

POISSON DIFFERENCE SCHEMES FOR HAMILTONIAN SYSTEMS ON POISSON MANIFOLDS

Wang Dao-liu

(Computing Center, Chinese Academy of Sciences, Beijing, China)

Abstract

In this paper a systematical method for the construction of Poisson difference schemes with arbitrary order of accuracy for Hamiltonian systems on Poisson manifolds is considered. The transition of such difference schemes from one time-step to the next is a Poisson map. In addition, these schemes preserve all Casimir functions and, under certain conditions, quadratic first integrals of the original Hamiltonian systems. Especially, the arbitrary order centered schemes preserve all Casimir functions and all quadratic first integrals of the original Hamiltonian systems.

§1. Introduction

For the Hamiltonian system

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

where $H(z) \in C^\infty(\mathbf{R}^{2n})$ is a Hamiltonian function, Feng Kang et al. have developed a general method for the construction of symplectic difference schemes via generating functions [3-6]. Such difference schemes preserve the symplecticity of the phase flow and the quadratic first integrals of the original Hamiltonian systems. The method used in [5] can be generalized to the following Hamiltonian system

$$\frac{dz}{dt} = K \nabla H(z), \quad z \in \mathbf{R}^n \quad (1)$$

where $H(z) \in C^\infty(\mathbf{R}^n)$, K is an anti-symmetric scale matrix, maybe singular. This system could appear such as in the semi-discretization of infinite dimensional Hamiltonian systems in space variables. The case of non-singular K has been considered in [12]. At that case n is even and a Poisson map coincides with a symplectic map. For a given generator map, a Poisson (or symplectic) map uniquely determines a gradient map, further a scalar function (up to a constant), and vice versa. So the scalar function is called a generating function. Here a given Poisson map can also determine a scalar function. This scalar function, in another way, can also determine a Poisson map. But we do not know if it is the original one. This is the present difficulty. Fortunately, for the phase flow of the system (1), we

* Received January 17, 1988.

¹⁾ The Project supported by National Natural Science Foundation of China.

can directly give its time-dependent generating function which satisfies a Hamilton Jacobi equation. When this result is obtained, the remainder is similar to [5].

In sec. 2 we consider some properties of the Hamiltonian system (1). Its phase flow is a one parameter group of Poisson maps. In sec. 3, it is shown that for the phase flow of the system (1) there exists generating functions and its generating functions satisfy some Hamilton Jacobi equation. This generating function can be expressed as a power series for analytic $H(z)$, whose coefficients can be recursively determined. Truncate it then Poisson difference schemes approximating to (1) with arbitrary order of accuracy are obtained (in sec. 4). Sec. 5 is about conservation laws. All Casimir functions and quadratic first integrals, under some conditions, are preserved. Especially, the arbitrary order centered schemes preserve all Casimir functions and quadratic first integrals of the original Hamiltonian systems.

We shall limit ourselves to the local case throughout the paper.

§2. Poisson Manifolds and Hamiltonian Systems

Let \mathbf{R}^n be an n -dim real space. The elements of \mathbf{R}^n are n -dim column vectors $z = (z_1, \dots, z_n)^T$. The superscript T represents the matrix transpose.

Let $C^\infty(\mathbf{R}^n)$ be the space of smooth real valued functions on \mathbf{R}^n . For $H(z) \in C^\infty(\mathbf{R}^n)$, we denote $\nabla H = \nabla_z H = (H_{z_1}, \dots, H_{z_n})^T$, $H_z = (H_{z_1}, \dots, H_{z_n})$ and $H_{z_i} = \partial H / \partial z_i$. So $\nabla H(z) = (H_z(z))^T$.

