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ON THE APPROXIMATION OF LINEAR HAMILTONIAN SYSTEMS*1)

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Abstract

When we study the oscillation of a physical system near its equilibrium and ignore dissipative effects, we may assume it is a linear Hamiltonian system (H-system), which possesses a special symplectic structure. Thus there arises a question: how to take this structure into account in the approximation of the H-system? This question was first answered by Feng Kang for finite dimensional H-systems[1-4].

We will in this paper discuss the symplectic difference schemes preserving the symplectic structure and its related properties, with emphasis on the infinite dimensional H-systems.

In the first section we propose the notion of symmetry of a difference scheme, and obtain the equivalence between symmetries and the conservation of first integrals. In the second section we discuss hyperbolic equations with constant coefficients in one space variable. This kind of H-system possesses not only a symplectic structure, but also a unitary structure. Our result is that a difference scheme is symplectic iff its amplification factors are of modulus one. In the third section we discuss symmetric hyperbolic equations with constant coefficients in several space variables. Although the antisymmtric operator of the symplectic structure is not invertible in that case, we obtain a similar conclusion. In the fourth section, we propose the notion of multiple-level symplectic difference schemes Finally, we derive the generating function for K-symplectic transformation, and construct a SDS for a hyperbolic equation with variable coefficients using the generating functions.

§1. Symmetries of Difference Schemes

a) Consider a linear Hamiltonian system with quadratic Hamiltonian $H(z)=\frac{1}{2}z^TAz$:

$$\frac{dz}{dt}=J^{-1}Az, \tag{0}$$

where $J=\begin{bmatrix}0 & I_n\\ -I_n & 0\end{bmatrix}$ and A is a $2n\times 2n$ symmetric matrix, and a difference scheme

$$z^{m+1}=\phi(J^{-1}A)z^m. \tag{1}$$

Definition. *We say* (1) *is a symplectic difference scheme if the matrix* $\phi=\phi(J^{-1}A)$ *is a symplectic matrix.*

Now we perform a canonical coordinate transformation $z\to w: z=Pw$, and the H-system written in the new coordinate w is

$$\frac{dw}{dt}=J^{-1}P^TAPw \tag{2}$$

and the scheme (1) is

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$$w^{m+1}=P^{-1}\phi(J^{-1}A)Pw^m. \tag{3}$$

Now we construct the difference scheme for the H-system (2)

$$w^{m+1}=\phi(J^{-1}P^TAP)w^m. \tag{4}$$

Then there arises a problem: Is scheme (3) equivalent to scheme (4)? The answer leads to the notion of symmetry.

Definition. *We say a scheme (1) is invariant under a group G of linear symplectic transformations if*

$$P^{-1}\phi(J^{-1}A)P=\phi(J^{-1}P^TAP)$$

for all A symmetric and all $P\in G$.

Another question of interest is: If a quadratic form $f(z)=\frac{1}{2}z^TBz$ is a first integral of the H-system, is it conserved by scheme (1), i.e.,

$$f(z^{m+1})=f(z^m)$$

for all $z^{m+1}=\phi(J^{-1}A)z^m$?

Example 1. Euler's mid-point scheme

$$z^{m+1}-z^m=\tau J^{-1}A((z^{m+1}+z^m)/2), \tag{5}$$

where τ is the time step, is symplectic and is invariant under the full symplectic group $S_p(2n)$. All the quadratic first integrals are conserved by the scheme (5)[2].

Theorem 1. *Let the quadratic form $f(z)=\frac{1}{2}z^TBz$ is a first integral of the H-system (0), $G^t=\exp(tJ^{-1}B)$ is the phase flow of the H-system with Hamiltonian $f(z)$, the scheme (1) is symplectic. Then f is conserved by (1) iff (1) is invariant under the phase flow G^t.*

Proof. By definition,

$$(G^t)^{-1}\phi(J^{-1}A)G^t=\phi((G^t)^{-1}J^{-1}AG^t)=\phi(J^{-1}(G^t)^TAx^t), \tag{6}$$

f is a first integral of the H-system. By the Noether theorem, $(G^t)^TAG^t=A$. Thus it follows from (6) that

$$(G^t)^{-1}\phi(J^{-1}A)G^t=\phi(J^{-1}A),\text{ or }\phi(J^{-1}A)G^t=G^t\phi(J^{-1}A).$$

