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THE CALCULUS OF GENERATING FUNCTIONS AND THE FORMAL ENERGY FOR HAMILTONIAN ALGORITHMS*[1)]

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Abstract

In [2–4], symplectic schemes of arbitrary order are constructed by generating functions. However the construction of generating functions is dependent on the chosen coordinates. One would like to know that under what circumstance the construction of generating functions will be independent of the coordinates. The generating functions are deeply associated with the conservation laws, so it is important to study their properties and computations. This paper will begin with the study of Darboux transformation, then in section 2, a normalization Darboux transformation will be defined naturally. Every symplectic scheme which is constructed from Darboux transformation and compatible with the Hamiltonian equation will satisfy this normalization condition. In section 3, we will study transformation properties of generator maps and generating functions. Section 4 will be devoted to the study of the relationship between the invariance of generating functions and the generator maps. In section 5, formal symplectic erengy of symplectic schemes are presented.

Key words: Generating function, calculus of generating functions, Darboux transformation cotangent bundles, Lagrangian submanifold, invariance of generating function, formal energy.

1. Darboux Transformation

Consider cotangent bundle $T^*R^n \simeq R^{2n}$ with natural symplectic structure

$$J_{2n} = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix} \tag{1.1}$$

and the product of cotangent bundles $(T^*R^n) \times (T^*R^n) \simeq R^{4n}$ with natural product symplectic structure

$$\tilde{J}_{4n} = \begin{bmatrix} -J_{2n} & 0 \\ 0 & J_{2n} \end{bmatrix}. \tag{1.2}$$

Correspondingly, we consider the product space $R^n \times R^n \simeq R^{2n}$. Its cotangent bundle, $T^*(R^n \times R^n) = T^*R^{2n} \simeq R^{4n}$ has natural symplectic structure

$$J_{4n} = \begin{bmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{bmatrix}. \tag{1.3}$$

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Choose symplectic coordinates $z=(p,q)$ on the symplectic manifold, then for symplectic transformation $g: T^*R^n \longrightarrow T^*R^n$, we have

$$\text{gra}(g)=\left\{\begin{bmatrix} g_z \\ z \end{bmatrix}, \quad z\in T^*R^n\right\}, \tag{1.4}$$

it is a Lagrangian submanifold of $T^*R^n\times T^*R^n$ in $\tilde{R}^{4n}=(R^{4n},\tilde{J}_{4n})$. Note that on R^{4n} there is a standard symplectic structure (R^{4n},J_{4n}). A generating map

$$\alpha: T^*R^n\times T^*R^n \longrightarrow T^*(R^n\times R^n)$$

maps the symplectic structure (1.2) to the standard one (1.3). In particular, α maps Lagrangian submanifolds in $(R^{4n},\tilde{J}_{4n})$ to Lagrangian submanifolds L_g in (R^{4n},J_{4n}). Suppose that α satisfies the transversality condition of g, then

$$L_g=\left\{\begin{bmatrix} d\phi_g(w) \\ w \end{bmatrix}, w\in R^{2n}\right\}. \tag{1.5}$$

ϕ_g is called generating function of g. We call this generating map α (linear case) or α_* (nonlinear case) Darboux transformation, in other words, we have the following definition.

Definition 1.1. A linear map

$$\alpha=\begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix}, \tag{1.6}$$

which acts as the followings

$$\begin{bmatrix} z_0 \\ z_1 \end{bmatrix}\in R^{4n}\longmapsto \alpha\begin{bmatrix} z_0 \\ z_1 \end{bmatrix}=\begin{bmatrix} A_\alpha z_0+B_\alpha z_1 \\ C_\alpha z_0+D_\alpha z_1 \end{bmatrix}=\begin{bmatrix} w_0 \\ w_1 \end{bmatrix}\in R^{4n}$$

is called a Darboux transformation, if

$$\alpha' J_{4n}\alpha=\tilde{J}_{4n}. \tag{1.7}$$

Denote

$$E_\alpha=C_\alpha+D_\alpha, \quad F_\alpha=A_\alpha+B_\alpha. \tag{1.8}$$

We have

Definition 1.2.

$$Sp(\tilde{J}_{4n},J_{4n})=\{\alpha\in GL(4n)|\alpha' J_{4n}\alpha=\tilde{J}_{4n}\}=Sp(\tilde{J},J);$$
$$Sp(J_{4n})=\{\beta\in GL(4n)|\beta' J_{4n}\beta=J_{4n}\}=Sp(4n);$$
$$Sp(\tilde{J}_{4n})=\{\gamma\in GL(4n)|\gamma'\tilde{J}_{4n}\gamma=\tilde{J}_{4n}\}=\widetilde{Sp}(4n).$$

Definition 1.3. A special case of Darboux transformation $\alpha_0=\begin{bmatrix} J_{2n} & -J_{2n} \\ \frac{1}{2}I_{2n} & \frac{1}{2}I_{2n} \end{bmatrix}$ is called Poincare transformation.

