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A NOTE ON CONSERVATION LAWS OF SYMPLECTIC DIFFERENCE SCHEMES FOR HAMILTONIAN SYSTEMS*1)

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Abstract

In this paper we consider the necessary conditions of conservation laws of symplectic difference schemes for Hamiltonian systems and give an example which shows that there does not exist any centered symplectic difference scheme which preserves all Hamiltonian energy.

§1. Introduction

It is well known that Hamiltonian systems have many intrinsic properties: preservation of phase are as and phase volume, conservation laws of energy and momenta, etc. In order to maintain the first property in numerical solution of Hamiltonian systems, Feng Kang first introduced in [1] a new notion — symplectic difference schemes of Hamiltonian systems and developed, with his colleagues, a systematical method — generating function method — to construct such schemes. This method has been further developed and widely extended [8, 10–12]. Meanwhile, symplectic difference schemes constructed in [2, 4] preserve a kind of quadratic first integrals of Hamiltonian systems. In particular, any centered symplectic difference scheme preserves all quadratic first integrals of Hamiltonian systems. But generally it can not preserve first integrals other than of quadratic form.

In Section 2, in order to fulfil the requirement of the next sections, we review the construction of the symplectic difference schemes of Hamiltonian systems by the generating function method developed in [2–4]. In Section 3, we give another proof of a theorem in [5] and prove that the sufficient condition of the theorem is also necessary for first order symplectic difference schemes. In addition, we give general conditions of first integrals of Hamiltonian systems and of conservation laws of centered symplectic difference schemes. In Section 4, we give a simple example. It shows that in general symplectic difference schemes cannot preserve the non-quadratic first integrals; especially, they cannot preserve the energy of a nonlinear Hamiltonian system.

§2. Review of the Construction of Symplectic Difference Schemes

Let R^{2n} be a $2n$-dimensional real space. Its elements are $2n$-dimensional column vectors $z = (z_1, \cdots, z_n, z_{n+1}, \cdots, z_{2n})^T = (p_1, \cdots, p_n, q_1, \cdots, q_n)^T$. The superscript T stands for

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the matrix transpose. Let $C^\infty(R^{2n})$ be the set of all real smooth functions on R^{2n}. $\forall H \in C^\infty(R^{2n})$, $\nabla H(z) = (H_{z_1}, \cdots, H_{z_{2n}})^T$, the gradient of H. Denote

$$J_{2n} = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad J^{-1} = J^T = -J, \tag{1}$$

where I_n and 0 represent unit and zero matrix respectively. A mapping $z \to \hat{z} = g(z)$ is said to be symplectic if its Jacobian is symplectic, i.e.,

$$g_z^T(z) J g_z(z) = J. \tag{2}$$

Consider the Hamiltonian system

$$\frac{dz}{dt} = J^{-1}\nabla H(z), \quad z \in R^{2n}, \tag{3}$$

where $H(z) \in C^\infty(R^{2n})$ is Hamiltonian. Its phase flow is denoted by $g^t(z) = g(z,t)$. It is a one-parameter (local) group of symplectic mappings. A function $F(z)$ is the first integral of the Hamiltonian system (3) if and only if their Poisson bracket is equal to zero, i.e.,

$$\{F, H\} = (\nabla F)^T J^{-1} \nabla H = 0. \tag{4}$$

A difference scheme approximating (3) is called symplectic if its transition from one time-step to the next is a symplectic mapping. [4] has proposed a method, called the generating function method, to construct systematically symplectic difference schemes of the Hamiltonian system (3). We now review the method. The details can be found in [4].