Taking derivative at $t=0$ and making use of $\left.\frac{d}{dt}\right|_{t=0}G^t=J^{-1}B$, we obtain

$$(\phi(J^{-1}A))^TB\phi(J^{-1}A)=(\phi(J^{-1}A))^TJ\phi(J^{-1}A)J^{-1}B=JJ^{-1}B=B.$$

Thus the symmetries imply conservations.

Now we assume conservations, i.e, $(\phi(J^{-1}A))^TB\phi(J^{-1}A)=B$. Then

$$J^{-1}B(\phi(J^{-1}A))=\phi(J^{-1}A)J^{-1}B,$$

and

$$\phi(J^{-1}A)\exp(J^{-1}Bt)=\exp(J^{-1}Bt)\phi(J^{-1}A).$$

Example 2. The generalized Euler scheme

$z^{m+1}=\phi(\tau J^{-1}A)z^m$, where $\phi_p(\lambda)$ is the p-th diagonal Pade approximant of $\exp\lambda$, is invariant under $S_p(2n)$. Hence all the first integrals of quadratic form are conserved by the difference scheme[1,2,4].

b) We will generalize the above notion to the nonlinear Hamiltonian system:

$$\frac{dz}{dt}=J^{-1}H_z \tag{(0)'}$$

Suppose we have a symplectic difference scheme derived according to a certain rule:

$$z^{m+1}=\phi_{J^{-1}H_z}(z^m) \tag{(1)'}$$

where $\phi_{J^{-1}H_z}$ is a nonlinear symplectic transformation (locally). Now we perform a nonlinear symplectic transformation $z=S(w)$. Then the H-system (0)′ written in the coordinate w is

$$\frac{dw}{dt}=J^{-1}\tilde{H}_w$$

where $\tilde{H}(w)=H(S(w))$.

Now the scheme (1)′ written in the new coordinate is

$$w^{m+1}=S^{-1}\circ\phi\circ S(w^m).$$

Definition. *We say the scheme* (1)′ *is invariant under a group G of symplectic transformations, if*

$$S^{-1}\circ\phi_{J^{-1}H_z}\circ S=\phi_{J^{-1}\tilde{H}_w},\qquad \forall S\in G.$$

Theorem 2. *Suppose f is a first integral of the* H-*system* (0)′, *and G^t is the phase flow of the Hamiltonian function f. Then f is conserved up to a constant by the scheme* (1)′

$$f\circ\phi_{J^{-1}H_z}(z)=f(z)+c,\quad c \textit{ is a constant},$$

iff the scheme (1)′ *is invariant under G^t.*

The proof will be given in subsection c.

Remark. If the scheme has a fixed point, i.e a point z, such that

$$\phi_{J^{-1}H_z}(z)=z,$$

then the constant $c=0$. This is often the case in practice.

Example 3. Euler's mid-point scheme

$$z^{n+1}-z^n=\tau J^{-1}H_z\left(\frac{z^n+z^{n+1}}{2}\right)$$

is invariant under any linear symplectic transformation. Thus every first integral of quadratic form are conserved by this scheme.

Example 4. The staggered explicit scheme for separable Hamiltonian function $H(p,q)=U(p)+V(q)$ (cf. [1])

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

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

is invariant under a canonical transformation of the form

$$\begin{bmatrix} A^{-T} & 0\\ 0 & A\end{bmatrix}.$$

Thus the linear momentum and angular momentum are conserved by the scheme.

c) The Proof of Theorem 2.

