SYMPLECTIC DIFFERENCE SCHEMES FOR HAMILTONIAN SYSTEMS IN GENERAL SYMPLECTIC STRUCTURE ①②

一般辛结构下的哈密尔顿系统的辛差分格式

Abstract

We consider the construction of phase flow generating functions and symplectic difference schemes for Hamiltonian systems in general symplectic structure with variable coefficients.

§1 Introduction

The standard symplectic structure w on $\mathbf{R}^{2n}$ is of the form

$$w = \sum_{i<j} J_{ij} dz_i \wedge dz_j, \quad J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}. \tag{1}$$

On such symplectic manifold, the Hamiltonian system has the simplest form

$$\frac{dz}{dt} = J^{-1} \Delta H(z) \tag{2}$$

with the Hamiltonian $H(z)$. The phase flow of the Hamiltonian system (2) preserves the symplectic structure (1). Therefore it preserves phase areas and the phase volume of the phase space. Feng Kang et al. in [2–4] developed a generating function method to construct systematically symplectic difference schemes with arbitrary order of accuracy to approximate the system (2). The transition of such difference schemes from one time-step to the next is a symplectic mapping. So they preserve the symplectic structure. It leads to the preservations of phase areas and the phase volume of the phase space.

Generally, a general symplectic structure on $\mathbf{R}^{2n}$ with variable coefficients

$$w = \sum_{i<j} K_{ij}(z) dz_i \wedge dz_j, \tag{3}$$

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which is a non-degenerate, closed 2-form. In this case, the Hamiltonian system of the form

$$\frac{dz}{dt} = K^{-1}(z)\nabla H(z), \quad K_{ji} = -K_{ij}, \tag{4}$$

where $H(z)$ is the Hamiltonian. As above, the phase flow of the system (4) preserves the symplectic structure (3). In numerical simulation for (4), usual discretization can not preserve the symplectic structure (3). By Darboux's theorem, we can, of course, transform (4) into (2) and then use the method in [2–4]. But (i) it is difficult to find out the transformation, and (ii) it is also interesting to discretize (4) directly such that the transition preserves the symplectic structure (3).

In this paper, we try to construct symplectic difference schemes in same way as in [4]. In [4], the key point is to introduce a linear transformation from the symplectic manifold $(\mathbf{R}^{4n}, \tilde{J}_{4n})$ into the symplectic manifold $(\mathbf{R}^{4n}, J_{4n})$ which transforms the $\tilde{J}_{4n}$-Lagrangian submanifold into J_{4n}-Lagrangian submanifold. Of course the inverse transformation transforms the J_{4n}-Lagrangian submanifolds into the $\tilde{J}_{4n}$-Lagrangian submanifolds. In fact, we can also take nonlinear transformations for the same purpose. This was first noted by Feng Kang and has been used in [5]. For other related developments, see [6–15]. In this paper, we use nonlinear transformations to reach our purpose.

In Section 2, we give the relationship between the $K(z)$-symplectic mappings and the gradient mappings. In Section 3, we consider the generating functions of the phase flow of the Hamiltonian system (4) and the corresponding Hamilton-Jacobi equation. When the Hamiltonian function is analytic, then the generating function can be expanded as a power series in t and its coefficients can be recursively determined. With the aid of such an expression, in Section 4 we give a systematic method to construct $K(z)$-symplectic difference schemes with arbitrary order of accuracy.

We shall only consider the local case throughout the paper.

§2 Generating Functions for $K(z)$-Symplectic Mappings

Let $\mathbf{R}^{2n}$ be a $2n$-dimensional real space. The elements of $\mathbf{R}^{2n}$ are $2n$-dimensional column vectors $z = (z_1, \cdots, z_n, z_{n+1}, \cdots, z_{2n})^T$. The superscript T represents the matrix transpose.