Let

$$\alpha = \begin{bmatrix} -J & J \\ \frac{1}{2}(I+V) & \frac{1}{2}(I-V) \end{bmatrix}, \quad \alpha^{-1} = \begin{bmatrix} \frac{1}{2}J(I+V^T) & I \\ -\frac{1}{2}J(I-V^T) & I \end{bmatrix}, \tag{5}$$

where $V^T J + JV = 0$, i.e., $V \in \mathrm{sp}(2n)$. Then α defines linear transformations

$$\begin{bmatrix} \hat{w} \\ w \end{bmatrix} = \alpha \begin{bmatrix} \hat{z} \\ z \end{bmatrix}, \quad \begin{bmatrix} \hat{z} \\ z \end{bmatrix} = \alpha^{-1} \begin{bmatrix} \hat{w} \\ w \end{bmatrix}, \tag{6}$$

i.e.,

$$\begin{aligned} \hat{w} &= J(z - \hat{z}), & \hat{z} &= w + \frac{1}{2}J(I+V^T)\hat{w}, \\ w &= \frac{1}{2}(\hat{z}+z) + \frac{1}{2}V(\hat{z}-z), & z &= w - \frac{1}{2}J(I-V^T)\hat{w}. \end{aligned} \tag{7}$$

If $\hat{z} = g(z,t)$ is the phase flow of the Hamiltonian system (3), then the equation

$$w + \frac{1}{2}J(I+V^T)\hat{w} = g(w - \frac{1}{2}J(I-V^T)\hat{w}, t) \tag{8}$$

defines implicitly a time-depednent gradient mapping $w \to \hat{w} = f(w,t)$, i.e., its Jacobian $f_w(w,t) \in \mathrm{Sm}(2n)$ everywhere. Hence there exists a scalar function, called the generating function, $\phi(w,t)$ such that

$$f(w,t) = \nabla\phi(w,t). \tag{9}$$

This generating function $\phi(w,t)$ satisfies the Hamilton Jacobi equation

$$\frac{\partial}{\partial t}\phi(w,t) = -H(w + A\nabla\phi(w,t)), \tag{10}$$

where $A = \frac{1}{2}J(I+V^T)$. The phase flow $\hat{z} = g(z,t)$ can be conversely determined by $\phi(w,t)$:

$$\hat{z} - z = -J^{-1}\nabla\phi\Big(\frac{1}{2}(\hat{z}+z) + \frac{1}{2}V(\hat{z}-z), t\Big). \tag{11}$$

Moreover, if $H(z)$ is analytic, then $\phi(w,t)$ can be expanded as a convergent power series in t for sufficiently small $|t|$:

$$\phi(w,t) = \sum_{k=1}^{\infty}\phi^{(k)}(w)t^k. \tag{12}$$

Its coefficients $\phi^{(k)}, k \geq 1$, can be determined by the following recursive formulas:

$$\phi^{(1)}(w) = -H(w), \tag{13}$$

$$\phi^{(k+1)}(w) = -\frac{1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{\substack{k_1+\cdots+k_m=k\\ k_i\geq 1}} D^m H(w)(A\nabla\phi^{(k_1)},\cdots,A\nabla\phi^{(k_m)}),\ k\geq 1. \tag{14}$$

Therefore in this case, the phase flow $\hat{z} = g(z,t)$ is the solution of the implicit equation

$$\hat{z} - z = -\sum_{k=1}^{\infty} t^k J^{-1}\nabla\phi^{(k)}\Big(\frac{1}{2}(\hat{z}+z) + \frac{1}{2}V(\hat{z}-z)\Big). \tag{15}$$

Taking its m-th approximant, we then get a symplectic difference scheme with m-th order of accuracy

$$\begin{aligned} z^{k+1} - z^k &= J\nabla\psi^{(m)}\Big(\frac{1}{2}(z^{k+1}+z^k) + \frac{1}{2}V(z^{k+1}-z^k), \tau\Big) \\ &= \sum_{i=1}^{m}\tau^i J\nabla\phi^{(i)}\Big(\frac{1}{2}(z^{k+1}+z^k) + \frac{1}{2}V(z^{k+1}-z^k)\Big), \end{aligned} \tag{16}$$

where $\tau > 0$ is the time-step. When $V = 0, \phi(w,t)$ is odd in t. Hence the symplectic difference scheme (16) is of even order $(m = 2l)$

$$z^{k+1} - z^k = \sum_{i=1}^{l}\tau^{(2i)}J\nabla\phi^{2i}\Big(\frac{1}{2}(z^{k+1}+z^k)\Big). \tag{17}$$

