THE SYMPLECTIC METHODS FOR THE COMPUTATION OF HAMILTONIAN EQUATIONS ①②

计算哈密尔顿方程的辛方法

Abstract

The present paper gives a brief survey of results from a systematic study, undertaken by the authors and their colleagues, on the symplectic approach to the numerical computation of Hamiltonian dynamical systems in finite and infinite dimensions. Both theoretical and practical aspects of the symplectic methods are considered. Almost all the real conservative physical processes can be cast in suitable Hamiltonian formulation in phase spaces with symplectic structure, which has the advantages to make the intrinsic properties and symmetries of the underlying processes more explicit than in other mathematically equivalent formulations, so we choose the Hamiltonian formalism as the basis, together with the mathematical and physical motivations of our symplectic approach for the purpose of numerical simulation of dynamical evolutions. We give some symplectic difference schemes and related general concepts for linear and nonlinear canonical systems in finite dimensions. The analysis confirms the expectation for them to behave more satisfactorily, especially in the desirable conservation properties, than the conventional schemes. We outline a general and constructive theory of generating functions and a general method of construction of symplectic difference schemes based on all possible generating functions. This is crucial for the developments of the symplectic methods. A generalization of the above theory and method to the canonical Hamiltonian eqs. in infinite dimensions is also given. The multi-level schemes, including the leapfrog one, are studied from the symplectic point of view. We give an application of symplectic schemes, with some indications of their potential usefulness, to the computation of chaos.

CONTENTS

§1 Introduction

§2 S-schemes for Linear and Nonlinear Hamiltonian Systems

§3 Constructive Theory of Generating Function and S-schemes

§4 S-schemes for Infinite Dimensional Hamiltonian Systems

§5 Multi-level S-schemes

§6 Numerical Examples

§7 S-schemes and Chaos

---

①Joint with Qin M Z

②In Zhu Y L, Guo Ben-yu, ed. Proc Conf on Numerical Methods for PDE's. Berlin: Springer, 1987. 1–37. Lect Notes in Math 1297

§1 Introduction

Recently it is evident that Hamiltonian formalism plays a fundamental role in the diverse areas of physics, mechanics, engineering, pure and applied mathematics, e.g. geometrical optics, analytical dynamics, nonlinear PDE's of first order, group representations, WKB asymptotics, pseudodifferential and Fourier integral operators, classification of singularities, integrability of non-linear evolution equations, optimal control theory, etc. It is also under extension to infinite dimensions for various field theories, including electrodynamics, plasma physics, elasticity, hydrodynamics etc. It is generally accepted that all real physical processes with negligible dissipation could be expressed, in some way or other, by Hamiltonian formalism, so the latter is becoming one of the most useful tools in the mathematical physics and engineering sciences.

Hamiltonian formalism has the important property of being area-preserving (symplectic) i.e. the sum of the areas of canonical variable pairs, projected on any two-dimensional surface in phase space, is time invariant. In numerically solving these equations one hopes that the approximating equation will hold this property.

In DD-5 Beijing Conference the first author [1] propose an approach for computing Hamiltonian equation from the viewpoint of symplectic geometry. This paper is a brief survey of considerations and developments [1-11, 15], obtained by the first author and his group, on the links between the Hamiltonian formalism and the numerical methods.

Now we will give a review of some facts from Hamiltonian mechanics which are fundamental to what follows. We consider the following canonical system of ordinary first order differential equations on R^{2n}

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad i = 1, 2, \cdots n, \tag{1.1}$$

where $H(p,q)$ is some real valued function. We call (1.1) a Hamiltonian system of differential equations (H-system). In the following, vectors are always represented by column matrices, matrix transpose is denoted by prime $'$. Let $z = (z_1, \cdots, z_n, z_{n+1}, \cdots, z_{2n})' = (p_1, \cdots, p_n, q_1, \cdots, q_n)'$, $H_z = \left[\frac{\partial H}{\partial p_1}, \cdots, \frac{\partial H}{\partial p_n}, \frac{\partial H}{\partial q_1}, \cdots, \frac{\partial H}{\partial q_n}\right]'$, $J_{2n} = J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, $J' = J^{-1} = -J$, where I_n is the $n \times n$ identity matrix. (1.1) can be written as

$$\frac{dz}{dt} = J^{-1} H_z, \tag{1.2}$$

defined in phase space R^{2n} with a standard symplectic structure given by the nonsingular anti-symmetric closed differential 2-form

$$\omega = \sum dz_i \wedge dz_{n+i} = \sum dp_i \wedge dq_i.$$

According to Darboux Theorem, the symplectic structure given by any non-singular anti-symmetric closed differential 2-form can be brought to the above standard form, at least locally, by suitable change of coordinates.

The right side of equation (1.2) gives a vector field. At each point (p,q) of the phase space, there is a $2n$-dimensional vector $(-H_q, H_p)$.

The fundamental theorem on Hamiltonian Formalism says that the solution $z(t)$ of the canonical system (1.2) can be generated by a one-parameter group $G(t)$, depending on given

Hamiltonian H, of canonical transformations of R^{2n} (locally in t and z) such that

$$z(t) = G(t)z(0).$$

This group is also called the phase flow

$$G(t) : (p(0), q(0)) \to (p(t), q(t))$$

where $p(t)$, $q(t)$ are the solution of Hamilton's system of equations (1.1).

A transformation $z \to \hat{z}$ of R^{2n} is called canonical, or symplectic, if it is a local diffeomorphism whose Jacobian $\frac{\partial \hat{z}}{\partial z} = M$ is every-where symplectic, i.e.

$$M'JM = J, \quad \text{i.e.} \quad M \in Sp(2n).$$

Linear canonical transformation is special symplectic transformation.

The canonicity of $G(t)$ implies the preservation of 2-form ω, 4-form $\omega \wedge \omega, \cdots$, $2n$-form $\omega \wedge \omega \wedge \cdots \wedge \omega$. They constitute the class of conservation laws of phase area of even dimensions for the Hamiltonian system (1.2).

Moreover, the Hamiltonian system possesses another class of conservation laws related to the energy $H(z)$. A function $\psi(z)$ is said to be an invariant integral of (1.2) if it is invariant under (1.2)

$$\psi(z(t)) \equiv \psi(z(0))$$

which is equivalent to

$$\{\psi, H\} = 0,$$

where the Poisson Brackets for any pair of differentiable functions ϕ and ψ are defined as

$$\{\phi, \psi\} = \phi_z' J^{-1} \psi_z.$$

H itself is always an invariant integral, see, e.g. [12].

For the numerical study, we are less interested in (1.2) as a general system of ODE per se, but rather as a specific system with Hamiltonian structure. It is natural to look for those discretization systems which preserve as much as possible the characteristic properties and inner symmetries of the original continuous systems. To this end the transition $\hat{z} \to z$ from the k-th time step $z^k = \hat{z}$ to the next $(k+1)$-th time step $z^{k+1} = z$ should be canonical for all k and, moreover, the invariant integrals of the original system should remain invariant under these transitions.

Thus, a difference scheme may be regarded as a transformation from time t^k to time t^{k+1}. We have the following

Definition 1. A difference scheme may be called symplectic or canonical scheme if its transitional transformation is symplectic.

We try to conceive, design, analyse and evaluate difference schemes and algorithms specifically within the framework of symplectic geometry. The approach proves to be quite successful as one might expect, we actually derive in this way numerous "unconventional" difference schemes.

An outline of the paper is as follows. In section 2 we review some symplectic difference schemes (S-scheme) for linear hamiltonian system (LH-system) and nonlinear hamiltonian system (NLH-system) and its related properties are given. In section 3, we systematically outline the general method of construction of S-schemes with any order accuracy via generating function. The constructive theory of generating function and the corresponding construction of S-schemes have been generalized to the case of phase space of infinite dimensions of the form $B^\star \times B$, where B is a reflexive Banach space, $B^\star$ its dual [3] [8]. Section 4 contains the main idea. The multi-level difference S-schemes of hamiltonian type are described in §5. In §6 we show some computational results and comparison with R-K method. The last section is S-scheme and chaos. It is well known that canonical transformation is an area preserving mapping. Therefore S-schemes are suitable tools for studying chaotic behavior in hamiltonian mechanics.

§2 S-schemes for Linear and Nonlinear Hamiltonian Systems

Consider the case for which the Hamiltonian is a quadratic form

$$H(z) = \frac{1}{2} z' S z, \quad S' = S, \quad H_z = Sz. \tag{2.1}$$

Then the canonical system

$$\frac{dz}{dt} = Lz, \qquad L = J^{-1} S \tag{2.2}$$

is linear, where L is infinitesimally symplectic, i.e. L satisfies $L'J + JL = 0$.

The solution of (2.2) is

$$z(t) = G(t) z(0)$$

where $G(t) = \exp tL$, as the exponential transform of infinitesimally symplectic tL, is symplectic.

It is easily seen that the weighted Euler scheme

$$\frac{1}{\tau}(z^{k+1} - z^k) = L(\alpha z^{k+1} + (1-\alpha) z^k)$$

for the linear system (2.2) is symplectic iff $\alpha = \frac{1}{2}$, i.e. it is the case of time centered Euler scheme with the transition matrix F_τ,

$$z^{k+1} = F_\tau z^k, \quad F_\tau = \psi(\tau L), \quad \psi(\lambda) = \frac{1 + \frac{\lambda}{2}}{1 - \frac{\lambda}{2}}, \tag{2.3}$$

F_τ, as the Cayley transform of infinitesimally symplectic τL, is symplectic.

In order to generalize the time-centered Euler scheme, we need, apart from the exponential or Cayley transforms, other matrix transforms carrying infinitesimally symplectic matrices into symplectic ones.

Theorem 1. *Let $\psi(\lambda)$ be a function of complex variable λ satisfying*

(I) $\psi(\lambda)$ *is analytic with real coefficients in a neighborhood D of $\lambda = 0$,*

(II) $\psi(\lambda)\psi(-\lambda) \equiv 1$ *in D,*

(III) $\psi'_\lambda(0) \neq 0$.

A is a matrix of order $2n$, then $(\psi(\tau L))' A \psi(\tau L) = A$ for all τ with sufficiently small $|\tau|$, iff

$$L'A + AL = 0.$$

If, more, $\exp \lambda - \psi(\lambda) = O(|\lambda|^{m+1})$, then

$$z^{k+1} = \psi(\tau L) z^k, \tag{2.4}$$

considered as an approximative scheme for the canonical system (2.2), is symplectic, of m-th order of accuracy and has the property that $z'Aw$ is invariant under $\psi(\tau L)$ iff it is invariant under G_t of (2.2).

Remark 1. The last property is remarkable in the sense that, all the bilinear invariants of the system (2.2), no more and no less, are kept invariant under the scheme (2.4), in spite of the fact that the latter is only approximate.

Remark 2. The approximative scheme in Theorem 1 becomes difference schemes only when $\psi(\lambda)$ is a rational function. As a concrete application to the construction of symplectic difference schemes, we take the diagonal Padè approximants to the exponential function

$$\exp\lambda - \frac{P_m(\lambda)}{P_m(-\lambda)} = O(|\lambda|^{2m+1})$$

where $P_0(\lambda) = 1$, $P_1(\lambda) = 2+\lambda$, $P_2(\lambda) = 12+16\lambda+\lambda^2$, $\cdots$, $P_m(\lambda) = 2(2m-1)P_{m-1}(\lambda) + \lambda^2 P_{m-2}(\lambda)$.

Theorem 1′. *Difference schemes*

$$z^{k+1} = \frac{P_m(\tau L)}{P_m(-\tau L)} z^k, \quad m = 1, 2, \cdots \tag{2.5}$$

for the eq. (2.2) *are symplectic, A-stable, of* $2m$*-th order of accuracy, and having the same set of bilinear invariants as that of eq.* (2.2), *and the case* $m = 1$ *is the centered Euler scheme* [5].