For a given anti-symmetric $n \times n$ matrix K (maybe singular), we can define a binary operation $\{\cdot, \cdot\}$ on $C^\infty(\mathbf{R}^n)$ by

$$\{F, H\} = (\nabla F)^T K \nabla H, \quad \forall F, H \in C^\infty(\mathbf{R}^n).$$

Evidently, it is bilinear, anti-symmetric and satisfies the Jacobi identity, i.e.,

$$\{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\} = 0, \quad \forall F, G, H \in C^\infty(\mathbf{R}^n).$$

From the definition it follows that it also satisfies Leibniz identity

$$\{FG, H\} = F\{G, H\} + \{F, H\}G.$$

So $\{\cdot, \cdot\}$ is a Poisson bracket on \mathbf{R}^n . \mathbf{R}^n equipped with the Poisson bracket is called a Poisson manifold, still denoted by \mathbf{R}^n .

A map $z \rightarrow \hat{z} = g(z) : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is called a Poisson map if it is a (local) diffeomorphism and preserves the Poisson bracket, i.e.,

$$\{F \circ g, H \circ g\} = \{F, H\} \circ g, \quad \forall F, H \in C^\infty(\mathbf{R}^n).$$

It is easy to verify that it is equivalent to

$$g_z(z) K (g_z(z))^T = K,$$

i.e., the Jacobian matrix g_z is everywhere Poisson; here a matrix M is called Poisson if

$$MKM^T = K.$$

Definition. A function $C(z) \in C^\infty(\mathbf{R}^n)$ is called a Casimir function if

$$\{C(z), F(z)\} = 0, \quad \forall F \in C^\infty(\mathbf{R}^n).$$

Proposition 1. $C(z) \in C^\infty(\mathbf{R}^n)$ is a Casimir function if and only if

$$K \nabla C(z) = 0, \quad \forall z \in \mathbf{R}^n.$$

By a Hamiltonian system on the Poisson manifold \mathbf{R}^n , we mean the following ordinary differential equation

$$\frac{dz}{dt} = K \nabla H(z), \quad z \in \mathbf{R}^n, \tag{2}$$

where $H(z) \in C^\infty(\mathbf{R}^n)$ is called a Hamiltonian function. Its phase flow is denoted by $g^t(z) = g(z, t) = g_H(z, t)$. It is a one parameter group of diffeomorphisms g^t , at least locally in t and z , i.e.,

$$g^0 = \text{identity}, \quad g^{t_1+t_2} = g^{t_1} \circ g^{t_2}.$$

If z_0 is taken as an initial value, then $z(t) = g^t(z_0)$ is the solution of (2) with the initial value z_0 .

Theorem 2. ([11]) *The phase flow $g^t(z)$ of the Hamiltonian system (2) is a one parameter group of Poisson maps, i.e.,*

$$\{F \circ g^t(z), G \circ g^t(z)\} = \{F, G\} \circ g^t(z), \quad \forall t \in \mathbf{R}, \forall F, G \in C^\infty(\mathbf{R}^n)$$

or

$$g_z^t(z) K (g_z^t(z))^T = K, \quad \forall t \in \mathbf{R}.$$

Theorem 3. *$F(z) \in C^\infty(\mathbf{R}^n)$ is a first integral of the Hamiltonian system (2) if and only if $\{F, H\} = 0$. Especially, every Casimir function is a first integral.*

§3. Generating Functions for Phase Flow of Hamiltonian Systems

Let $\alpha = \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix} \in \mathbf{GL}(2n)$ satisfy

$$\alpha \begin{bmatrix} 0 & K \\ K & 0 \end{bmatrix} \alpha^T = \begin{bmatrix} K & 0 \\ 0 & -K \end{bmatrix}. \tag{3}$$

Expanding it, we get

$$\begin{aligned} B_\alpha K A_\alpha^T + A_\alpha K B_\alpha^T &= K, & B_\alpha K C_\alpha^T + A_\alpha K D_\alpha^T &= 0, \\ D_\alpha K A_\alpha^T + C_\alpha K B_\alpha^T &= 0, & D_\alpha K C_\alpha^T + C_\alpha K D_\alpha^T &= -K. \end{aligned} \tag{4}$$

Left multiplying (3) by α^{-1} , we have

$$\begin{aligned} A^\alpha K &= K B_\alpha^T, & B^\alpha K &= -K D_\alpha^T, \\ C^\alpha K &= K A_\alpha^T, & D^\alpha K &= -K C_\alpha^T, \end{aligned} \tag{5}$$

where $\alpha^{-1} = \begin{bmatrix} A^\alpha & B^\alpha \\ C^\alpha & D^\alpha \end{bmatrix}$.

