

A SYMPLECTIC DIFFERENCE SCHEME FOR THE INFINITE DIMENSIONAL HAMILTON SYSTEM^{*1)}

LI CHUN-WANG (李春旺) QIN MENG-ZHAO (秦孟兆)

(Computing Center, Academia Sinica, Beijing, China)

Abstract

Symplectic geometry plays a very important role in the research and development of Hamilton mechanics, which has been attracting increasing interest^{[1],[4]}. Consequently, the study of the numerical methods with symplectic nature becomes a necessity.

Feng Kang introduced in [5] the concept of symplectic scheme of the Hamilton equation, and used the generating function methods to construct the symplectic scheme with arbitrarily precise order in the finite dimensional case, which can be applied to the ordinary differential equation, such as the two body problem^[1]. He also widened the traditional concept of generating function.

The authors in this paper use the method in the infinite dimensional case following [6], that is, using generating function methods to construct the difference scheme of arbitrary order of accuracy for partial differential equations which can be written as Hamilton system in the Banach space.

First, the Hamilton equation of infinite dimensions is briefly reviewed. Then, we introduce symplectic manifold and symplectic structure in the Banach space. Thirdly, Hamilton vector field and its flow are discussed. Fourthly, we put forward the generating functional and symplectic difference scheme. Fifthly, the application of this result in various Banach spaces, such as Toda lattice equation, wave equation, compressible flow equation and electromagnetic flow equation, is described.

§ 1. An Infinite Dimensional Hamilton Equation

Suppose B is a reflexive Banach space and B^* its dual space. E^n is an Euclidean space and n its dimension. The generalized coordinate in the Banach space is function $q(r, t): E^n \times R \rightarrow B, \forall t \in R$. We have $q(r, t) \in B$. B corresponds to the configuration space. We introduce $p(r, t)$, the generalized moment, where $r \in E^n, t \in R$. For $\forall t \in R, P(r, t) \in B^*$. $B \times B^*$ constitutes a phase space.

Let H be an energy function in Hamilton mechanics. We have the Hamilton equation in $B \times B^*$ ^[2]

$$\begin{aligned} \frac{dp}{dt} &= -\frac{\delta H}{\delta q}(p, q, t), \\ \frac{dq}{dt} &= \frac{\delta H}{\delta p}(p, q, t). \end{aligned} \quad (1)$$

Let T be a mapping: $B \times B^* \rightarrow B \times B^*$. We call T the canonical transformation, if in $D \subset B \times B^*$, where D is an open set, we have

$$\int p dq - \int P dQ = dS(p, q, t), \quad (2)$$

where $\begin{pmatrix} P \\ Q \end{pmatrix} = T \begin{pmatrix} p \\ q \end{pmatrix}$ and S is a function in $B \times B^*$, which has Frecht derivative in D .

* Received December 10, 1986.

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

Let

$$K(P, Q, t) = H + \frac{\partial S}{\partial t} + \int P \frac{dQ}{dt} d_\mu |_{(p, q) \rightarrow (P, Q)} \tag{3}$$

Considering (2), we have

$$\int p dq - H dt = \int P dQ - K dt + dS. \tag{4}$$

In the new variable, the Hamilton equation has the form:

$$\begin{aligned} \dot{P} &= -\frac{\delta K}{\delta Q}, \\ \dot{Q} &= \frac{\delta K}{\delta P}. \end{aligned} \tag{5}$$

Suppose the moment P can be represented in q and Q . The functional $S_1 = S(q, P(q, Q, t), t)$ is called generating functional, when $\frac{\delta^2 S_1}{\delta q \delta Q}$ is nonsingular.

