DIFFERENCE SCHEMES FOR HAMILTONIAN FORMALISM AND SYMPLECTIC GEOMETRY*1)

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§ 1. Introduction

The present program [1] that the author and his group have started is a systematic study of the numerical methods for the solution of differential equations of mathematical physics expressed in Hamiltonian formalism. As is well known, Hamiltonian canonical systems serve as the basic mathematical formalism, for diverse areas of physics, mechanics, engineering, as well as pure and applied mathematics, e.g., geometrical optics, analytical dynamics, non-linear PDE's of first order, group representations, WKB asymptotics, pseudo-differential and Fourier integral operators, electrodynamics, plasma physics, elasticity, hydrodynamics, relativity, control theory, etc. It is generally accepted that all real physical processes with negligible dissipation could be expressed, in some way or other, in suitable Hamiltonian forms. So the general methods developed for the numerical solution of Hamiltonian equations, if good, would have wide applications.

Since symplectic geometry is the mathematical foundation of Hamiltonian formalism, a wealth of theoretical results is already accumulated which should be and could be explored for numerical purposes. So the proper mode of research in this area should be geometrical. 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, and we actually derive in this way numerous "unconventional" difference schemes.

Due to historical reasons, classical symplectic geometry, however, lacks the "computational" component in the modern sense. Our present study might be considered as an attempt to fill the blank. We got a number of results (e.g. Th. 1, § 2) which are crucial for the construction of symplectic difference schemes on the one hand and which have independent theoretical interest in themselves on the other hand.

In this paper, we consider the canonical system in finite dimensions

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

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

In the following, vectors are always represented by column matrices, and matrix transpose is denoted by prime. Let $z=(z_1, \cdots, z_n, z_{n+1}, \cdots, z_{2n})'=(p_1, \cdots, p_n,$

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$q_1, \cdots, q_n)'$, $H_z=(H_{z_1}, \cdots, H_{z_{2n}})'$. (1.1) can be written as

$$\frac{dz}{dt}=J^{-1}H_z, \quad J=\begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \tag{1.2}$$

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

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

The Fundamental Theorem on Hamiltonian Formalism says that the solution of the canonical system (1.2) can be generated by a one-parameter group G_t of canonical transformations of R^{2n} (locally in t and z) such that

$$G_{t_1}G_{t_2}=G_{t_1+t_2},$$

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

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

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

Linear canonical transformations are simply symplectic transformations.

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 $\phi(z)$ is said to be an invariant integral of (1.2) if it is invariant under (1.2)

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

which is equivalent to

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

where the Poisson bracket for two functions $\phi(z)$, $\psi(z)$ are defined as

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

H itself is always an invariant integral, see, e.g., [2].

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 many as possible the characteristic properties and inner symmetries of the original continuous systems. We hope that this might lead to more satisfactory theoretical foundation and practical performance.

The above digressions on Hamiltonian systems suggest the following guideline for difference schemes to be constructed. The transition from the k-th time step z^k to the next $(k+1)$-th time step z^{k+1} should be canonical for all k and, moreover, the invariant integrals of the original system should remain invariant under these transitions.

§2. Some Difference Schemes for Hamiltonian Systems

2.1. *The Centered Euler Scheme and Its Generalizations*

Consider first the case for which the Hamiltonian is a quadratic form

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

Then the canonical system is linear

$$\frac{dz}{dt}=Lz, \tag{2.2}$$

where $L=J^{-1}S$ is infinitesimally symplectic, i.e.

$$L'J+JL=0.$$

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.

Proposition 1. 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 if and only if $\alpha=\frac{1}{2}$, i.e. it is the case of time-centered Euler scheme with the transition.

For the time-centered case, the transition matrix

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

where F_τ is 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 $|\tau|$, if and only if

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

If, moreover, $\exp\lambda-\psi(\lambda)=0(|\lambda|^{m+1})$, 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 accuracy and has the property that $z'Aw$ is invariant under $\psi(\tau L)$ if and only if it is invariant under G_t of (2.2) ([5]).