Proposition 1.4. *If* $\alpha \in Sp(\tilde{J}_{4n}, J_{4n})$, $\beta \in Sp(4n)$, $\gamma \in \widetilde{Sp}(4n)$, *then* $\beta\alpha\gamma \in Sp(\tilde{J}_{4n}, J_{4n})$.

Proposition 1.5. $Sp(\tilde{J}_{4n}, J_{4n}) = Sp(4n)\alpha_0 = \alpha_0\widetilde{Sp}(4n)$ *and* $Sp(\tilde{J}_{4n}, J_{4n}) = Sp(4n)\alpha = \alpha\widetilde{Sp}(4n)$, $\forall\alpha \in Sp(\tilde{J}_{4n}, J_{4n})$.

Proposition 1.6. *If* $\alpha = \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix} \in Sp(\tilde{J}_{4n}, J_{4n})$, *then*

$$\alpha^{-1} = \begin{bmatrix} -J_{2n}C'_\alpha & J_{2n}A'_\alpha \\ J_{2n}D'_\alpha & -J_{2n}B'_\alpha \end{bmatrix} = \begin{bmatrix} A_{\alpha^{-1}} & B_{\alpha^{-1}} \\ C_{\alpha^{-1}} & D_{\alpha^{-1}} \end{bmatrix}.$$

We have the following well known theorem.

Theorem 1.7[2–5]**.** *If* $\alpha \in Sp(\tilde{J}_{4n}, J_{4n})$ *satisfies transversality condition* $|C_\alpha + D_\alpha| \neq 0$, *then for all symplectic diffeomorphisms,* $z \longrightarrow g(z)$ *in* R^{2n}, $g \sim I_{2n}$ *(near identity),* $g_z \in Sp(2n)$ *there exists a generating function* $\phi_{\alpha;g}$: $R^{2n} \longrightarrow R$ *such that* $A_\alpha g(z) + B_\alpha z = \nabla\phi_{\alpha;g}(C_\alpha g(z) + D_\alpha z)$, *i.e.,* $(A_\alpha \circ g + B_\alpha)(C_\alpha \circ g + D_\alpha)^{-1} z = \nabla\phi_{\alpha;g}(z)$ *identically in* z.

2. Normalization of Darboux Transformation

Denote $M \equiv Sp(\tilde{J}_{4n}, J_{4n})$ a submanifold in $GL(4n)$, dim $M = \dfrac{1}{2}4n(4n+1) = 8n^2 + 2n$. Denote $M^* \equiv \{\alpha \in M \mid |E_\alpha| \neq 0\}$ an open submanifold of M, dimM^* =dim$M$. Denote $M' \equiv \{\alpha \in M \mid E_\alpha = I_n, F_\alpha = 0\} \subset M^* \subset M$.

Definition 2.1. Darboux transformation is called normalization Darboux transformation if (1) $E_\alpha = I_{2n}$ and (2) $F_\alpha = O_{2n}$.

The following theorem answers the question about how to construct a normalization Darboux transformation from a given one.

Theorem 2.2. $\forall\alpha \in M^*$, *there exists*

$$\beta_1 = \begin{bmatrix} I_{2n} & P \\ 0 & I_{2n} \end{bmatrix} \in Sp(4n), \quad |T| \neq 0, \quad \beta_2 = \begin{bmatrix} T'^{-1} & 0 \\ 0 & T \end{bmatrix} \in Sp(4n),$$

such that $\beta_2\beta_1\alpha \in M'$.

Proof. We only need take $P = -F_\alpha E_\alpha^{-1} = -(A_\alpha + B_\alpha)(C_\alpha + D_\alpha)^{-1}$, $T = E_\alpha^{-1}$, then

$$\begin{aligned} \beta_2 \cdot \beta_1 \cdot \alpha &= \begin{bmatrix} E'_\alpha & 0 \\ 0 & E_\alpha^{-1} \end{bmatrix} \begin{bmatrix} I & -F_\alpha E_\alpha^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix} = \begin{bmatrix} A_{\beta_2\beta_1\alpha} & B_{\beta_2\beta_1\alpha} \\ C_{\beta_2\beta_1\alpha} & D_{\beta_2\beta_1\alpha} \end{bmatrix} \\ &= \alpha_1 = \begin{pmatrix} E'_\alpha(A_\alpha - F_\alpha E_\alpha^{-1}C_\alpha) & E'_\alpha(B_\alpha - F_\alpha E_\alpha^{-1}D_\alpha) \\ E_\alpha^{-1}C_\alpha & E_\alpha^{-1}D_\alpha \end{pmatrix}. \end{aligned} \tag{2.1}$$

It's easy to calculate that $A_{\beta_2\beta_1\alpha} + B_{\beta_2\beta_1\alpha} = O_{2n}$, $C_{\beta_2\beta_1\alpha} + D_{\beta_2\beta_1\alpha} = I_{2n}$.