From (4), we have

$$\begin{aligned} p &= \frac{\delta}{\delta q} S_1(q, Q, t) \\ P &= -\frac{\delta}{\delta Q} S_1(q, Q, t). \end{aligned} \tag{6}$$

Example. Let $S_1(q, Q) = \int_D q \cdot Q d_\mu$. Then

$$\begin{aligned} p &= \frac{+\delta S_1}{\delta q} = Q, \\ P &= \frac{-\delta S_1}{\delta Q} = -q, \end{aligned}$$

$$K(P, Q, t) = H(Q, -P, t).$$

There are other kinds of generating functional: $S_2(p, Q, t)$, $S_3(q, P, t)$ and $S_4(p, P, t)$. For convenience, we give a list below:

G-F	Nonsingular condition	New variable
$S_1(q, Q, t)$	$\frac{\delta^2 S_1}{\delta q \delta Q} \neq 0$	$p = \frac{\delta S_1}{\delta q}(q, Q, t)$ $P = -\frac{\delta S_1}{\delta Q}(q, Q, t)$
$S_2(p, Q, t)$	$\frac{\delta^2 S_2}{\delta p \delta Q} \neq 0$	$q = -\frac{\delta S_2}{\delta p}(p, Q, t)$ $P = -\frac{\delta S_2}{\delta Q}(p, Q, t)$
$S_3(q, P, t)$	$\frac{\delta^2 S_3}{\delta q \delta P} \neq 0$	$p = \frac{\delta S_3}{\delta q}(q, P, t)$ $Q = \frac{\delta S_3}{\delta P}(q, P, t)$
$S_4(p, P, t)$	$\frac{\delta^2 S_4}{\delta p \delta P} \neq 0$	$q = \frac{\delta S_4}{\delta p}(p, P, t)$ $Q = -\frac{\delta S_4}{\delta P}(p, P, t)$

Generating functional S plays a key role and its more general form will be given below.

The infinite dimensional Hamilton-Jacobi equation can be written as

$$\frac{\partial S}{\partial t} + H\left(\frac{\delta S}{\delta q}, q, t\right) = 0. \quad (7)$$

The functional $S(q, t)$ is unknown, and is called the first integral of (7), if S satisfies (7), and $\frac{\delta^2 S}{\delta q \delta Q}$ is nonsingular, where $Q(\tau)$ is an arbitrary function.

From the Jacobi theorem, we know that if the first integral of (7) is solved, then the solution of (1) can be obtained from

$$p = \frac{\delta S}{\delta q}(q, Q, t),$$

$$P = -\frac{\delta S}{\delta Q}(q, Q, t),$$

where $P(\tau)$ and $Q(\tau)$ are functions in E^n .

§ 2. Symplectic Manifold and Its Structure

Let B be a reflexive Banach space. $\varepsilon: B \times B \rightarrow R$ is a continuous bilinear mapping.

Define

$$\varepsilon^b: B \rightarrow B^*,$$

$$\varepsilon^b(e) \cdot f = \varepsilon(e, f).$$

Then ε^b is a linear mapping. We say ε is weakly nondegenerate, if ε^b is an injection. We call ε nondegenerate, if ε^b is a bijection.

Let P be the manifold modelled on B . ω is a 2-form on P , such that:

a) ω is closed: $d\omega = 0$,

b) $\forall x \in P$, $\omega_x: T_x P \times T_x P \rightarrow R$ is nondegenerate.

We call (P, ω) the symplectic manifold and ω the symplectic form.

Theorem 1 (Darboux, Weinstein)^[4]. *Let (P, ω) be symplectic. For $\forall x \in P$, there is a local coordinate of x under which ω is a constant.*

Suppose that M is modelled on B . T^*M is its cotangent bundle. $\tau^*: T^*M \rightarrow M$ is a natural projection. θ is the canonical 1-form on T^*M defined by:

$$\theta(\alpha_m) \cdot W = -\alpha_m \cdot (T\tau^*(W)),$$

where $\alpha_m \in T_m^*M$ and $W \in T_{\alpha_m}(T^*M)$.