A symplectic form w on $\mathbf{R}^{2n}$ is a non-degenerate, closed 2-form, defined by

$$w = \frac{1}{2}\sum_{i,j=1}^{2n} K_{ij}(z) dz_i \wedge dz_j. \tag{5}$$

Denote the entries of $K(z)$ by $K_{ij}(z)$, $i, j = 1, \cdots, 2n$. Then $K(z)$ is anti-symmetric. The non-degeneracy and closedness of w imply that $\det K(z) \neq 0$ and $K_{ij}(z)$ is subject to the condition

$$\frac{\partial K_{ij}(z)}{\partial z_l} + \frac{\partial K_{jl}(z)}{\partial z_i} + \frac{\partial K_{li}(z)}{\partial z_j} = 0, \qquad i, j, l = 1, \cdots, 2n. \tag{6}$$

From now on, we always identify the symplectic form w with $K(z)$.

Denote

$$J_{4n} = \begin{bmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{bmatrix}, \quad \tilde{K}(\hat{z}, z) = \begin{bmatrix} K(\hat{z}) & 0 \\ 0 & -K(z) \end{bmatrix}.$$

Evidently they define two symplectic structures on $\mathbf{R}^{4n}$:

$$\Omega = \sum_{i=1}^{2n} dw_i \wedge dw_{2n+i}, \quad \tilde{\Omega} = \frac{1}{2}\sum_{i,j=1}^{2n} (k_{ij}(\hat{z})d\hat{z}_i \wedge d\hat{z}_j - k_{ij}(z)dz_i \wedge dz_j).$$

A $2n$-dimensional submanifold $L \subset \mathbf{R}^{4n}$ is a J_{4n}-and $\tilde{K}(\hat{z}, z)$-Lagrangian submanifold if $i_L^*\Omega = 0$ and $i_L^*\tilde{\Omega} = 0$, where $i_L : L \to \mathbf{R}^{4n}$ is the inclusion. Suppose that in local coordinates L has the expression

$$L = \left\{ \begin{pmatrix} \hat{z} \\ z \end{pmatrix} \in \mathbf{R}^{4n} \mid z = z(x),\ \hat{z} = \hat{z}(x),\ x \in U \subset \mathbf{R}^{2n},\ \text{open set} \right\}.$$

Then L is a J_{4n}-Lagrangian submanifold if and only if

$$(T_x L)^T J_{4n} T_x L = 0,$$

i.e.,

$$(\hat{z}_x^T(x), z_x^T(x)) \begin{bmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{bmatrix} \begin{pmatrix} \hat{z}_x(x) \\ z_x(x) \end{pmatrix} = \hat{z}_x^T(x) z_x(x) - z_x^T(x)\hat{z}_x(x) = 0,$$

where $T_x L$ is the tangent space to L at x. L is a $\tilde{K}(\hat{z}, z)$-Lagrangian submanifold if and only if

$$(T_x L)^T \tilde{K}(\hat{z}(x), z(x)) T_x L = 0,$$

i.e.,

$$(\hat{z}_x^T(x), z_x^T(x)) \begin{bmatrix} K(\hat{z}(x)) & 0 \\ 0 & -K(z(x)) \end{bmatrix} \begin{pmatrix} \hat{z}_x(x) \\ z_x(x) \end{pmatrix}$$
$$= \hat{z}_x^T(x) K(\hat{z}(x))\hat{z}_x(x) - z_x^T(x) K(z(x)) z_x(x) = 0.$$

A smooth mapping $g : z \to \hat{z} = g(z)$ from $\mathbf{R}^{2n}$ to itself is called $K(z)$-symplectic if its Jacobian $M(z) = g_z(z)$ satisfies

$$M^T(z) K(g(z)) M(z) = K(z). \tag{7}$$

Therefore its graph

$$\Gamma_g = \left\{ \begin{bmatrix} \hat{z} \\ z \end{bmatrix} \in \mathbf{R}^{4n} | \hat{z} = g(z), z \in \mathbf{R}^{2n} \right\}$$

is a $\tilde{K}(\hat{z}, z)$-Lagrangian submanifold for

$$(T_z\Gamma_g)^T\ \tilde{K}(g(z), z) T_z \Gamma_g = (M^T(z), I) \begin{bmatrix} K(g(z)) & 0 \\ 0 & -K(z) \end{bmatrix} \begin{pmatrix} M(z) \\ I \end{pmatrix}$$
$$= M^T(z) K(g(z)) M(z) - K(z) = 0.$$

