $c_3 = 1, \alpha_{33} = 1/2$ , method (5.3) is of order 5 and given by

$$c^\top = \left( \frac{4 - \sqrt{6}}{10}, \frac{4 + \sqrt{6}}{10}, 1 \right), \quad b^\top = \left( \frac{9 + \sqrt{6}}{36}, \frac{9 - \sqrt{6}}{36}, 0 \right), \quad d^\top = \left( \frac{16 - \sqrt{6}}{36}, \frac{16 + \sqrt{6}}{36}, \frac{1}{9} \right),$$

$$\alpha_{13} = \frac{47}{60} - \frac{2}{3}\bar{g}_6, \quad \alpha_{23} = -\frac{3}{2} + \bar{g}_6, \quad \bar{g}_6 = 6 \sum_{i=1}^3 d_i c_i^5.$$

From Section 4, we easily show that method (5.3) is singly-implicit iff

$$\alpha_{13} = 12\lambda^3, \quad \alpha_{23} = -18\lambda^2, \quad \alpha_{33} = 3\lambda, \tag{5.7a}$$

$$\phi(\lambda) = 6\lambda^3 - 6\lambda^2 + \frac{3}{4}\lambda - \frac{1}{60} = 0, \quad \bar{g}_6 = \frac{9}{10} (-20\lambda^2 + 4\lambda + 1). \tag{5.7b}$$

It follows from (5.7b) that  $\bar{g}_6 \neq 1$ , i.e.,  $BD(6)$  cannot hold. Therefore, a one-parameter (i.e.,  $c_3$ ) family of three-stage five-order symplectic singly-implicit RKN methods is given by (5.3), (5.4a), (5.5), (5.7a), and  $\lambda$  satisfying  $\phi(\lambda) = 0$ , i.e.,  $\lambda \approx 0.8581, 0.1133, 0.0286$ .

From Section 4, we also easily show that method (5.3) is multiply implicit iff

$$\frac{\hat{\beta}^2}{4} + \frac{\hat{\alpha}^3}{27} < 0, \tag{5.8}$$

where

$$\begin{aligned} \hat{\alpha} &= -\frac{1}{3}\alpha_{33}^2 + \frac{1}{5}\alpha_{33} - \frac{1}{6}\bar{g}_6 - \frac{3}{20}, \\ \hat{\beta} &= -\frac{2}{27}\alpha_{33}^3 + \frac{1}{15}\alpha_{33}^2 - \left(\frac{1}{18}\bar{g}_6 - \frac{1}{40}\right)\alpha_{33} + \frac{1}{18}\bar{g}_6 - \frac{19}{360}. \end{aligned}$$

Inequality (5.8) implies  $\hat{\alpha} < 0$ . When  $\bar{g}_6 = 1$ ,  $\hat{\alpha} < 0$  is equivalent to  $\alpha_{33} > 1/2$  or  $\alpha_{33} < 1/10$ . For example, let  $\alpha_{33} = 0$ , the three-stage six-order multiply-implicit RKN method (5.3) is given by (5.6), and

$$\alpha_{13} = \frac{19}{30}, \quad \alpha_{23} = -\frac{9}{10}, \quad \alpha_{33} = 0. \tag{5.9}$$