In the local chart $U \subset B$, we have

$$\theta(x, \alpha) \cdot (e, \beta) = -(x, \alpha) \cdot (x, e) = -\alpha(e)$$

in which $(x, \alpha) \in U \times B^*$, $(e, \beta) \in B \times B^*$.

The canonical 2-form ω is defined by: $\omega = d\theta$. In local chart:

$$\omega(x, \alpha)[(e_1, \alpha_1), (e_2, \alpha_2)] = \{\alpha_2(e_1) - \alpha_1(e_2)\}.$$

For such ω , we have

Theorem 2. a) ω is the weak symplectic form on $P = T^*M$,

b) ω is symplectic iff B is reflexive.

Proof. See [4].

Let (P, ω) be a symplectic manifold a smooth mapping $P \rightarrow P$ is called

canonical or symplectic if

$$f^*\omega = \omega.$$

§ 3. The Hamilton Vector Field and the Hamilton System

Let (P, ω) be a symplectic manifold. $H: P \rightarrow R$ is a given smooth function. $\phi: TP \rightarrow T^*P$ is the diffeomorphism induced from ω :

$$\phi(x) \cdot \alpha = \omega(x, \alpha),$$

where $x, \alpha \in TP$.

$\phi^{-1}dH$ is called the Hamilton vector field with energy H . If $\phi^{-1}dH$ is denoted by X_H , then X_H is defined by

$$\omega_x(X_H(x), V) = dH_x \cdot V,$$

where $x \in P, V \in T_xP$, i.e. $i_{X_H}\omega = dH$.

Theorem 3. *Let $c(t)$ be the integral curve of X_H . Then $H(c(t))$ is constant for any t .*

Proof. From the chain law, we have

$$H(c(t)) = dH_{c(t)} \cdot c'(t) = \omega_{c(t)}(X_H(t), X_H(t)) = 0.$$

In the general case, suppose that M is modelled on $B, P = T^*M$ and H is a smooth function on P . Then, locally

$$X_H = (D_2H, -D_1H)$$

in which H maps from $U \times B^*$ to R . So $D_2H(x, \alpha): B^* \rightarrow R \in B^{**} \approx B \cdot D_1H \in B^*$.

If we denote the element of TP by (x, α) , then in the local chart, X_H can be written as $\left(\frac{\delta H}{\delta \alpha}, -\frac{\delta H}{\delta x}\right)$.

The Hamilton system has the form

$$\frac{dZ}{dt} = X_H(Z).$$

Theorem 4. *Suppose (P, ω) is symplectic. $H: P \rightarrow R$. Let F_t be the flow of X_H . Then for any t, F_t is symplectic.*

$$F_t^*\omega = \omega.$$

Proof.

$$\frac{d}{dt} F_t^*\omega = F_t^*L_{X_H}\omega = F_t^*(di_{X_H} + i_{X_H}d)\omega = F_t^*d^2H(x) + F_t^*i_{X_H}d\omega = 0.$$

If we define the operator J as

$$J: B \times B^* \rightarrow (B \times B^*)^* = B^* \times B,$$

$$J(x, \alpha) = (-\alpha, x),$$

then it is easy to prove that $J \in GL((B \times B^*), (B \times B^*)^*)$.

$$J = \begin{pmatrix} 0 & -I_{B^*} \\ I_B & 0 \end{pmatrix}, \quad J^{-1} = \begin{pmatrix} 0 & I_B \\ -I_{B^*} & 0 \end{pmatrix}.$$

$I_B: B \rightarrow B$ identity operator,

$I_{B^*}: B^* \rightarrow B^*$ identity operator.

We write them briefly as I .

Then the Hamilton System has the form

$$\frac{dZ}{dt} = J^{-1}H_z,$$

where $H_z = (D_1H, D_2H)$.

Canonical 2-form:

$$\omega(\alpha_1, \alpha_2) = \langle J\alpha_1, \alpha_2 \rangle,$$

where in the local chart at $P = T^*M$, $\alpha_1, \alpha_2 \in B \times B^*$, and \langle, \rangle is a dual product.