Similarly, let $w \to \hat{w} = f(w)$ be a gradient mapping from $\mathbf{R}^{2n}$ to itself. Then the graph of f

$$\Gamma_f = \left\{ \begin{bmatrix} \hat{w} \\ w \end{bmatrix} \in \mathbf{R}^{4n} | \hat{w} = g(w), \quad w \in \mathbf{R}^{2n} \right\}$$

is a J_{4n}-Lagrangian submanifold[4].

Define nonlinear transformation from $\mathbf{R}^{4n}$ to itself

$$\alpha : \begin{pmatrix} \hat{z} \\ z \end{pmatrix} \to \begin{pmatrix} \hat{w} \\ w \end{pmatrix} = \alpha \begin{pmatrix} \hat{z} \\ z \end{pmatrix}, \quad \alpha^{-1} : \begin{pmatrix} \hat{w} \\ w \end{pmatrix} \to \begin{pmatrix} \hat{z} \\ z \end{pmatrix} = \alpha \begin{pmatrix} \hat{w} \\ w \end{pmatrix} \tag{8}$$

i.e.,

$$\begin{aligned} \hat{w} &= \alpha_1(\hat{z}, z), \qquad & \hat{z} &= \alpha^1(\hat{w}, w), \\ w &= \alpha_2(\hat{z}, z), \qquad & z &= \alpha^2(\hat{w}, w). \end{aligned} \tag{9}$$

Denote

$$\alpha_*(\hat{z}, z) = \begin{bmatrix} \dfrac{\partial \hat{w}}{\partial \hat{z}} & \dfrac{\partial \hat{w}}{\partial z} \\ \dfrac{\partial w}{\partial \hat{z}} & \dfrac{\partial w}{\partial z} \end{bmatrix} = \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix},$$

$$\alpha_*^{-1}(\hat{w}, w) = \begin{bmatrix} \dfrac{\partial \hat{z}}{\partial \hat{w}} & \dfrac{\partial \hat{z}}{\partial w} \\ \dfrac{\partial z}{\partial \hat{w}} & \dfrac{\partial z}{\partial w} \end{bmatrix} = \begin{bmatrix} A^\alpha & B^\alpha \\ C^\alpha & D^\alpha \end{bmatrix},$$

where α_* is the Jacobian of α.

Let α be a diffeomorphism from $\mathbf{R}^{4n}$ to itself and satisfy the condition

$$\alpha_*^T J_{4n} \alpha_* = \tilde{K}(\hat{z}, z), \tag{10}$$

i.e.,

$$\begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix}^T \begin{bmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{bmatrix} \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix} = \begin{bmatrix} K(\hat{z}) & 0 \\ 0 & -K(z) \end{bmatrix}. \tag{11}$$

It follows from (11) that

$$\begin{aligned} A^\alpha &= -K^{-1}(\hat{z}) C_\alpha^T, \quad & B^\alpha &= K^{-1}(\hat{z}) A_\alpha^T, \\ C^\alpha &= K^{-1}(z) D_\alpha^T, \quad & D^\alpha &= -K^{-1}(z) B_\alpha^T. \end{aligned} \tag{12}$$

By Darboux's theorem, such diffeomorphism exists, at least locally.

Theorem 1. *Let α be a diffeomorphism of $\mathbf{R}^{4n}$ satisfying* (10) *as above. Then α carries every $\tilde{K}$-Lagrangian submanifold into a J_{4n}-Lagrangian submanifold and conversely α^{-1} carries every J_{4n}-Lagrangian submanifold into a $\tilde{K}$-Lagrangian submanifold.*

Proof. Let L be a $\tilde{K}$-Lagrangian submanifold. The image of L under α is $\alpha(L)$. Its tangent space is

$$T_*(\alpha(L)) = \alpha_* \cdot T_* L.$$

So by (10),

$$T_*(\alpha(L))^T J_{4n} T_*(\alpha(L)) = (T_* L)^T \alpha_*^T J_{4n} \alpha_* T_* L = (T_* L)^T \tilde{K} T_* L = 0.$$

The converse is similar.