For the general non-linear canonical system (1.2), the time-centered Euler scheme is

$$\frac{1}{\tau}(z^{k+1} - z^k) = J^{-1}H_z(\frac{1}{2}(z^{k+1} + z^k)). \tag{2.6}$$

The transition $z^{k+1} \to z^k$ is canonical with Jacobian

$$F_\tau = [I - \frac{\tau}{2}J^{-1}H_{zz}(\frac{1}{2}(z^{k+1}+z^k))]^{-1}[I + \frac{\tau}{2}J^{-1}H_{zz}(\frac{1}{2}(z^{k+1}+z^k))]$$

symplectic everywhere. However, unlike the linear case, the invariant integrals ψ, not quadratic in z, including $H(z)$, are conserved only approximately:

$$\psi(z^{k+1}) - \psi(z^k) = O(\tau^3).$$

For the general non-linear separable system for which $H(p,q) = U(p) + V(q)$, U, V, being kinetic and potential energies respectively, we define the staggered scheme

$$\begin{aligned} &\frac{1}{\tau}(p^{k+1} - p^k) = -V_q(q^{k+\frac{1}{2}}), \\ &\frac{1}{\tau}(q^{k+1+\frac{1}{2}} - q^{k+\frac{1}{2}}) = U_p(p^{k+1}). \end{aligned} \tag{2.7}$$

The p's are set at integer times $t = k\tau$, q's at half-integer times $t = (k+\frac{1}{2})\tau$. The transition

$$\begin{aligned} &w^k = \begin{bmatrix} p^k \\ q^{k+\frac{1}{2}} \end{bmatrix} \to \begin{bmatrix} p^{k+1} \\ q^{k+1+\frac{1}{2}} \end{bmatrix} = w^{k+1} = F_\tau w^k, \\ &F_\tau = \begin{bmatrix} I & 0 \\ -\tau M & I \end{bmatrix}^{-1} \begin{bmatrix} I & -\tau L \\ 0 & I \end{bmatrix}, \\ &M = U_{pp}(p^{k+1}), \qquad L = V_{qq}(q^{k+\frac{1}{2}}), \end{aligned}$$

is symplectic of 2nd order accuracy and practically explicit, since p, q are computed at different times, we have to use certain synchronization, e.g. using

$$q^k = \frac{1}{2}(q^{k-\frac{1}{2}} + q^{k+\frac{1}{2}})$$

to compute the invariant integrals $\psi(p,q)$

$$\psi(p^{k+1}, q^{k+1}) - \psi(p^k, q^k) = O(\tau^3).$$

In [1, 9], a class of energy conservative schemes was constructed using the differencing of the Hamiltonian function, however, the symplectic property was not satisfactory. The problem of compatibility of energy conservation with phase area conservative in difference schemes is solved successfully for linear canonical system (Theorem 1). It seems difficult, however, for the general nonlinear system.

Suppose that the Hamiltonian function $H(p,q)$ does not depend on time

$$H + h = 0, \tag{2.8}$$

where h is a constant, is the integral of energy of the system.

We assume that (in some region) the equation (2.8) can be solved for some variable (no loss of generality) for example p_1, $H_{p_1} = \frac{dq_1}{dt} \neq 0$, so (2.8) is solved by

$$K(p_2, p_3, \cdots, p_n, q_1, \cdots, q_n, h) + p_1 = 0 \tag{2.9}$$

and $t \to q_1(t)$ has an inverse $q_1 \to t(q_1)$, so we can use q_1 instead of t as "time". Equations (1.1) can be written as

$$\frac{dq_r}{dq_1} = \frac{\partial K}{\partial p_r}, \quad \frac{dp_r}{dq_1} = -\frac{\partial K}{\partial q_r}, \quad (r = 2, 3, \cdots, n), \tag{2.10}$$

$$\frac{dt}{dq_1} = \frac{\partial K}{\partial h}, \quad \frac{dh}{dq_1} = 0 = -\frac{\partial K}{\partial t}. \tag{2.11}$$

The last two equations can be separated from the rest of the system, since the first $(2n-2)$ equations do not involve t, and h is a constant. The phase trajectories of (1.1) on the energy surface $H(z) + h = 0$ satisfy (2.10). Moreover (2.11), (2.10) combine into a new H-system $dw/dq_1 = J^{-1}K_w$ in "time" q_1 in the modified phase space with new canonical variables $w = (h, p_2, \cdots, p_n; t, q_2, \cdots, q_n)$ with "time"-dependent Hamiltonian $K(w; q_1)$. Since K is independent of $w_{n+1} = t$, its conjugate variable $w_1 = h$ is constant. We use the Euler scheme

$$\frac{1}{\Delta q_1}(w^{m+1} - w^m) = J^{-1}K_w(\frac{1}{2}(w^{m+1} + w^m); \ \frac{1}{2}(q_1^{m+1} + q_1^m)), \quad q_1^{m+1} = q_1^m + \Delta q_1.$$

The transition $w^m \to w^{m+1}$ is symplectic and preserves $w_1 = h$, i.e. $h^m = h^{m+1}$. We compute, in addition, $K^m = K(w^m; q_1^m)$, $p_1^m = -K^m$. Owing to the identity

$$H(-K(p_2, \cdots, p_n, q_1, q_2, \cdots, q_n, h), p_2, \cdots, p_n, q_1, \cdots, q_n) + h \equiv 0,$$

we have $H^m = H(p_1^m, p_2^m, \cdots, q_n^m) = -h^m = -h^{m+1} = H^{m+1}$. So we get energy conservative scheme which is also symplectic in a modified sense. Here the computed time steps $t^{m+1} - t^m$ are in general variable under the fixed "time" step Δq_1. This agrees with an idea of T.D. Lee [16], where time steps are to be solved to make energy conservative. The above approach to make S-schemes energy conservative is due to Qin Meng-zhao.

The problem of preservation of first integrals of system (1.2) under a S-scheme

$$z^{m+1} = S_H^\tau(z^m),$$

where S_H^τ is a symplectic transformation depending on $H(z)$ and step τ, is closely related to the invariance properties of S_H^τ under groups of symplectic transformations [7]. The scheme S_H^τ is said to be invariant under a group G of symplectic transformations if

$$g^{-1} \circ S_H^\tau \circ g = S_{H \circ g}, \quad \forall g \in G.$$

Theorem 2. *Let F be a first integral of system $dz/dt = J^{-1}H_z$. Then F is preserved up to a constant by the scheme S_H^τ, i.e.*

$$F(z) \equiv F(S_H^\tau(z)) + c, \qquad c = const.$$

iff S_H^τ is invariant under the 1-parameter group G_F^t of the phase flow of the system $dz/dt = J^{-1}F_z$. The constant $c = 0$ if S_H^τ has a fixed point.

It is known that all linear first integrals (e.g., linear momenta) of H-system are preserved by any compatible difference scheme, symplectic or not. However for quadratic first integrals (e.g., angular momenta), this is by far not case. In this aspect the symplectic schemes are distinguished as shown above at least for linear H-systems.

For general non-linear H-systems and for symplectic Euler schemes of arbitrary $2m$-th order (the case $m = 1$ is (2.6), for higher order schemes see Theorem 8, §3), Ge Zhong, Wang Dao-liu, and Wu Yu-hua have proved the physically significant property of preservation of all the quadratic first integrals. This is easily seen for the case $m = 1$: Let $F(z) = \frac{1}{2}z'Bz$, $B' = B$, be a first integral of (1.2), then $\{f, H\} = (Bz)'J^{-1}H_z(z) = 0$ for all z. Multiply (2.6) by $(B\frac{1}{2}(z^{k+1} + z^k))'$, we get $\frac{1}{\tau}\frac{1}{2}(z^{k+1} + z^k)'B(z^{k+1} - z^k) = 0$, then $F(z^{k+1}) = F(z^k)$.

§3 Constructive Theory of Generating Functions and S-schemes

In this section we reproduce almost verbally the results from [4]. The generalization to Poisson maps was done in [11]. The generalization to infinite dimensions was done in [8] and will be outlined in §4.

In order to develop a general method of construction of canonical difference schemes we first give a constructive generalization of the classical theory of generating function and Hamilton-Jacobi equations. Our approach in this part was inspired by the early works of Siegel [13] and Hua [14]. Every matrix

$$A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \in M(4n, 2n), \; A_1, A_2 \in M(2n), \quad \text{rank } A = 2n$$

defines in R^{4n} a $2n$-dimensional subspace $\{A\}$ spanned by its column vectors. $\{A\} = \{B\}$ iff $A \sim B$, i.e.

$$AP = B, \quad \text{i.e.} \quad \begin{bmatrix} A_1P \\ A_2P \end{bmatrix} = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \quad \text{for some } P \in GL(2n).$$

The spaces of symmetric and symplectic matrices of order $2n$ will be denoted by $Sm(2n)$, $Sp(2n)$ respectively. Let

$$J_{4n} = \begin{bmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{bmatrix}, \qquad \widetilde{J}_{4n} = \begin{bmatrix} -J_{2n} & 0 \\ 0 & J_{2n} \end{bmatrix}$$

$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} \in M(4n, 2n), \text{ of rank } 2n.$$

Subspace $\{X\} \subset R^{4n}$ is called J_{4n}-Lagrangian (and $\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$ is called a symmetric pair) if

$$X' J_{4n} X = O_{2n}, \quad \text{i.e.} \quad X_1' X_2 - X_2' X_1 = O_{2n}.$$

If, moreover, $|X_2| \neq 0$, then $X_1 X_2^{-1} = N \in Sm(2n)$ and $\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim \begin{bmatrix} N \\ I \end{bmatrix}$, where N is determined uniquely by the subspace $\{X\}$. Similarly, subspace $\{Y\} \subset R^{4n}$ is called $\widetilde{J}_{4n}$-Lagrangian (and $\begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix}$ is called a symplectic pair) if

$$Y' \widetilde{J}_{4n} Y = O_{2n}, \text{ i.e.,} \quad Y_1' J_{2n} Y_1 - Y_2' J_{2n} Y_2 = O_{2n}.$$

If, moreover, $|Y_2| \neq 0$, then $Y_1 Y_2^{-1} = M \in Sp(2n)$ and $\begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} \sim \begin{bmatrix} M \\ I \end{bmatrix}$, where M is determined uniquely by the subspace $\{Y\}$.

A $2n$-dimensional submanifold $U \subset R^{4n}$ is called J_{4n}-Lagrangian (respectively $\widetilde{J}_{4n}$-Lagrangian) if the tangent plane of U is a J_{4n}-Lagrangian (respectively $\widetilde{J}_{4n}$-Lagrangian) subspace of the tangent space at each point of U.

Let $z \to \hat{z} = g(z)$ be a canonical transformation in R^{2n}, with Jacobian $g_z = M(z) \in Sp(2n)$. The graph of g,

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

is a $\widetilde{J}_{4n}$-Lagrangian submanifold, whose tangent plane is spanned by the symplectic pair $\begin{bmatrix} M(z) \\ I \end{bmatrix}$.

Similarly, let $w \to \hat{w} = f(w)$ be a gradient transformation in R^{2n}, the Jacobian $f_w = N(w) \in Sm(2n)$. This is equivalent to the (local) existence of a scalar function $\phi(w)$ such that $f(w) = \phi_w(w)$. The graph of f,

$$U = \left\{ \begin{bmatrix} \hat{w} \\ w \end{bmatrix} \in R^{4n} | \hat{w} = f'(w) \right\},$$

is a J_{4n}-Lagrangian submanifold with tangent planes spanned by the symmetric pair $\begin{bmatrix} N(w) \\ I \end{bmatrix}$.

Theorem 3. *$T \in GL(4n)$ carries every $\widetilde{J}_{4n}$-Lagrangian submanifold into J_{4n}-Lagrangian submanifold if and only if*

$$T' J_{4n} T = \mu \widetilde{J}_{4n}, \quad \textit{for some } \mu \neq 0,$$

i.e.

$$\begin{aligned} A_1 &= -\mu^{-1} J_{2n} C', \quad B_1 = \mu^{-1} J_{2n} A', \\ C_1 &= \mu^{-1} J_{2n} D', \quad D_1 = -\mu^{-1} J_{2n} B', \\ A &= \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \quad T^{-1} = \begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix}. \end{aligned} \tag{3.1}$$

The totality of T's in Theorem 3 will be denoted by $CSp(\widetilde{J}_{4n}, J_{4n})$, the subset with $\mu = 1$ by $Sp(\widetilde{J}_{4n}, J_{4n})$. The latter is not empty since $\widetilde{J}_{4n}$ is congruent to J_{4n}. Fix $T_0 \in Sp(\widetilde{J}_{4n}, J_{4n})$; then every $T \in CSp(\widetilde{J}_{4n}, J_{4n})$ is a product

$$T = MT_0, \quad M \in CSp(4n) = \text{conformal symplectic group}.$$

T^{-1} for $T \in CSp(\widetilde{J}_{4n}, J_{4n})$ carries J_{4n}-Lagrangian submanifolds into $\widetilde{J}_{4n}$-Lagrangian submanifolds.

A major component of the transformation theory in symplectic geometry is the method of generating functions. Canonical transformations can in some way be expressed in implicit form, as gradient transformations with generating functions via suitable linear transformations. The graphs of canonical and gradient transformations in R^{4n} are $\widetilde{J}_{4n}$-Lagrangian and J_{4n}-Lagrangian submanifolds respectively. Theorem 3 leads to the existence and construction of the generating functions, under some transversality conditions, for the canonical transformations.