We will work in the general context of a phase manifold P (cf. [5]) with a symplectic 2-form ω. Recall that a function f on P determines a Hamiltonian vector field $J^{-1}df$ such that

$$\langle df, x\rangle = \omega(x, J^{-1}df) \quad \forall x \in TP.$$

First we assume the symmetry, changing the notation $\phi_{J^{-1}H_z} = \phi_{J^{-1}dH}$ for convenience,

$$(G^t)^{-1} \circ \varphi_{J^{-1}dH} \circ G^t = \varphi_{J^{-1}(G^t)^*dH}.$$

Since f is a first integral of the system $(0)'$,

$$(G^t)^* dH = d(H \circ G^t) = dH.$$

Thus

$$G^t_f \circ \phi_{J^{-1}dH} = \phi_{J^{-1}dH} \circ G^t.$$

Taking derivative at $t=0$, $a \in P$, we have

$$J^{-1}df \circ \phi_{J^{-1}dH}(a) = (\phi_{J^{-1}dH})_* J^{-1}df(a).$$

Then for $x \in T_{\phi(a)}P$, $\phi = \phi_{J^{-1}dH}$,

$$\omega(J^{-1}df(a), (\phi^{-1})_* x) = \phi^* \omega(J^{-1}df(a), (\phi^{-1})_* x)$$
$$= \omega((\phi)_* J^{-1}df(a), x) = \omega(J^{-1}df \circ \phi(a), x),$$
$$\langle (\phi^{-1})^* df(a), x\rangle = \langle df(a), (\phi^{-1})_* x\rangle = \omega((\phi^{-1})_* x, J^{-1}df(a))$$
$$= \omega(x, J^{-1}df \circ \phi(a)) = \langle df \circ \phi(a), x\rangle.$$

Hence

$$((\phi^{-1})^* df - df)(\phi(a)) = 0,$$

or,

$$d(f \circ \phi) - df = 0,$$
$$f \circ \phi = f + c \ (c \text{ constant}).$$

Now we assume the conservation

$$f \circ \phi_{J^{-1}dH} = f + c.$$

We can prove that

$$(\phi_{J^{-1}dH})_* J^{-1}df = J^{-1}df \circ \phi_{J^{-1}dH}.$$

The phase flows of the vector fields $J^{-1}df$ and $(\phi_{J^{-1}dH})J^{-1}df \circ \phi^{-1}_{J^{-1}dH}$ are G^t, $\phi_{J^{-1}dH} \circ G^t \circ \phi^{-1}_{J^{-1}dH}$ respectively. Therefore

$$G^t = \phi_{J^{-1}dH} \circ G^t \circ \phi^{-1}_{J^{-1}dH}.$$

§ 2. Symplectic Difference Schemes for Hyperbolic Equations

Because the H system treated here possesses a unitary structure, we will make use of the language of complex number.

a) Consider the phase space $\mathbf{R}^{2n}$ with a canonical coordinates p_i, q_i. We can regard it as an n-dimensional complex space $\mathbf{C}^n$, with the coordinates $z_j = p_j + iq_j$.

Recall that an $n \times n$ complex matrix can be realized as a $2n \times 2n$ real matrix. On the other hand, a $2n \times 2n$ real matrix A can be complexified into an $n \times n$ complex matrix $C(A)$ such that

$$c(Az) = C(A)c(z), \quad \forall z \in \mathbf{R}^{2n}$$

iff A is of the form

$$A=\begin{bmatrix} A_1 & -B_1 \\ B_1 & A_1 \end{bmatrix},\ C(A)=A_1+iB_1,\ z=\begin{bmatrix} p \\ q \end{bmatrix},\ c(z)=p+iq.$$

In particular, $C(J_{2n}^{-1})=I_n i$.

A symplectic matrix can be complexified iff it is an orthogonal matrix at the same time, and $C(A)$ is a unitary matrix. On the other hand, a complexifiable matrix is symplectic iff it is unitary

$$U(n)=\mathrm{Sp}(2n)\cap O(2n)=\mathrm{Sp}(2n)\cap GL(n, C).$$

b) Consider a hyperbolic equation with periodic boundary condition:

$$\frac{\partial u}{\partial t}=\frac{\partial u}{\partial x}. \tag{7}$$

Here the antisymmetric operator is $D=\frac{\partial}{\partial x}$, the symplectic form is $\omega(w, v)=\int_0^{2\pi} wDv dx$ and the Hamiltonian functional is $H(u)=\frac{1}{2}\int_0^{2\pi} u^2 dx$ with functional derivative $H_u=u$. So (7) is an infinite dimensional H-system (cf. [6])

$$\frac{\partial u}{\partial t}=DH_u.$$

Using complex Fourier expansion for the real periodic $u(x, t)$, we have

$$u(x, t)=\sum_{-\infty}^{\infty} c_k(t)e^{ikx},\ c_{-k}=\bar{c}_k,\ \frac{dc_k}{dt}=\sum_{-\infty}^{\infty} ikc_k.$$