We now introduce a lemma in [4].

Lemma 2. *Let $\left[\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right] \in \mathrm{GL}(4n)$. Denote $\left[\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right]^{-1} = \left[\begin{smallmatrix} A_1 & B_1 \\ C_1 & D_1 \end{smallmatrix}\right]$. Define a linear fractional transformation as follows.*

$$\sigma : \begin{array}{l} \mathbf{M}(2n) \to \mathbf{M}(2n), \\ M \to N = \sigma(M) = (AM + B)(CM + D)^{-1} \end{array} \tag{13}$$

under the transversality condition

$$|CM + D| \neq 0.$$

Then the following four conditions are equivalent mutually:

$$|CM + D| \neq 0, \tag{14}$$

$$|MC_1 - A_1| \neq 0, \tag{15}$$

$$|C_1N + D_1| \neq 0, \tag{16}$$

$$|NC - A| \neq 0. \tag{17}$$

The linear fractional transformation defined by (13) *can be represented as*

$$N = \sigma(M) = (MC_1 - A_1)^{-1}(B_1 - MD_1). \tag{18}$$

In this case, the inverse transformation must exist and can be represented as

$$M = \sigma^{-1}(N) = \begin{cases} (A_1N + B_1)(C_1N + D_1)^{-1}, & (19) \\ (NC - A)^{-1}(B - ND). & (20) \end{cases}$$

Theorem 3. *Let α be defined as above. Let $z \to \hat{z} = g(z)$ be a $K(z)$-symplectic mapping in (some neighborhood of) $\mathbf{R}^{2n}$ with Jacobian $g_z(z) = M(z)$. If (in some neighborhood of $\mathbf{R}^{2n}$) M satisfies the transversality condition*

$$|C_\alpha(g(z), z)M(z) + D_\alpha(g(z), z)| \neq 0, \tag{21}$$

then there exists uniquely in (some neighborhood of) $\mathbf{R}^{2n}$ *a gradient mapping $w \to \hat{w} = f(w)$ with Jacobian $f_w(w) = N(w)$ and a scalar function-generating function-$\phi(w)$ such that*

$$f(w) = \nabla\phi(w), \tag{22}$$

$$\alpha_1(g(z), z) = f(\alpha_2(g(z), z)) = \nabla\phi(\alpha_2(g(z), z)), \quad \textit{identically in } z, \tag{23}$$

$$N = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}, \quad M = (A^\alpha N + B^\alpha)(C^\alpha N + D^\alpha)^{-1}. \tag{24}$$

Proof. The image of the graph Γ_g under α is

$$\alpha(\Gamma_g) = \left\{ \begin{pmatrix} \hat{w} \\ w \end{pmatrix} \in \mathbf{R}^{4n} | \hat{w} = \alpha_1(g(z), z), \quad w = \alpha_2(g(z), z) \right\}.$$

By (21),

$$\frac{\partial w}{\partial z} = \frac{\partial \alpha_2}{\partial \hat{z}} \cdot \frac{\partial \hat{z}}{\partial z} + \frac{\partial \alpha_2}{\partial z} = C_\alpha M + D_\alpha$$

is nonsingular. So by the inverse function theorem, $w = \alpha_2(g(z), z)$ is invertible. The inverse function is denoted by $z = z(w)$. Set

$$\hat{w} = f(w) = \alpha_1(g(z), z)|_{z=z(w)}. \tag{25}$$

Then

$$N = \frac{\partial f}{\partial w} = \Big(\frac{\partial \alpha_1}{\partial \hat{z}}\frac{\partial g}{\partial z} + \frac{\partial \alpha_1}{\partial z}\Big)\Big(\frac{\partial \alpha_2}{\partial \hat{z}}\frac{\partial g}{\partial z} + \frac{\partial \alpha_2}{\partial z}\Big)^{-1} = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}.$$