Theorem 4. *Let* $T = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$, $T^{-1} = \begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix}$, $T \in CSp(\widetilde{J}_{4n}, J_{4n})$, *which define linear transformations*

$$\hat{w} = A\hat{z} + Bz, \quad \hat{z} = A_1\hat{w} + B_1 w,$$
$$w = C\hat{z} + Cz, \quad z = C_1\hat{w} + D_1 w.$$

Let $z \to \hat{z} = g(z)$ *be a canonical transformation in (some neighborhood of)* R^{2n}, *with Jacobian* $g_z = M(z) \in Sp(2n)$ *and graph*

$$V^{2n} = \left\{ \begin{bmatrix} \hat{z} \\ z \end{bmatrix} \in R^{4n} | \hat{z} - g(z) = 0 \right\}.$$

If (in some neighborhood of R^{4n}*)*

$$|CM + D| \neq 0, \tag{3.2}$$

then there exists in (some neighborhood of) R^{2n} *a gradient transformation* $w \to \hat{w} = f(w)$ *with Jacobian* $f_w = N(w) \in Sm(2n)$ *and graph*

$$U^{2n} = \left\{ \begin{bmatrix} \hat{w} \\ w \end{bmatrix} \in R^{4n} | \hat{w} - f(w) = 0 \right\}$$

and a scalar function — generating function — $\phi(w)$ *such that*

(1) $f(w) = \phi_w(w)$;

(2) $N = (AM + B)(CM + D)^{-1}$, $M = (NC - A)^{-1}(B - ND)$;

(3) $T(V^{2n}) = U^{2n}$, $V^{2n} = T^{-1}(U^{2n})$.

This corresponds to the fact that, under the transversality condition (3.2),

$$[\hat{w} - \phi_w(w)]_{\hat{w} = A\hat{z} + Bz, w = C\hat{z} + Dz} = 0$$

gives the implicit representation of the canonical transformation $\hat{z} = g(z)$ via linear transformation T and generating function ϕ.

For the time-dependent canonical transformation, related to the time-evolution of the solutions of a canonical system (1.2) with Hamiltonian function $H(z)$, we have the following general theorem on the existence and construction of the time-dependent generating function and Hamilton-Jacobi equation depending on T and H under some transversality condition.

Theorem 5. *Let T be such as in Theorems 3 and 4. Let $z \to \hat{z} = g(z,t)$ be a time-dependent canonical transformation (in some neighborhood) of R^{2n} with Jacobian $g_z(z,t) = M(z,t) \in Sp(2n)$ such that*

(a) *$g(\star, 0)$ is a linear canonical transformation $M(z,0) = M_0$, independent of z,*

(b) *$g^{-1}(\star, 0) g(\star, t)$ is the time-dependent canonical transformation carrying the solution $z(t)$ at moment t to $z(0)$ at moment $t = 0$ for the canonical system. If*

$$|CM_0 + D| \neq 0, \tag{3.3}$$

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

(1) *$[\hat{w} - f(w,t)]_{\hat{w}=A\hat{z}+Bz, w=C\hat{z}+Dz} = 0$ is the implicit representation of the canonical transformation $\hat{z} = g(z,t)$;*

(2) *$N = (AM+B)(CM+D)^{-1}$, $M = (NC-A)^{-1}(B-ND)$;*

(3) *$\phi_w(w,t) = f(w,t)$;*

(4) *$\phi_t(w,t) = -\mu H(C_1 \phi_w(w,t) + D_1 w)$, $w = C\hat{z} + Dz$.*

Equation (4) is the most general Hamilton-Jacobi equation abbreviated as H.J. equation for the Hamiltonian canonical system (1.2) and linear transformation $T \in CSp(\widetilde{J}_{4n}, J_{4n})$.

Special types of generating functions:

$$\text{(I)} \qquad T = \begin{bmatrix} -I_n & 0 & 0 & 0 \\ 0 & 0 & I_n & 0 \\ 0 & I_n & 0 & 0 \\ 0 & 0 & 0 & I_n \end{bmatrix}, \ \mu = 1, \ M_0 = J_{2n}, \ |CM_0 + D| \neq 0;$$

$$w = \begin{bmatrix} \hat{q} \\ q \end{bmatrix}, \quad \phi = \phi(\hat{q}, q, t);$$

$$\hat{w} = \begin{bmatrix} -\hat{p} \\ p \end{bmatrix} = \begin{bmatrix} \phi_{\hat{q}} \\ \phi_q \end{bmatrix}, \quad \phi_t = -H(\phi_q, q)$$

are the generating function and H-J equation of the first kind [12].

$$\text{(II)} \qquad T = \begin{bmatrix} -I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & -I_n \\ 0 & I_n & 0 & 0 \\ 0 & 0 & I_n & 0 \end{bmatrix}, \ \mu = 1, \ M_0 = I_{2n}, \ |CM_0 + D| \neq 0;$$

$$w = \begin{bmatrix} \hat{q} \\ p \end{bmatrix}, \quad \phi = \phi(\hat{q}, p, t);$$

$$\hat{w} = \begin{bmatrix} -\hat{p} \\ -q \end{bmatrix} = \begin{bmatrix} \phi_{\hat{q}} \\ \phi_p \end{bmatrix}, \quad \phi_t = -H(p, -\phi_p)$$

are the generating function and H-J equation of the second kind [2].

$$
\begin{aligned}
&\text{(III)} \quad T = \begin{bmatrix} -J_{2n} & J_{2n} \\ \frac{1}{2}I_{2n} & \frac{1}{2}I_{2n} \end{bmatrix}, \ \mu = -1, \ M_0 = I_{2n}, \ |CM_0 + D| \neq 0; \\
&w = \frac{1}{2}(z + \hat{z}), \quad \phi = \phi'(w,t); \\
&\hat{w} = J(z - \hat{z}) = \phi_w, \quad \phi_t = H(w - \frac{1}{2}J\phi_w)
\end{aligned}
$$

are a new type of generating functions and H-J equations, not encountered in the classical literature.

By recursions we can determine explicitly all possible time-dependent generating functions for analytic Hamiltonians [6].

Theorem 6. *Let $H(z)$ depend analytically on z. Then $\phi(w,t)$ in Theorem 5 can be expressed as convergent power series in t for sufficiently small $|t|$:*

$$
\begin{aligned}
\phi(w,t) &= \sum_{k=0}^{\infty} \phi^{(k)}(w) t^k, \\
\phi^{(0)}(w) &= \frac{1}{2} w' N_0 w, \quad N_0 = (AM_0 + B)(CM_0 + D)^{-1}, \\
\phi^{(1)}(w) &= -\mu H(E_0 w), \ E_0 = (CM_0 + D)^{-1}, \\
k \geq 1: \quad \phi^{(k+1)}(w) &= \frac{-\mu}{k+1} \sum_{m=1}^{k} \frac{1}{m!} \sum_{i_1,\cdots,i_m=1}^{2n} H_{z_{i_1},\cdots,z_{i_m}}(E_0 w) \\
&\times \sum_{\substack{k_1+\cdots+k_m=k \\ k_j \geq 1}} \Big(C_1 \phi_w^{(k_1)}(w)\Big)_{i_1} \cdots \Big(C_1 \phi_w^{(k_m)}(w)\Big)_{i_m}.
\end{aligned} \tag{3.4}
$$

Generating functions play the central role for the construction of canonical difference schemes for Hamiltonian systems. The general methodology for the latter is as follows: Choose some suitable type of generating function (Theorem 5) with its explicit expression (Theorem 6). Truncate or approximate it in some way and take gradient of this approximate generating function. Then we get automatically the implicit representation of some canonical transformation for the transition of the difference scheme. In this way one can get an abundance of canonical difference schemes. This methodology is unconventional in the ordinary sense, but natural from the point of view of symplectic geometry [6]. As an illustration we construct a family of canonical difference schemes of arbitrary order from the truncations of the Taylor series of the generating functions for each choice of $T \in CSp(\widetilde{J}_{4n}, J_{4n})$ and $M_0 \in Sp(2n)$ satisfying (3.3).

Theorem 7. *Using Theorems* 5 *and* 6, *for sufficiently small $\tau > 0$ as the time-step, we define*

$$
\psi^{(m)}(w,\tau) = \sum_{k=0}^{m} \phi^{(k)}(w)\tau^k, \ m = 1, 2, \cdots. \tag{3.5}
$$

Then the gradient transformation

$$
w \to \hat{w} = \psi_w^{(m)}(w,\tau) \tag{3.6}
$$

with Jacobian $N^{(m)}(w,\tau) \in Sm(2m)$ *satisfies*

$$|N^{(m)}C - A| \neq 0 \tag{3.7}$$

and defines implicitly a canonical difference scheme $\hat{z} = z^k \to z^{k+1} = z$ *of* m*-th order accuracy upon substitution*

$$\hat{w} = Az^k + Bz^{k+1}, \quad w = Cz^k + Dz^{k+1}. \tag{3.8}$$

For the special case of type (III), the generating function $\phi(w,t)$ is odd in t. Then Theorem 7 leads to a family of canonical difference schemes of arbitrary even order accuracy, generalizing the centered Euler scheme, as follows.

Theorem 8. *Using Theorems* 5 *and* 6, *for sufficiently small* $\tau > 0$ *as the time-step, we define*

$$\psi^{(2m)}(w,\tau) = \sum_{k=1}^{m} \phi^{(2k-1)}(w)\tau^{2k-1}, \; m = 1, 2, \cdots. \tag{3.9}$$

Then the gradient transformation

$$w \to \hat{w} = \psi_w^{(2m)}(w,\tau) \tag{3.10}$$

with Jacobian $N^{(2m)}(w,\tau) \in Sm(2n)$ *satisfies*

$$|N^{(2m)}C - A| \neq 0$$

and defines implicitly a canonical difference scheme $\hat{z} = z^k \to z^{k+1} = z$ *of* $2m$*-th order accuracy upon substitution* (3.8). *The case* $m = 1$ *is the centered Euler scheme* (2.6).

For linear canonical system (2.1), (2.2) the type (III) generating function is the quadratic form

$$\phi(w,\tau) = \frac{1}{2}w'(2J\tanh(\frac{\tau}{2}L)), \; L = J^{-1}S, \; S' = S, \tag{3.11}$$

where

$$\tanh\lambda = \lambda - \frac{1}{3}\lambda^3 + \frac{2}{15}\lambda^5 - \frac{17}{312}\lambda^7 + \cdots = \sum_{k=1}^{\infty} a_{2k-1}\lambda^{2k-1}.$$

$$a_{2k-1} = 2^{2k}(2^{2k}-1)B_{2n}/(2k)!, \quad B_{2k} \text{ — Bernoulli numbers,}$$

$$2J\tanh(\frac{\tau}{2}L) \in Sm(2n).$$

(3.10) becomes symplectic difference schemes

$$z^{k+1} - z^k = \Big(\sum_{k=1}^{m} a_{2k-1}(\frac{\tau}{2}L)^{2k-1}\Big)(z^{k+1} + z^k). \tag{3.12}$$

The case $m = 1$ is the centered Euler scheme (2.3).

Several specific S-schemes up to fourth order accuracy are given in Appendix 1.

§4 S-scheme for Infinite Dimensional Hamiltonian Systems

4.1 An infinite dimensional hamiltonian equation

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

Let H be a functional in Hamiltonian mechanics. We have the Hamiltonian equation in $B \times B^\star$:

$$\begin{aligned} \frac{dp}{dt} &= -\frac{\delta H}{\delta q}(q,p,t), \\ \frac{dq}{dt} &= \frac{\delta H}{\delta p}(q,p,t), \end{aligned} \tag{4.1}$$

where $\frac{\delta}{\delta q}$, $\frac{\delta}{\delta p}$ are functional derivatives.

We denote $z = (q,p) \in B \times B^\star$, then we get formally the form of (4.1)

$$\frac{dz}{dt} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} H_z.$$

We define the operator J as

$$\begin{aligned} J: \quad & B \times B^\star \to (B \times B^\star)^\star = B^\star \times B \\ & J(q,p) = (-p,q) \end{aligned}$$

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

$$J = \begin{bmatrix} 0 & -I_{B^\star} \\ I_B & 0 \end{bmatrix} \qquad J^{-1} = \begin{bmatrix} 0 & I_B \\ -I_{B^\star} & 0 \end{bmatrix},$$

$$I_B : B \to B \text{ identity operator,}$$

$$I_{B^\star} : B^\star \to B^\star \text{ identity operator,}$$

we write them briefly as I.

Then the H-system has the form

$$\frac{dz}{dt} = J^{-1} H_z, \tag{4.2}$$

where $H_z = (\frac{\delta H}{\delta q}, \frac{\delta H}{\delta p})$, with canonical 2-form:

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

where $\alpha_1, \alpha_2 \in B \times B^\star$, and $\langle , \rangle$ is the dual product.

