ON DIFFERENCE SCHEMES AND SYMPLECTIC GEOMETRY [①]

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§1 Introductory Remarks

In this paper we present some considerations and results of a preliminary study, specifically within the framework of symplectic geometry, of difference schemes for numerical solution of the canonical system of equations

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

with given Hamiltonian function $H(p_1, \cdots, p_n, q_1, \cdots, q_n)$.

The canonical system (1) with remarkable elegance and symmetry was first introduced by Hamilton in 1824 as a general mathematical scheme for problems of geometrical optics. The success of this approach was evidenced by the subsequent theoretical prediction and experimental confirmation of the phenomenon of conical refraction. The approach was then successfully applied by Hamilton himself in 1834 to an entirely different area—analytical dynamics. It was immediately followed and analytically developed by Jacobi into a well-established mathematical formalism for mechanics, which is an alternative of, and equivalent to, the Newtonian and Lagrangian formalisms. The proper geometrization of Hamiltonian formalism was started by Poincaré in 1890's, his contributions, together with the later ones by Cartan, Birkhoff, Weyl, Siegel, et al., in the 20th century, gave rise to a new discipline, called symplectic geometry, which serves as the mathematical foundation of Hamiltonian formalism.

For a certain long period of time, however, Hamiltonian formalism and symplectic geometry had not attracted deserved attention from the general mathematical community, their theoretical as well as practical significance remained not fully recognized. A turn of interest was triggered first by Kolmogorov-Arnold-Moser's researches on the invariance of conditional periodicity under small perturbation of the Hamiltonian around the integrable system, which brought to light the potential of the symplectic approach. This was followed by Keller-Maslov's contribution to the symplectic-geometrical foundation of the WKB asymptotic method for solving wave and Schrödinger equations and extending thereby the validity of the method beyond the caustic singularities. Since then, in the recent 2 decades

[①] In Feng K, ed. Proc 1984 Beijing Symp Diff Geometry and Diff Equations. Beijing: Science Press, 1985. 42–58

there is an ever growing interest of research and realization of the importance of Hamiltonian formalism in many different areas of pure and applied mathematics. It is known that, Hamiltonian formalism, apart from its classical links with analytical mechanics, geometrical optics, calculus of variations and non-linear PDE of first order, has inherent connections also with unitary representations of Lie groups and geometric quantization (Kirillov, Kostant, et al.), with linear PDE and pseudodifferential operators (Hörmander, Egorov, et al.), with classification of singularities (Arnold, et al.), with integrability theory of non-linear evolution equations with soliton solutions, with optimal control theory, etc. It is also under extension to infinite dimensions for various field theories, including hydrodynamics, elasticity, electrodynamics, plasma physics, relativity, etc. Now it is almost certain that all real physical processes with negligible dissipation can be described, in some way or other, by Hamiltonian formalism, so the latter is becoming one of the most useful tools in the mathematical arsenal of physical and engineering sciences. In this way, a systematic study of physical methods of Hamiltonian systems is motivated and would eventually lead to more general applicability and more direct accessibility of the Hamiltonian formalism.

§2 Digressions on Hamiltonian Formalism

We give here a brief summary of the Hamiltonian formalism and its basic geometrical properties. For simplicity we use the usual coordinate description and consider only the classical phase space R^{2n} of a dynamical system with n degrees of freedom. For details, see, e.g., [1]. $R^{2n} = R^n_p \times R^n_q$, $z = [z_1, \cdots, z_{2n}]' \in R^{2n}$ splits into $z = \begin{bmatrix} p \\ q \end{bmatrix}$, $q = [q_1, \cdots, q_n]' = [z_{n+1}, \cdots, z_{2n}]' \in R^n_q$, R^n_q is the configuration space, whose "points" q represents positions of the system; $p = [p_1 \cdots, p_n]' = [z_1, \cdots, z_n]' \in R^n_p$, R^n_p is the momenta space, whose "vectors" p represents the momenta of the system.