For a given $\alpha \in \mathbf{GL}(2n)$, we can define a linear fractional transformation

$$\begin{aligned} \sigma_{\alpha^{-1}} : \mathbf{M}(n) &\longrightarrow \mathbf{M}(n), \\ N = \sigma_{\alpha^{-1}}(M) &= (A^\alpha M + B^\alpha)(C^\alpha M + D^\alpha)^{-1}, \end{aligned} \tag{6}$$

under the transversality condition

$$|C^\alpha M + D^\alpha| \neq 0. \tag{7}$$

Its inverse transformation is $\sigma_{\alpha^{-1}} = \sigma_{\alpha}$:

$$M = \sigma_{\alpha}(N) = (A_{\alpha}N + B_{\alpha})(C_{\alpha}N + D_{\alpha})^{-1}$$

for

$$|C_{\alpha}N + D_{\alpha}| \neq 0. \quad (8)$$

The conditions (7) and (8) are equivalent [5].

By direct verification, we can obtain

Lemma 4. *Let $\alpha \in \mathbf{GL}(2n)$ satisfy the condition (3). Then M is a Poisson matrix and satisfies (7) if and only if $N = \sigma_{\alpha^{-1}}(M)$ satisfies (8) and $NK \in \mathbf{Sm}(n)$.*

Theorem 5. *Let $\alpha \in \mathbf{GL}(2n)$ satisfy the condition (3). Let $z \rightarrow \hat{z} = g(z) : \mathbf{R}^n \rightarrow \mathbf{R}^n$ be a Poisson map and its Jacobian $M(z) = g_z(z)$ satisfy the transversality condition (7). Then there exists a map $w \rightarrow \hat{w} = f(w) : \mathbf{R}^n \rightarrow \mathbf{R}^n$ with Jacobian $N(w) = f_w(w) = \sigma_{\alpha^{-1}}(M(z))$ and a scalar function $\phi(\bar{w})$ (depending on α and g) such that*

$$A^{\alpha}g(z) + B^{\alpha}z = f(C^{\alpha}g(z) + D^{\alpha}z), \quad (9)$$

$$f(K\bar{w}) \text{ is a gradient map, } NK = \sigma_{\alpha^{-1}}(M)K \in \mathbf{Sm}(n), \quad (10)$$

$$f(K\bar{w}) = \nabla\phi(\bar{w}). \quad (11)$$

Proof. Set

$$\hat{w} = A^{\alpha}g(z) + B^{\alpha}z, \quad w = C^{\alpha}g(z) + D^{\alpha}z.$$

By assumption, $|C^{\alpha}M(z) + D^{\alpha}| \neq 0$. So by Inverse Implicit Theorem, $w = C^{\alpha}g(z) + D^{\alpha}z$ is invertible. Denote its inverse as $z = z(w)$. Set $\hat{w} = f(w) = (A^{\alpha}g(z) + B^{\alpha}z)|_{z=z(w)} = A^{\alpha}g(z(w)) + B^{\alpha}z(w)$. Then its Jacobian is

$$\begin{aligned} N(w) = f_w(w) &= \frac{\partial \hat{w}}{\partial w} = \frac{\partial \hat{w}}{\partial z} \frac{\partial z}{\partial w} = \frac{\partial \hat{w}}{\partial z} \left(\frac{\partial w}{\partial z} \right)^{-1} \\ &= (A^{\alpha}M(z) + B^{\alpha})(C^{\alpha}M(z) + D^{\alpha})^{-1} = \sigma_{\alpha^{-1}}(M(z)). \end{aligned}$$