Notice that the image $\alpha(\Gamma_g)$ is a J_{4n}-Lagrangian submanifold. That is, the tangent space $T_*(\alpha(\Gamma_g))$ is J_{4n}-Lagrangian. It means

$$((A_\alpha M + B_\alpha)^T, (C_\alpha M + D_\alpha)^T) \begin{pmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{pmatrix} \begin{pmatrix} A_\alpha M + B_\alpha \\ C_\alpha M + D_\alpha \end{pmatrix}$$

$$= (A_\alpha M + B_\alpha)^T(C_\alpha M + D_\alpha) - (C_\alpha M + D_\alpha)^T(A_\alpha M + B_\alpha) = 0,$$

i.e.,

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

It shows that $\hat{w} = f(w)$ is a gradient mapping. By the Poincare lemma, there is a scalar function $\phi(w)$ such that

$$f(w) = \nabla \phi(w).$$

That is (22). (23) follows from the construction of $f(w)$ and $z(w)$. In fact by (25),

$$f(w) = \alpha_1(g(z), z) \circ z(w). \tag{26}$$

Since $z(w) \circ \alpha_2(g(z), z) \equiv z$, substituting $w = \alpha_2(g(z), z)$ into (26), we get (23) at once.

Proposition 4. *$f(w)$ obtained in Theorem 3 is also the solution of the following implicit equation*

$$\alpha^1(f(w), w) = g(\alpha^2(f(w), w)). \tag{27}$$

Theorem 5. *Let α be as in Theorem 3. Let $w \to \hat{w} = f(w)$ be a gradient mapping in (some neighborhood of) $\mathbf{R}^{2n}$ with Jacobian $f_w(w) = N(w)$. If in some neighborhood of $\mathbf{R}^{2n}, N$ satisfies the condition*

$$|C^\alpha(f(w), w)N(w) + D^\alpha(f(w), w)| \neq 0, \tag{28}$$

then there exists uniquely, in some neighborhood of $\mathbf{R}^{2n}$, a $K(z)$-symplectic mapping $z \to \hat{z} = g(z)$ with Jacobian $g_z(z) = M(z)$ such that

$$\alpha^1(f(w), w) = g(\alpha^2(f(w), w)), \tag{29}$$

$$M = (A^\alpha N + B^\alpha)(C^\alpha N + D^\alpha)^{-1}, \quad N = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}. \tag{30}$$

Similarly to Proposition 4, $g(z)$ is the solution of the implicit equation

$$\alpha_1(g(z), z) = f(\alpha_2(g(z), z)). \tag{31}$$

The proof is similar to that of Theorem 3 and is omitted here.

§3 Generating Functions for the Phase Flow of Hamiltonian Systems

We now consider the general Hamiltonian system

$$\frac{dz}{dt} = K^{-1}(z)\nabla H(z), \quad z \in \mathbf{R}^{2n}, \tag{32}$$

with the Hamiltonian $H(z)$. Its phase flow is denoted by $g^t(z) = g(z,t) = g_H(z,t)$. $g(z,t)$ is a one-parameter group of $K(z)$-symplectic mappings, at least local in z and t, 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 condition, then $z(t) = g^t(z_0) = g(z_0, t) = g_H(z_0, t)$ is the solution of (32) with the initial value z_0; in addition

$$g_z^T(z,t)K(g(z,t))g_z(z,t) = K(z), \quad \forall t \in \mathbf{R}. \tag{33}$$

Theorem 6. *Let α be as above and $z \to \hat{z} = g(z,t)$ be the phase flow of the Hamiltonian system* (32) *with Jacobian $M(z,t) = g_z(z,t)$. If at some point z_0,*

$$|C_\alpha(z_0, z_0) + D_\alpha(z_0, z_0)| \neq 0, \tag{34}$$

then there exists, for sufficiently small $|t|$ and in some neighborhood of $\mathbf{R}^{2n}$, a time-dependent gradient mapping $w \to \hat{w} = f(w,t)$ with Jacobian $N(w,t) = f_w(w,t)$ symmetric and a time-dependent generating function $\phi_{\alpha,H}(w,t) = \phi(w,t)$ such that