4.2 Generating functional and difference schemes

Suppose f: $B \times B^\star \to (B \times B^\star)^\star$

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

We call f a gradient transformation, or potential operator, if there is ϕ: $B \times B^\star \to R$ such that:

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

Let g: $B \times B^\star \to B \times B^\star$ be a canonical transformation

$$z \to \hat{z} = g(z)$$

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

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

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

Lemma 1 ([17]). *If the following conditions are satisfied:*

1. *F is an operator: $E \to E^\star$, E is a reflexive Banach space,*
2. *F has Gateaux differential $DF(x,h)$ in U which belongs to E and is defined by $|x - x_0| < r$,*
3. *functional $\langle DF(x,h_1),h_2\rangle$ is continuous in U, then F is a potential operator iff $\langle DF(x,h_1),h_2\rangle$ is symmetric for $\forall x \in U$:*

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

Theorem 3′. *T carries every symplectic transformation into gradient transformation, if:*

$$T^\star \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} T = \mu \begin{bmatrix} -J & 0 \\ 0 & J \end{bmatrix}$$

i.e.,

$$\begin{aligned} &A_1 = -\mu^{-1}JC^\star, \quad B_1 = \mu^{-1}JA^\star, \\ &C_1 = \mu^{-1}JA^\star, \qquad D_1 = -\mu^{-1}JB^\star, \\ &T = \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \quad T^{-1} = \begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix}. \end{aligned} \tag{4.3}$$

With the aid of the above theorem, like the finite dimensional case, we have

Theorem 5′. *Let T be defined as above. $z \to \hat{z} = g(z,t)$ is a canonical transformation. $z(t)$ is the solution of* (4.2).

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

1) *$g(\star,0)$ is a linear canonical transformation, $M(z,0) = M_0$ is independent of z.*

2) *$g^{-1}(z,0)g(\star,t)$ is a canonical transformation dependent on t, and carries $z(t)$ into $z(0)$.*

3) *$CM_0 + D$ is nonsingular,*

then there is a gradient transformation dependent on t: $w \to \hat{w} = f(w,t)$ and a generating functional $\phi(w,t)$ for sufficiently small $|t|$, such that:

(1) $\quad [\hat{w} - f(w,t)]_{\hat{w}=A\hat{z}+Bz,w=C\hat{z}+Dz} = 0.$

(2) $\quad \phi_t(w,t) = -\mu H(C_1\phi_w(w,t) + D_1 w)|_{w=C\hat{z}+Dz}. \qquad (4.4)$

Like the finite dimensional case, we can determine by recursion all possible time-dependent generating functionals for Hamiltonians $H(z)$ analytic in z.

$$
\begin{aligned}
\phi(w,t) &= \sum_{k=0}^{\infty} \phi^{(k)}(w)t^k, \\
\phi^{(0)}(w,t) &= \frac{1}{2}\langle w^\star, N_0 w\rangle, \quad N_0 = (AM_0+B)(CM_0+D)^{-1}, \\
\phi^{(1)}(w) &= -\mu H(E_0 w), \quad E_0 = (CM_0+D)^{-1}, \\
k \geq 1: \quad \phi^{(k+1)}(w) &= -\frac{1}{k+1}\sum_{m=1}^{k}\frac{\mu}{m!}\sum_{k_1+k_2+\cdots+k_m=k} H^{(m)}(E_0 w) \\
&\quad \times \left(C_1\phi_w^{(k_1)}(w)\right)\cdots\left(C_1\phi_w^{(k_m)}(w)\right).
\end{aligned} \tag{4.5}
$$

Remark. All conclusion concerning construction of S-scheme via generating functional is true when the J-symplectic form is replaced by K-symplectic form in finite or infinite dimensional case.

Remark. When we take $B = R^n$, $q = (q_1, \cdots, q_n) \in R^n$, $p = (p_1, \cdots, p_n) \in (R^n)^\star = R^n$, equations (4.1) become the canonical Hamiltonian equations (1.1). All the conclusion of the finite dimensional case can be regarded as a special case of infinite dimensional case.

Remark. Using above method, we get a semi-discrete S-scheme (involving time discretization only), in other words, we obtained an ∞-dim symplectic transformation in space $B \times B^\star$. In order to obtain a fully discrete S-scheme in $R^n \times R^n$, we must approximate spatial derivative by central difference. As we have done in §6, a fully discrete S-scheme for wave equation is obtained.

Another way is a method of lines: discretizing spatial derivatives, then we get a system of Hamiltonian ODE's. For fully discrete S-scheme, we use methods of constructing S-schemes for finite dimensional H-system [1, 25].

§5 Multi-level S-schemes

We first consider an LH-system

$$\frac{du}{dt} = J^{-1}Au, \tag{5.1}$$

where A is a symmetric matrix. For this system we consider a three-level difference scheme

$$u^{n+1} - \phi_1 u^n - \phi_2 u^{n-1} = 0. \tag{5.2}$$

Introducing a new variable $v^n = u^{n-1}$, we obtain an equivalent two-level scheme

$$\begin{bmatrix} u^{n+1} \\ v^{n+1} \end{bmatrix} = \begin{bmatrix} \phi_1 & \phi_2 \\ I & 0 \end{bmatrix} \begin{bmatrix} u^n \\ v^n \end{bmatrix}. \tag{5.3}$$

In this case an equivalent H-system is given by

$$\frac{d}{dt}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & J^{-1} \\ J^{-1} & 0 \end{bmatrix} \begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}. \tag{5.4}$$

Rewrite it in the form

$$\frac{dz}{dt} = K^{-1}Az \tag{5.5}$$

where

$$K^{-1} = \begin{bmatrix} 0 & J^{-1} \\ J^{-1} & 0 \end{bmatrix}.$$

We call scheme (5.2) a S-scheme, if scheme (5.3) is K-symplectic, i.e.

$$\begin{bmatrix} \phi_1^T & I_n \\ \phi_2^T & 0 \end{bmatrix} \begin{bmatrix} 0 & J \\ J & 0 \end{bmatrix} \begin{bmatrix} \phi_1 & \phi_2 \\ I_n & 0 \end{bmatrix} = \begin{bmatrix} 0 & J \\ J & 0 \end{bmatrix}. \tag{5.6}$$

After a short computation, we can prove

Lemma 2 ([7]). *Scheme* (5.3) *is a S-scheme, iff* ϕ_1 *is an infinitesimal symplectic matrix,* $\phi_2 = I$.

Theorem 9. *Scheme*

$$u^{n+1} = u^{n-1} + 2\mathrm{sh}\,(\tau J^{-1}A)u^n \tag{5.7}$$

is a S-scheme with any order of accuracy, where

$$\mathrm{sh}\,(\lambda) = \lambda + \frac{\lambda^3}{3!} + \frac{\lambda^5}{5!} + \cdots + \frac{\lambda^{2m-1}}{(2m-1)!} + \cdots.$$

$m = 1$: It is the usual leap-frog scheme of second order

$$u^{n+1} = u^{n-1} + 2\tau J^{-1}Au^n. \tag{5.8}$$

$m = 2$: It is the generalized leap-frog scheme of fourth order

$$u^{n+1} = u^{n-1} + 2\tau J^{-1}Au^n + \frac{\tau^3}{3!}(J^{-1}A)^3u^n. \tag{5.9}$$

Leap-frog scheme for LH-systems can be generalized to the NLH-System (1.2). Consider a three-level scheme

$$Z^{n+1} - \phi_1(Z^n) - \phi_2(Z^{n-1}) = 0 \tag{5.10}$$

Introducing a new variable $V^n = Z^{n-1}$, then

$$T: \quad \begin{aligned} Z^{n+1} &= \phi_1(Z^n) + \phi_2(V^n) \\ V^{n+1} &= Z^n \end{aligned} \tag{5.10$'$}$$

We say (5.10) is a S-scheme if the Jacobian

$$dT = \frac{\partial(Z^{n+1}, V^{n+1})}{\partial(Z^n, V^n)} \quad \text{satisfies}$$

$$(dT)' \begin{bmatrix} 0 & J^{-1} \\ J^{-1} & 0 \end{bmatrix} (dT) = \begin{bmatrix} 0 & J^{-1} \\ J^{-1} & 0 \end{bmatrix}.$$

Lemma 2′. *Scheme* (5.10) *is a S-scheme, iff* $\frac{\partial\phi_1}{\partial Z^n}$ *is an infinitesimal symplectic matrix,* $\frac{\partial\phi_2}{\partial Z^n} = I$.

For example, the leap-frog scheme is a S-scheme:

$$Z^{n+1} = Z^{n-1} - 2\tau J^{-1}H_Z(Z^n).$$

As an application we consider two forms of H-system for wave equation $w_{tt} = w_{xx}$. The first form is to take its H-Functional as

$$H(v,u) = \frac{1}{2}\int(v^2 + u_x^2)dx, \text{where } u = w,\ v = w_t.$$

We write the H-system

$$\frac{dz}{dt} = J^{-1}Az, \tag{5.11}$$

where

$$J^{-1}A = \begin{bmatrix} 0 & \frac{\partial^2}{\partial x^2} \\ 1 & 0 \end{bmatrix}, \quad z = \begin{bmatrix} v \\ u \end{bmatrix}, \quad A = \begin{bmatrix} 1 & 0 \\ 0 & -\frac{\partial^2}{\partial x^2} \end{bmatrix}.$$

Another form is to put $v = w_t$, $u = w_x$,

$$\frac{dz}{dt} = \mathcal{D}\frac{\delta H}{\delta z}, \qquad H(v,u) = \frac{1}{2}\int (v^2+u^2)dx, \tag{5.12}$$

where $\mathcal{D} = \begin{bmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{bmatrix}$, obviously it is a skew-adjoint operator. Rewrite it in form

$$\frac{dz}{dt} = K^{-1}Az, \tag{5.13}$$

where

$$K^{-1}A = \begin{bmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{bmatrix}, \quad A = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}, \quad K^{-1} = \mathcal{D}.$$

Let

$$\Delta_2 u_m = \frac{u(m+1) - 2u(m) + u(m-1)}{\Delta x^2} \tag{5.14}$$

$$\Delta_4 u_m = \frac{-u(m+2) + 16u(m+1) - 30u(m) + 16u(m-1) - u(m-2)}{12\Delta x^2} \tag{5.15}$$

$$\nabla_2 u_m = \frac{u(m+1) - u(m-1)}{2\Delta x} \tag{5.16}$$

$$\nabla_4 u_m = \frac{-u(m+2) + 8u(m+1) - 8u(m-1) + u(m-2)}{12\Delta x} \tag{5.17}$$

For the first kind of equation (5.11), the schemes (5.8), (5.9) have forms respectively

$$\begin{bmatrix} v^{n+1} \\ u^{n+1} \end{bmatrix} = \begin{bmatrix} v^{n-1} \\ u^{n-1} \end{bmatrix} + 2\Delta t \begin{bmatrix} 0 & M \\ I & 0 \end{bmatrix} \begin{bmatrix} v^n \\ u^n \end{bmatrix}, \tag{5.18}$$

$$\begin{bmatrix} v^{n+1} \\ u^{n+1} \end{bmatrix} = \begin{bmatrix} v^{n-1} \\ u^{n-1} \end{bmatrix} + 2\Delta t \begin{bmatrix} 0 & M \\ I & 0 \end{bmatrix} \begin{bmatrix} v^n \\ u^n \end{bmatrix} + \frac{\Delta t^3}{3} \begin{bmatrix} 0 & M \\ I & 0 \end{bmatrix}^3 \begin{bmatrix} v^n \\ u^n \end{bmatrix}. \tag{5.19}$$

Here I is $n \times n$ identity matrix, M is $n \times n$ matrix. According to (5.14), (5.15) it may be put in two forms

$$M_1 : \quad \frac{1}{\Delta x^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & 1 \\ 1 & -2 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & -2 & 1 \\ 1 & 0 & \cdots & 1 & -2 \end{bmatrix}$$

$$M_2 : \quad \frac{1}{12\Delta x^2}\begin{bmatrix} -30 & 16 & -1 & 0 & \cdots & -1 & 16 \\ 16 & -30 & 16 & -1 & \cdots & 0 & -1 \\ -1 & 16 & -30 & 16 & -1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -1 & 0 & 0 & \cdots & 16 & -30 & 16 \\ 16 & -1 & 0 & \cdots & -1 & 16 & -30 \end{bmatrix}$$

In scheme (5.18) if $M = M_1$ we express this scheme with accuracy $O(\Delta t^2 + \Delta x^2)$ by SLFM $(2,2)$ and if $M = M_2$ we express it by SLFM $(2,4)$.

In scheme (5.19), if $M = M_1$ we express it by SLFM $(4,2)$ and if $M = M_2$ we express it by SLFM $(4,4)$.

