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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

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