Now consider a difference scheme approximating (7):

$$P_1(E)u^{n+1}=P_2(E)u^n \tag{8}$$

where $P_1(\lambda)$ and $P_2(\lambda)$ are functions of the form

$$\sum a_k\lambda^k,\quad k \text{ are integers}$$

and E is the shift operator: $(Eu)(x)=u(x+h)$; h is the space step.

Expand the functions u^n, u^{n+1} in Fourier series

$$u^n=\sum c_k^n e^{ikx},\quad u^{n+1}=\sum c_k^{n+1}e^{ikx},$$

and substitute them into (8). Then

$$P_1(e^{ikh})c_k^{n+1}=P_2(e^{ikh})c_k^n.$$

Hence the transformation $u^n\to u^{n+1}$ can be complexified. From the discussion in subsection a, we have

Theorem 3. *The difference scheme (8) is symplectic iff the amplification factors are of modulus one*

$$|P_2(e^{ikh})/P_1(e^{ikh})|=1.$$

c) Consider the following hyperbolic system with periodic boundary condition

$$\frac{\partial U}{\partial t}=\frac{\partial}{\partial x}(AU), \tag{9}$$

where $U=(u_1, \cdots, u_m)$, A is a constant real symmetric matrix, the antisymmetric operator is $D=I_m\frac{\partial}{\partial x}$, the H functional is $\frac{1}{2}\int U^T AU\, dx$, and the symplectic two-form is

$$\omega(U, V)=\int U^T DV\,dx.$$

We have similar Fourier expansions as in subsection b, but with complex vector coefficients C_k instead. Now consider a difference scheme

$$P_1(E)U^{n+1}=P_2(E)U^n \tag{10}$$

where $P_1(\lambda)$, $P_2(\lambda)$ are $n\times n$ matrices, their elements are functions of the form

$$\sum a_k\lambda^k.$$

Let C_k^n, C_k^{n+1} be the Fourier coefficients of U^n, U^{n+1} respectively, then

$$P_1(e^{ikh})C_k^{n+1}=P_2(e^{ikh})C_k^n.$$

Theorem 4. *The scheme* (10) *is symplectic iff the amplification matrices*

$$P_1^{-1}(e^{ikh})P_2(e^{ikh})$$

are unitary.

§ 3. The Case for Hyperbolic Equations in Several space Variables

a) Consider an equation

$$\frac{\partial u}{\partial t}=\frac{\partial u}{\partial x}+2\frac{\partial u}{\partial y}.$$

Here the H operator is $D=\frac{\partial}{\partial x}+2\frac{\partial}{\partial y}$, which is not invertible. Therefore the notion of canonical transformation needs reconsideration.

b) Consider a scalar hyperbolic equation in several periodic space variables

$$\frac{\partial U}{\partial t}=\left(A_1\frac{\partial}{\partial x_1}+A_2\frac{\partial}{\partial x_2}+\cdots+A_n\frac{\partial}{\partial x_n}\right)U.$$

Let antisymmetric operator $D=A_1\frac{\partial}{\partial x_1}+\cdots+A_n\frac{\partial}{\partial x_n}$, and the action of D on $e^{iK\cdot X}$ is $D\cdot e^{iK\cdot X}=iA\cdot Ke^{iK\cdot X}$, with the notations

$$A=(A_1, \cdots, A_n),\ K=(k_1, \cdots, k_n)\quad A\cdot K=A_1k_1+\cdots+A_nk_n.$$

We say an index K is resonant if $A\cdot K=0$; otherwise it is non-resonant.