For the second kind of equation (5.13), the schemes (5.8), (5.9) become

$$\begin{bmatrix} v^{n+1} \\ u^{n+1} \end{bmatrix} = \begin{bmatrix} v^{n-1} \\ u^{n-1} \end{bmatrix} + 2\Delta t \begin{bmatrix} 0 & M \\ M & 0 \end{bmatrix} \begin{bmatrix} v^{n} \\ u^{n} \end{bmatrix},$$

$$\begin{bmatrix} v^{n+1} \\ u^{n+1} \end{bmatrix} = \begin{bmatrix} v^{n-1} \\ u^{n-1} \end{bmatrix} + 2\Delta t \begin{bmatrix} 0 & M \\ M & 0 \end{bmatrix} \begin{bmatrix} v^{n} \\ u^{n} \end{bmatrix} + \frac{\Delta t^3}{3}\begin{bmatrix} 0 & M \\ M & 0 \end{bmatrix}^3 \begin{bmatrix} v^{n} \\ u^{n} \end{bmatrix}.$$

Here M is $n \times n$ matrix, according to (5.16), (5.17) they are

$$M_3 : \quad \frac{1}{2\Delta x}\begin{bmatrix} 0 & 1 & 0 & \cdots & -1 \\ -1 & 0 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & 0 & 1 \\ 1 & 0 & \cdots & -1 & 0 \end{bmatrix}$$

$$M_4 : \quad \frac{1}{12\Delta x}\begin{bmatrix} 0 & 8 & -1 & 0 & \cdots & 1 & -8 \\ -8 & 0 & 8 & -1 & \cdots & 0 & 1 \\ 1 & -8 & 0 & 8 & -1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -1 & 0 & \cdots & \cdots & -8 & 0 & 8 \\ 8 & -1 & 0 & \cdots & 1 & -8 & 0 \end{bmatrix}$$

In scheme (5.18), if $M = M_3$ we express it by KLFM $(2,2)$ and if $M = M_4$ we express it by KLFM $(2,2)$, and if $M = M_4$ we express it by KLFM $(2,4)$.

In scheme (5.19), if $M = M_3$ we express it by KLFM $(4,2)$ and if $M = M_4$ we express it by KLFM $(4,4)$.

Lemma 3. *Eigenvalues of matrices*

$$\begin{bmatrix} 0 & M_1 \\ I & 0 \end{bmatrix}, \begin{bmatrix} 0 & M_2 \\ I & 0 \end{bmatrix}, \begin{bmatrix} 0 & M_3 \\ M_3 & 0 \end{bmatrix}, \begin{bmatrix} 0 & M_4 \\ M_4 & 0 \end{bmatrix}$$

are

$$\begin{aligned} \mu_k^{(1)} &= \pm \frac{2i}{\Delta x} \sin(\frac{\pi k}{2N}), \quad \mu_k^{(2)} = \pm \frac{i}{\Delta x} \sqrt{4 \sin^2 \frac{\pi k}{2N} + \frac{4}{3} \sin^4 \frac{\pi k}{2N}} \\ \mu_k^{(3)} &= \pm \frac{i}{\Delta x} \sin(\frac{\pi k}{2N}), \quad \mu_k^{(4)} = \pm \frac{i}{\Delta x} (\frac{1}{6} \sin \frac{2\pi k}{2N} - \frac{8}{6} \sin \frac{\pi k}{2N}) \\ &k = 0, 1, \cdots, 2N-1, \end{aligned}$$

respectively.

Above eigenvalues and criterions in [20] are used to derive the stability conditions in the following Table 1.

Using above scheme, numerical solutions of problem (6.4) have been done, we will list the numerical results and test of stability in Appendix 2 Table (2-5).

Remark. Under the condition that the eigenvalues of infinitesimally symplectic matrices J^{-1} A are purely imaginary the region of stability of the generalized leap-frog scheme (5.6) tends to the full real axis as the orders of accuracy increase to infinity [10].

Table 1

H-eq.	scheme	error of approximation	stability condition
$\frac{d}{dt}\begin{bmatrix} v \\ u \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} v \\ -u_{xx} \end{bmatrix}$	SLFM(2,2)	$o(\Delta t^2 + \Delta x^2)$	$\Delta t/\Delta x \le 1/2$
	SLFM(2,4)	$o(\Delta t^2 + \Delta x^4)$	$\Delta t/\Delta x \le 0.4330$
	SLFM(4,2)	$o(\Delta t^4 + \Delta x^2)$	$\Delta t/\Delta x \le 1.4237$
	SLFM(4,4)	$o(\Delta t^4 + \Delta x^4)$	$\Delta t/\Delta x \le 1.2330$
$\frac{d}{dt}\begin{bmatrix} v \\ u \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix}$	KLFM(2,2)	$o(\Delta t^2 + \Delta x^2)$	$\Delta t/\Delta x \le 1/2$
	KLFM(2,4)	$o(\Delta t^2 + \Delta x^4)$	$\Delta t/\Delta x \le 0.7287$
	SLFM(4,2)	$o(\Delta t^4 + \Delta x^2)$	$\Delta t/\Delta x \le 2.8473$
	SLFM(4,4)	$o(\Delta t^4 + \Delta x^4)$	$\Delta t/\Delta x \le 2.0750$

§6 Numerical Examples

6.1 Two-body problem

In celestial mechanics, the simplest and famous example is the two-body problem. We outline its arguments here

(i) $M = R^2 \times \{R^2 - (0)\}$, phase space.

(ii) $m \in M$, initial data.

(iii) Hamiltonian, $H(p, q) = \|p\|^2/2 - 1/\|q\|$.

It has been proved that if angular momentum $G \neq 0$ the path is an ellipse, parabola, or hyperbola according to $E < 0$, $E = 0$, $E > 0$. The case $G = 0$ is degenerate, the path is a straight line.

We choose (A-III-4)

$$z^{n+1} = z^n + \tau J^{-1} H_z\left(\frac{z^{n+1} + z^n}{2}\right) + \frac{\tau^3}{24}((J^{-1}H_z)' H_{zz}(J^{-1}H_z))_z\left(\frac{z^{n+1} + z^n}{2}\right), \tag{6.1}$$

where $z^n = \begin{pmatrix} p^n \\ q^n \end{pmatrix}$, τ is step length. This scheme is fourth order. Because the scheme is symplectic, we keep $G = q_1 p_2 - p_1 q_2$ constant, i.e., keep the path's curvature unchanged. We have computed all the kinds of paths. The paths are the same as the theory predicts. In elliptic case, the R-K method cannot be carried through. As a matter of fact, it will overflow after short time. Because scheme (6.1) is A-stable, it gives good result in all cases. In Appendix 2 Table 6 we will list comparison data between R-K method and S-schemes (fourth order and second order).

6.2 Wave equation

Let $B = H^1$, $P = H^1 \times H^{-1}$. In $H^2 \times H^1$, a subspace of P, we have the Hamiltonian functional

$$H(u, v) = \int_{R^2} \frac{1}{2}(v^2 + (\nabla u)^2) dx.$$

The corresponding Hamiltonian vector field is $(v, \Delta u)$. The associated H-equation is

$$\begin{aligned} \frac{dv}{dt} &= -\frac{\delta H}{\delta u} = \Delta u, \\ \frac{du}{dt} &= \frac{\delta H}{\delta v} = v. \end{aligned} \tag{6.2}$$

Choosing $T = \begin{bmatrix} -J & +J \\ \frac{1}{2}I & \frac{1}{2}I \end{bmatrix}$, we get a S-scheme (A-III-4) of fourth order for wave equation [8]

$$z^{n+1} = z^n + \tau J^{-1} H_z - \frac{2\tau^3}{4!} J^{-1} H_{zz} J^{-1} H_{zz} J^{-1} H_z, \tag{6.3}$$

e.g.

$$\begin{bmatrix} v \\ u \end{bmatrix}^{n+1} = \begin{bmatrix} v \\ u \end{bmatrix}^{n} + \tau \begin{bmatrix} 0 & \Delta \\ I & 0 \end{bmatrix} \begin{bmatrix} \bar{v} \\ \bar{u} \end{bmatrix} - \frac{\tau^3}{12} \begin{bmatrix} 0 & \Delta \\ I & 0 \end{bmatrix}^3 \begin{bmatrix} \bar{v} \\ \bar{u} \end{bmatrix},$$

where $\bar{v} = \frac{1}{2}(v^{n+1} + v^n)$, $\bar{u} = -\frac{1}{2}(u^{n+1} + u^n)$.

If we take Δ as the fourth-order centered difference approximation, using periodic boundary condition we get

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

where

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

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

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

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, $h = \frac{2\pi}{N}$.

Computations were done. The initial and boundary conditions are taken to be

$$\begin{aligned} &u(0,x) = \sin x \quad \text{for } 0 \le x \le 2\pi, \\ &u_t(0,x) = \cos x \quad \text{for } 0 \le x \le 2\pi, \\ &u(t,0) = u(t,2\pi). \end{aligned} \tag{6.4}$$

The exact solution is $u(t,x) = \sin(x+t)$.

We list the numerical and corresponding exact results in Appendix 2 table 7.

§7 S-schemes and Chaos

Most systems with two or more degrees of freedom have some chaotic motions and some regular motions. The regular motions occur then the system is far away from resonances of low order. This is in accord with the conclusion of the KAM theorem. On the other hand, when the system is near such resonances, chaotic motion occurs.

Hénon and Heiles [21] considered a system with two degrees of freedom with coordinates $q_1(t)$ and $q_2(t)$ and conjugate momenta $p_1(t)$ and $p_2(t)$. Their Hamiltonian is

$$H(q_1,q_2,p_1,p_2) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2 + 2q_1^2 q_2 - \frac{2}{3}q_2^3). \tag{7.1}$$

They found that for total energy E less than $1/12$, the solutions were regular for most initial conditions. As E increased the fraction of initial condition leading to chaotic solutions increased.

For (7.1), its canonical equations are

$$\frac{d}{dt}\begin{bmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} p_1 \\ p_2 \\ q_1 + 2q_1 q_2 \\ q_2 + q_1^2 - q_2^2 \end{bmatrix}. \tag{7.2}$$

Using the explicit scheme (A-II-1), we obtain

$$\begin{aligned} p_1^{n+1} &= p_1^n - \tau(q_1^n + 2q_1^n q_2^n), \\ p_2^{n+1} &= p_2^n - \tau(q_2^n + (q_1^2)^n - (q_2^2)^n), \\ q_1^{n+1} &= q_1^n + \tau p_1^{n+1}, \\ q_2^{n+1} &= q_2^n + \tau p_2^{n+1}. \end{aligned} \tag{7.3}$$

Obviously this scheme is a symplectic transformation, approximating original system in second order precision, of course, it is regarded as an area-preserving mapping. As the time step we selected $\tau = 0.0005$ for 20000 cycles, the CPU time was 10 minutes (IBM-4341). The results obtained are in agreement with the results of Hénon-Heiles (1964).

In Appendix 2 Fig. 1, we list the graphics of surfaces of section computed with scheme (7.3) for $E(\text{or } H) = 1/24, 1/12, 1/8, 1/6$. Good results are also obtained by the implicit S-scheme (fourth order) (A-III-4).

Hénon [22] accepted Kruskal's suggestion [21] to study an area-preserving mapping directly.

$$\begin{aligned} T: \quad x_{n+1} &= 1 - ax_n^2 + y_n \\ y_{n+1} &= bx_n \end{aligned} \tag{7.4}$$

describes conservative system, dissipative system and logistic system when $|b| = 1$, $|b| < 1$ and $|b| = 0$ respectively.

In the case $b = \pm 1$, T is an area-preserving mapping and may be thought of as the Poincare section for a H-system with two degrees of freedom.

Remark. The research of dynamical system with three degrees of freedom can be reduced to the study of a four dimensional mapping. Scheme (7.3) is an area preserving mapping, therefore it is a good tool for studying dynamical system with three degrees of freedom.

Now we consider the equation

$$\frac{du}{dt} = u(1-u) \tag{7.5}$$

with initial condition $u(0) = u_0$. Using leap-frog scheme (5.8), we get a difference equation

$$\frac{u_{n+1} - u_{n_1}}{2h} = u_n(1 - u_n), \tag{7.6}$$

with initial condition $u(0) = u_0$ and $u_1 = u_0 + hu_0(1 - u_0)$ computed by Euler's forward difference scheme. Using leap-frog method described in (5.10), we obtain

$$\begin{aligned} u_{n+1} &= 2hu_n(1 - u_n) + v_n \\ v_{n+1} &= u_n. \end{aligned} \tag{7.7}$$

Thus we have a mapping $\bar{T}$: $R^2 \to R^2$ defined by

$$\begin{aligned} X &= 2hx(1-x) + y \\ Y &= x \end{aligned} \tag{7.8}$$

Scheme (7.6), in the sense of (5.6), is a S-scheme. The Jacobian matrix T is given by

$$d\bar{T} = \frac{\partial(X,Y)}{\partial(x,y)} = \begin{bmatrix} 2h(1-2x) & 1 \\ 1 & 0 \end{bmatrix}$$

Obviously $|d\bar{T}| = -1$, therefore it is an area-preserving scheme.