Evidently, f and g satisfy (9). Set $\tilde{f}(\bar{w}) = f(w)|_{w=K\bar{w}} = f(K\bar{w})$. Then, by Lemma 4, $\tilde{f}_{\bar{w}} = f_w \cdot K = \sigma_{\alpha^{-1}}(M) \cdot K \in \mathbf{Sm}(n)$. That is, $\tilde{f}(\bar{w}) = f(K\bar{w})$ is a gradient map. So by Poincare Lemma, there exists a scalar function $\phi(\bar{w})$, such that

$$\nabla\phi(\bar{w}) = \tilde{f}(\bar{w}) = f(K\bar{w}).$$

Analogous to [5], it is easy to get the following

Theorem 6. *Let $\alpha \in \mathbf{GL}(2n)$ satisfy (3). Let $z \rightarrow \hat{z} = g(z, t)$ be the phase flow of the Hamiltonian system (2) with the Jacobian $M(z, t) = g_z(z, t)$ and*

$$|C^{\alpha} + D^{\alpha}| \neq 0. \quad (12)$$

Then there exists, for sufficiently small $|t|$ and in (some neighbourhood of) \mathbf{R}^n , a time-dependent map $w \rightarrow \hat{w} = f(w, t) : \mathbf{R}^n \rightarrow \mathbf{R}^n$ with the Jacobian $N(w, t) = f_w(w, t) = \sigma_{\alpha^{-1}}(M)$ and a time-dependent scalar function $\phi(\bar{w}, t)$ such that

$$A^{\alpha}g(z, t) + B^{\alpha}z = f(C^{\alpha}g(z, t) + D^{\alpha}z, t), \text{ identically in } z$$

$$\tilde{f}(\bar{w}, t) = f(w, t)|_{w=K\bar{w}} = f(K\bar{w}, t) \text{ is a time-dependent gradient map,}$$

$$NK = \sigma_{\alpha^{-1}}(M)K \in \mathbf{Sm}(n),$$

$$\tilde{f}(\bar{w}, t) = f(K\bar{w}, t) = \nabla\phi(\bar{w}, t),$$

$$\frac{\partial \phi}{\partial t} = \phi_t(\bar{w}, t) = -H(A_{\alpha}\nabla\phi(\bar{w}, t) + B_{\alpha}K\bar{w}).$$

From Theorem 5, we know that if K is non-singular, then $g(z)$ and $\phi(\bar{w})$ have the relation

$$A^\alpha g(z) + B^\alpha z = \nabla_{\bar{w}} \phi(K^{-1}(C^\alpha g(z) + D^\alpha z)).$$

So a Poisson map $g(z)$ uniquely determines a scalar function $\phi(\bar{w})$ (up to a constant), and vice versa. In this case, $\phi(\bar{w})$ is called a generating function of $g(z)$. Consequently the phase flow $g(z, t)$ of a Hamiltonian system corresponds to a time-dependent generating function (for fixed α) which satisfies some Hamilton Jacobi equation. For the case of the singular K , given a Poisson map, we can get a scalar function. But the above relation is not valid. Of course, for a given scalar function $\tilde{\phi}(\bar{w})$, there corresponds a Poisson map, defined by

$$A^\alpha \tilde{g}(z) + B^\alpha z = K^T \nabla_{\bar{w}} \tilde{\phi}(C^\alpha \tilde{g}(z) + D^\alpha z)$$

under the condition

$$|C_\alpha K^T \tilde{\phi}_{\bar{w}\bar{w}}(\bar{w}) + D_\alpha| \neq 0.$$

Even though we take $\tilde{\phi}(\bar{w}) = \phi(\bar{w})$, we do not know if $\tilde{g}(z)$ coincides with $g(z)$. Hence we can not use $\phi(\bar{w}, t)$ in Theorem 6 to determine the phase flow $g(z, t)$. In order to overcome the difficulty, we make the slight change of ϕ and directly give Hamilton Jacobi equation. Below we consider α in a subset, i.e., it is of the form

$$\alpha = \begin{bmatrix} \frac{1}{2}(I - V) & I \\ -\frac{1}{2}(I + V) & I \end{bmatrix}, \quad \alpha^{-1} = \begin{bmatrix} I & -I \\ \frac{1}{2}(I + V) & \frac{1}{2}(I - V) \end{bmatrix}, \quad (13)$$

where

$$KV^T + VK = 0.$$

It is easy to verify that such an α satisfies (3).