Now the given equation is a H-system with Hamiltonian functional $H(U)=\frac{1}{2}\int U^2dX$ and symplectic form $\omega(U, V)=\int U\,DV\,dX$.

Definition. *A linear bounded invertible transformation T is a symplectic transformation if*

1) $\omega(TU, TV)=\omega(U, V)$ *holds for all U, V;*

2) *if $DU=0$, then $TU=U$.*

c) Consider a difference scheme

$$P_1(E)U^{m+1}=P_2(E)U^m \tag{11}$$

where $P_1(\lambda)$, $P_2(\lambda)$ are functions of the form

$$\sum a_K\lambda_1^{k_1}\cdots\lambda_n^{k_n}=\sum a_K\lambda^K$$

with the notations $E=(E_1, \cdots, E_n)$, $E_iU(X)=U(X+h_ie_i)$; $h=(h_1, \cdots, h_n)$. Then

$$P_1(E)e^{iK\cdot X}=P_1(e^{iK\cdot h})e^{iK\cdot X}.$$

Now assume that $U^{m+1}=\sum C_K^{m+1}e^{iK\cdot X}$, $U^m=\sum C_K^m e^{iK\cdot X}$. Substituting them into (11), we have

$$P_1(e^{iK\cdot H})C_K^{m+1}=P_2(e^{iK\cdot H})C_K^m.$$

Theorem 5. *The scheme* (11) *is symplectic iff* $|(P_1(e^{iK\cdot H}))^{-1}P_2(e^{iKH})|=1$ *if* K *is non-resonant and* $P_1(e^{iKH})=P_2(e^{iKH})$ *otherwise.*

Proof. Suppose the condition of the theorem is satisfied. Denote the matrix $(P_1(e^{iKh}))^{-1}P_2(e^{iKh})$ by F_K,

$$U^m=\sum B_K e^{iKX},\ U^{m+1}=\sum F_K B_K e^{iKX},$$
$$V^m=\sum C_K e^{iKX},\ V^{m+1}=\sum F_K C_K e^{iKX},$$
$$\omega(U^m,\ V^m)=\sum_{k_1>0}\mathrm{Im}(B_K\bar{C}_K)(A\cdot K)(2\pi)^n,$$
$$\omega(U^{m+1},\ V^{m+1})=\sum_{k_1>0}\mathrm{Im}(B_K F_K\bar{F}_K\bar{C}_K)(A\cdot K)(2\pi)^n.$$

If K is non-resonant, $F_K\bar{F}_K=1$; otherwise $A\cdot K=0$. therefore

$$\omega(U^m,\ V^m)=\omega(U^{m+1},\ V^{m+1}).$$

If $DV^m=0$, then $V^m=\sum_{K\in R}C_K e^{iK\cdot X}$, where R is the set of K satisfying $A\cdot K=0$, $V^{m+1}=\sum_{K\in R}F_K C_K e^{iK\cdot X}=V^m$.

The converse is easy to prove.

§ 4. Multiple-level Symplectic Difference Schemes

a) We first consider a H-system

$$\frac{\partial z}{\partial t}=J^{-1}Az.$$

Let $v(t)=z(t-\tau)$; then

$$\frac{d}{dt}\begin{bmatrix} z\\ v\end{bmatrix}=\begin{pmatrix}0 & J^{-1}\\ J^{-1} & 0\end{pmatrix}\begin{pmatrix}0 & A\\ A & 0\end{pmatrix}\begin{pmatrix}z\\ v\end{pmatrix},$$

where the antisymmtric operator is $\begin{bmatrix}0 & J^{-1}\\ J^{-1} & 0\end{bmatrix}$.