Let $u_{2m}=p_m$, $u_{2m-1}=q_m$. Rewrite the equation in the following form [9] [23]

$$S: \quad \begin{aligned} \frac{p_m-p_{m-1}}{2h} &= q_m(1-q_m) \\ \frac{q_{m+1}-q_m}{2h} &= p_m(1-p_m) \end{aligned} \tag{7.9}$$

The above system is H-system with $H(p,q)=\frac{1}{2}(p^2-q^2)-\frac{1}{3}(p^3-q^3)$. Symplectic transformation (7.9) can be regarded as a composition transformation $\bar{T}\cdot\bar{T}$.

In general we must use the central difference for conservative systems. On the contrary, in order to describe a dissipative system we must employ mixed difference [24]

$$(1-\theta)\frac{u_{n+1}-u_{n-1}}{2h}+\theta\frac{u_{n+1}-u_n}{h}=u_n(1-u_n), \quad 0\le\theta\le 1, \tag{7.10}$$

or equivalently, a mapping

$$T_\theta: \quad \begin{aligned} u_{n+1} &= \tfrac{1-\theta}{1+\theta}v_n+\tfrac{2}{1+\theta}[(\theta+h)u_n-hu_n^2] \\ v_{n+1} &= u_n. \end{aligned} \tag{7.11}$$

Its Jacobian is

$$dT_\theta=\begin{bmatrix} 2(\theta+h-2hu_n)/(1+\theta) & (1-\theta)/(1+\theta) \\ 1 & 0 \end{bmatrix}.$$

Transform the mapping (7.11) by an affine transformation

$$\begin{aligned} u_n &= \frac{\theta+h}{2h}\left[(\frac{h-\theta}{1+\theta})x_n+1\right] \\ v_n &= \frac{\theta+h}{2h}\left[(\frac{h-\theta}{1+\theta})y_n+1\right] \end{aligned}$$

into the form (7.4) with $a=(h^2-\theta^2)/(1+\theta)^2$, $b=(1-\theta)/(1+\theta)$. In particular, we select $h=1.898, \theta=0.538$ then the corresponding map (7.4) with $a=1.4$ and $b=1.3$ is a Hénon's strange attractor [24], see Fig.3(c) in Appendix 2.

The step length $h=1.898$ is too large as time step for numerical integration. But it is still significant in studying an area mapping.

Appendix 1

In this Appendix we collect S-schemes for H-system (1.2) with precision up to fourth order. According to method of construction of S-schemes described in §3, we have

$$\begin{aligned} \phi^{(0)}(w) =& \frac{1}{2}w'N_0w, \\ \phi^{(1)}(w) =& -\mu H(E_0w), \\ \phi^{(2)}(w) =& -\frac{\mu}{2}H_{z_i}(C_1\phi_w^{(1)})_i, \\ \phi^{(3)}(w) =& -\frac{\mu}{3}\Big(\frac{1}{2!}H_{z_{i_1}z_{i_2}}(C_1\phi_w^{(1)})_{i_1}(C_1\phi_w^{(1)})_{i_2}+H_{z_i}(C_1\phi_w^{(2)})_i\Big), \\ \phi^{(4)}(w) =& -\frac{\mu}{4}\Big(\frac{1}{3!}H_{z_{i_1}z_{i_2}z_{i_3}}(C_1\phi_w^{(1)})_{i_1}(C_1\phi_w^{(1)})_{i_2}(C_1\phi_w^{(1)})_{i_3} \\ &+H_{z_{i_1}z_{i_2}}(C_1\phi_w^{(2)})_{i_1}(C_1\phi_w^{(1)})_{i_2}+H_{z_1}(C_1\phi_w^{(3)})_i\Big). \end{aligned} \tag{A-0}$$

In §3 case II, $M_0 = I_{2n}$, $\mu = 1$, by (3.1), we have

$$w = \begin{vmatrix} \hat{q} \\ p \end{vmatrix}, \quad C_1 = \begin{bmatrix} 0 & 0 \\ 0 & -I \end{bmatrix}, \quad D_1 = \begin{bmatrix} 0 & I \\ 0 & 0 \end{bmatrix}, \quad \text{H-J equation is} \phi_t = -H(p, -\phi_p).$$

As matrices in theorem 6, N_0, E_0 are

$$N_0 = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}, \quad E_0 = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}, \quad E_0 w = \begin{bmatrix} p \\ \hat{q} \end{bmatrix}.$$

Substituting μ, N_0, E_0, C_1 into (A-0) yields

$$\phi^{(0)}(w) = \frac{1}{2} w' N_0 w = \frac{1}{2} \hat{q}_i p_i,$$

where repeated subscripts i subject to Einstein summation convention.

$$\begin{aligned}
\phi^{(1)}(w) =& - H(p\hat{q}), \\
\phi^{(2)}(w) =& - \frac{1}{2!} H_{q_i} H_{p_i}, \\
\phi^{(3)}(w) =& - \frac{1}{3!} \Big(H_{q_i q_j} H_{p_i} H_{p_j} + H_{q_i p_j} H_{p_i} H_{q_j} + H_{p_i p_j} H_{q_i} H_{q_j} \Big), \\
\phi^{(4)}(w) =& - \frac{1}{4!} \Big(H_{q_i q_j q_k} H_{p_i} H_{p_j} H_{p_k} + H_{q_i q_j p_k} H_{p_i} H_{p_j} H_{q_k} \\
&+ H_{q_i p_j p_k} H_{p_i} H_{q_j} H_{q_k} + H_{p_i p_j p_k} H_{q_i} H_{q_j} H_{q_k} \\
&+ 5 H_{q_i q_j} H_{p_j p_k} H_{p_i} H_{q_k} + H_{q_i p_j} H_{q_j p_k} H_{p_i} H_{q_k} \\
&+ 3 H_{q_i p_j} H_{p_i p_k} H_{q_j} H_{q_k} + 3 H_{q_i q_j} H_{q_k p_i} H_{p_j} H_{p_k} \Big).
\end{aligned}$$

Scheme of first order: Using (3.5), (3.6), we have

$$\begin{aligned}
&\psi^{(1)}(w,\tau) = \phi^{(0)}(w) + \phi^{(1)}(w)\tau \\
&\hat{w} = \psi^{(1)}_w(w,\tau) = \phi^{(0)}_w(w) + \tau \phi^{(1)}_w(w) \\
&\begin{bmatrix} -\hat{p} \\ -q \end{bmatrix} = - \begin{bmatrix} p \\ \hat{q} \end{bmatrix} + \tau \begin{bmatrix} -H_q(p,\hat{q}) \\ -H_p(p,\hat{q}) \end{bmatrix},
\end{aligned}$$

where $\hat{p} = p^0$, $\hat{q} = q^0$. Thus we obtain scheme of first order accuracy

$$\begin{aligned}
p &= p^0 - \tau H_q(p, q^0), \\
q &= q^0 + \tau H_p(p, q^0).
\end{aligned} \tag{A-II-1}$$

Remark. This scheme will have 2nd-order accuracy when computing p in the $(n+1)$-th time step and q in the $(n+1+\frac{1}{2})$-th step. Especially, for separable H-system it is the staggered explicit scheme (2.7).

By similar derivation, we have scheme of second order:

$$\begin{aligned}
\psi^{(2)}(w,\tau) =& \psi^{(1)}(w,\tau) + \tau^2 \phi^{(2)}(w), \\
\hat{w} =& \psi^{(2)}_w(w,\tau) = \psi^{(1)}_w(w,\tau) + \tau^2 \phi^{(2)}_w(w). \\
p_i =& p_i^0 - \tau H_{q_i}(p, q^0) - \frac{\tau^2}{2} [H_{q_j q_i} H_{p_j} + H_{q_j} H_{p_j q_i}], \\
q_i =& q_i^0 + \tau H_{p_i}(p, q^0) + \frac{\tau^2}{2} [H_{q_j p_i} H_{p_j} + H_{q_j} H_{p_j p_i}].
\end{aligned} \tag{A-II-2}$$

Scheme of third order:

$$\begin{aligned}
\psi^{(3)}(w,\tau) =& \psi^{(2)}(w,\tau) + \tau^3\phi^{(3)}(w),\\
\hat{w} =& \psi_w^{(3)}(w,\tau) = \psi_w^{(2)}(w,\tau) + \tau^3\phi_w^{(3)}(w).\\
p_i =& p_i^0 - \tau H_{q_i}(p,q^0) - \frac{\tau^2}{2!}(H_{q_j q_i}H_{p_j} + H_{p_j q_i}H_{p_j})\\
&- \frac{\tau^3}{3!}[H_{q_k q_j q_i}H_{p_k}H_{p_j} + H_{q_k p_j q_i}H_{p_k}H_{q_j} + H_{p_k p_j q_i}H_{q_k}H_{q_j}\\
&+ H_{q_j p_k}(H_{p_j q_i}H_{q_k} + H_{p_j}H_{q_k q_i}) + 2H_{p_j p_k}H_{q_j q_i}H_{q_k}\\
&+ 2H_{q_j q_k}H_{p_j q_i}H_{p_k}], \qquad \text{(A-II-3)}\\
q_i =& q_i^0 + \tau H_{p_i}(p,q^0) + \frac{\tau^2}{2!}(H_{q_j p_i}H_{p_j} + H_{p_j p_i}H_{q_j})\\
&+ \frac{\tau^3}{3!}[H_{q_j p_k p_i}H_{p_j}H_{q_k} + H_{p_j p_k p_i}H_{q_j}H_{q_k} + H_{q_j q_k q_i}H_{p_j}H_{p_k}\\
&+ H_{q_j p_k}(H_{p_j p_i}H_{q_k} + H_{p_j}H_{q_k p_i}) + 2H_{p_j p_k}H_{q_j p_i}H_{q_k}\\
&+ 2H_{q_j q_k}H_{p_j p_i}H_{p_k}].
\end{aligned}$$

Scheme of fourth order:

$$\begin{aligned}
\psi^{(4)}(w,\tau) &= \psi^{(3)}(w,\tau) + \tau^4\phi^{(4)}(w),\\
\hat{w} &= \psi_w^{(4)}(w,\tau) = \psi_w^{(3)}(w,\tau) + \tau^4\phi_w^{(4)}(w).
\end{aligned} \qquad \text{(A-II-4)}$$

In §3, case III, $\mu = -1$, $M_0 = I$, $w = \frac{1}{2}(z+\hat{z})$, $\hat{w} = J(z-\hat{z})$, by (3.1) we have $C_1 = \frac{1}{2}J^{-1} = \frac{1}{2}\begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}$, $D_1 = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}$. H-J equation is $\phi_t = H(w - \frac{1}{2}J\phi_w)$,

$$N_0 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, E_0 = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}, E_0 w = \frac{1}{2}(z+\hat{z}) = \frac{1}{2}(z+z^0).$$

Substituting μ, N_0, E_0, C_1 into (A-0) yields

$$\begin{aligned}
\phi^{(0)}(w) &= 0,\\
\phi^{(1)}(w) &= H(w),\\
\phi^{(2)}(w) &= \frac{1}{2}H_z'(\frac{1}{2}J^{-1}H_z) = 0,\\
\phi^{(3)}(w) &= \frac{1}{3}H_{z_i}(w)(C_1\phi_w^{(2)})_i + \frac{1}{6}H_{z_i z_j}(C_1\phi_w^{(1)})_i(C_1\phi_w^{(1)})_j\\
&= \frac{1}{6}H_{z_i z_j}(C_1\phi_w^{(1)})_i(C_1\phi_w^{(1)})_j\\
&= \frac{1}{4!}\{H_{p_i p_j}H_{q_i}H_{q_j} - 2H_{p_i q_j}H_{p_j}H_{q_i} + H_{q_i q_j}H_{p_i}H_{p_j}\}, \quad \phi^{(4)}(w) = 0.
\end{aligned}$$

By similar derivation as above, we have scheme of second order:

$$\begin{aligned}
\psi^{(2)}(w,\tau) &= \psi^{(1)}(w,\tau) + \tau^2\phi^{(2)}(w) = \psi^{(1)}(w,\tau) = \phi^{(0)}(w) + \tau\phi^{(1)}(w),\\
\hat{w} &= \psi^{(2)}(w,\tau) = \tau\phi_w^{(1)}(w) = \tau H_z(w).
\end{aligned}$$

i.e.