Later, we will assume α to be a normalization Darboux transformation if we do not point out specifically.

Theorem 2.3. *A Darboux transformation can be written in the standard form as*

$$\alpha = \begin{bmatrix} J_{2n} & -J_{2n} \\ \frac{1}{2}(I+V) & \frac{1}{2}(I-V) \end{bmatrix}, \quad V \in sp(2n).$$

It's not difficult to show

$$\forall \alpha_1 \in M \Longrightarrow \exists \beta \in Sp(4n), \quad \beta = \begin{bmatrix} A_\beta & B_\beta \\ C_\beta & D_\beta \end{bmatrix},$$

such that $\alpha_1 = \beta\alpha_0$, where α_0 is Poincare transformation. By computation, we get

$$\alpha_1 = \begin{bmatrix} A_\beta J + \frac{1}{2}B_\beta & -A_\beta J + \frac{1}{2}B_\beta \\ C_\beta J + \frac{1}{2}D_\beta & -C_\beta J + \frac{1}{2}D_\beta \end{bmatrix}.$$

Because $\alpha_1 \in M'$, we have $D_\beta = I_{2n}, B_\beta = 0$, i.e., $\beta = \begin{bmatrix} A_\beta & 0 \\ C_\beta & I_{2n} \end{bmatrix}$. Since $\beta \in Sp(4n)$, we have $\beta = \begin{bmatrix} I_{2n} & 0 \\ Q & I_{2n} \end{bmatrix}$, $Q \in Sm(2n)$. Thus

$$\alpha_1 = \begin{bmatrix} I_{2n} & 0 \\ Q & I_{2n} \end{bmatrix} \begin{bmatrix} J & -J \\ \frac{1}{2}I & \frac{1}{2}I \end{bmatrix} = \begin{bmatrix} J & -J \\ \frac{1}{2}I + QJ & \frac{1}{2}I - QJ \end{bmatrix} = \begin{bmatrix} J & -J \\ \frac{1}{2}(I+V) & \frac{1}{2}(I-V) \end{bmatrix},$$

where $Q' = Q, V = 2QJ$. We shall write

$$\alpha_V = \begin{bmatrix} J_{2n} & -J_{2n} \\ \frac{1}{2}(I+V) & \frac{1}{2}(I-V) \end{bmatrix}, \quad \alpha_V^{-1} = \begin{bmatrix} -\frac{1}{2}(I-V)J & I_{2n} \\ \frac{1}{2}(I+V)J & I_{2n} \end{bmatrix}.$$

Corollary 2.4. *Every* $\alpha = \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix} \in M^*$ *has a normalized form* $\alpha_V \in M'$ *with* $V = (C_\alpha + D_\alpha)^{-1}(C_\alpha - D_\alpha) \in sp(2n)$.

This result can be derived from (2.1).

From the following theorem, we can show that the normalization condition is natural.

Theorem 2.5. G^τ *is a consistent difference scheme for* $\dot{z} = J^{-1}H_z$, $\forall H$, *i.e.,*

(1) $G^\tau(z)|_{\tau=0} = z, \quad \forall z, H;$

(2) $\frac{\partial G^\tau(z)}{\partial z}\Big|_{\tau=0} = J^{-1}H_z(z) \quad \forall z, H;$

iff generating Darboux transformation is normalized with $A = -J$.

Proof. We take symplectic difference scheme of first order via generating function of type $\alpha = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$. We have

$$AG^\tau(z) + Bz = -\tau H_w(CG^\tau(z) + Dz). \tag{2.2}$$

At first, we prove the only if part of the theorem. When take $\tau = 0$, we have

$$AG^0(z) + Bz = (A+B)z = 0, \quad \forall z \Longrightarrow A + B = 0,$$
$$A\frac{\partial G^\tau(z)}{\partial \tau}\Big|_{\tau=0} = -H_z((C+D)z).$$

Since we know $\left(\frac{\partial G^{\tau}(z)}{\partial \tau}\right)\Big|_{\tau=0} = J^{-1}H_z(z)$, then $AJ^{-1}H_z(z) = -H_z((C+D)z)$, $\forall H, z$. We have $H(z) = z'b \Longrightarrow AJ^{-1}b = -b$, $\forall b \Longrightarrow A = -J$. On the other hand since $H_z(z) = H_w((C+D)z)$, $\forall H, z$, we have

$$H = \frac{1}{2}z'z \Longrightarrow z = (C+D)z, \quad \forall z \Longrightarrow C+D = I.$$

