CANONICAL DIFFERENCE SCHEMES FOR HAMILTONIAN CANONICAL DIFFERENTIAL EQUATIONS[①]

哈密尔顿典则方程的典则差分格式

The present program[1] that the author and his group have started is a systematic study, within the framework of symplectic geometry, 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, pseudodifferential 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.

We consider the canonical system in finite dimensions

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

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

In the following, vectors are always represented by column matrices, matrix transpose is denoted by a prime $'$. Let $z = (z_1, \ldots, z_n, z_{n+1}, \ldots, z_{2n})' = (p_1, \ldots, p_n, q_1, \ldots, q_n)'$, (1) can be written as

$$\frac{dz}{dt} = J^{-1}H_z, \quad J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \tag{2}$$

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 (2) can be generated by a one-parameter group G_t of canonical transformations of R^{2n} (locally in t and z) such that

$$G_{t_1}G_{t_2} = G_{t_1+t_2}$$
$$z(t) = G_t z(0).$$

①In Proc Inter Workshop on Applied Diff Equations. Singapore: World Scientific. 1986: 59–73

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 symplectic everywhere, 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 $\omega \wedge \omega \cdots \wedge \omega$. They constitute the class of conservation laws of phase area of even dimensions for the Hamiltonian system (2).

Moreover, the Hamiltonian systems possesses another class of conservation laws related to the energy $H(z)$. A function $\phi(z)$ is said to be an invariant integral of (2) if it is invariant under (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

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

H itself is always an invariant integral. See, e.g., Refs. 5 and 6.

For the numerical study, we are less interested in (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. 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.

We give a brief survey of some of our preliminary results[1−4].

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

$$H(z) = \frac{1}{2} z'Sz, \quad S' = S, \quad H_z = S(z). \tag{3}$$

Then the canonical system is linear

$$\frac{dz}{dt} = Bz, \tag{4}$$

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

$$B'J + JB = 0.$$

The solution is

$$z(t) = G_t z(0),$$

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

Theorem 0. *The weighted Euler scheme*

$$\frac{z^{k+1}-z^k}{\tau}=B(\alpha z^{k+1}+(1-\alpha)z^k) \tag{5}$$

for the linear system (4) *is symplectic if and only if* $\alpha=1/2$, *i.e. it is the case of time-centered Euler Scheme with the transition.*

For the time-centered case, the transition matrix

$$z^{k+1}=F_\tau z^k,\quad F_\tau=\phi(\tau B),\quad \phi(\lambda)=\frac{1+\frac{\lambda}{2}}{1-\frac{\lambda}{2}} \tag{6}$$

F_τ, as Cayley transform of infinitesimally symplectic τB, 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) $\psi(0)\neq 0$.

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

$$B'A+AB=0.$$

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

$$z^{k+1}=\psi(\tau B)z^k, \tag{7}$$

considered as an approximative scheme for the canonical system (4), *is symplectic, of m-th order of accuracy and has the property that $z'Aw$ is invariant under $\psi(\tau B)$ if and only if it is invariant under G_τ of* (4).

Remark 1. The last property is remarkable in the sense that, all the bilinear invariants of the system (4), no more and no less, are kept invariant under the scheme (7), 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 for the construction of symplectic difference schemes, take the diagonal Padé approximants to the exponential function

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

Theorem 2. *The difference schemes*

$$z^{k+1}=\frac{P_m(\tau B)}{P_m(-\tau B)}z^k,\quad m=1,2,\ldots \tag{8}$$

for the system (4) *are symplectic, A-stable, of $2m$-th order of accuracy, and having the same set of bilinear invariants as that of system* (4). *The case $m=1$ is the centered Euler scheme.*

For the general non-linear canonical system (2), the time-centered Euler scheme is

$$\frac{1}{\tau}(z^{k+1}-z^k)=J^{-1}H_z(\frac{1}{2}(z^{k+1}+z^k)). \tag{9}$$

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

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

symplectic everywhere. However, unlike the linear case the invariant integrals $\varphi(z)$ of system (2), including $H(z)$, are conserved only approximately

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

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

$$\begin{aligned}
&\frac{1}{\tau}(p^{k+1} - p^k) = -V_q(q^{k+\frac{1}{2}}),\\
&\frac{1}{\tau}(q^{k+1+\frac{1}{2}} - q^{k+\frac{1}{2}}) = U_q(q^{k+1}).
\end{aligned} \tag{10}$$

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

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

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

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

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

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

For the comparison of stability for the linear system (4) with separable Hamiltonian with the canonical schemes in Theorems 1, 2 the staggered scheme and the application of the latter to the wave equation see Ref 1. In Ref 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 to be difficult, however, for the general non-linear systems.