§3. On Conservation Laws

Theorem 1[5]. *If $F(z) = \frac{1}{2}z^TSz, S\in \mathrm{Sm}(2n)$ is a quadratic first integral of the Hamiltonian system* (3) *and*

$$V^TS + SV = 0, \tag{18}$$

then $F(z)$ is also the invariant of the symplectic difference scheme (16), *i.e.*,

$$F(z^{k+1}) = F(z^k), \quad k \geq 0. \tag{19}$$

For $V = 0$, i.e., the case of centered symplectic difference schemes, (18) is always valid. So all centered symplectic difference schemes preserve all quadratic first integrals of the Hamiltonian system (3). This result was first noticed by Ge Zhong, Wu Yu-hua and Wang Dao-liu. For the general case, the result was obtained in [5]. Here we give another proof.

Proof of Theorem 1. Since $F(z)$ is the first integral of the system (3),

$$\frac{1}{2}\hat{z}^T S \hat{z} = \frac{1}{2} z^T S z.$$

It can be rewritten as

$$\frac{1}{2}(\hat{z} + z)^T S(\hat{z} - z) = 0. \tag{20}$$

From (18), it follows that

$$\begin{aligned}\frac{1}{2}(V(\hat{z} - z))^T S(\hat{z} - z) &= \frac{1}{2}(\hat{z} - z)^T V^T S(\hat{z} - z) \\ &= \frac{1}{4}(\hat{z} - z)^T (V^T S + SV)(\hat{z} - z) = 0, \quad \forall \hat{z},\ z \in R^{2n}.\end{aligned}$$

Combining it with (20), we have

$$\left(\frac{1}{2}(\hat{z} + z) + \frac{1}{2}V(\hat{z} - z)\right)^T S(\hat{z} - z) = 0.$$

Using (15), it becomes

$$\left(\frac{1}{2}(\hat{z} + z) + \frac{1}{2}V(\hat{z} - z)\right)^T SJ \sum_{j=1}^{\infty} t^j \nabla\phi^{(j)} \left(\frac{1}{2}(\hat{z} + z) + \frac{1}{2}V(\hat{z} - z)\right) = 0.$$

From this we get

$$w^T SJ\nabla\phi^{(j)}(w) = 0, \quad \forall j \geq 1, \quad \forall w \in R^{2n}.$$

Then, when we take $w = \frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k)$, we have

$$w^T S(z^{k+1} - z^k) = \sum_{j=1}^{m} \tau^j w^T SJ\nabla\phi^{(j)}(w) = 0.$$

Since

$$\begin{aligned}w^T S(z^{k+1} - z^k) &= \left(\frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k)\right)^T S(z^{k+1} - z^k) \\ &= \frac{1}{2}(z^{k+1})^T S z^{k+1} - \frac{1}{2}(z^k)^T S z^k,\end{aligned}$$

$F(z)$ is the quadratic invariant of the symplectic difference scheme (16).

We now take

$$V = \begin{bmatrix} (1 - 2\theta)I_n & 0 \\ 0 & -(1 - 2\theta)I_n \end{bmatrix}. \tag{21}$$

It can be easily verified that $V^TJ + JV = 0$, i.e., $V \in \mathbf{sp}(2n)$. Let $S \in \mathbf{Sm}(2n)$. Denote $S = \begin{bmatrix} A & B \\ B^T & D \end{bmatrix}$, $A^T = A$, $D^T = D$. Then

$$V^TS + SV = 2\begin{bmatrix} (1-2\theta)A & 0 \\ 0 & -(1-2\theta)D \end{bmatrix}.$$

Hence (18) is equivalent to

$$(1-2\theta)A = 0, \quad (1-2\theta)D = 0.$$

It means that either $\theta = 1/2$ or $A = D = 0$. When $\theta = 1/2$, the scheme (16) is centered. It preserves all quadratic first integrals of the Hamiltonian system (3). When $\theta \neq 1/2$, the symplectic difference scheme (16) only preserves the quadratic first integrals with the form p^TBq of the Hamiltonian system (3).