Now we show the if part, take

$$A + B = 0, \quad A = -J, \quad C + D = I \tag{2.3}$$

then $A(G^{\tau}(z) - z) = -\tau H_z(CG^{\tau}(z) + Dz)$, $A = -J$, $\tau = 0 \Longrightarrow G^{\tau}(z)|_{\tau=0} = z$. On the other hand

$$A\left(\frac{\partial G^{\tau}(z)}{\partial \tau}\right)_{\tau=0} = -H_z((C+D)z) \Longrightarrow \left(\frac{\partial G^{\tau}(z)}{\partial \tau}\right)_{\tau=0} = J^{-1}H_z(z), \quad \forall z, H.$$

Theorem 2.6. *A normalized Darboux transformation with $A = -J$ iff can be written in the standard form*

$$\alpha = \begin{bmatrix} -J & J \\ \frac{1}{2}(I-V) & \frac{1}{2}(I+V) \end{bmatrix}, \quad \forall \quad V \in sp(2n)$$

with $\mu = 1$.

3. Transform Properties of Generator Maps and Generating Functions

Let $\alpha = \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix} \in Sp(\tilde{J}_{4n}, J_{4n})$. Define $E_\alpha = C_\alpha + D_\alpha$, $F_\alpha = A_\alpha + B_\alpha$. Suppose $g \in$ *Sp-Diff*, $g \sim I_{2n}$. In the future, we assume that transversality condition $|E_\alpha| \neq 0$ is satisfied.

Theorem 3.2. *$\forall\ T \in GL(2n)$, define $\beta_T = \begin{bmatrix} T'^{-1} & 0 \\ 0 & T \end{bmatrix} \in Sp(4n)$, $\beta_T\alpha \in Sp(\tilde{J}_{4n}, J_{4n})$, we have*

$$\phi_{\beta_T \circ \alpha}, g \cong \phi_{\alpha,g} \circ T^{-1}. \tag{3.1}$$

Proof. Since

$$\beta_T\alpha = \begin{bmatrix} T'^{-1}A_\alpha & T'^{-1}B_\alpha \\ TC_\alpha & TD_\alpha \end{bmatrix} = \begin{bmatrix} A_{\beta_T\alpha} & B_{\beta_T\alpha} \\ C_{\beta_T\alpha} & D_{\beta_T\alpha} \end{bmatrix},$$

we have

$$A_\alpha g(z) + B_\alpha z = \nabla\phi_{\alpha,g} \circ (C_\alpha g(z) + D_\alpha z) \tag{3.2}$$

identically in z, and

$$T'^{-1}A_\alpha g(z) + T'^{-1}B_\alpha z = \nabla\phi_{\beta_T\alpha,g} \circ (TC_\alpha g(z) + TD_\alpha z)$$

$\Longleftrightarrow$

$$A_\alpha g(z) + B_\alpha z = T'(\nabla\phi_{\beta_T\alpha,g}) \circ T(C_\alpha g(z) + D_\alpha z) = \nabla(\phi_{\beta_T\alpha}, g \circ T)(C_\alpha g(z) + D_\alpha z) \tag{3.3}$$

identically in z.

Compare (3.2) with (3.3), we find

$$\nabla\phi_{\alpha,g}(C_\alpha g(z)+D_\alpha z)=\nabla(\phi_{\beta_T\alpha,g}\circ T)(C_\alpha g(z)+D_\alpha z)$$

identically in z. Thus we obtain $\phi_{\alpha,g}\cong\phi_{\beta_T\alpha,g}\circ T$, or $\phi_{\alpha,g}\circ T^{-1}\cong\phi_{\beta_T\alpha,g}$.

Theorem 3.2. *$\forall S\in Sp(2n)$, define $\gamma_S=\begin{bmatrix}S&0\\0&S\end{bmatrix}\in\tilde{S}p(4n)$, then we have*

$$\phi_{\alpha\gamma_S,g}\cong\phi_{\alpha,S\circ g\circ S^{-1}}. \tag{3.4}$$

Proof. Since

$$\alpha\gamma_S=\begin{bmatrix}A_\alpha S&B_\alpha S\\C_\alpha S&D_\alpha S\end{bmatrix}=\begin{bmatrix}A_{\alpha\gamma_S}&B_{\alpha\gamma_S}\\C_{\alpha\gamma_S}&D_{\alpha\gamma_S}\end{bmatrix}$$

and

$$A_\alpha S\circ g\circ S^{-1}(z)+B_\alpha z=\nabla\phi_{\alpha,S\circ g\circ S^{-1}}(C_\alpha S\circ g\circ S^{-1}(z)+D_\alpha z)$$

identically in z, because S nonsingular, we may replace z by $S(z)$, so we get

$$A_\alpha S\circ g(z)+B_\alpha Sz=\nabla\phi_{\alpha,S\circ g\circ S^{-1}}(C_\alpha Sg(z)+D_\alpha Sz),\quad\forall z. \tag{3.5}$$