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 [illegible]

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

$$\exp\lambda-\frac{P_m(\lambda)}{P_m(-\lambda)}=0(|\lambda|^{2m+1}),$$

where

$$\begin{aligned}
&P_0(\lambda)=1,\\
&P_1(\lambda)=2+\lambda,\\
&P_2(\lambda)=12+6\lambda+\lambda^2,\\
&P_3(\lambda)=120+60\lambda+12\lambda^2+\lambda^3,\\
&\cdots\cdots\\
&P_m(\lambda)=2(2m-1)P_{m-1}(\lambda)+\lambda^2P_{m-2}(\lambda), \text{ etc.}
\end{aligned}$$

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

For the comparison of stability properties of (2.4) and (2.2), we consider the simple case of separable Hamiltonian

$$S=\begin{bmatrix} S_1 & 0\\ 0 & S_2\end{bmatrix}, \quad L=J^{-1}S=\begin{bmatrix} 0 & -S_2\\ S_1 & 0\end{bmatrix},$$
$$S_1=S_1' \text{ pos. def.}; \ S_2=S_2'.$$

The eigenvalue λ of L is related to the eigenvalue μ of the pencil $S_2-\mu S_1^{-1}$ by $\lambda^2=-\mu$, where μ is real, $\mu=0$ or $+\omega^2$ or $-a^2$ $(\omega>0,\ a>0)$. The Jordan normal form of L, G_τ, F_τ consists of n diagonal blocks of order 2 of the following three possible types:

	type 1	type 2	type 3
L	$\begin{bmatrix}0&0\\0&0\end{bmatrix}$	$\begin{bmatrix}i\omega&0\\0&-i\omega\end{bmatrix}$	$\begin{bmatrix}a&0\\0&-a\end{bmatrix}$
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	$\begin{bmatrix}1&0\\0&1\end{bmatrix}$	$\begin{bmatrix}\frac{P_m(i\omega\tau)}{P_m(-i\omega\tau)}&0\\0&\frac{P_m(-i\omega\tau)}{P_m(i\omega\tau)}\end{bmatrix}$	$\begin{bmatrix}\frac{P_m(a\tau)}{P_m(-a\tau)}&0\\0&\frac{P_m(-a\tau)}{P_m(a\tau)}\end{bmatrix}$

When type 3 is missing, all eigenvalues of both G_τ and F_τ are unimodular with linear elementary divisors. Type 3 leads to instability for both G_τ and F_τ.

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

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

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

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

everywhere symplectic. However, unlike the linear case the invariant integrals $\phi(z)$ of system (1.2), including $H(z)$, are conserved only approximately

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

The analogous averaged Euler scheme

$$\frac{1}{\tau}(z^{k+1}-z^k)=J^{-1}\Big[\frac{1}{2}H_z(z^{k+1})+\frac{1}{2}H_z(z^k)\Big]$$

which reduces, like (2.6), to the same symplectic scheme (2.4) for linear systems, is not canonical in general.

2.2. *Staggered Explicit Schemes for Separable Hamiltonians*

For the non-linear separable system we have

$$\frac{1}{\tau}(p^{k+1}-p^k)=-V_q(q^{k+1/2}),$$

$$\frac{1}{\tau}(q^{k+1+1/2}-q^{k+1/2})=U_p(p^{k+1}).$$

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

$$w^k=\begin{bmatrix} p^k \\ q^{k+1/2}\end{bmatrix}\to\begin{bmatrix} p^{k+1} \\ q^{k+1+1/2}\end{bmatrix}=w^{k+1}=F_\tau w^k,$$

$$F_\tau=\begin{bmatrix} I & 0 \\ -\tau S_1 & I\end{bmatrix}^{-1}\begin{bmatrix} I & -\tau S_2 \\ 0 & I\end{bmatrix},\ S_1=U_{pp}(p^{k+1}),\ S_2=V_{qq}(q^{k+1/2}),$$

is symplectic, of 2nd order accuracy and practically explicit. Since p, q are computed at different times, we need synchronization, e.g. using

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

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

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

For the comparison of stability for the linear system (2.2) with separable Hamiltonian with the staggered scheme and the application of the latter to the wave equation, see [1]. In [1], a class of energy-conservative schemes was constructed using the differencing of the Hamiltonian function; the symplectic property is not satisfactory. The problem of compatibility of energy conservation with phase area conservation in difference schemes is solved successfully for linear canonical systems (Theorem 1); it seems difficult, however, for the general non-linear systems.