The phase space R^{2n} is equipped with a standard symplectic structure defined by a "fundamental" differential 2-form on R^{2n}:

$$\omega_J = \sum_{i=1}^{n} dp_i \wedge dq_i = \sum_{i=1}^{n} dz_i \wedge dz_{n+1}, \tag{2}$$

i.e., to each $z \in R^{2n}$ a bilinear antisymmetric form

$$\omega_J(\xi, \eta)_z = \xi' J \eta \tag{3}$$

for each pair of tangent vectors $\xi = [\xi_1, \cdots, \xi_{2n}]'$, $\eta = [\eta_1, \cdots, \eta_{2n}]'$ at z, J is the standard antisymmetric matrix

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad J' = -J = J^{-1}, \quad \det J = 1.$$

The fundamental 2-form ω_J is non-singular and closed, i.e., $d\omega_J = 0$.

Let w: $R^{2n} \to R^{2n}$ be a differential mapping, $z \in R^{2n} \to w(z) \in R^{2n}$, the corresponding

Jacobi matrix is denoted by

$$\frac{\partial w}{\partial z} = \begin{bmatrix} \frac{\partial w_1}{\partial z_1} & \cdots & \frac{\partial w_1}{\partial z_{2n}} \\ \vdots & & \vdots \\ \frac{\partial w_{2n}}{\partial z_1} & \cdots & \frac{\partial w_{2n}}{\partial z_{2n}} \end{bmatrix}$$

mapping w induces, for each $z \in R^{2n}$, a linear mapping w_* of the tangent space at z into the tangent space at $w(z)$ by

$$\xi = [\xi_1, \cdots, \xi_{2n}]' \to w_*\xi = \frac{\partial w}{\partial z}\xi$$

w also induces, for each 2-form ω on R^{2n}, a 2-form $w^*\omega$ on R^{2n} by the formula

$$w^*\omega(\xi, \eta)_z = \omega(\frac{\partial w}{\partial z}\xi, \frac{\partial w}{\partial z}\eta)_{w(z)}.$$

If $\omega(\xi, \eta)_z = \xi A(z)\eta$, $A'(z) = -A(z)$, then $w^*\omega(\xi, \eta) = \xi B(z)\eta$, where

$$B(z) = (\frac{\partial w}{\partial z})' A(w(z))\frac{\partial w}{\partial z}.$$

A diffeomorphism (differentiable, one-one, onto mapping) of R^{2n} is called a canonical transformation if w preserves the standard symplectic structure, i.e., $w^*\omega_J = \omega_J$, i.e.,

$$(\frac{\partial w}{\partial z})' J(\frac{\partial w}{\partial z}) = J \tag{4}$$

i.e., the Jacobian $\frac{\partial w}{\partial z}$ is a symplectic matrix for each z.

For every pair of smooth functions $\phi(z)$, $\psi(z)$ on R^{2n}, we associate a smooth function $\chi(z) = \{\phi, \psi\}$, called the Poisson bracket by

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

where $\phi'_z = [\frac{\partial \phi}{\partial z_1}, \cdots, \frac{\partial \phi}{\partial z_n}]$. The Poisson brackets are anti-symmetric and satisfy Jacobi identity.

Choose a smooth function $H(z) = H(z_1, \cdots, z_{2n}) = H(p_1, \cdots, p_n, q_1, \cdots, q_n)$. The equations (1), or written alternatively as

$$\frac{dz}{dt} = J^{-1}H_z, \tag{5}$$

is called the canonical system of equations with Hamiltonian $H(z)$. According to the general theory of ODE, for each Hamiltonian system (5), there corresponds a one-parameter group of diffeomorphisms g^t at least locally in t and z, of R^{2n} such that