$$f(w,t) = \nabla\phi(w,t), \tag{35}$$

$$\frac{\partial\phi(w,t)}{\partial t} = -H(\hat{z}(\nabla\phi(w,t), w)) = -\hat{H}(\nabla\phi(w,t), w), \tag{36}$$

$$\alpha_1(g(z,t), z) = \nabla\phi(\alpha_2(g(z,t), z), t), \text{ identically in some neighborhood of } z_0, \tag{37}$$

$$N = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}, \quad M = (A^\alpha N + B^\alpha)(C^\alpha N + D^\alpha)^{-1}, \tag{38}$$

where $\hat{H}(\hat{w}, w) = H(\hat{z}) \circ \alpha^1(\hat{w}, w)$.

(36) is also called the Hamilton-Jacobi equation for the Hamiltonian system (32) and the nonlinear transformation α.

Theorem 7. *Let $H(z)$ and α be analytic. Then the generating function $\phi_{\alpha,H}(w,t) = \phi(w,t)$ can be expanded as a convergent power series in t for sufficiently small $|\,t\,|$*

$$\phi(w,t) = \sum_{k=0}^{\infty} \phi^{(k)}(w)t^k, \tag{39}$$

and $\phi^{(k)}(w), k \geq 0$, can be recursively determined by the following equations

$$\phi^{(0)}(w) = \int f(w,0)dw + \text{ const. }, \tag{40}$$

$$\phi^{(1)}(w) = -\hat{H}(f(w,0), w), \tag{41}$$

$$\phi^{(k+1)}(w) = -\frac{1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{\substack{k_1+\cdots k_m = k\\ k_i \geq 1}} D^m_{\hat{w}}\hat{H}(\nabla\phi^{(k_1)}(w), \cdots, \nabla\phi^{(k_m)}(w)), \quad k \geq 1, \tag{42}$$

where the integral of (40) *is taken on the curve connecting w and $w_0 = \alpha_2(z_0, z_0)$, $\hat{H}(\hat{w}, w) = H \circ \alpha^1(\hat{w}, w)$. Here we have used the notation of multi-linear forms,* e.g.,

$$\begin{aligned} &D^m_{\hat{w}}\hat{H}(f(w,0), w)(\nabla\phi^{(k_1)}, \cdots, \nabla\phi^{(k_m)}) \\ &\quad = \sum_{i_1,\cdots,i_m=1}^{2n} \hat{H}_{\hat{w}_{i_1},\cdots,\hat{w}_{i_m}}(f(w,0), w)(\nabla\phi^{(k_1)})_{i_1}\cdots(\nabla\phi^{(k_m)})_{i_m}. \end{aligned}$$

$(\nabla\phi^{(k_l)})_{i_l}$ is the i_l-th component of the column vector $\nabla\phi^{(k_l)}$.

Proof. Differentiating (39) with respect to w and t, we get

$$\nabla\phi(w,t) = \sum_{k=0}^{\infty}\nabla\phi^{(k)}(w)t^k, \tag{43}$$

$$\frac{\partial\phi(w,t)}{\partial t} = \sum_{k=0}^{\infty}(k+1)t^k\phi^{(k+1)}(w). \tag{44}$$

By (35),

$$\nabla\phi^{(0)}(w) = \nabla\phi(w,0) = f(w,0).$$

So we can take $\phi^{(0)}(w) = \int_{w_0}^{w} f(w,0)dw$. Expanding $\hat{H}(f(w,t),w)$ in $(f(w,0),w)$ and gathering the terms with the same order, we get

$$\begin{aligned}\hat{H}(\nabla\phi(w,t),w) &= \hat{H}\Big(f(w,0)+\sum_{k=1}^{\infty} t^k \nabla\phi^{(k)}(w), w\Big)\\ &= \hat{H}(f(w,0),w) + \sum_{k=1}^{\infty} t^k \sum_{m=1}^{k} \frac{1}{m!} \sum_{\substack{k_1+\cdots+k_m=k\\ k_i\geq 1}} D_{\hat{w}}^m \hat{H}(f(w,0),w)(\nabla\phi^{(k_1)},\cdots,\nabla\phi^{(k_m)}).\end{aligned}$$

Using the Hamilton-Jacobi equation (36) and comparing with (44), we get (41) and (42).