On the other hand

$$(A_\alpha S)g(z)+(B_\alpha S)z=\nabla\phi_{\alpha\gamma_S},g[(C_\alpha S)g(z)+D_\alpha S)z],\quad\forall z. \tag{3.6}$$

Compare (3.5) with (3.6) and note that $|C_\alpha+D_\alpha|\neq0\iff|C_\alpha S+D_\alpha S|\neq0\iff|C_\alpha Sg_z(z)+D_\alpha S|\neq0$, we obtain $\nabla\phi_{\alpha\gamma_S,g}=\nabla\phi_{\alpha,S\circ g\circ S^{-1}}$, i.e., $\phi_{\alpha\gamma_S,g}\cong\phi_{\alpha,S\circ g\circ S^{-1}}$.

Theorem 3.3. *Take $\beta=\begin{bmatrix}I_{2n}&P\\0&I_{2n}\end{bmatrix}\in Sp(4n)$, $P\in Sm(2n)$, $\alpha\in Sp(\tilde{J}_{4n},J_{4n})$, then*

$$\phi_{\beta\alpha,g}\cong\phi_{\alpha,g}+\psi_P \tag{3.7}$$

where $\psi_P=\frac{1}{2}w'Pw$(function independent of g).

Proof.

$$\beta\alpha=\begin{bmatrix}I_{2n}&P\\0&I_{2n}\end{bmatrix}\begin{bmatrix}A_\alpha&B_\alpha\\C_\alpha&D_\alpha\end{bmatrix}=\begin{bmatrix}A_\alpha+PC_\alpha&B_\alpha+PD_\alpha\\C_\alpha&D_\alpha\end{bmatrix}.$$

Obviously, $E_{\beta\alpha}=E_\alpha,F_{\beta\alpha}=F_\alpha+PE_\alpha$, so

$$A_{\beta\alpha}g(z)+B_{\beta\alpha}z=\nabla\phi_{\beta\alpha,g}(C_{\beta\alpha}g(z)+D_{\beta\alpha}z), \tag{3.8}$$

$$A_\alpha g(z)+B_\alpha z+(PC_\alpha g(z)+PD_\alpha z)=\nabla\phi_{\beta\alpha,g}(C_\alpha g(z)+D_\alpha z). \tag{3.9}$$

On the other hand

$$\nabla\psi_P(C_\alpha g(z)+D_\alpha z)=P(C_\alpha g(z)+D_\alpha z). \tag{3.10}$$

Inserting (3.10) into (3.9), we obtain

$$A_\alpha g(z)+B_\alpha z=\nabla\phi_{\beta\alpha,g}(C_\alpha g(z)+D_\alpha z)-\nabla\psi_P(C_\alpha g(z)+D_\alpha z)$$

$$= (\nabla(\phi_{\beta\alpha,g} - \psi_P))(C_\alpha g(z) + D_\alpha z). \tag{3.11}$$

Compare (3.11) and $A_\alpha g(z)+B_\alpha z = \nabla\phi_{\alpha,g}(C_\alpha g(z)+D_\alpha z)$, we obtain $\phi_{\beta\alpha,g}-\psi_P \cong \phi_{\alpha,g}$. Analogically, if we take $\beta = \begin{bmatrix} I_{2n} & 0 \\ Q & I_{2n} \end{bmatrix} \in Sp(4n)$, $Q \in Sm(2n)$, we have the following result.

Theorem 3.4.

$$\phi_{\alpha,g} + \frac{1}{2}(\nabla_w\phi_{\alpha,g}(w))'Q(\nabla_w\phi_{\alpha,g}(w)) \cong \phi_{\beta\alpha,g}(w + Q\nabla\phi_{\alpha,g}(w)). \tag{3.12}$$

Theorem 3.5.

$$\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix},g^{-1}} \cong -\phi_{\begin{bmatrix} -B & -A \\ D & C \end{bmatrix},g}. \tag{3.13}$$

Proof. Since $A_\alpha g^{-1}(z) + B_\alpha z = \nabla\phi_{\alpha,g^{-1}}(C_\alpha g^{-1}(z) + D_\alpha z)$, replace z by $g(z)$, we have

$$A_\alpha z + B_\alpha g(z) = \nabla\phi_{\alpha,g^{-1}}(C_\alpha z + D_\alpha g(z)). \tag{3.14}$$

Comparing

$$-B_\alpha g(z) - A_\alpha z = \nabla\phi_{\begin{bmatrix} -B_\alpha & -A_\alpha \\ D_\alpha & C_\alpha \end{bmatrix},g}(D_\alpha g(z) + C_\alpha z)$$

with (3.14) concludes our proof.

Theorem 3.5′. *If* $\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix},g^{-1}} = -\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix},g}$, $\forall g$, *then* $A + B = 0, C = D$.