### 6. NUMERICAL EXPERIMENTS

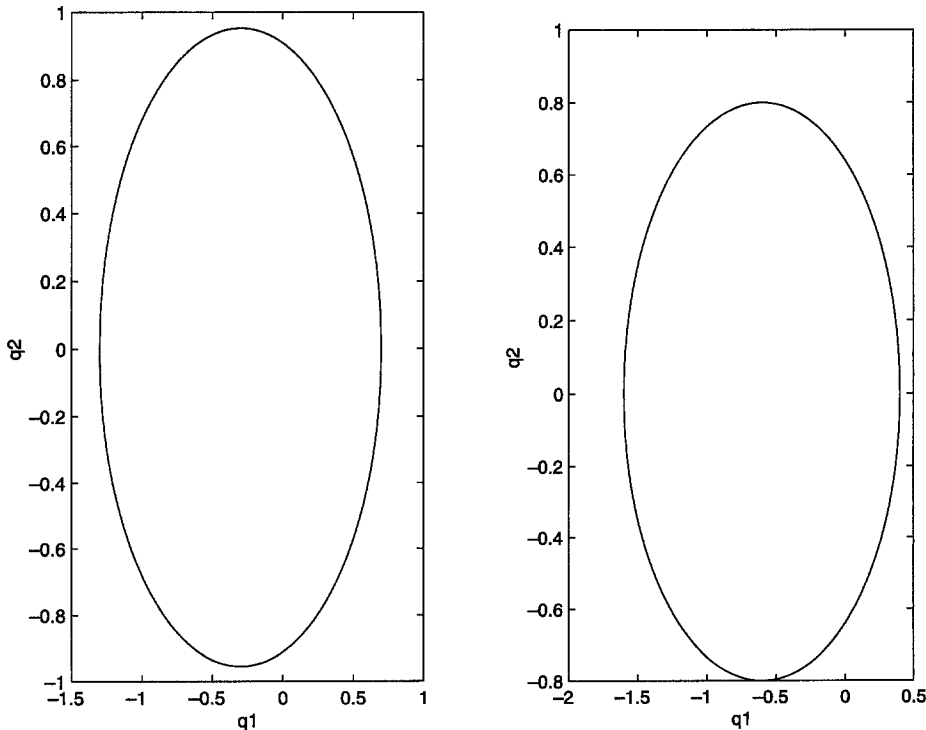
We solve the Kepler problem

$$q'(t) = H_p(p, q), \quad p'(t) = -H_q(p, q), \quad t \in [tb, te], \tag{6.1}$$

where  $q = (q1, q2)^\top$ ,  $p = (p1, p2)^\top$  and the Hamiltonian

$$H(p, q) = H(p1, p2, q1, q2) = \frac{1}{2}((p1)^2 + (p2)^2) - \frac{1}{\sqrt{(q1)^2 + (q2)^2}} = \text{Const},$$

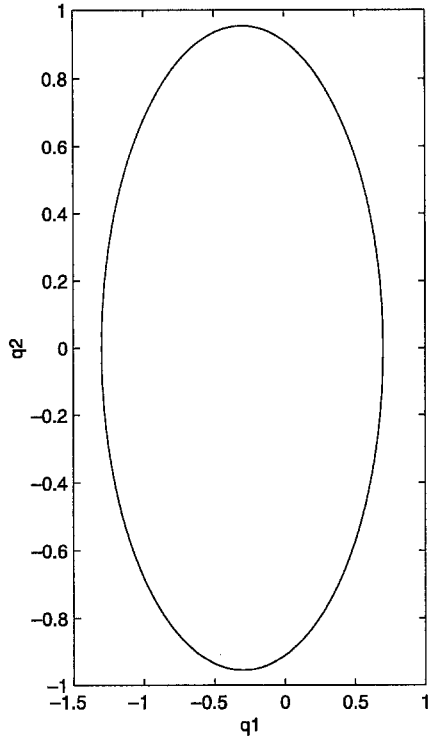
by using the following symplectic RKN methods.



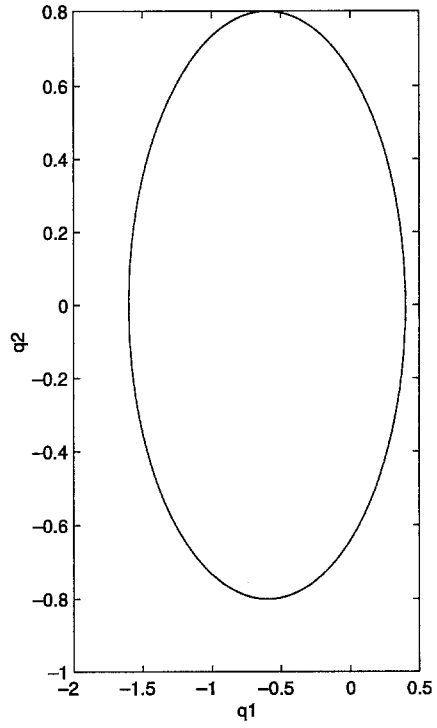
(a)  $e = 0.3$ .