Consider a 3-level difference scheme of the form

$$z^{n+1}-\phi_1 z^n-\phi_2 z^{n-1}=0, \tag{12}$$

By introducing a new variable $v^n=z^{n+1}$, (12) can be written in the form

$$\begin{bmatrix}z^{k+1}\\ v^{k+1}\end{bmatrix}=\begin{bmatrix}\phi_1 & \phi_2\\ I_n & 0\end{bmatrix}\begin{bmatrix}z^k\\ v^k\end{bmatrix}.$$

Definition. *We say a difference scheme* (12) *is symplectic if*

$$\begin{bmatrix}\phi_1 & \phi_2\\ I_n & 0\end{bmatrix}^T\begin{bmatrix}0 & J^{-1}\\ J^{-1} & 0\end{bmatrix}\begin{bmatrix}\phi_1 & \phi_2\\ I_n & 0\end{bmatrix}=\begin{bmatrix}0 & J^{-1}\\ J^{-1} & 0\end{bmatrix}.$$

After a short computation, we can prove

Lemma 1. *Scheme* (12) *is symplectic iff* ϕ_1 *is an infinitesimal symplectic matrix and* $\phi_2=I$.

For example, the following schemes are symplectic,

$$z^{n+1}-\phi_m(\tau J^{-1}A)z^n-z^{n-1}=0$$

where

$$\phi_0(\lambda)=2\lambda,$$

$$\phi_m(\lambda)=2\sum_{k=0}^{m}\frac{\lambda^{2k+1}}{(2k+1)!}.$$

b) A real vector $z\in\mathbb{R}^{2n}$ can also be regarded as a complex vector $c(z)$. Then, from

$$z^{n+1}-\phi z^n-z^{n-1}=0$$

we have

$$c(z^{n+1})-c(\phi z^n)-c(z^{n-1})=0.$$

If matrix ϕ can be complexified as $C(\phi)$, the above can be written as

$$c(z^{n+1})-C(\phi)c(z^n)-c(z^{n-1})=0.$$

Lemma 2. *The necessary and sufficient condition that an infinitesimal symplectic matrix can be complexified is that it is an infinitesimal orthogonal matrix, and the complexified matrix is an infinitesimal unitary matrix.*

Lemma 3. *A complex matrix is an infinitesimal symplectic matrix iff it is an infinitesimal unitary matrix.*

The proofs of these lemmas are easy.

c) Consider a three-level difference scheme for $\frac{\partial u}{\partial t}=\frac{\partial u}{\partial x}$:

$$u^{n+1}-2\tau P_1(E)u^n-P_2(E)u^{n-1}=0.$$

It is easy to prove that it is symplectic iff $P(E)$ is a centered differencing $P(E^{-1})=-P(E)$, $P(E)=I$.

Note that the well known leap-frog scheme is symplectic. Another one with accuracy $O(\tau^4+h^4)$ is

$$\frac{u^{n+1}(x)-u^{n-1}(x)}{2\tau}+\frac{1}{12h}(u^n(x+2h)-8u^n(x+h)+8u^n(x-h)-u^n(x-2h))$$

$$=\frac{\tau^2}{36h^3}(u^n(x+2h)-2u^n(x+h)+2u^n(x-h)-u^n(x-2h)).$$

d) The above notion can be generalized to the non-linear H-system

$$\frac{dz}{dt}=J^{-1}H_z.$$

Consider a three-level difference scheme

$$z^{n+1}-\phi_1(z^n)-\phi_2(z^{n-1})=0. \tag{13}$$

Introduce a new variable $v^n=z^{n-1}$, then

$$z^{n+1}=\phi_1(z^n)+\phi_2(v^n),$$
$$v^{n+1}=z^n.$$

We say (13) is symplectic if the Jacobian $Q=\frac{\partial(z^{n+1},\ v^{n+1})}{\partial(z^n,\ v^n)}$, satisfies

$$Q^T\begin{bmatrix}0 & J^{-1}\\ J^{-1} & 0\end{bmatrix}Q=\begin{bmatrix}0 & J^{-1}\\ J^{-1} & 0\end{bmatrix}$$

Theorem 6. *Scheme (D) is symplectic iff $\frac{\partial\phi_1}{\partial z^n}$ is an infinitesimal symplectic* matrix, $\frac{\partial \phi_2}{\partial z^{n-1}}=I$.

For example, the leap-frog scheme

$$z^{n+1}-2\tau J^{-1}H_z(z^n)-z^{n-1}=0$$

is symplectic.