Proof. Since by Theorem 3.5 and uniqueness theorem 4.2, we have

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \pm \begin{bmatrix} -B & -A \\ D & C \end{bmatrix}.$$

We only consider the case "+", in this case we have $A + B = 0$, $C = D$.

Remark. For Poincare map $\alpha_0 = \begin{bmatrix} J & -J \\ \frac{1}{2}I & \frac{1}{2}I \end{bmatrix}$, we have $\phi_{\alpha_0,g^{-1}} \cong -\phi_{\alpha_0,g}$, $\forall g \in$ *Sp-diff.*

Theorem 3.6. *Let* g_H^t *be the phase flow of Hamiltonian system* $H(z)$*, then the generating function of* g_H^t *under Poincare map* α_0 *is an odd in* t*, i.e.,* $\phi_{\alpha_0,g_H^t}(w,t) = -\phi_{\alpha_0,g_H^t}(w,-t)$, $\forall w \in R^{2n}, t \in R$.

Proof.

$$g_H^{-t} = (g_H^t)^{-1}, \quad \phi_{\alpha_0,g_H^{-t}}(w,t) = \phi_{\alpha_0,g_H^t}(w,-t) = \phi_{\alpha_0,(g_H^t)^{-1}}(w,t) = -\phi_{\alpha_0,g_H^t}(w,t).$$

Theorem 3.7. *If* $S \in Sp(2n)$, $\alpha \in Sp(\tilde{J}_{4n}, J_{4n})$, $\gamma_1 = \begin{bmatrix} S & 0 \\ 0 & I \end{bmatrix}$, *then*

$$\alpha\gamma_1 = \begin{bmatrix} A_\alpha S & B_\alpha \\ C_\alpha S & D_\alpha \end{bmatrix}.$$

Assume $|E_{\alpha\gamma}| = |C_\alpha S + D_\alpha| \neq 0$, we have

$$\phi_{\alpha,S\cdot g} \cong \phi_{\alpha\gamma_1,g}, \tag{3.15}$$

i.e.,

$$\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, S\cdot g} \cong \phi_{\begin{bmatrix} AS & B \\ CS & D \end{bmatrix}, g}.$$

Theorem 3.8. *If*

$$\gamma_2 = \begin{bmatrix} I & 0 \\ 0 & S \end{bmatrix}, \quad \alpha \in Sp(\tilde{J}_{4n}, J_{4n}), \quad \alpha\gamma_2 = \begin{bmatrix} A_\alpha & B_\alpha S \\ C_\alpha & D_\alpha S \end{bmatrix},$$

assume $|B_\alpha + D_\alpha S| \neq 0$, *we have*

$$\phi_{\alpha, g\circ S^{-1}} \cong \phi_{\alpha\gamma_2, g}, \tag{3.16}$$

i.e.,

$$\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g\circ S^{-1}} = \phi_{\begin{bmatrix} A & BS \\ C & DS \end{bmatrix}, g}.$$

Proof. Since

$$Ag(S^{-1}z) + Bz = \nabla\phi_{\alpha, g\circ S^{-1}}(Cg(S^{-1}z) + Dz), \quad \forall z,$$

replace z by Sz, we get

$$Ag(z) + BSz = \nabla\phi_{\alpha, g\circ S^{-1}}(Cg(z) + DSz) = \nabla\phi_{\begin{bmatrix} A & BS \\ C & DS \end{bmatrix}, g}(Cg(z) + DSz),$$

$$\phi_{\begin{bmatrix} A & BS \\ C & DS \end{bmatrix}, g} \cong \phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g\circ S^{-1}}.$$

Proof of (3.7) is similar.

Theorem 3.9. *If*

$$\beta = \begin{bmatrix} \lambda I_{2n} & 0 \\ 0 & I_{2n} \end{bmatrix} \in CSp(4n), \quad \alpha \in Sp(\tilde{J}_{4n}, J_{4n}), \quad \lambda \neq 0,$$
$$\beta\alpha = \begin{bmatrix} \lambda A & \lambda B \\ C & D \end{bmatrix} \in CSp(\tilde{J}_{4n}, J_{4n}), \quad \mu(\beta\alpha) = \lambda,$$

then we have

$$\phi_{\begin{bmatrix} \lambda A & \lambda B \\ C & D \end{bmatrix}} \cong \lambda\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g} \tag{3.17}$$

Theorem 3.10. *Suppose*

$$\beta = \begin{bmatrix} I_{2n} & 0 \\ 0 & \lambda I_{2n} \end{bmatrix} \in CSp(J_{4n}), \quad \lambda \neq 0, \quad \alpha \in Sp(\tilde{J}_4 n, J_{4n}),$$
$$\beta\alpha = \begin{bmatrix} A & B \\ \lambda C & \lambda D \end{bmatrix} \in CSp(\tilde{J}_{4n}, J_{4n}), \quad \mu(\beta\alpha) = \lambda,$$

then we have

$$\phi_{\begin{bmatrix} A & B \\ \lambda C & \lambda D \end{bmatrix}, g} \cong \lambda\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g} \circ \lambda^{-1} I_{2n} \tag{3.18}$$