(b)  $e = 0.6$ .

Figure 2.

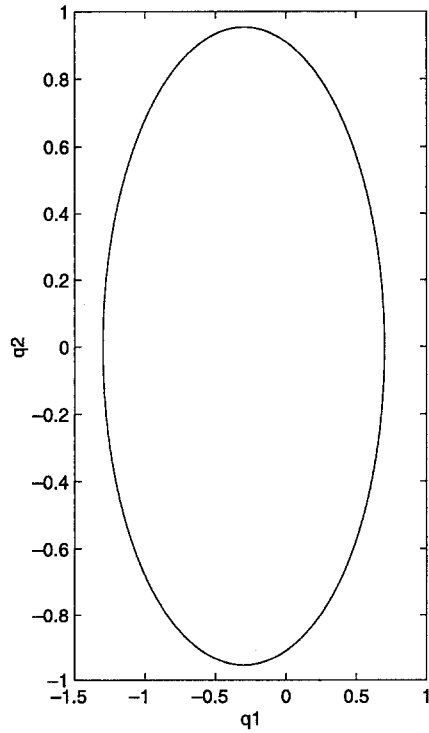


(a)  $e = 0.3$ .

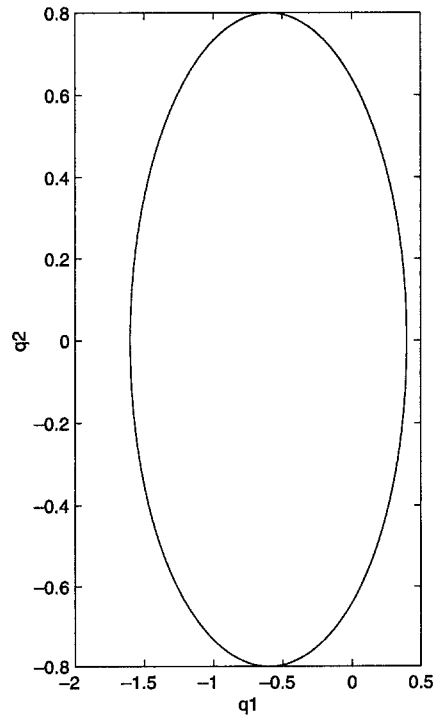


(b)  $e = 0.6$ .

Figure 3.



(a)  $e = 0.3$ .



(b)  $e = 0.6$ .

Figure 4.

(1) METHOD I. The two-stage four-order symplectic multiply-implicit RKN method (5.1) with

$$c^T = \left( \frac{3 - \sqrt{3}}{6}, \frac{3 + \sqrt{3}}{6} \right), \quad d^T = \left( \frac{1}{2}, \frac{1}{2} \right), \quad b^T = \left( \frac{3 + \sqrt{3}}{12}, \frac{3 - \sqrt{3}}{12} \right), \quad (6.2)$$

$$\alpha_{12} = \frac{1}{36}, \quad \alpha_{22} = \frac{1}{12}.$$

(2) METHOD II. The two-stage four-order symplectic singly-implicit RKN method (5.1) with equation (6.2) and

$$\alpha_{12} = -2\lambda^2, \quad \alpha_{22} = 2\lambda, \quad \lambda = \frac{4 + \sqrt{10}}{12}.$$

(3) METHOD III. The three-stage six-order symplectic multiply-implicit RKN method (5.3) with (5.6) and (5.9).

We consider that  $tb = 0$ ,  $te = 800$ , the step size  $h = 0.01$ , and the initial conditions

$$q1(0) = 1 - e, \quad q2(0) = 0, \quad p1(0) = 0, \quad p2(0) = \sqrt{\frac{1+e}{1-e}}.$$

Here  $e$  is the eccentricity and we choose  $e = 0.3, 0.6$ . Figures 2–4 exhibit the correct qualitative behaviors for long-time integration of problem (6.1), where Figures 2a and 2b, Figures 3a and 3b, and Figures 4a and 4b correspond to Methods I–III, respectively.

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