Theorem 7. Let $\alpha \in \mathbf{GL}(2n)$ be as in (13). Let $\psi(w, t)$ be the solution of the following partial differential equation

$$\frac{\partial \psi}{\partial t} = \psi_t(w, t) = -H(w - A_\alpha K \nabla \psi(w, t)), \quad (14)$$

where $A_\alpha = \frac{1}{2}(I - V)$, with the initial condition $\psi(w, 0) = 0$. Then, for sufficiently small t and in (some neighbourhood of) \mathbf{R}^n , the phase flow $g(z, t)$ of the Hamiltonian system (2) satisfies

$$g(z, t) - z = -K \nabla_w \psi(C^\alpha g(z, t) + D^\alpha z, t), \quad \text{identically in } z, \quad (15)$$

where $C^\alpha = \frac{1}{2}(I + V)$, $D^\alpha = \frac{1}{2}(I - V)$.

The scalar function $\psi(w, t)$ is called the generating function of the phase flow $g(z, t)$. The equation (14) is called the Hamilton Jacobi equation of the Hamiltonian system (2).

Proof. Evidently, the initial-value problem always has a solution locally [9]. So we only need to prove that the solution of (15) satisfies (2). Differentiating (15) with respect to t , we get

$$\frac{dg(z, t)}{dt} = -K \psi_{ww}(w, t) \cdot C^\alpha \frac{dg(z, t)}{dt} - K (\nabla_w \psi)_t(w, t), \quad (16)$$

where $w = C^\alpha g(z, t) + D^\alpha z$, $\psi_{ww}(w, t)$ is the Hessian of $\psi(w, t)$ with respect to w . By (14),

$$(\nabla_w \psi)_t(w, t) = -(I - A_\alpha K \psi_{ww}(w, t))^T \nabla H(\hat{z}),$$

where $\hat{z} = w - A_\alpha K \nabla \psi(w, t)$. Substituting it into (16), we have

$$\begin{aligned} (I + K \psi_{ww} C^\alpha) \frac{dg(z, t)}{dt} &= K(I + \psi_{ww} K A_\alpha^T) \nabla H(\hat{z}) \\ &= (I + K \psi_{ww} C^\alpha) K \nabla H(\hat{z}) \quad (\text{by (7)}). \end{aligned}$$

Since $\psi_{ww}(w, 0) = 0$, $I + K \psi_{ww} C^\alpha$ is non-singular for sufficiently small t and in (some neighbourhood of) \mathbb{R}^n . It reduces

$$\frac{dg(z, t)}{dt} = K \nabla H(\hat{z}), \quad (17)$$

Since $w = C^\alpha g(z, t) + D^\alpha z$, then by (15),

$$g(z, t) - z = -K \nabla_w \psi(w, t).$$

So

$$\begin{aligned} \hat{z} &= w - A_\alpha K \nabla \psi(w, t) = C^\alpha g(z, t) + D^\alpha z + A_\alpha (g(z, t) - z) \\ &= (C^\alpha + A_\alpha) g(z, t) + (D^\alpha - A_\alpha) z = g(z, t). \end{aligned}$$

Combining with (17), we get

$$\frac{dg(z, t)}{dt} = K \nabla H(g(z, t)).$$

For $t = 0$, $\psi(w, 0) = 0$, so $g(z, 0) - z = 0$, i.e., $g(z, 0) = z$. Therefore, $g(z, t)$ defined by (15) is really the phase flow of the Hamiltonian system (2).