§4 $K(z)$-Symplectic Difference Schemes

In the previous section, we have established the relationship between the phase flow $g(z,t)$ and the generating function $\phi(w,t)$. And when H and α are analytic, the generating function has a power series expansion. With the aid of the expansion, we can systematically construct $K(z)$-symplectic difference schemes, i.e., the transition of such difference schemes from one time-step to the next is $K(z)$-symplectic.

Theorem 8. *Let α be given as in Theorem 7 and $H(z)$ analytic. For sufficiently small $\tau > 0$ as the time-step. Take*

$$\psi^{(m)}(w,\tau) = \sum_{i=0}^{m} \phi^{(i)}(w)\tau^i, \quad m = 1,2,\cdots, \tag{45}$$

where $\phi^{(i)}(w)$ are determined by (40), (41) and (42). Then $\psi^{(m)}(w,\tau)$ defines a $K(z)$-symplectic difference scheme $z = z^k \to z^{k+1} = \hat{z}$,

$$\alpha_1(z^{k+1},z^k) = \nabla_w \psi^{(m)}(\alpha_2(z^{k+1},z^k),\tau) \tag{46}$$

of m-th order of accuracy.

Proof. By hypothesis,

$$|C(z_0,z_0) + D(z_0,z_0)| \neq 0.$$

So by Lemma 2, $|C^\alpha N + D^\alpha| \neq 0$ where $N = (A_\alpha + B_\alpha)(C_\alpha + D_\alpha)^{-1} = \phi_{ww}(w_0,0) = \psi_{ww}^{(m)}(w_0,0)$, the Hessians of $\phi(w_0,0)$ and $\psi^{(m)}(w_0,0)$ respectively, and $w_0 = \alpha_2(z_0,z_0)$. Thus for sufficiently small τ and in some neighborhood of w_0, $|C^\alpha N^{(m)}(w,\tau) + D^\alpha| \neq 0$, where $N^{(m)}(w,\tau) = \psi_{ww}^{(m)}(w,\tau)$. By Theorem 5, $\nabla\psi^{(m)}(w,\tau)$ defines a time-dependent $K(z)$-symplectic mapping which is expressed by (31). It means that (46) is a $K(z)$-symplectic difference scheme.

Since $\psi^{(m)}(w,\tau)$ is the m-th approximate to $\phi(w,\tau)$, so is $f^{(m)}(w,\tau) = \nabla\psi^{(m)}(w,\tau)$ to $f(w,t)$. It follows that the difference scheme (46) is of m-th order of accuracy.

Example. Take $n = 1$ and

$$K = \begin{bmatrix} 0 & p \\ -p & 0 \end{bmatrix}, \quad H(p,q) = \frac{1}{2}(p^2 - q^2). \tag{47}$$

The corresponding Hamiltonian system is

$$\frac{dz}{dt} = K^{-1}\nabla H = \begin{bmatrix} 0 & -p^{-1} \\ p^{-1} & 0 \end{bmatrix} \begin{bmatrix} p \\ -q \end{bmatrix} = \begin{bmatrix} p^{-1}q \\ 1 \end{bmatrix},$$