Because the Hamilton System in the local chart of the manifold has the same form as in the phase space, in the subsequent sections we discuss only $B \times B^*$ and use the theorems in the symplectic manifold, if we regard $B \times B^*$ as a symplectic manifold with natural symplectic structure.

§ 4. Generating Functional and Difference Schemes

Suppose $f: B \times B^* \rightarrow (B \times B^*)^*$,

$$\hat{W} = f(W).$$

We call f a gradient transformation, or potential operator, if there is $\phi: B \times B^* \rightarrow R$ such that

$$\hat{W} = \phi_w(W).$$

Let $g: B \times B^* \rightarrow B \times B^*$ be a canonical transformation

$$Z \rightarrow \hat{Z} = g(Z),$$

$T \in GL((B \times B^*) \times (B \times B^*), (B \times B^*)^* \times (B \times B^*)^*)$,

$$T = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

in which $A, B \in GL(B \times B^*, (B \times B^*)^*)$, $C, D \in GL((B \times B^*)^*, B \times B^*)$.

Let

$$\hat{W} = A\hat{Z} + BZ,$$

$$W = C\hat{Z} + DZ.$$

Then

$$\begin{pmatrix} \hat{W}_w \\ I \end{pmatrix} = T \begin{pmatrix} \hat{Z}_z \\ I \end{pmatrix} Z_w.$$

Lemma 1 ^[9]. *If the following conditions are satisfied:*

1. F is an operator: $B \rightarrow B^*$,

2. F has Gateaux differentiation $DF(x, h)$ in D : $|x - x_0| < r$,

3. functional $(DF(x, h_1), h_2)$ is continuous in D ,

then F is a potential operator iff $(DF(x, h_1), h_2)$ is symmetric for any $x \in D$:

$$(DF(x, h_1), h_2) = (DF(x, h_2), h_1), \quad \forall h_1, h_2 \in E.$$

Because $\hat{Z} = g(Z)$ is symplectic, we get

$$\left\langle \begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix} \cdot \begin{pmatrix} \hat{Z}_{z_1} \\ I \end{pmatrix}, \begin{pmatrix} \hat{Z}_{z_2} \\ I \end{pmatrix} \right\rangle = 0,$$

where $\begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix}$ is a mapping:

$$(B \times B^*) \times (B \times B^*) \rightarrow (B \times B^*)^* \times (B \times B^*)^*.$$

If $\hat{W} = f(W)$ is a gradient transformation, from Lemma 1, we get

$$\left\langle \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \hat{W}_w \\ I \end{pmatrix}, \begin{pmatrix} \hat{W}_w \\ I \end{pmatrix} \right\rangle = 0.$$

For the condition of T , we have

Theorem 5. T carries every symplectic transformation into a gradient transformation, if:

$$T^* \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} T = \mu \begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix}$$

i.e.,

$$A_1 = -\mu^{-1} J^{-1} O^*, \quad B_1 = \mu^{-1} J^{-1} A^*,$$

$$C_1 = \mu^{-1} J^{-1} A^*, \quad D_1 = -\mu^{-1} J^{-1} B^*,$$

$$T = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad T^{-1} = \begin{pmatrix} A_1 & B_1 \\ C_1 & D_1 \end{pmatrix}.$$

Proof. From Lemma 1, we only need to prove that if $\hat{Z} = f(Z)$ is symplectic, then \hat{W}_w is symmetric.