§ 5. Symplectic Schemes Based on Generating Functions

We will extend the construction of symplectic difference schemes based on the generating functions in [2].

Suppose K is an invertible skew-symmetric matrix. We say a transformation T is a K-symplectic transformation if its Jacobian matrix is a K-symplectic matrix.

Lemma 4. *A K-symplectic transformation, not too far from the identity, can be given by a generating function ϕ of Euler type*

$$\tilde{w}=T(w),\ K(\tilde{w}-w)=\phi_w\left(\frac{w+\tilde{w}}{2}\right).$$

Proof. There exists a non-singular matrix P s.t., $P^TKP=J$. Let $z=Pw$, $\tilde{z}=P\tilde{w}$. Then the transformation $z\to\tilde{z}=P^{-1}\circ T\circ P(z)$ is a J-symplectic transformation, which can be given by a generating function $\tilde{\phi}$:

$$J(\tilde{z}-z)=\tilde{\phi}_z\left(\frac{\tilde{z}+z}{2}\right).$$

Let $\phi(w)=\tilde{\phi}(Pw)$; then from above,

$$K(\tilde{w}-w)=\phi_w\left(\frac{\tilde{w}+w}{2}\right).$$

b) Now we are going to construct a symplectic scheme for the following hyperbolic equation with variable coefficient $a(x)$

$$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}(au).$$

We first discretize in the time direction (cf. [2]),

$$(12-6\tau D+\tau^2D^2)u^{n+1}=(12+6\tau D+\tau^2D^2)u^n,\ D=\frac{\partial}{\partial x},$$

which can be written in terms of a generating functional ϕ

$$(u^{n+1}-u^n)=\frac{\partial}{\partial x}\phi_u\left(\frac{u^{n+1}+u^n}{2}\right),$$

where $\phi_u=\frac{\delta\phi}{\delta u}$ is the variational derivative of

$$\phi(u)=6\tau\int ua(12-6\tau D+\tau^2D^2)^{-1}u\,dx.$$

We approximate $\frac{\partial}{\partial x}$ by $P_1(E)=-\frac{1}{12}(E-8E+8E^{-1}-E^{-2})$, $\phi(u)$ by $\phi_n(u)=6\tau\int ua(12-6\tau(P_1(E)a)+\tau^2(P_2(E)a)^2)^{-1}u\,dx$, $P_2(E)=\frac{1}{h^2}(E-2I+E^{-1})$. Then $\phi_n(u)$ gives rise to a symplectic transformation $u^n\to u^{n+1}$ by

$$u^{n+1}-u^n=P_1(E)\frac{\delta\phi_n}{\delta u}\left(\frac{u^{n+1}+u^n}{2}\right)$$

or,

$$
\begin{aligned}
&(12-6\tau P_1(E)a+\tau^2(P_2(E)a)^2)u^{n+1}\\
&=(12+6\tau P_1(E)a+\tau^2(P_2(E)a)^2u^n.
\end{aligned}
$$

This is symplectic and of accuracy (τ^4+h^4).

References

[1] Feng, Kang: On difference schemes and symplectic geometry, Proceedings of 1984 Beijing International Symposium on Diffenential Geometry and Differential Equations, Ed-Feng Kang, Science Press, 1985, 42—58,

[2] Feng, Kang: Difference schemes for Hamiltonian formalism and symplectic geometry, *Jour. of Computational Mathematics*, **4**: 3 (1986), 279—289.

[3] Feng, Kang: Symplectic geometry and numerical methods in fluid dynamics, Proceedings of Tenth International Conference on Numerical Methods in Fluid Dynamics, Lecture Notes in Physics, 264, Springer-Verlag, Berlin, 1986, 1—7.

[4] Feng, Kang; Wu, Hua-mo; Qing Meng-zhao: Symplectic difference schemes for the linear Hamiltonian canonical systems, to appear.

[5] Arnold, V. I.: Mathematical Methods of Classical Mechanics, Springer-Verlag, Berlin, 1978.

[6] Benjamin, T. Brooke: Impulse, flow forces and variational principles, *IMA Jour. of Applied Mathematics*, **32** (1984), 3—68.