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

such that, if $z(0)$ is taken as the initial condition, then the solution of (5) is generated by

$$z(t) = g^t z(0).$$

The basic property of Hamiltonian system (1) is that g^t are canonical transformations

$$g^{t*}\omega_J = \omega_J, \tag{6}$$

for all t. This leads to the following class of phase-area conservation laws

$$\begin{aligned} \int_{g^t\sigma^2} \omega_J &= \int_{\sigma^2} \omega_J, \quad \text{every 2-chain } \sigma^2 \subset R^{2n}, \\ \int_{g^t\sigma^4} \omega_J \wedge \omega_J &= \int_{\sigma^4} \omega_J \wedge \omega_J, \quad \text{every 4-chain } \sigma^4 \subset R^{2n}, \\ &\cdots \\ \int_{g^t\sigma^{2n}} \omega_J \wedge \cdots \wedge \omega_J &= \int_{\sigma^{2n}} \omega_J \wedge \cdots \wedge \omega_J, \quad \text{every } 2n\text{-chain } \sigma^{2n} \subset R^{2n}, \end{aligned} \tag{7}$$

the last one is the Liouville's phase-volume conservation law.

Another class of conservation law is related to energy and all the first integrals. A smooth function $\varphi(z)$ is said to be a first integral if $\varphi(g^t z) = \varphi(z)$ for all t, z, the latter is equivalent to the condition $\{\phi, H\} = 0$. H, usually representing the energy, is itself a first integral.

The above situations can be generalized. A symplectic structure in R^{2n} is specified by a non-degenerate, closed 2 form $\omega_K = \sum k_{ij}(z) dz_i \wedge dz_j$

$$\omega_K(\xi, \eta)_z = \frac{1}{2}\xi' K(z)\eta, \quad K'(z) = -K(z), \quad \det K(z) \neq 0.$$

A differentiable mapping w: $R^{2n} \to R^{2n}$ is called K-canonical if $w^*\omega_K = \omega_K$, i.e.

$$(\frac{\partial w}{\partial z})' K(w(z)) \frac{\partial w}{\partial z} = K(z). \tag{8}$$

The Poisson bracket is defined as

$$\{\phi, \psi\}_K = \phi_z' K^{-1}(z) \psi_z,$$

which is anti-symmetric and satisfies the Jacobi identity. The equations of the form

$$\frac{dz}{dt} = K^{-1} H_z \tag{9}$$

is called the K-canonical system with Hamiltonian H, whose solutions are generated by a one-parameter group g^t, which consists of K-canonical transformations. The conservation laws of (7) remain true with J replaced by K, while the Liouville's theorem remains unchanged. The condition of first integrals for (9) is analogous, H is also among the first integrals.

Darboux theorem establishes the equivalence between all symplectic structures: Every non-singular closed 2-form ω_K can be brought to the standard form

$$\sum k_{ij}(z) dz_i \wedge dz_j = \sum dw_i \wedge dw_{n+1}$$

locally by suitable coordinate transformation $z \to w(z)$.

§3 Difference Schemes for Linear Canonical Systems

Take the Hamiltonian to be a quadratic form

$$H(z) = \frac{1}{2} z' S z, \qquad S' = S, \tag{10}$$

and K be an anti-symmetric non-singular constant matrix, then the K-canonical system (9) becomes linear

$$\frac{dz}{dt} = Bz, \qquad B = K^{-1}S, \tag{11}$$

the generating one-parameter group is a group of linear transformations which coincides with their own Jacobians

$$z(t) = G(t)z(0), \qquad G(t) = \exp tB. \tag{12}$$

The matrix B is infinitesimally K-symplectic

$$KB + B'K = 0, \tag{13}$$

its exponential transform exp tB is K-symplectic and S-orthogonal

$$(\exp tB)'K(\exp tB) = K, \quad (\exp tB)'S(\exp tB) = S, \tag{14}$$

i.e., both the symplectic structure and the energy are conserved.