Theorem 8. *Let $H(z)$ depend analytically on z . Then the generating function $\psi(w, t)$ can be expressed as a convergent power series in t for sufficiently small $|t|$*

$$\psi(w, t) = \sum_{k=1}^{\infty} \psi^{(k)}(w) t^k. \quad (18)$$

The coefficients $\psi^{(k)}(w)$, $k = 1, 2, \dots$ can be recursively determined by the following equations

$$\psi^{(1)}(w) = -H(w),$$

$$\psi^{(k+1)}(w) = \frac{-1}{k+1} \sum_{m=1}^k \frac{1}{m!} \sum_{\substack{k_1 + \dots + k_m = k \\ k_i \geq 1}} D_z^m H(w) (A_\alpha K^T \nabla \psi^{(k_1)}(w), \dots, A_\alpha K^T \nabla \psi^{(k_m)}(w)), \quad k \geq 1,$$

where we use the notation of multi-linear forms, e.g.,

$$\begin{aligned} &D_z^m H(w) (A_\alpha K^T \nabla \psi^{(k_1)}(w), \dots, A_\alpha K^T \nabla \psi^{(k_m)}(w)) \\ &= \sum_{i_1, \dots, i_m=1}^n H_{z_{i_1}, \dots, z_{i_m}}(w) (A_\alpha K^T \nabla \psi^{(k_1)}(w))_{i_1} \dots (A_\alpha K^T \nabla \psi^{(k_m)}(w))_{i_m}. \end{aligned}$$

$(A_\alpha K^T \nabla \psi^{(k_i)}(w))_{i_i}$ is the i_i -th component of the column vector $A_\alpha K^T \nabla \psi^{(k_i)}(w)$.

Proof. Differentiating (18) with respect to w and t , we get

$$\nabla_w \psi(w, t) = \sum_{k=1}^{\infty} \nabla \psi^{(k)}(w) t^k, \quad (19)$$

$$\frac{\partial \psi}{\partial t} = \psi_t(w, t) = \sum_{k=0}^{\infty} (k+1) t^k \psi^{(k+1)}(w). \quad (20)$$

Substituting them into the Hamilton Jacobi equation, expanding it and comparing the terms of the same order with respect to t , we can get above recursive formula.

From (15) and (19) it follows that $\hat{z} = g(z, t)$ is the solution of the following implicit equation

$$\hat{z} - z = -K \sum_{k=1}^{\infty} t^k \nabla \psi^{(k)} \left(\frac{1}{2}(\hat{z} + z) + \frac{1}{2}V(\hat{z} - z) \right). \tag{21}$$

For $V = 0$, the Hamilton Jacobi equation is

$$\psi_t(w, t) = -H \left(w - \frac{1}{2}K \nabla_w \psi(w, t) \right).$$

and the generating function $\psi(w, t)$ is odd in t . So

$$\psi(w, t) = \sum_{k=1}^{\infty} \psi^{(2k-1)}(w) t^{2k-1}.$$

§4. Construction of Poisson Difference Schemes for Hamiltonian Systems

In this section we use the power series expression of the generating function $\psi_{\alpha, H}(w, t)$ to construct Poisson difference schemes for the Hamiltonian system (2).

Theorem 9. *Let $\alpha \in \text{GL}(2n)$ be as in (13). Using Theorem 8, for sufficiently small $\tau > 0$ as the time step, the m -th truncation of $\psi(w, t)$*

$$\psi^{(m)}(w, \tau) = \sum_{j=1}^m \psi^{(j)}(w) \tau^j, \quad m = 1, 2, \dots$$

defines an implicit Poisson difference scheme $z = z^k \rightarrow z^{k+1} = \hat{z}$,

$$\begin{aligned} z^{k+1} - z^k &= -K \nabla \psi^{(m)} \left(\frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k), \tau \right) \\ &= -K \sum_{j=1}^m \tau^j \nabla \psi^{(j)} \left(\frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k) \right) \end{aligned} \tag{22}$$

with m -th order of accuracy. The transition of such scheme is a Poisson map.

Proof. For sufficiently small τ and in some neighbourhood of \mathbf{R}^n , $I + K \psi_{ww}^{(m)} C^\alpha$ is non-singular. Hence the implicit equation

$$\hat{z} - z = -K \nabla \psi^{(m)} \left(\frac{1}{2}(\hat{z} + z) + \frac{1}{2}V(\hat{z} - z), \tau \right)$$

defines a map $z \rightarrow \hat{z} = g^{(m)}(z, \tau)$, i.e., it satisfies the identity

$$g^{(m)}(z, \tau) - z \equiv -K \nabla \psi^{(m)}(C^\alpha g^{(m)}(z, \tau) + D^\alpha z, \tau).$$

Set $z = z^k$ and $\hat{z} = z^{k+1}$. Then we get the scheme (22).