§ 3. A General Theory of Generating Functions and Hamilton–Jacobi Equations

Our approach in this part was inspired by the early works of Siegel [3] and Hua [4]. Every matrix

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

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

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

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

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

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

Subspace $\{X\}\subset R^{4n}$ is called J_{4n}-Lagrangian $\left(\text{and}\ \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}\ \text{is called a symmetric pair}\right)$ 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 $X_1X_2^{-1}=N\in Sm(2n)$ 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 $\mathcal{J}_{4n}$-Lagrangian $\left(\text{and}\ \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix}\ \text{is called a symplectic pair}\right)$ if

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

If, moreover, $|Y_2|\neq 0$, then $Y_1Y_2^{-1}=M\in Sp(2n)$ 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 $\mathcal{J}_{4n}$-Lagrangian) if the tangent plane of U is a J_{4n}-Lagrangian (respectively $\mathcal{J}_{4n}$-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

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

of g is a $\mathcal{J}_{4n}$-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

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

of f 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 $\tilde{J}_{4n}$-Lagrangian submanifold into J_{4n}-Lagrangian submanifold if and only if*

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

i.e.

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

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

$$T = M T_0, \ M \in CSp(4n) = \text{conformal symplectic group.}$$

T^{-1} for $T \in CSp(\tilde{J}_{4n}, J_{4n})$ carries J_{4n}-Lagrangian submanifolds into $\tilde{J}_{4n}$-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 $\tilde{J}_{4n}$-Lagrangian and J_{4n}-Lagrangian submanifolds respectively. Theorem 3 leads to the existence and construction of the generating functions, under non-exceptional conditions, for the canonical transformations.

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

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

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})

$$|CM + D| \neq 0, \tag{3.1}$$

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

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

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 (3.1),

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

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

(b) *$g^{-1}(*, 0)\ g(*, t)$ 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*

$$|CM_0 + D| \neq 0, \tag{3.2}$$

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 $T \in CSp(\tilde{J}_{4n}, J_{4n})$.

Special types of generating functions:

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

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

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

This is the generating function and H. J. equation of the first kind [2].

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

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

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

This is the generating function and H. J. equation of the second kind [2].

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

$$w=\frac{1}{2}(z+\hat{z}),\ \phi=\phi(w,\ t);$$

$$\hat{w}=J(z-\hat{z})=\phi_w,\quad \phi_t=H\left(w-\frac{1}{2}J\phi_w\right).$$

This is 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 is expressible as convergent power series in t for sufficiently small $|t|$:*

$$\phi(w,\ t)=\sum_{k=1}^{\infty}\phi^{(k)}(w)t^k,$$

$$\phi^{(0)}(w)=\frac{1}{2}w'N_0w,\quad N_0=(AM_0+B)(CM_0+D)^{-1},$$

$$\phi^{(1)}(w)=-\mu H(E_0w),\quad E_0=(CM_0+D)^{-1},$$

$$k\geq 1:\qquad \phi^{(k+1)}(w)=\frac{1}{k+1}\sum_{m=1}^{k}\frac{\mu}{m!}\sum_{i_1,\dots,i_m=1}^{2n}H_{z_{i_1},\dots,z_{i_m}}(E_0w)\times\sum_{\substack{k_1+\dots+k_m=k\\ k_j\geq 1}}(C_1\phi_w^{(k_1)}(w))_{i_1}\cdots(C_1\phi_w^{(k_m)}(w))_{i_m}.$$

§ 4. Construction of Canonical Difference Schemes via Generating Functions

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 $T\in CSp(\tilde{J}_{4n}, J_{4n})$ and $M_0\in Sp(2n)$ satisfysng (3.2).

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

$$\psi^{(m)}(w, \tau)=\sum_{k=0}^{m}\phi^{(k)}(w)\tau^k, \quad m=1, 2, \cdots. \tag{4.1}$$

Then the gradient transformation

$$w\to\hat{w}=\psi_w^{(m)}(w, \tau) \tag{4.2}$$

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

$$|N^{(m)}C-A|\neq 0 \tag{4.3}$$

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

$$\hat{w}=Az^k+Bz^{k+1}, \quad w=Cz^k+Dz^{k+1}. \tag{4.4}$$

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.

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

$$\psi^{(2m)}(w, \tau)=\sum_{k=1}^{m}\phi^{(2k-1)}(w)\tau^{2k-1}, \quad m=1, 2, \cdots. \tag{4.5}$$

Then the gradient transformation

$$w\to\hat{w}=\psi_w^{(2m)}(w, \tau) \tag{4.6}$$

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 (4.4). 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

$$\phi(w, t)=\frac{1}{2}w'\left(2J\tanh\frac{\tau}{2}L\right)w, \quad L=J^{-1}S, \quad S'=S, \tag{4.7}$$

where

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

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

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

(4.6) becomes symplectic difference schemes

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

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

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