Proof of (3.9): Since

$$\alpha \in Sp(\tilde{J}_{4n}, J_{4n}) \Longrightarrow Ag(z) + Bz = \nabla \phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g}(Cg(z) + Dz),$$

$$\beta \in CSp(\tilde{J}_{4n}, J_{4n}) \Longrightarrow \lambda Ag(z) + \lambda Bz = \nabla \phi_{\begin{bmatrix} \lambda A & \lambda B \\ C & D \end{bmatrix}, g}(Cg(z) + Dz)$$

$$\text{L.H.S} = \lambda Ag(z) + \lambda Bz = \lambda \nabla \phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g}(Cg(z) + Dz),$$

$$\text{R.H.S} = \nabla \phi_{\begin{bmatrix} \lambda A & \lambda B \\ C & D \end{bmatrix}, g}(Cg(z) + Dz),$$

then we have

$$\nabla \phi_{\begin{bmatrix} \lambda A & \lambda B \\ C & D \end{bmatrix}, g}(Cg(z) + Dz) = \lambda \nabla \phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g}(Cg(z) + Dz),$$

$$\phi_{\begin{bmatrix} \lambda A & \lambda B \\ C & D \end{bmatrix}, g} \cong \lambda \phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g}.$$

Proof of (3.10): From

$$\begin{bmatrix} A & B \\ \lambda C & \lambda D \end{bmatrix} \in CSp(\tilde{J}_{4n}, J_{4n})$$

it follows that

$$Ag(z) + Bz = \nabla \phi_{\begin{bmatrix} A & B \\ \lambda C & \lambda D \end{bmatrix}, g}(\lambda Cg(z) + \lambda Dz).$$

$$\text{L.H.S} = \nabla \phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g}(Cg(z) + Dz),$$

$$\begin{aligned} \text{R.H.S} &= (\phi_{\begin{bmatrix} A & B \\ \lambda C & \lambda D \end{bmatrix}, g}) \circ \lambda I_{2n}(Cg(z) + Dz) \\ &= \lambda^{-1} \nabla (\phi_{\begin{bmatrix} A & B \\ \lambda C & \lambda D \end{bmatrix}, g} \circ \lambda I_{2n})(Cg(z) + Dz). \end{aligned}$$

Hence

$$\phi_{\begin{bmatrix} A & B \\ C & D \end{bmatrix}, g} \cong \lambda^{-1} \phi_{\begin{bmatrix} A & B \\ \lambda C & \lambda D \end{bmatrix}, g} \circ \lambda I_{2n}.$$

At the end of this section, we give out two conclusive theorems which can include the contents of the seven theorems given before. They are easy to prove and the proofs are omitted here.

Let

$$\alpha \in CSp(\tilde{J}_{4n}, J_{4n}), \quad \beta \in CSp(J_{4n}), \quad \beta = \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$

obviously, $\beta\alpha \in CSp(\tilde{J}_{4n}, J_{4n})$, $\mu(\beta\alpha) = \lambda(\beta)\mu(\alpha)$. We have the following theorem.

Theorem 3.11.

$$\begin{aligned} &\phi_{\beta\alpha,g}(C\nabla_w \phi_{\alpha,g}(w) + dw) \cong \lambda(\beta)\phi_{\alpha,g}(w) \\ &\quad + \Big\{\frac{1}{2}w'(d'b)w + (\nabla_w \phi_{\alpha,g}(w))'(c'b)w \frac{1}{2}(\nabla_w \phi_{\alpha,g}(w))'(c'a)(\nabla_w \phi_{\alpha,g}(w))\Big\}. \end{aligned} \tag{3.19}$$

We now formulate the other one. Let $\alpha \in CSp(\tilde{J}_{4n}, J_{4n})$, $\gamma \in CSp(\tilde{J}_{4n}) \Longleftrightarrow \gamma' \tilde{J}_{4n} \gamma = \upsilon(\gamma) \tilde{J}_{4n} \Longrightarrow \alpha\gamma \in CSp(\tilde{J}_{4n},\, J_{4n})$, $\mu(\alpha\gamma) = \mu(\alpha)\upsilon(\gamma)$, $\gamma = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$.

Theorem 3.12.

$$\phi_{\alpha\gamma, g} \cong \phi_{\alpha, (a\cdot g + b)\circ(c \cdot g + d)^{-1}}. \tag{3.20}$$

4. Invariance of Generating Functions and Commutativity of Generator Maps

First we give out the uniqueness theorem of linear fractional transformation.