The Jacobian of $-K \nabla \psi^{(m)}(w, \tau)$ is $N^{(m)}(w, \tau) = -K \psi_{ww}^{(m)}(w, \tau)$. Evidently, $N^{(m)}K \in \text{Sm}(n)$. Thus by Lemma 4, $M^{(m)}(z, \tau) = g_z^{(m)}(z, \tau) = \sigma_\alpha(N^{(m)}(w, \tau))$ is a Poisson matrix. So $g^{(m)}(z, \tau)$ is a Poisson map. Since $\psi^{(m)}(w, \tau)$ is the m -th approximant to $\psi(w, t)$,

$g_z^{(m)}(z, \tau)$ is also the m -th approximant to $g(z, t)$. Therefore the Poisson difference scheme given by (22) is of m -th order of accuracy.

For $V = 0$, and for sufficiently small $\tau > 0$ as the time-step,

$$\psi^{(2m)}(w, \tau) = \sum_{i=1}^m \psi^{(2i-1)}(w) \tau^{2i-1}, \quad m = 1, 2, \dots,$$

defines a $2m$ -th order centered scheme

$$z^{k+1} = z^k - K \sum_{i=1}^m \nabla \psi^{(2i-1)} \left(\frac{1}{2}(z^{k+1} + z^k) \right) \tau^{2i-1}. \quad (23)$$

Take $m = 1$, $\psi^{(1)} = -H$. We get the 2-nd order centered Euler scheme

$$z^{k+1} = z^k + \tau K \nabla H \left(\frac{1}{2}(z^{k+1} + z^k) \right).$$

Take $m = 2$,

$$\begin{aligned} \psi^{(3)}(w) &= -\frac{1}{6} H_{zz} \left(\frac{1}{2} K^T \nabla \psi^{(1)}, \frac{1}{2} K^T \nabla \psi^{(1)} \right) (w) \\ &= \frac{1}{24} ((\nabla H)^T K H_{zz} K \nabla H)(w) = \frac{1}{24} \sum_{i,j=1}^n (K H_{zz} K)_{ij} H_{z_i} H_{z_j}, \end{aligned}$$

where all derivatives of H is evaluated at $w = \frac{1}{2}(\hat{z} + z)$. Thus the 4-th order centered scheme is

$$z^{k+1} = z^k + \tau K \nabla H \left(\frac{1}{2}(z^{k+1} + z^k) \right) - \frac{\tau^3}{24} K \sum_{i,j=1}^n \nabla ((K H_{zz} K)_{ij} H_{z_i} H_{z_j}) \left(\frac{1}{2}(z^{k+1} + z^k) \right).$$

§5. Conservation Laws

In this section we consider the conservation laws of Poisson difference schemes (22). Naturally we hope that the Poisson difference schemes can preserve the conservation laws of the original Hamiltonian systems as many as possible. Here we will show that the Poisson difference schemes (22) can preserve all Casimir functions and, under some additional condition, quadratic first integrals of the original Hamiltonian system (2).

Theorem 10. *The general Poisson difference schemes (22) preserve all Casimir functions. That is, if $C(z) \in C^\infty(\mathbf{R}^n)$ is a Casimir function, then*

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

Proof. By Proposition 1,

$$K \nabla C(z) = 0, \quad \forall z \in \mathbf{R}^n.$$

Hence

$$\begin{aligned} C(z^{k+1}) - C(z^k) &= (\nabla C(z^*))^T (z^{k+1} - z^k) \\ &= -(\nabla C(z^*))^T K \nabla \psi^{(m)} \left(\frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k), \tau \right) = 0. \end{aligned}$$