Theorem 1 for the first order symplectic difference scheme has a converse. Presicely speaking, we have the following theorem.

Theorem 2. *Let $F(z) = \frac{1}{2}z^TSz$, where $S \in \mathbf{Sm}(2n)$ is a quadratic first integral of the Hamiltonian system (3), and in some neighborhood of R^{2n} the Hessian of H, H_{zz}, is non-degenerate. If $F(z)$ is also an invariant of the first order symplectic difference scheme*

$$z^{k+1} - z^k = \tau J^{-1}\nabla H\Big(\frac{1}{2}(z^{k+1}+z^k) + \frac{1}{2}V(z^{k+1}-z^k)\Big), \tag{22}$$

i.e., $F(z^{k+1}) = F(z^k), k \geq 0$, then

$$V^TS + SV = 0. \tag{23}$$

Proof. By assumption, F is the first integral of (3); then

$$\{F, H\} = z^TSJ^{-1}\nabla H(z) = 0, \quad \forall z \in R^{2n}.$$

Hence

$$\Big(\frac{1}{2}(z^{k+1}+z^k) + \frac{1}{2}V(z^{k+1}-z^k)\Big)^T S(z^{k+1}-z^k) = \tau w^TSJ^{-1}\nabla H(w) = 0, \tag{24}$$

where $w = \frac{1}{2}(z^{k+1}+z^k) + \frac{1}{2}V(z^{k+1}-z^k)$. By hypothesis, $F(z)$ is also the invariant of (22). It means

$$\frac{1}{2}(z^{k+1})^TSz^{k+1} = \frac{1}{2}(z^k)^TSz^k,$$

i.e.,

$$\frac{1}{2}(z^{k+1}+z^k)^TS(z^{k+1}-z^k) = 0. \tag{25}$$

Combining (24) and (25), we get

$$\frac{1}{2}(z^{k+1}-z^k)^TV^TS(z^{k+1}-z^k) = \frac{1}{4}(z^{k+1}-z^k)^T(V^TS+SV)(z^{k+1}-z^k) = 0.$$

Because H_{zz} is non-degenerate in some neighborhood of R^{2n}, $z^{k+1} \neq z^k$ for sufficiently small τ. Hence we get the conclusion (23).

Lemma 3. *$V \in \mathbf{sp}(2n)$ such that*

$$V^T S + SV = 0, \quad \forall S \in \mathbf{Sm}(2n) \cap \mathbf{GL}(2n)$$

if and only if $V = 0$.

Theorem 4. *There does not exist first order symplectic difference scheme with the form (22) which preserves all Hamiltonian energy.*

The proof follows from Theorem 2, Lemma 3 and Theorem 6 in the next section.

We now consider the conservation properties of centered symplectic difference schemes (17). In this case, $V = 0$. Thus (7) becomes

$$\hat{z} = w + \frac{1}{2} J\hat{w}, \quad z = w - \frac{1}{2} J\hat{w}.$$

Set

$$u_k = \frac{1}{2} J\nabla\phi^{(k)}(w), k \geq 1; \quad u = \frac{1}{2} J\nabla\phi(w,t) = \sum_{k=1}^{\infty} \frac{1}{2} J\nabla\phi^{(k)}(w) t^k = \sum_{k=1}^{\infty} u_k t^k;$$

$$\tilde{u} = \frac{1}{2} J\dot{\nabla}\psi^{(m)}(w,\tau) = \sum_{k=1}^{m} \frac{1}{2} J\nabla\phi^{(k)}(w)\tau^k = \sum_{k=1}^{m} u_k t^k.$$

Since the generating function $\phi(w,t)$ is odd in t, $u_{2k} = 0$.