In a wider context let $\psi(\lambda)$ be a meromorphic function, in case the matrix B has no eigenvalue at the poles of $\psi(\lambda)$— we then say that B is non-exceptional—, the transform $\psi(B)$ is well-determined. It can be shown that, in order that $\psi(B)$ be K-symplectic for all non-exceptional infinitesimal K-symplectic matrices tB, it is necessary and sufficient that

$$\psi(\lambda)\psi(-\lambda) = 1. \tag{15}$$

When this is satisfied, we have, we have, for all integers $m \geq 0$,

$$(\psi(tB))'KB^m(\psi(tB)) = KB^m. \tag{16}$$

Let

$$K_i = KB^{2i-2}, \quad S_i = KB^{2i-1}, \qquad i = 1, 2, 3, \cdots, n. \tag{17}$$

$K_1 = K$, K_i are anti-symmetric, $S_1 = S$, S_i are symmetric, then (14) is extended to

$$(\psi(tB))'K_i(\psi(tB)) = K_i, \qquad (\psi(tB))'S_i(\psi(tB)) = S_i. \tag{18}$$

The independency of the sets K_i and S_i depends on the degree of the minimal polynomial of B. Thus the K-canonical transformation $\psi(tB)$ has many conservation laws of phase-areas and symplectic structures as well as many quadratic first integrals $\varphi_i(z) = \frac{1}{2}z'S_iz$. The exponential transform $\psi(\lambda) = \exp \lambda \to \exp B$ and Cayley transform $\psi(\lambda) = \frac{1+\lambda}{1-\lambda} \to \frac{I+B}{I-B}$ satisfy the condition (15).

In our study of numerical methods, we are interested in the Hamiltonian equations less as a system of ODE's per se, but rather as a specific system with Hamiltonian structure. It is natural to look forward to those discrete systems which preserve as much as possible the intrinsic properties of the continuous system. We hope this would lead to more satisfactory practical performance and theoretical foundation.

Consider now three kinds of difference schemes for linear Hamiltonian system (11). Let τ be the time-step, $z(n\tau) \sim z^n$, $n = 0, 1, 2, \cdots$. Scheme I — Centered implicit Euler scheme

$$\frac{1}{\tau}(z^{m+1} - z^m) = B\frac{1}{2}(z^{m+1} + z^m), \quad B = K^{-1}S. \tag{19}$$

The transition $z^m \to z^{m+1}$ is given by the following linear transformation F_τ which coincides with its own Jacobian

$$z^{m+1} = F_\tau z^m, \quad F_\tau = (I - \frac{\tau}{2}B)^{-1}(I + \frac{\tau}{2}B) = \psi(-\frac{\tau}{2}B), \tag{20}$$

where $\psi(\lambda) = \frac{1-\lambda}{1+\lambda}$, the Cayley transform function. Note that the corresponding transition $z(m\tau) \to z((m+1)\tau)$ for the true solution at the same time-step τ is given by

$$z((m+1)\tau) = G_\tau z(m\tau), \quad G_\tau = \exp \tau B.$$

So G_τ and F_τ are the exponential and Cayley transforms respectively of the same B, so they have the same sets of invariant "symplectic structures" K_i and invariant "energies" S_i as given by (17). Even more than that, it can be easily proved that each function of anyone of the following types

(a) Quadratic form $f(z)$,

(b) Bilinear form $g(z, w)$,

(c) Linear form $\ell(z)$

is invariant under the differential equations (11) if and only if it is invariant under the difference equations (19). So the conservation properties of (11) and (19) are the same.

For the comparison of the stability properties of (11) and (19), we take, for simplicity, $K = J$ and the "separable" Hamiltonian

$$H(p, q) = U(p) + V(q) = \text{kinetic energy} + \text{potential energy},$$

where

$$U(p) = \frac{1}{2} p' M p, \quad M = M', \quad \text{positive definite},$$
$$V(q) = \frac{1}{2} q' L q, \quad L = L', \quad \text{not necessarily positive definite},$$

so that

$$S = \begin{bmatrix} M & 0 \\ 0 & L \end{bmatrix}, \quad B = J^{-1} S = \begin{bmatrix} 0 & -L \\ M & 0 \end{bmatrix},$$

and systems (11), (19) can be written as

$$\frac{dp}{dt} = -Lq, \quad \frac{dq}{dt} = Mp, \tag{21}$$

$$\frac{1}{\tau}(p^{m+1} - p^m) = -L\frac{1}{2}(q^{m+1} + q^m), \quad \frac{1}{\tau}(q^{m+1} - q^m) = M\frac{1}{2}(p^{m+1} + p^m). \tag{22}$$