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 functions and Hamilton-Jacobi equations. Our approach is in part inspired by the early works of Siegel[7] and Hua[8]. Every $4n \times 2n$ matrix

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

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.

$$AP = B, \quad \text{i.e.,} \quad \begin{pmatrix} A_1 P \\ A_2 P \end{pmatrix} = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}, \quad \text{for some } P \in GL(2n).$$

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

$$J_{4n} = \begin{pmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{pmatrix}, \quad \tilde{J}_{4n} = \begin{pmatrix} -J_{2n} & 0 \\ 0 & +J_{2n} \end{pmatrix}$$

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

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

$$X' J_{4n} X = 0_{2n}, \quad \text{i.e.} \quad X_1' X_2 - X_2' X_1 = 0_{2n}.$$

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

$$Y' \tilde{J}_{4n} Y = 0_{2n}, \quad \text{i.e.} \quad Y_1' J_{2n} Y_1 - Y_2' J_{2n} Y_2 = 0_{2n}.$$

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

A $2n$-dimensional submanifold $U \subset R^{4n}$ is called J_{4n}-Lagrangian (resp. $\tilde{J}_{4n}$-Lagrangian) if the tangent plane of U is a J_{4n}-Lagrangian (resp. $\tilde{J}_{4n}$-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,

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

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

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,

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

is a J_{4n}-Lagrangian submanifold, whose tangent plane is spanned by the symmetric pair $\binom{N(w)}{I}$. The following algebraic theorem is crucial for our construction.

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

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

i.e.

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

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

The totality of $T's$ in Theorem 3 will be denoted by $CSp(\tilde{J}_{4n}, J_{4n})$. 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 certain transversality condition, for the canonical transformations.

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

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

If (in some neighborhood of R^{4n}) the transversality condition

$$| CM + D | \neq 0, \tag{11}$$

holds, then there exists in (some neighborhood of) R^{4n} a gradient transformation $w \to \hat{w} = f(w)$ with Jacobian $f_w = N(w) \subset Sm(2n)$ and graph

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

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 (11)

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

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 (2) with Hamiltonian function $H(z)$, we have the following general theorem on the existence and construction of time-dependent generating function and Hamilton-Jacobi equation depending on T and H under the 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, $M(z,0) = M_0$ be 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 (2). If*

$$| CM_0 + D | \neq 0.$$

then for sufficiently small $| t |$, the transversality condition (11) holds and there exists 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) $\phi_t(w,t) = -\mu H(C_1\phi_w(w,t) + D_1 w)$, $w = C\hat{z} + D_z$.

The last equation is the most general Hamilton-Jacobi equation for the canonical system with Hamiltonian $H(z)$ and linear transformation $T \in CS_p(\tilde{J}_{4n}, J_{4n})$.

By recursions we can determine explicitly the power series expansions for all possible time-dependent generating functions for analytic Hamiltonians.

Theorem 6. *Let $H(z)$ depends analytically on z, then $\phi(w,t)$ in Theorem 5 is expressible as convergent power series in t for sufficiently small $|t|$:*

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

Examples of special types of generating functions:

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

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

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

This is the generating function and H.J. equation of the first kind for the "free" canonical transformations[5].

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

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

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

This is the generating function and H.J. equation of the second kind[5].

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

$$w = \begin{pmatrix} \frac{1}{2}(\hat{p} + p) \\ \frac{1}{2}(\hat{q} + q) \end{pmatrix} = \begin{pmatrix} \bar{p} \\ \bar{p} \end{pmatrix} = \text{mean values}, \quad \phi = \phi(\bar{p}, \bar{q}, t),$$

$$\hat{w} = \begin{pmatrix} q - \hat{q} \\ \hat{p} - p \end{pmatrix} = \begin{pmatrix} \phi_{\bar{p}} \\ \phi_{\bar{q}} \end{pmatrix}, \quad \phi_t = -H(\bar{p} + \frac{1}{2}\phi_{\bar{q}}, \bar{q} - \frac{1}{2}\phi_{\bar{p}})$$

This is a new type of generating functions and H.J. equations, not encountered in the classical literature. $\phi(\bar{p}, \bar{q}, t)$ is an odd function in t.

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 it or approximate it in some way, take the 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. As an illustration we construct a generalization of centered Euler scheme with arbitrarily high order of accuracy.

Theorem 7. *Choose the generating function of Example* (III) *with its m-th truncation*

$$\phi(\bar{p},\bar{q},\tau)=\sum_{k=0}^{\infty}\phi^{(2k+1)}(\bar{p},\bar{q},)\tau^{2k+1},$$

$$\phi_m(\bar{p},\bar{q},\tau)=\sum_{k=0}^{m-1}\phi^{(2k+1)}(\bar{p},\bar{q},)\tau^{2k+1},\quad m=1,2,\ldots,$$

with $\tau>0$ small enough as the time-step, $\phi(\tau)-\phi_m(\tau)=O(\tau^{2n})$. Let $\hat{z}=z^k$, $z=z^{k+1}$, $\bar{z}=\frac{1}{2}(z^k+z^{k+1})$, then

$$\hat{q}-q=\sum_{k=0}^{m-1}\phi_{\bar{p}}^{(2k+1)}(\bar{p},\bar{q})\tau^{2k+1},$$

$$p-\hat{p}=\sum_{k=0}^{m-1}\phi_{\bar{q}}^{(2k+1)}(\bar{p},\bar{q})\tau^{2k+1}$$

is a canonical difference scheme of $2m$-th order of accuracy, $m=1$ is the centered Euler scheme (9).

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

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

4 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

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

6 Abraham R, Marsden J. Foundations of Mechanics. 2nd ed. Mass: Addison-Wesley, Reading. 1978

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

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