Because

$$\begin{aligned} &= \left\langle \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \hat{W}_w \\ I \end{pmatrix}, \begin{pmatrix} \hat{W}_w \\ I \end{pmatrix} \right\rangle \\ &= \left\langle \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} T \begin{pmatrix} \hat{Z}_z \\ I \end{pmatrix} Z_w, T \begin{pmatrix} \hat{Z}_z \\ I \end{pmatrix} \cdot Z_w \right\rangle \end{aligned}$$

for the nonexceptional condition that Z_w is nonsingular, if

$$T^* \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} T = \mu \begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix},$$

then

$$\left\langle \begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix} \begin{pmatrix} \hat{Z}_z \\ I \end{pmatrix}, \begin{pmatrix} \hat{Z}_z \\ I \end{pmatrix} \right\rangle = 0$$

implies

$$\left\langle \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \hat{W}_w \\ I \end{pmatrix}, \begin{pmatrix} \hat{W}_w \\ I \end{pmatrix} \right\rangle = 0.$$

As a matter of fact, the condition is necessary and sufficient.

Theorem 6. Suppose T satisfies the condition of the above theorem. $\hat{Z} = g(Z)$ is a canonical transformation and $C\hat{Z}_z + D$ is nonsingular. Then there is a gradient transformation $W \rightarrow \hat{W} = f(W)$ and functional $\phi(W)$ such that $f(W) = \phi_w(W)$.

Proof. This is obvious from Theorem 5 because f is symmetric. So, from Lemma 1, there is $\phi(W)$ such that

$$f(W) = \phi_w(W).$$

$\phi(W)$ is called generating functional. For the H dependent on t , we have

Theorem 7. Let T be defined as above. $Z \rightarrow \hat{Z} = g(Z, t)$ is a canonical transformation. $Z(t)$ is phase flow.

$$M(Z, t) = g_z(Z, t).$$

- 1) $g(*, 0)$ is a linear canonical transformation, $M(Z, 0) = M_0$ is independent of Z ,
- 2) $g^{-1}(*, 0)g(*, t)$ is a canonical transformation dependent on t , and carries $Z(t)$ into $Z(0)$,
- 3) $OZ_z(0) + D$ is nonsingular.

Then there are a gradient transformation dependent on t : $W \rightarrow \hat{W} = f(W, t)$ and a generating functional $\phi(W, t)$ for sufficiently small $|t|$. Such that

- (1) $[\hat{W} - f(W, t)]_{\hat{W} = AZ + BZ, W = CZ + DZ} = 0$,
 - (2) $\phi_t(W, t) = \mu H(O_1\phi_w(W, t) + D_1W) |_{W = CZ + DZ}$,
- (2) is a general Hamilton-Jacobi equation.

Proof. Denote (Z, t) by \tilde{Z} , (W, t) by \tilde{W} . Similarly we have \tilde{Z} and \tilde{W} . $\tilde{W} = \begin{pmatrix} \hat{W} \\ H \end{pmatrix}$.

Then

$$\begin{pmatrix} \tilde{W} \\ \tilde{W} \end{pmatrix} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} \begin{pmatrix} \tilde{Z} \\ \tilde{Z} \end{pmatrix},$$

where

$$\tilde{A} = \begin{pmatrix} A & 0 \\ 0 & 1 \end{pmatrix}, \quad \tilde{B} = \begin{pmatrix} B & 0 \\ 0 & 1 \end{pmatrix},$$

$$\tilde{C} = \begin{pmatrix} C & 0 \\ 0 & 1 \end{pmatrix}, \quad \tilde{D} = \begin{pmatrix} D & 0 \\ 0 & 1 \end{pmatrix}.$$

As in Theorem 5, it is sufficient to show that $\frac{\delta(\hat{W}, H)}{\delta(W, t)}$ is symmetric and

$$\frac{\delta(\hat{W}, H)}{\delta(W, t)} = \begin{pmatrix} \hat{W}_w & D_w H \\ \frac{\partial \hat{W}}{\partial t} & \frac{\partial H}{\partial t} \end{pmatrix}.$$

Via direct calculation and by use of the equation $T^* \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} T = \begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix}$,

we get

$$D_w H = \frac{\partial \hat{W}}{\partial t}.$$

So there is a $\phi(W, t)$ such that

$$\begin{pmatrix} \hat{W} \\ H \end{pmatrix} = \frac{\delta \phi}{\delta(W, t)}.$$

So $H(O_1\phi_w(W, t) + D_1W, t) = \phi_t(W, t)$.