The eigenvalue λ of B is related to the eigenvalue μ of the Pencil $L - \mu M^{-1}$ by $\lambda^2 = -\mu$, where μ is real, $\mu = 0$ or $-\omega^2$ or $+a^2$, where ω and a are positive. The Jordan normal form of the matrices B, G_τ and F_τ consists of n diagonal blocks of order 2 of the following three possible types

	Type 1	Type 2	Type 3
B	$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$	$\begin{bmatrix} i\omega & 0 \\ 0 & -i\omega \end{bmatrix}$	$\begin{bmatrix} a & 0 \\ 0 & -a \end{bmatrix}$
G_τ	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} e^{i\omega\tau} & 0 \\ 0 & e^{-i\omega\tau} \end{bmatrix}$	$\begin{bmatrix} e^{a\tau} & 0 \\ 0 & e^{-a\tau} \end{bmatrix}$
F_τ	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} \frac{1+i\omega\tau/2}{1-i\omega\tau/2} & 0 \\ 0 & \frac{1-i\omega\tau/2}{1+i\omega\tau/2} \end{bmatrix}$	$\begin{bmatrix} \frac{1+a\tau/2}{1-a\tau/2} & 0 \\ 0 & \frac{1-a\tau/2}{1+a\tau/2} \end{bmatrix}$

When type 3 is missing in B, all eigenvalues of both (20) and (21) are unimodular with linear elementary divisors. Type 3 leads to instability for both (20) and (21).

Note that

$$G_\tau = \exp\tau \begin{bmatrix} 0 & -L \\ M & 0 \end{bmatrix} = \begin{bmatrix} G_{\tau,11} & G_{\tau,12} \\ G_{\tau,21} & G_{\tau,22} \end{bmatrix},$$

$$\begin{aligned} G_{\tau,11} &= \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!}(\tau)^{2m}(LM)^m, \quad G_{\tau,12} = -\sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)!}(\tau)^{2m+1}(LM)^m L, \\ G_{\tau,21} &= \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)!}(\tau)^{2m+1}(ML)^m M, \quad G_{\tau,22} = \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m)!}(\tau)^{2m}(ML)^m. \end{aligned} \tag{23}$$

Scheme II, Staggered explicit scheme for separable Hamiltonian systems (20)

$$\begin{aligned} \frac{1}{\tau}(p^{m+1} - p^m) &= -Lg^{m+1/2}, \\ \frac{1}{\tau}(q^{m+1+1/2} - q^{m+1/2}) &= Mp^{m+1}. \end{aligned} \tag{24}$$

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

In this case the transition

$$w^m = \begin{bmatrix} p^m \\ q^{m+1/2} \end{bmatrix} \to w^{m+1} = \begin{bmatrix} p^{m+1} \\ q^{m+1+1/2} \end{bmatrix}$$

is given by the linear transformation

$$w^{m+1} = F_\tau w^m, \quad F_\tau = \begin{bmatrix} I & 0 \\ -\tau M & I \end{bmatrix}^{-1} \begin{bmatrix} I & -\tau L \\ 0 & I \end{bmatrix}. \tag{25}$$

In order to analyze this scheme we introduce a linear transformation for the true solutions

$$z(t) = \begin{bmatrix} p(t) \\ q(t) \end{bmatrix} \to w(t) = \begin{bmatrix} p(t) \\ q(t+\frac{\tau}{2}) \end{bmatrix},$$

$$w(t) = Tz(t), \quad T = \begin{bmatrix} I & 0 \\ G_{\frac{\tau}{2},21} & G_{\frac{\tau}{2},22} \end{bmatrix}, \quad z(t) = T^{-1}w(t).$$