$$J(z-\hat{z}) = \tau H_z(\frac{z+\hat{z}}{2}),$$
$$z = z^0 + \tau J^{-1} H_z(\frac{z+z^0}{2}). \tag{A-III-1}$$

i.e.

$$p = p^0 - \tau H_q(\frac{p+p^0}{2}, \frac{q+q^0}{2}),$$
$$q = q^0 + \tau H_p(\frac{p+p^0}{2}, \frac{q+q^0}{2}). \tag{A-III-2}$$

Scheme of fourth order:

$$\begin{aligned}\hat{w} =& \psi_w^{(4)}(w,\tau) = \tau\phi_w^{(1)}(w) + \tau^3\phi_w^{(3)}(w)\\ =& \tau H_z(w) + \frac{\tau^3}{4!}[(J^{-1}H_z)' H_{zz}(J^{-1}H_z)]_z(w),\end{aligned} \tag{A-III-3}$$

$$\begin{aligned}p_i =& p_i^0 - \tau H_{q_i}(\frac{p+p^0}{2}, \frac{q+q^0}{2}) - \frac{\tau^3}{4!}\{H_{p_j p_k q_i} H_{q_j} H_{q_k} + 2H_{p_j p_k} H_{q_j q_i} H_{q_k}\\ &- 2H_{p_j q_k q_i} H_{p_k} H_{q_j} - 2H_{p_k q_j} H_{p_j q_i} H_{q_k} - 2H_{p_k q_j} H_{p_j} H_{q_k q_i}\\ &+ 2H_{q_j q_k} H_{p_j q_i} H_{p_k} + H_{q_j q_k q_i} H_{p_j} H_{p_k}\},\\ q_i =& q_i^0 + \tau H_{p_i}(\frac{p+p^0}{2}, \frac{q+q^0}{2}) + \frac{\tau^3}{4!}\{H_{p_j p_k p_i} H_{q_j} H_{q_k} + 2H_{p_j p_k} H_{q_j p_i} H_{q_k}\\ &- 2H_{p_j q_k p_i} H_{p_k} H_{q_j} - 2H_{p_k q_j} H_{p_j p_i} H_{q_k} - 2H_{p_k q_j} H_{p_j} H_{q_k p_i}\\ &+ 2H_{q_j q_k p_i} H_{p_j} H_{p_k} + 2H_{q_j q_k} H_{p_j p_i} H_{p_k}\}.\end{aligned} \tag{A-III-4}$$

Appendix 2

This Appendix consists of Tables 2-7 and Figures 1-3, which give some computer results.

Table 2. Comparison of the exact solutions with the numerical solutions of eq. (5.11) with (6.4) and of (5.12) with initial data $u(0,x) = v(0,x) = \sin x$, using different leap-frog schemes, where $u(n,m)$ denotes value of $u(t,x)$ at $t = nDt$, $x = mDx$. Courant number $C = Dt/Dx = 0.4$, $Dx = \frac{2}{40}$.

Table 3. Similar results as in Table 2, but only with schemes, SLFM $(4,4)$ and KLFM $(4,4)$ under $C = 1.1$.

Table 4. Numerical tests of stability of scheme KLFM $(4,4)$ with $C = 2.09$ and 2.07, (critical $C = 2.075$).

Table 5. Numerical tests of stability of scheme SLFM $(4,4)$ with $C = 1.23$ and 1.24, (critical $C = 1.233$).

Table 6. Comparison of numerical results for 2-body problem by 5-6-th order R-K scheme and by 4-th and 2-nd order S-schemes. This shows that lower order S-schemes are comparable in precision with higher order R-K schemes.

Table 7. Comparison of the exact solution with the numerical results of eq. (5.11) with (6.4) using the scheme (6.3) adapted from A-III-4 scheme.

Fig. 1. Intersections of the orbits of Hénon-Heiles system with the Poincare section, computed by 2-nd order S-schemes. (A): $H = \frac{1}{24}$, all motions are regular. (B): $H = \frac{1}{12}$, all motions are regular. (C): $H = \frac{1}{8}$, most of the motions are regular but chaotic motions appear. (D): $H = \frac{1}{6}$, almost all motions are chaotic.

Fig. 2. Orbit of the conservative system (7.11) with $\theta = 0$, (A): $h = 0.4$, $u_0 = 0.58$. There are 2 rings, each ring contains 11 archipelagoes, each archipelago consists basically of 5 isles, (B): $h = 0.1$, $u_0 = 0.54$. There are 2 rings with simple, regular structure. (C): $h = 0.4$, $u_0 = 0.5$. (D): $h = 0.4$, $u_0 = 0.6$. In (C), (D) the structure are grossly similar to that of (A), but more irregular, especially in (D).

Fig. 3. Orbit of dissipative system (7.11) with $\theta > 0$, arising from mixed leap-frog schemes (7.10) for system (7.5). (A): $h = 1.898$, $\theta = 0.538$, $u_0 = 0.58$. This is the strange attractor of the Hénon map. (B): $h = 0.1$, $\theta = 0.01$, $u_0 = 0.6$. (C): $h = 0.4$, $\theta = 0.01$, $u_0 = 0.56$. (D): $h = 0.5$, $\theta = 0.01$, $u_0 = 0.56$. The last 3 graphs show interesting spiral structures. Here (B) is a dissipative counterpart of Fig. 2 (B), with 2 rings changed into 2 contracting spirals. In (C), (D), the spirals have more complicated structures than that of (B). Note that the number of branches of the contracting spiral is 8 in (C), 6 in (D).

Fig. 2 (A,C,D) and Fig. 3 (B,C,D) contain some interesting features, which seems, to the authors' knowledge, to be new.

Table 2

$Dt = 0.06283$		$Dx = 0.15708$		$C = Dt/Dx = 0.4$
SCHEME	$u(99,0)$	$u(99,10)$	$u(99,20)$	$u(99,30)$
KLFM(4,2)	0.06279	0.99777	−0.06778	−0.99777
KLFM(4,4)	0.06279	0.99815	−0.06279	−0.99815
KLFM(2,2)	0.04109	0.99149	−0.04109	−0.99149
KLFM(2,4)	0.03701	0.99930	−0.03701	−0.99930
SLFM(2,2)	0.06047	0.99817	−0.06048	−0.99817
SLFM(2,4)	0.05636	0.99841	−0.05635	−0.99841
SLFM(4,2)	0.06277	0.99803	−0.06277	−0.99803
SLFM(4,4)	0.06277	0.99803	−0.06279	−0.99803
Analytical Solution	0.06279	0.99803	−0.06279	−0.99803

Table 3

$Dt = 0.17279$		$Dx = 0.15708$		$C = Dt/Dx = 1.1$
SCHEME	$u(99,0)$	$u(99,10)$	$u(99,20)$	$u(99,30)$
KLFM(4,4)	−0.98519	0.17145	0.98519	−0.17145
SLFM(4,4)	−0.98520	0.17111	0.98532	−0.17109
Analytical Solution	−0.98511	0.17191	0.98512	−0.17192

Table 4

	$Dt = 0.15708$	KLFM(4,4)		
C-number	$u(30,0)$	$u(99,0)$	$u(30,10)$	$u(99,10)$
2.09	-0.68332	overflow	-0.73430	overflow
2.07	-0.63119	0.99853	-0.77565	0.05482
Analytical Solution	-0.63208	0.99870	-0.77490	0.05089

Table 5

	$Dt = 0.15708$	SLFM(4,4)		
C-number	$u(30,0)$	$u(99,0)$	$u(30,10)$	$u(99,10)$
1.23	-0.23288	0.75542	-0.97253	0.65509
1.24	0.09666	overflow	-0.55163	overflow
Analytical Solution	-0.23344	0.75630	-0.97237	0.65423

Table 6

Runge-Kutta-Verner method (5 or 6 order)

Initial data 1, 1, 1, 1. Step length: 0.05

	p^1	p^2	q^1	q^2
$t = 0.5$	0.88041	0.88041	1.46630	1.46630
$t = 2.0$	0.74699	0.74699	2.66716	2.66716
$t = 4.0$	0.68254	0.68254	4.08757	4.08757
$t = 7.0$	0.63992	0.63992	6.06290	6.06290
$t = 10.0$	0.61794	0.61794	7.94673	7.94673

S-Scheme 4 order (A-III-4)

Initial data 1, 1, 1, 1. Step length: 0.05

	p^1	p^2	q^1	q^2
$t = 0.5$	0.88041	0.88041	1.46629	1.46629
$t = 2.0$	0.74699	0.74699	2.66713	2.66713
$t = 4.0$	0.68254	0.68254	4.08750	4.08750
$t = 7.0$	0.63991	0.63991	6.06281	6.06281
$t = 10.0$	0.61793	0.61793	7.94660	7.94660

S-Scheme 2 order (A-III-2)

Initial data 1, 1, 1, 1. Step length: 0.05

	p^1	p^2	q^1	q^2
$t = 0.5$	0.88045	0.88045	1.46635	1.46635
$t = 2.0$	0.74706	0.74706	2.66732	2.66732
$t = 4.0$	0.68262	0.68262	4.08789	4.08789
$t = 7.0$	0.64001	0.64001	6.06348	6.06348
$t = 10.0$	0.61803	0.61803	7.94756	7.94756

Table 7

$h = 2 * 3.14159/40 \quad t = 1.0$

$X = M * h$	$\sin(x + t)$	A-III-4 $Dt = 0.15$	A-III-4 $Dt = 0.3$
$M = 0$	−0.54402	−0.54419	−0.54470
$M = 2$	−0.77668	−0.77679	−0.77717
$M = 4$	−0.93332	−0.93335	−0.93358
$M = 6$	−0.99859	−0.99855	−0.99861
$M = 8$	−0.96611	−0.96600	−0.96591
$M = 10$	−0.83907	−0.83890	−0.83870
$M = 12$	−0.62989	−0.62967	−0.62940
$M = 14$	−0.35906	−0.35878	−0.35850
$M = 16$	−0.05307	−0.05279	−0.05251
$M = 18$	0.25811	0.25835	0.25657
$M = 20$	0.54402	0.54422	0.54434
$M = 22$	0.77668	0.77682	0.77680
$M = 24$	0.93332	0.93337	0.93320
$M = 26$	0.99886	0.99857	0.99823
$M = 28$	0.96611	0.96601	0.96552
$M = 30$	0.83907	0.83916	0.83829
$M = 32$	0.62989	0.62968	0.62900
$M = 34$	0.35906	0.35881	0.35809
$M = 36$	0.05307	0.05282	0.05212
$M = 38$	−0.25811	−0.25832	−0.25896
$M = 40$	−0.54402	−0.54419	−0.54471