Depending on $\phi(W, t)$, we can get general symplectic difference schemes.

Theorem 8. Let H be a analytical function. Then $\phi(W, t)$ can be expressed as a series of t . For sufficiently small $|t|$, the series is convergent.

$$\phi(W, t) = \sum_{k=0}^{\infty} \phi^{(k)}(W) t^k,$$

$$\phi^{(0)}(W, t) = \frac{1}{2} W^* \hat{W}_w(0) W, \quad \hat{W}_w(0) = (AZ_z(0) + B)(OZ_z(0) + D)^{-1},$$

$$\phi^{(k)}(W) = \mu H(E_0 W), \quad E_0 = (O\hat{Z}_z(0) + D)^{-1}, \quad k \geq 1.$$

$$\phi^{(k+1)}(W) = \frac{1}{k+1} \sum_{m=1}^k \frac{\mu}{m!} \sum_{\substack{k_1+\dots+k_m=k \\ k_i \geq 1}} (H)^{(m)}(E_0 W) (C_1 \phi_W^{(k_1)}) \dots (C_1 \phi_W^{(k_m)}(W)).$$

Proof. We substitute $\phi(W, t) = \sum_{k=1}^{\infty} \phi^{(k)}(W) t^k$ into

$$\phi_t = \mu H(C_1 \phi_W + D_1 W, t).$$

Comparing the coefficient of t^n , we get the representation easily. We can select several form of T .

[I]

$$T = \begin{pmatrix} -I & 0 & 0 & 0 \\ 0 & 0 & 0 & -I \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \end{pmatrix},$$

$$\mu = -1, \quad M_0 = I.$$

$CM_0 + D$ is nonsingular,

$$W = \begin{pmatrix} \hat{q} \\ p \end{pmatrix}, \quad \hat{W} = \begin{pmatrix} -\hat{p} \\ -q \end{pmatrix},$$

$$\phi = \phi(\hat{p}, q, t).$$

The Hamilton-Jacobi equation: $\phi_t = -H(q, -\phi_q)$.

[II]

$$T = \begin{pmatrix} -J & J \\ \frac{1}{2}I & \frac{1}{2}I \end{pmatrix},$$

$$\mu = 1, \quad M_0 = I,$$

$CM_0 + D$ is nonsingular,

$$W = \frac{1}{2} \begin{pmatrix} \hat{p} + p \\ \hat{q} + q \end{pmatrix}, \quad \hat{W} = \begin{pmatrix} q - \hat{q} \\ \hat{p} - p \end{pmatrix},$$

Denote $(\hat{p} + p)/2$ by \bar{p} , $(\hat{q} + q)/2$ by \bar{q} .

Then, the Hamilton-Jacobi equation is

$$\phi_t = H\left(\bar{p} - \frac{1}{2} \phi_q, \bar{q} + \frac{1}{2} \phi_p\right).$$

Remark 1. If B is a Hilbert space $B = B^*$, we have more generating functionals such as

[III]

$$T = \begin{pmatrix} -I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{pmatrix},$$

$$\mu = -1, \quad M_0 = J,$$

$CM_0 + D$ is nonsingular,

$$W = \begin{pmatrix} \hat{q} \\ q \end{pmatrix}, \quad \hat{W} = \begin{pmatrix} -\hat{p} \\ p \end{pmatrix}.$$

The generating functional is $\phi = \phi(\hat{q}, q, t)$; correspondingly the Hamilton-Jacobi equation is

$$\phi_t = -H(\phi_q, q).$$

§ 5. Applications

1. When we take $B = R^n$, $q = (q_1, \dots, q_n) \in R^n$, $p = (p_1, \dots, p_n) \in (R^n)^* = R^n$, equation (1) becomes the canonical Hamilton equation. Because R^n is a Hilbert space, from Remark 1, all the conclusions of the finite dimensional case can be regarded as a special case of what is in Hilbert space.