Define

$$K = T^{-1'}JT^{-1} = [k_{ij}(z)], \quad K' = -K.$$

It can be shown that $d(\sum k_{ij}(z)dz_i \wedge dz_j) = 0$ and det $k \neq 0$, so K actually defines a symplectic structure. Then $w(t)$ satisfies the K-canonical system

$$\frac{dw}{dt} = K^{-1}\widetilde{H}_w = K^{-1}\widetilde{S}w \tag{26}$$

with Hamiltonian $\widetilde{H}(w) = H(T^{-1}w) = \frac{1}{2}w'\widetilde{S}w$,

$$\widetilde{S} = T^{-1'}ST^{-1},$$

so the transition

$$\widetilde{G}_\tau : w(t) = \begin{bmatrix} p(t) \\ q(t+\frac{\tau}{2}) \end{bmatrix} \to w(t+\tau) = \begin{bmatrix} p(t+\tau) \\ q(t+\tau+\frac{\tau}{2}) \end{bmatrix}$$

is linear and K-symplectic, i.e., $\widetilde{G}'_\tau K\widetilde{G}_\tau = K$.

It can be proved that F_τ is also K-symplectic as is expected. However, the energy conservation properties are somehow different, F_τ does preserve $\widetilde{H}(w)$, which is the true energy after synchronizing p^m, $q^{m+\frac{1}{2}}$ at staggered moments by T^{-1} to p^m, q^m at the same moment. F_τ preserves, instead, a modified Hamiltonian $\hat{H}(w) = \frac{1}{2}w'\hat{S}w$, $\hat{S} = T^{-1'}JT^{-1}\begin{bmatrix} I & -\frac{\tau}{2}B \\ -\frac{\tau}{2}A & I \end{bmatrix}^{-1}\begin{bmatrix} 0 & -B \\ A & 0 \end{bmatrix}$. Note that in practical computation, the synchronization is done by defining $q^m = \frac{1}{2}(q^{m-\frac{1}{2}} + q^{m+\frac{1}{2}})$, then all the first integrals $\varphi(p,q)$, including the Hamiltonian $H(p,q)$ are conserved approximately as

$$\phi(p^{m+1}, q^{m+1}) = \phi(p^m, q^m) \mod O(\tau^3).$$

The eigenvalue λ of F_τ is related to the eigenvalue μ of the pencil $L - \mu M^{-1}$ by $\lambda^2 + \lambda(\tau^2\mu - 2) + 1 = 0$, this leads to the Jordan normal form of F, consisting again of three possible types

	Type 1	Type 2
F_τ	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 + \dfrac{\omega^2\tau^2}{2} + \dfrac{i\omega\tau}{2}\sqrt{4-\omega^2\tau^2} & 0 \\ 0 & 1 + \dfrac{\omega^2\tau^2}{2} - \dfrac{i\omega\tau}{2}\sqrt{4-\omega^2\tau^2} \end{bmatrix}$

	Type 3
F_τ	$\begin{bmatrix} 1 + \dfrac{a^2\tau^2}{2} + \dfrac{a\tau}{2}\sqrt{4+a^2\tau^2} & 0 \\ 0 & 1 + \dfrac{a^2\tau^2}{2} + \dfrac{a\tau}{2}\sqrt{4+a^2\tau^2} \end{bmatrix}$

Type 2: When $\tau < \frac{2}{\omega}$, the two eigenvalues are unimodular, complex-conjugate, distinct. They collide at -1 when $\tau = \frac{2}{\omega}$. As $\tau > \frac{2}{\omega}$ they become distinct and real, one with modulus > 1 and other with modulus < 1. Type 3: the two eigenvalues are real and distinct, one with modulus > 1 and other with modulus < 1. In case L being non-negative definite, Type 3 is missing, then all eigenvalues of F_τ are unimodular and belonging to linear elementary divisors when $\tau < \frac{2}{\omega_{\max}}$

We apply the above scheme to the 1-D wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1, \quad u(0,t) = u(l,t) = 0$$

with finite element semi-discretization

$$\frac{d^2 u_k}{dt^2} = \frac{c^2}{h^2}\left[u_{k-1} - 2u_k + u_{k+1}\right], \quad k = 1, \cdots, n;$$
$$u_0 = u_{n+1} = 0, \quad h = \frac{1}{n+1}.$$