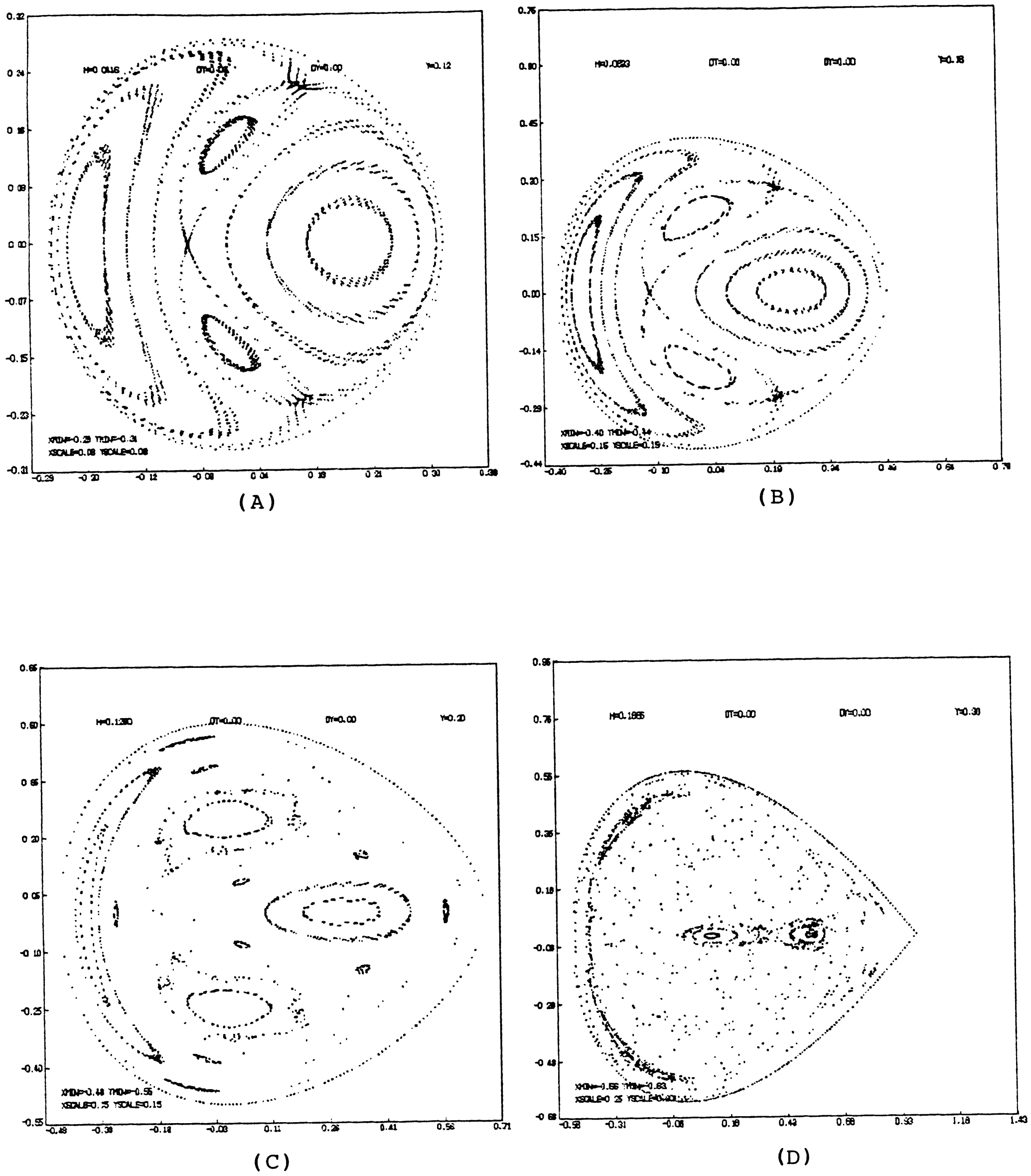

Fig. 1

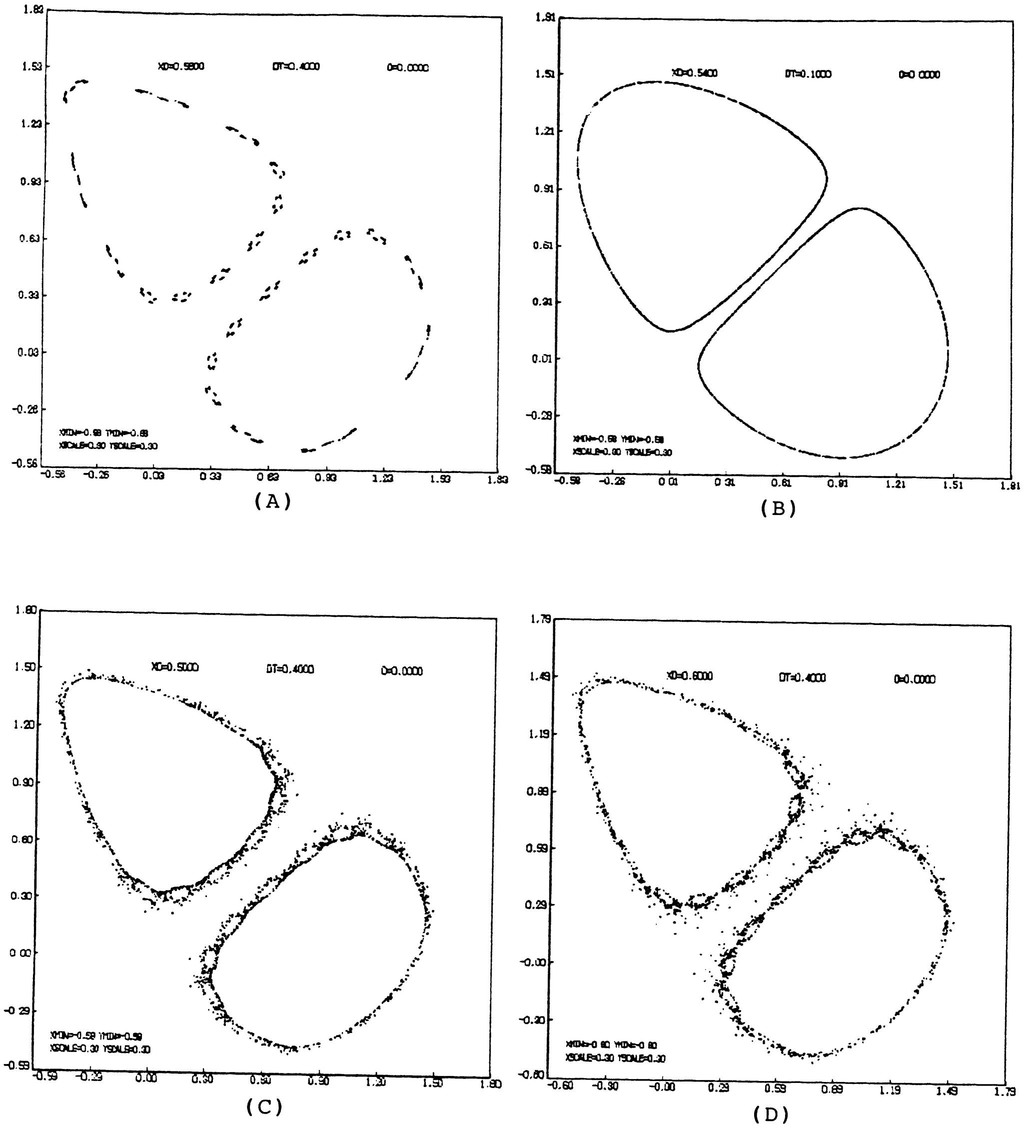

Fig. 2

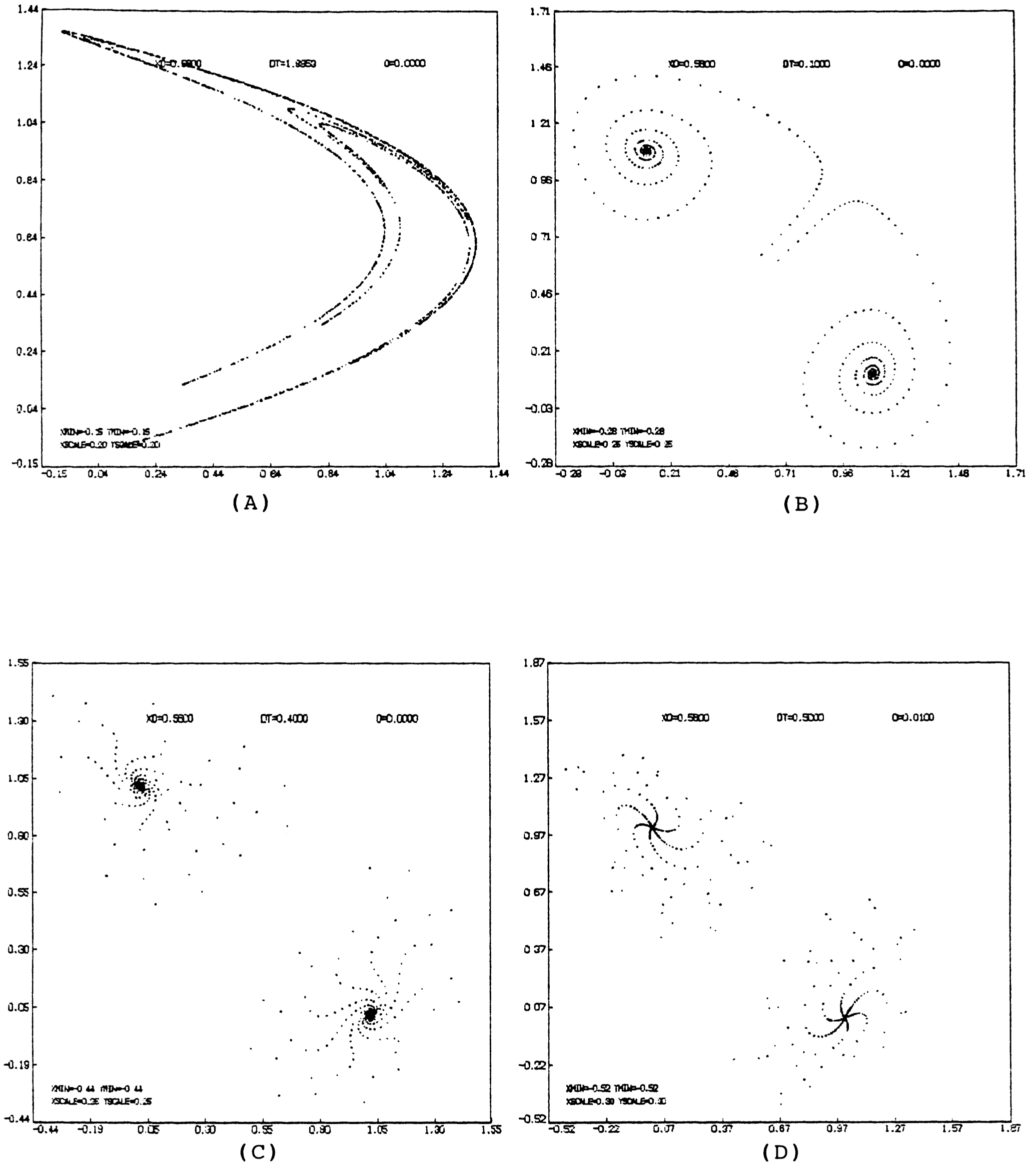

Fig. 3

References

1 Feng K. On difference schemes and symplectic geometry. In Feng K, ed. Proc 1984 Beijing Symp Diff Geometry and Diff Equations. Beijing: Science Press, 1985. 42–58

2 Feng K. Canonical difference schemes for Hamiltonian canonical differential equation. In Xiao S, ed. Inter workshop on applied differential equation. Singapore: World Scientific. 1985: 59–71

3 Feng K. Symplectic geometry and numerical methods in fluid dynamics. In Zhuang F G, Zhu Y L, eds. Proc 10th Inter Conf on Numerical Methods in Fluid Dynamics. Lecture Notes in Physics 264. Berlin: Springer Verlag. 1986: 1–7

4 Feng K. Difference schemes for Hamiltonian formalism and symplectic geometry. J Comp Math. 1986 4(3): 279–289

5 Feng K, Wu H M, Qin M Z. Symplectic difference schemes for linear Hamiltonian canonical systems. J Comp Math. 1990 8(4): 371–380

6 Feng K, Wu H M, Qin M Z, Wang D L. Construction of canonical difference schemes for Hamiltonian formalism via generating functions. J Comp Math. 1989 7(1): 71–96

7 Ge Z, Feng K. On the approximation of Hamiltonian systems. J Comp Math. 1988 6(1): 88–97

8 Li C W, Qin M Z. Symplectic difference schemes for infinite dimensional Hamiltonian systems. J Comp Math. 1988 6(2): 164–174

9 Qin M Z. A difference scheme for the Hamiltonian equation. J Comp Math. 1987 5

10 Qin M Z. Leap-frog schemes for wave equation. J Comp Math.

11 Ge Z. Generating functions for the Poisson map: [Preprint]. Beijing: CAS. Computing Center, 1987

12 Arnold V I. Mathematical Methods of Classical Mechanics. New York: Springer. 1978

13 Siegel C L. Symplectic geometry. Amer J Math. 1943 65: 1–86.

14 Hua L K. On the theory of automorphic functions of a matrix variable I, II. Amer J Math. 1944 66: 470–488, 531–563

15 Li C W. Numerical calculation for the Hamiltonian System: [Master dissertation]. Beijing: CAS. Computing Center, 1986

16 Lee T D. Discrete Mechanics. CU-TP-267. A series of four Lectures given at the International School of Subnuclear Physics, Erice, August 1983.

17 Vainberg M. Variational method in nonlinear operator analysis. San Francisco: Holden Day. 1964

18 Abraham R, Marsden J. Foundation of Mechanics. Mass: Addison-Wesley, Reading. 1978

19 Chernoff P R, Marsden J E. Properties of infinite dimensional Hamiltonian. Lecture Notes in Mathematics 425. Berlin: Springer.

20 Miller J H. On the Location of zeros of certain classes of polynomials with application to numerical analysis. J Inst Math Appl. 1971 8: 397–406

21 Hènon M, Heiles C. The applicability of the third integral of motion. Astron J. 1964 69: 73

22 Hènon M. A two-dimensional mapping with a strange attractor. Comm Math Phys. 1976 50: 69–77

23 Sanz-Serna J M. Studies in numerical nonlinear instability I. SIAM J Sci Stat Comp. 1985 6(4): 923–938

24 Yamaguti M, Ushiki S. Chaos in numerical analysis of ordinary differential equations. Phys 3D. 1981: 618–626

25 Huang M Y. Hamiltonian approximation for the nonlinear wave equation. In this Proceedings.