2. Toda Lattice

$$(p, q) = (p_n, q_n), \quad n = \dots - k, \dots, k, \dots.$$

Its 2-form is $\Omega = \sum_n dp_n \wedge dq_n$.

The Hamilton function has the form

$$H = \frac{1}{2} \sum p_n^2 + \sum_n [\exp(q_n - q_{n-1}) - 1 - q_n + q_{n-1}].$$

Let

$$p = \{p_n\}, \quad q = \{q_n\}.$$

Then $p \in E^\infty$, $q \in E^\infty$. We write the equation as

$$\begin{aligned} \frac{dq}{dt} &= p, \\ \frac{dp}{dt} &= Aq \end{aligned}$$

in which $Aq \in E^\infty$. $(Aq)_n = \exp(q_n - q_{n-1}) - \exp(q_{n+1} - q_n)$.

This equation is introduced by Toda as the model of lattice of interesting oscillators^[8]. Because E^∞ is a Hilbert space, generating functionals [I], [II] and [III] can be taken. If we take [II], the second order accuracy scheme is

$$\begin{aligned} q^{n+1} &= q^n + \frac{\Delta t}{2} (p^n + p^{n+1}), \\ p^{n+1} &= p^n + \frac{\Delta t A}{2} (q^n + q^{n+1}). \end{aligned}$$

3. Wave equation. Let

$$B = H^1, \quad P = H^1 \times H^{-1}.$$

In $H^2 \times H^1$, a subspace of P , we have the Hamilton functional:

$$H(\phi, \dot{\phi}) = \int_{R^3} \frac{1}{2} \{ \dot{\phi}^2 + (\nabla \phi)^2 + m^2 \phi^2 \} + F\{\phi\} dx,$$

$$dH = \dot{\iota}_{X_H} \omega,$$

$$X_H(\phi, \dot{\phi}) \equiv (\dot{\phi}, \Delta \phi - m^2 \phi - F'(\phi)).$$

So, setting $u = \phi$ and $v = \dot{\phi}$ we have

$$\frac{dv}{dt} = -\frac{\delta H}{\delta u},$$

$$\frac{du}{dt} = \frac{\delta H}{\delta v}.$$

For B being the reflexive Banach space, we choose

$$T = \begin{pmatrix} J & -J \\ \frac{1}{2}I & \frac{1}{2}I \end{pmatrix}$$

briefly for $m=0$ and $F = \text{constant}$. We construct a difference scheme which is of fourth order accuracy.

$$Z^{n+1} = Z^n + \tau J^{-1} H_z \left(\frac{Z^{n+1} + Z^n}{2} \right) - \frac{2\tau^3}{3!4} J^{-1} H_{zz} \cdot (J^{-1} H_{zz}) J^{-1} H_z \left(\frac{Z^{n+1} + Z^n}{2} \right),$$

$$\begin{pmatrix} v^{n+1} \\ u^{n+1} \end{pmatrix} = \begin{pmatrix} v^n \\ u^n \end{pmatrix} + \tau \begin{pmatrix} 0 & \Delta \\ I & 0 \end{pmatrix} \begin{pmatrix} \bar{v} \\ \bar{u} \end{pmatrix} - \frac{\tau^3}{3!4} \begin{pmatrix} 0 & \Delta \\ I & 0 \end{pmatrix} \begin{pmatrix} 0 & \Delta \\ I & 0 \end{pmatrix} \begin{pmatrix} 0 & \Delta \\ I & 0 \end{pmatrix} \begin{pmatrix} \bar{v} \\ \bar{u} \end{pmatrix}$$