Lemma 5. *$F(z)$ is the first integral of the Hamiltonian system (3) if and only if*

$$\sum_{j=1,\text{odd}}^{k} \frac{1}{j!} \sum_{\substack{k_1+\cdots+k_j=k \\ k_i \geq 1,\text{odd}}} D^j F(w)(u_{k_1}, \cdots, u_{k_j}) = 0, \quad \forall \text{ odd } k. \tag{26}$$

$F(z)$ is preserved by the centered symplectic difference scheme (17) with m-th order of accuracy if and only if

$$\sum_{j=1,\text{odd}}^{k} \frac{1}{j!} \sum_{\substack{k_1+\cdots+k_j=k \\ 1 \leq k_i \leq m,\text{odd}}} D^j F(w)(u_{k_1}, \cdots, u_{k_j}) = 0, \quad \forall \text{ odd } k. \tag{27}$$

Proof. Suppose that $F(z)$ is a first integral of the Hamiltonian system (3). Then

$$F(\hat{z}) = F(z),$$

i.e.,

$$F(w+u) = F(w-u). \tag{28}$$

Expanding the left and right hand sides of the equation above, we get

$$F(w+u) = F(w) + \sum_{k=1}^{\infty} t^k \sum_{j=1}^{k} \frac{1}{j!} \sum_{\substack{k_1+\cdots+k_j=k \\ k_i \geq 1,\text{odd}}} D^j F(w)(u_{k_1}, \cdots, u_{k_j}),$$

$$F(w-u) = F(w) + \sum_{k=1}^{\infty} t^k \sum_{j=1}^{k} \frac{(-1)^j}{j!} \sum_{\substack{k_1+\cdots+k_j=k \\ k_i \geq 1,\text{odd}}} D^j F(w)(u_{k_1}, \cdots, u_{k_j}).$$

Hence (28) is equivalent to

$$\sum_{j=1,\mathrm{odd}}^{k}\frac{1}{j!}\sum_{\substack{k_1+\cdots+k_j=k\\ k_i\geq 1,\mathrm{odd}}} D^jF(w)(u_{k_1},\cdots,u_{k_j})=0,\quad \forall k\geq 1. \tag{29}$$

Similarly, the symplectic difference scheme (17) preserves $F(z)$ if and only if

$$F(w+\tilde{u})=F(w-\tilde{u}). \tag{30}$$

It is equivalent to

$$\sum_{j=1,\mathrm{odd}}^{k}\frac{1}{j!}\sum_{\substack{k_1+\cdots+k_j=k\\ 1\leq k_i\leq m,\mathrm{odd}}} D^jF(w)(u_{k_1},\cdots,u_{k_j})=0,\quad \forall k\geq 1. \tag{31}$$

As k is even, the second summation of (29) or (31) is empty. So for even k, (29) and (31) are always valid.

When $F(z)$ is of quadratic form, $D^mF=0$, $m\geq 3$. In this case, (26) and (27) become respectively

$$DF(u_k)=0,\quad \forall\ k\geq 1, \tag{32}$$

and

$$DF(u_k)=0,\quad \forall\ m\geq k\geq 1. \tag{33}$$

Of course, (32) implies (33). We thus obtain the conclusion again: all centered symplectic difference schemes preserve all quadratic first integrals of the Hamiltonian system (3).

§4. An Example

We now give an example. It shows that in general, only the first integral of quadratic form of Hamiltonian systems can been preserved by symplectic difference schemes.

Theorem 6. *Let $n=1$, and $H(p,q)=p^2q$ be Hamiltonian. Then any centered symplectic difference scheme (17) can not preserve H.*

Lemma 7. *Let H be as above. Then $\phi^{(2k-1)}(w), k\geq 1$, determined by (13) and (14), have the expression*

$$\phi^{(2k-1)}(w)=C_kp^{2k}q,\quad k\geq 1, \tag{34}$$

where $C_k=(-1)^k|C_k|$, $k\geq 1$, are determined by the following recursive formula

$$C_1=-1,\quad C_k=\frac{(-1)^k}{4}\sum_{j=1}^{k-1}|C_j|\,|C_{k-j}|,\quad k\geq 1. \tag{35}$$

Proof. By induction with respect to k.