i.e.,

$$\frac{dp}{dt} = p^{-1}q, \quad \frac{dq}{dt} = 1. \tag{48}$$

The phase flow $\hat{p} = g_1(p,q,t), \hat{q} = g_2(p,q,t)$ is

$$\hat{p}^2 = p^2 + 2qt + t^2, \quad \hat{q} = q + t. \tag{49}$$

Take the transformation α as

$$\begin{bmatrix} \hat{z} \\ z \end{bmatrix} \to \begin{bmatrix} \hat{w} \\ w \end{bmatrix} = \alpha \begin{bmatrix} \hat{z} \\ z \end{bmatrix}: \quad \begin{array}{l} \hat{P} = \frac{1}{4}\hat{p}^2 + \hat{q} - q, \quad \hat{Q} = \frac{1}{4}\hat{p}^2 + \hat{q} + q, \\ P = -\frac{1}{4}p^2 + \hat{q} - q, \quad Q = \frac{1}{4}p^2 + \hat{q} + q, \end{array} \tag{50}$$

where $\hat{w} = (\hat{P},\hat{Q})^T, w = (P,Q)^T$. Its inverse transformation α^{-1} is

$$\begin{bmatrix} \hat{w} \\ w \end{bmatrix} \to \begin{bmatrix} \hat{z} \\ z \end{bmatrix} = \alpha^{-1} \begin{bmatrix} \hat{w} \\ w \end{bmatrix}: \quad \begin{array}{l} \hat{p}^2 = 2(\hat{P} + \hat{Q} - P - Q), \quad \hat{q} = \frac{1}{2}(P+Q), \\ p^2 = 2(\hat{P} - \hat{Q} - P + Q), \quad q = \frac{1}{2}(\hat{Q} - \hat{P}). \end{array} \tag{51}$$

The Jacobian of α is

$$\alpha_* = \begin{bmatrix} \frac{2}{3}\hat{p} & 1 & \frac{1}{2}p & -1 \\ \hat{p} & 1 & 0 & 1 \\ \hat{p} & 1 & 0 & -1 \\ \frac{1}{2}\hat{p} & 1 & \frac{1}{2}p & 1 \end{bmatrix}. \tag{52}$$

By direct computation, we can immediately know that α satisfies (10), α also satisfies (34) as

$$|C_\alpha + D_\alpha| = -\frac{1}{2}p \neq 0 \quad \text{for } p \neq 0.$$

It follows from (50) that

$$\hat{H}(\hat{P},\hat{Q},P,Q) = \hat{P} - \hat{Q} - P + Q - \frac{1}{8}(\hat{P} - \hat{Q})^2, \quad \nabla\phi^{(0)}(w) = f(w,0) = \begin{pmatrix} -P \\ Q \end{pmatrix}.$$

So $\phi^{(0)}(P,Q) = \frac{1}{2}(Q^2 - P^2)$,

$$\phi^{(1)}(P,Q) = -\hat{H}(\nabla\phi^{(0)}(P,Q),P,Q) = 2P + \frac{1}{8}(P+Q)^2,$$

$$\nabla\phi^{(1)}(P,Q) = \begin{pmatrix} 2 + \frac{1}{4}(P+Q) \\ \frac{1}{4}(P+Q) \end{pmatrix}.$$

The first-order scheme is

$$\frac{1}{4}(p^{k+1})^2 + q^{k+1} - q^k = \frac{1}{4}(p^k)^2 - q^{k+1} + q^k + \tau(2 + \frac{1}{4}(P+Q)),$$
$$\frac{1}{4}(p^{k+1})^2 + q^{k+1} + q^k = \frac{1}{4}(p^k)^2 + q^{k+1} + q^k + \frac{\tau}{4}(P+Q),$$

i.e.,

$$(p^{k+1})^2 = (p^k)^2 + 2\tau q^{k+1}, \quad q^{k+1} = q^k + \tau. \tag{53}$$

Referring to (49), we have seen that (53) is indeed its first order approximation. Its transition matrix is $\begin{bmatrix} (p^{k+1})^{-1}p^k & \tau(p^{k+1})^{-1} \\ 0 & 1 \end{bmatrix}$. Direct computation gives that it is $K(z)$-symplectic.

Discussion. The difficulty of this method is to find out nonlinear transformations α satisfying (10). It in fact is to realize Darboux's theorem in $4n$ dimensions. It seems as difficult as to directly transform $K(z)$ into J_{2n}. But in our case, we have more parameters to select. Hence we hope the problem will be easier than the original one.

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