Let $q_k = u_k$, $p_k = \frac{\partial u_k}{\partial t}$, we get a canonical system (24) with

$$M = I, \quad L = \frac{c^2}{h^2} \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}.$$

The types 1 and 3 are missing, $\omega_k = \frac{2c}{h} \cos \frac{k\pi}{2n+1} < \omega_1 = \frac{2c}{h} \cos \frac{\pi}{2n+1} < \frac{2c}{h}$. So the Courant condition $\tau \leq \frac{h}{c}$ ensures stability of (24). The scheme is in fact equivalent to the classical 5-point scheme for the wave equation, see [2]. There is an interesting study [3], with further references there, on computer simulation of fluids base on Hamiltonian formalism with spatiotemporal staggered scheme.

Schemes III. Energy-conservative schemes by Hamiltonian differencing. For simplicity, we illustrate the cases only by $n = 2$. Let $z = z^m$, $\widetilde{z} = z^{m+1}$,

$$\begin{aligned} \frac{1}{\tau}(\widetilde{p}_1 - p_1) &= -\frac{1}{\widetilde{q}_1 - q}\{H(p_1 p_2 \widetilde{q}_1 q_2) - H(p_1 p_2 q_1 q_2)\}, \\ \frac{1}{\tau}(\widetilde{p}_2 - p_2) &= -\frac{1}{\widetilde{q}_2 - q_2}\{H(\widetilde{p}_1 p_2 \widetilde{q}_1 \widetilde{q}_2) - H(\widetilde{p}_1 p_2 \widetilde{q}_1 q_2)\}, \\ \frac{1}{\tau}(\widetilde{q}_1 - q_2) &= \frac{1}{\widetilde{p}_1 - p_1}\{H(\widetilde{p}_1 p_2 \widetilde{q}_1 q_2) - H(p_1 p_2 \widetilde{q}_1 q_2)\}, \\ \frac{1}{\tau}(\widetilde{q}_2 - q_2) &= \frac{1}{\widetilde{p}_2 - p_2}\{H(\widetilde{p}_1 \widetilde{p}_2 \widetilde{q}_1 \widetilde{q}_2) - H(\widetilde{p}_1 p_2 \widetilde{q}_1 \widetilde{q}_2)\}. \end{aligned} \tag{27}$$

By addition and cancellation we have energy conservation for arbitrary Hamiltonian $H(\widetilde{p}_1 \widetilde{p}_2 \widetilde{q}_1 \widetilde{q}_2) = H(p_1 p_2 q_1 q_2)$.

For quadratic Hamiltonian, $H = \frac{1}{2} z' S z$, we get

$$\frac{1}{\tau}(z^{m+1} - z^m) = J^{-1} S \frac{1}{2}(z^{m+1} + z^m) - \frac{1}{2} J R (z^{m+1} - z^m),$$

where

$$S = \begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ & s_{22} & s_{23} & s_{24} \\ & * & s_{33} & s_{34} \\ & & & s_{44} \end{bmatrix} = S', \quad R = \begin{bmatrix} 0 & -s_{12} & s_{13} & -s_{14} \\ & 0 & s_{23} & s_{24} \\ & * & 0 & -s_{34} \\ & & & 0 \end{bmatrix} = -R',$$

and

$$z^{m+1} = F_\tau z^m, \quad F_\tau = (I + \frac{\tau}{2} J R - \frac{\tau}{2} J^{-1} S)^{-1} (I + \frac{\tau}{2} J R + \frac{\tau}{2} J^{-1} S).$$

Let $\bar{K} = J - \frac{\tau}{2} R$, $\bar{B} = \bar{K}^{-1} S$, we can prove that F_τ is the Cayley transform

$$F_\tau = \psi(-\frac{\tau}{2} \bar{B}), \quad \psi(\lambda) = \frac{1 - \lambda}{1 + \lambda},$$

so we have invariant "symplectic structures" $\bar{K}_1 = \bar{K}$, $\bar{K}_2, \bar{K}_3, \cdots$ and invariant "energies" $\bar{S}_1, = S$, $\bar{S}_2, \bar{S}_3, \cdots$ like (17), (18).