For $k=1$, by (13), $\phi^{(1)}(w)=-H(p,q)=-p^2q$; (34) and (35) are valid. Suppose for $k-1,k-2,\cdots$, (34) and (35) are also valid. Then since H is a polynomial of degree 3, $D^mH=0, m\geq 4$. Using the notation above, $u_{2j}=0$,

$$u_{2j-1}=\frac{1}{2}J\nabla\phi^{(2j-1)}=\frac{1}{2}C_j\begin{bmatrix}p^{2j}\\ -2jp^{2j-1}q\end{bmatrix},\quad j=1,\cdots,k,$$

$$D^2H(u_{2j-1},u_{2(k-j+1)-1})=(u_{2j-1})^TH_{zz}u_{2(k-j+1)-1}=-\frac{1}{2}(2k+1)C_jC_{k-j+1}p^{2(k+1)}q.$$

Hence by (14),

$$\phi^{(2k+1)} = -\frac{1}{2k+1}\sum_{m=1}^{2k}\frac{1}{m!}\sum_{\substack{k_1+\cdots+k_m=2k\\ k_i\geq 1,\text{odd}}} D^m H(w)(u_{k_1},\cdots,u_{k_m})$$

$$= -\frac{1}{2(2k+1)}\sum_{j+i=k+1} D^2 H(u_{2j-1},u_{2i-1})$$

$$= -\frac{1}{2(2k+1)}\sum_{j=1}^{k} D^2 H(u_{2j-1},u_{2(k+1-j)-1}) = \frac{1}{4}\sum_{j=1}^{k} C_j C_{k+1-j} p^{2(k+1)} q.$$

$$C_{k+1} = \frac{1}{4}\sum_{j=1}^{k} C_j C_{k+1-j} = \frac{1}{4}\sum_{j=1}^{k}(-1)^j|C_j|(-1)^{k+1-j}|C_{k+1-j}|$$

$$= \frac{(-1)^{k+1}}{4}\sum_{j=1}^{k}|C_j|\ |C_{k+1-j}|.$$

Proof of Theorem 6. Since H is Hamiltonian, it is of course the first integral of the Hamiltonian system (3). By Lemma 5, we have

$$DH(u_k) + \frac{1}{3!}\sum_{\substack{k_1+k_2+k_3=k\\ k_i\geq 1,\text{ odd}}} D^3 H(w)(u_{k_1},u_{k_2},u_{k_3}) = 0, \quad \forall \text{ odd } k. \tag{36}$$

But H is preserved by the centered symplectic difference scheme (17) if and only if

$$DH(u_k) + \frac{1}{3!}\sum_{\substack{k_1+k_2+k_3=k\\ 1\leq k_i\leq m,\text{ odd}}} D^3 H(w)(u_{k_1},u_{k_2},u_{k_3}) = 0, \quad 1\leq k\leq m,\text{odd}, \tag{37}$$

$$\frac{1}{3!}\sum_{\substack{k_1+k_2+k_3=k\\ 1\leq k_i\leq m,\text{ odd}}} D^3 H(w)(u_{k_1},u_{k_2},u_{k_3}) = 0, \quad k>m,\text{odd}. \tag{38}$$

Consider the term of $k = m+1 = 2l+1$. By Lemma 7,

$$DH(u_{2l+1}) = \frac{1}{2}C_{l+1}(2pq,p^2)\begin{pmatrix} p^{2l+2} \\ -2(l+1)p^{2l+1}q \end{pmatrix} = -lC_{l+1}p^{2l+3}q \neq 0.$$

Hence (38) is not valid for $k = m+1$. It implies that the centered symplectic difference scheme (17) does not preserve $H(p,q)$.

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