Theorem 11. Let $F(z) = \frac{1}{2}z^T S z$, $S \in \mathbf{Sm}(n)$ be the first integral of the system (2). If

$$V^T S + S V = 0, \quad (24)$$

then F is also a first integral of the Poisson difference scheme (22), i.e.,

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

Proof. By assumption, $F(\hat{z}) = F(z)$, where $\hat{z} = g(z, t)$, i.e.,

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

It can be rewritten as

$$\frac{1}{2}(\hat{z} + z)^T S (\hat{z} - z) = 0. \quad (25)$$

From the condition (24), it follows that

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

Combining with (25), we have

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

Using (21), it becomes

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

It follows that

$$w^T S K \nabla \psi^{(j)}(w) = 0, \quad \forall j \geq 1, \forall w \in \mathbf{R}^n.$$

Hence for the Poisson difference scheme (22), taking

$$w = \frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k),$$

we obtain

$$\begin{aligned} \frac{1}{2}(z^{k+1} + z^k)^T S (z^{k+1} - z^k) &= \left(\frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k) \right)^T S (z^{k+1} - z^k) \\ &= - \left(\frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k) \right)^T S K \\ &\quad \times \sum_{j=1}^m \nabla \psi^{(j)} \left(\frac{1}{2}(z^{k+1} + z^k) + \frac{1}{2}V(z^{k+1} - z^k) \right) \tau^j = 0. \end{aligned}$$

It is just

$$\frac{1}{2}(z^{k+1})^T S z^{k+1} = \frac{1}{2}(z^k)^T S z^k$$

i.e.,

$$F(z^{k+1}) = F(z^k).$$

When we take $V = 0$, (24) always holds. Therefore we have the following

Corollary 12. All centered Euler difference schemes (23) preserve all Casimir functions and quadratic first integrals of the original Hamiltonian systems.

Acknowledgement. The author would be grateful to Prof. Feng Kang for his enthusiastic guidance, Wu Yu-hua for his helpful suggestions and other members of our research group for their valuable discussion.

References

- [1] R. Abraham and J. Marsden, *Foundations of Mechanics*, Addison-Wesley, Reading, Mass, 1978.
- [2] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer, New York, 1978.
- [3] Feng Kang, On difference schemes and symplectic geometry, *Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations—Computation of Partial Differential Equations*, Ed. Feng Kang, Science Press, Beijing, 1985, 42–58.
- [4] Feng Kang, Difference schemes for Hamiltonian formalism and symplectic geometry, *J. Comput. Math.*, **4** : 3 (1986), 279–289.
- [5] Feng Kang and Qin Meng-zhao, The symplectic methods for the computation of Hamiltonian equations, *Proc. of 1st Chinese Conf. on Numerical Methods of PDE's*, March 1986, Shanghai, *Lecture Notes in Mathematics*, No. 1297, 1–37, ed. Zhu You-lan and Gu Ben-yu, Springer, Berlin, 1987.
- [6] Feng Kang, Wu Hua-mo, Qin Meng-zhao and Wang Dao-liu, Construction of canonical difference schemes for Hamiltonian formalism via generating functions, *J. Comput. Math.*, **7** : 1 (1989), 71–96.
- [7] Feng Kang, Wu Hua-mo and Qin Meng-zhao, Symplectic difference schemes for the linear Hamiltonian canonical systems, *J. Comput. Math.*, **8** : 4 (1990), 371–380.
- [8] Ge Zhong and Feng Kang, On the approximation of linear H-systems, *J. Comput. Math.*, **6** : 1 (1988), 88–97.
- [9] P. Hartman, *Ordinary Differential Equations*, John Wiley & Sons, New York, 1964.
- [10] Li Chun-wang and Qin Meng-zhao, A symplectic difference scheme for the infinite dimensional Hamilton system, *J. Comput. Math.*, **6** : 2 (1988), 164–174.
- [11] A. Weinstein, The local structure of Poisson manifolds, *J. Diff. Geometry*, **18** (1983), 523–557.
- [12] Wu Yu-hua, Symplectic transformations and symplectic difference schemes, *Mathematica Numerica Sinica*, **11** (1989), 359–366 (in Chinese); *Chin. J. Num. Math. Appl.*, **12** (1990), 23–31.