§4 Difference Schemes for General Canonical Systems

The three kinds of schemes for linear systems in the previous section can be generalized to the general non-linear case.

Scheme I. For the general canonical system (1), we put

$$\frac{1}{\tau}(z^{m+1}-z^m)=J^{-1}H_z(\frac{1}{2}z^{m+1}+\frac{1}{2}z^m). \tag{28}$$

The transition $z^m\to z^{m+1}$ is non-linear in general. By differentiation,

$$\frac{\partial z^{m+1}}{\partial z^m}-I=\tau J^{-1}H_{zz}(\frac{z^{m+1}+z^m}{2})\left[\frac{1}{2}\frac{\partial z^{m+1}}{\partial z^m}+\frac{1}{2}I\right],$$

here $H_{zz}(\frac{z^{m+1}+z^m}{2})$ is the Hessian matrix of the function $H(z)$, evaluated at $z=\frac{z^{m+1}+z^m}{2}$, $\frac{\partial z^{m+1}}{\partial z^m}$ is the Jacobian matrix F_τ, so

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

When z remains bounded and take τ sufficiently small we can keep the infinitesimally symplectic matrix $\frac{\tau}{2}J^{-1}H_{zz}(\frac{z^{m+1}+z^m}{2})$ non-exceptional, then F_τ, as a Cayley transform, is symplectic. Thus all the conservation laws for phase areas remain true. However, unlike the linear case, the first integrals $\phi(z)$ including H itself are not conserved exactly. Instead, the approximate conservation

$$\varphi(z^{m+1})=\varphi(z^m)\mod O(\tau^3)$$

can be shown.

We remark that the analogous averaged implicit Euler scheme

$$\frac{1}{\tau}(z^{m+1}-z^m)=J^{-1}\left[\frac{1}{2}H_z(z^{m+1})+\frac{1}{2}H_z(z^m)\right], \tag{29}$$

which reduces, like (28), to the same symplectic scheme (19) with $K=J$ for linear problems.

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

which is not symplectic in general.

Scheme II. For the canonical system with general separable Hamiltonian $H(p,q)=U(p)+V(q)$, we have

$$\begin{aligned}&\frac{1}{\tau}(p^{m+1}-p^m)=-V_q(q^{m+1/2}),\\&\frac{1}{\tau}(q^{m+1+1/2}-q^{m+1/2})=U_p(p^{m+1}).\end{aligned} \tag{30}$$

The transition $\begin{bmatrix}p^m\\q^{m+1/2}\end{bmatrix}\to\begin{bmatrix}p^{m+1}\\q^{m+1+1/2}\end{bmatrix}$ has Jacobian

$$F_\tau=\begin{bmatrix}I&0\\-\tau M&I\end{bmatrix}^{-1}\begin{bmatrix}I&-\tau L\\0&I\end{bmatrix},$$

which can be shown to K-symplectic as for (24), (26), but with

$$M=U_{pp}(p^{m+1}),\quad L=V_{qq}(q^{m+1/2}).$$

This leads to a class of modified conservation laws of phase areas, but with Liouville's theorem unchanged.

The first integrals $\phi(p,q)$, including $H(p,q)$, are approximately conserved as

$$\phi(p^{m+1}, \frac{1}{2}(q^{m+1+1/2} + q^{m+1/2})) = \phi(p^m, \frac{1}{2}(q^{m+1/2} + q^{m-1/2}), \quad \bmod O(\tau^3).$$

Scheme III. This has already been constructed for the nonlinear case in the previous section, the Hamiltonian $H(z)$ is always conserved exactly. However, the first integrals $\phi(z)$, other than the Hamiltonian, are approximately conserved to a lower order as

$$\phi(z^{m+1}) = \phi(z^m), \quad \bmod O(\tau^2)$$

due to some kind of asymmetry in the algorithm. Moreover, except in the linear systems, symplectic properties for the Jacobian of transition could not be established in general.

The details of the results and some other developments will be published elsewhere.

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