If we take Δ as the fourth-order centered difference approximation we get

$$Z^{n+1} = Z^n + \tau B \bar{Z} - \frac{\tau^3}{12} B^3 \bar{Z},$$

where

$$B = \begin{bmatrix} 0 & M \\ I & 0 \end{bmatrix},$$

$$M = \frac{1}{12h^2} \begin{bmatrix} -30 & 16 & -1 & 0 & 0 \\ 16 & -30 & 16 & -1 & 0 \\ -1 & 16 & -30 & 16 & -1 \\ \dots & \dots & \dots & \dots & \dots \\ -1 & 16 & -30 & 16 & -1 \end{bmatrix},$$

$$\bar{Z} = \frac{Z^{n+1} + Z^n}{2}.$$

τ is the time step length, h is the space step length, M is an $n \times n$ matrix, I is the $n \times n$ unit matrix $n = \frac{2\pi}{h} + 1$.

This scheme has been computed on the computer, and the result is very satisfactory. Its detail will be discussed in another paper [7].

4. For compressible flow.

$$H = C \cdot \rho^r + (\sigma \nabla \mu + \rho \nabla \phi)^2 / 2\rho,$$

where $(\rho, \phi) (\sigma, \mu)$ is conjugate variable,

$$\sigma = -\rho \lambda.$$

For flow field: $v = \lambda \nabla \mu - \nabla \phi$, λ, u are vortex labels. The equation has the form

$$\frac{\partial \rho}{\partial t} = -\frac{\partial H}{\partial \phi},$$

$$\frac{\partial \phi}{\partial t} = \frac{\partial H}{\partial \rho},$$

$$\frac{\partial \mu}{\partial t} = \frac{\partial H}{\partial \sigma},$$

$$\frac{\partial \sigma}{\partial t} = -\frac{\partial H}{\partial \mu}.$$

Denote $p = (\rho, \sigma)$, $q = (\phi, \mu)$. We have $\frac{\partial}{\partial t} \begin{pmatrix} p \\ q \end{pmatrix} = J^{-1} \begin{pmatrix} \frac{\partial H}{\partial p} \\ \frac{\partial H}{\partial q} \end{pmatrix}$.

We choose the generating functional of first kind with second-order accuracy. Then

$$\begin{aligned} p^{n+1} &= p^n - \tau H_q(p^n, q^{n+1/2}), \\ q^{n+1+1/2} &= q^{n+1/2} + \tau H_p(p^{n+1}, q^{n+1/2}). \end{aligned}$$

References

- [1] Abraham R.; Marsden J.: *Foundation of Mechanics*, Benjamin-Cummings, New York, 1978.
- [2] Abraham R.; Marsden J.: *Manifold, Tensor Analysis, and Applications*, Addison-Wesley Publishing Company, INC.
- [3] Buneman O.: Compressible flow simulation using Hamilton's equation and Clebsch-type vortex parameters, *Phys. Fl.*, **23**: 8 (1980), 1716.
- [4] Chernoff P.; Marsden J.: *Properties of Infinite Dimensional Hamilton System*, Lecture Notes in Math. 425, Springer, New York.
- [5] Feng Kang: On difference Schemes and Symplectic geometry, *Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations*, Ed. Feng Kang, Science Press, Beijing, 1985.
- [6] Feng Kang: Difference scheme for Hamilton formalism and symplectic geometry, *J. Comp. Math.*, **4**: 3 (1986), 279—289.
- [7] Qin Meng-zhao; Li Chun-wang: The symplectic difference scheme of fourth order for the wave equation, to appear.
- [8] Toda M.: Wave propagation in anharmonic lattices, *J. Phy. Soc. Jap.*, **23** (1967), 501—506.
- [9] Vainberg M.: *Variational Methods in Nonlinear Operator Analysis*, Holden-Day, San Francisco, 1964.