Theorem 4.1. *Suppose*

$$\alpha = \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix}, \quad \overline{\alpha} = \begin{bmatrix} A_{\overline{\alpha}} & B_{\overline{\alpha}} \\ C_{\overline{\alpha}} & D_{\overline{\alpha}} \end{bmatrix} \in Sp(\tilde{J}_{4n}, J_{4n}), \quad |E_\alpha| \neq 0, \quad |E_{\overline{\alpha}}| \neq 0.$$

If

$$(A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1} = (A_{\overline{\alpha}} M + B_{\overline{\alpha}})(C_{\overline{\alpha}} M + D_{\overline{\alpha}})^{-1}, \quad \forall M \sim I_{2n},\ M \in Sp(2n),$$

then $\overline{\alpha} = \pm\alpha$.

Proof. Let

$$N_0 = (A_\alpha I + B_\alpha)(C_\alpha I + D_\alpha)^{-1} = (A_{\overline{\alpha}} I + B_{\overline{\alpha}})(C_{\overline{\alpha}} I + D_{\overline{\alpha}})^{-1}.$$

Suppose $\beta \in Sp(4n)$, first we prove that

$$(A_\beta N + B_\beta)(C_\beta N + D_\beta)^{-1} = N, \quad \forall N \sim N_0, \quad N \in Sm(2n),$$

then $\beta = \pm I_{4n}$.

1° : $(A_\beta N_0 + B_\beta)(C_\beta N_0 + D_\beta)^{-1} = N_0 \Longrightarrow A_\beta N_0 + B_\beta = N_0 C_\beta N_0 + N_0 D_\beta$.

2° : Take $N = N_0 + \varepsilon I \Longrightarrow A_\beta(N_0 + \varepsilon I) + B_\beta = (N_0 + \varepsilon I) C_\beta (N_0 + \varepsilon I) + (N_0 + \varepsilon I) D_\beta$.

From 1°, 2° $\Longrightarrow \varepsilon A_\beta = \varepsilon N_0 C_\beta + \varepsilon C_\beta N_0 + \varepsilon D_\beta + \varepsilon^2 C_\beta$, $\forall \varepsilon \Longrightarrow A_\beta - D_\beta - N_0 C_\beta - C_\beta N_0 = \varepsilon C_\beta \Longrightarrow C_\beta = 0$, then $A_\beta = D_\beta$.

From 1°, we have $B = \begin{bmatrix} A_\beta & B_\beta \\ 0 & A_\beta \end{bmatrix}$, $B_\beta = B_\beta'$. Therefore, from 1° we have

$$A_\beta N A_\beta^{-1} = N - B_\beta A_\beta^{-1}.$$

Subtract this formula by $A_\beta N_0 A_\beta^{-1} = N_0 - B_\beta A_\beta^{-1}$, we get

$$A_\beta (N - N_0) = (N - N_0) A_\beta.$$

Take $N - N_0 = \varepsilon S, S \in Sm(2n) \Longrightarrow A_\beta S = S A_\beta$, $\forall S \in Sm(2n) \Longrightarrow A_\beta = \lambda I_{2n}$. (This can be proved by mathematical induction).

Then from 1°, $A_\beta N_0 + B_\beta = N_0 A_\beta \Longrightarrow B_\beta = 0$, and

$$\beta = \begin{bmatrix} A_\beta & 0 \\ 0 & A_\beta \end{bmatrix} = \lambda I_{4n} \in Sp(4n) \Longrightarrow \lambda = \pm 1.$$

Let $\beta = \overline{\alpha}\alpha^{-1}$, then the fractional transformation of β leaves all symmetric $N \sim N_0$. Because $\alpha \in Sp(\tilde{J}, J)$, $\alpha^{-1} \in Sp(J, \tilde{J})$, $\overline{\alpha}\alpha^{-1} \in Sp(J, J) = Sp(4n)$.

We now give the uniqueness theorem for Darboux transformations.

Theorem 4.2. *Suppose* $\alpha, \overline{\alpha} \in Sp(\tilde{J}, J)$, *then*

$$\phi_{\alpha,g} \cong \phi_{\overline{\alpha},g}, \quad \forall g \in Sp-Diff, \quad g \sim I_{2n} \Longrightarrow \overline{\alpha} = \pm\alpha.$$

Proof. From hypothesis, we have

$$\phi_{\alpha,g} \cong \phi_{\overline{\alpha},g} \Longrightarrow \text{ Hessian of } \phi_{\alpha,g} = (\phi_{\alpha,g})_{ww} = (A_\alpha g(z) + B_\alpha)(C_\alpha g(z) + D_\alpha)^{-1},$$
$$(\phi_{\overline{\alpha},g})_{ww} = (A_{\overline{\alpha}} g(z) + B_{\overline{\alpha}})(C_{\overline{\alpha}} g(z) + D_{\overline{\alpha}})^{-1}, \quad \forall g_z \in Sp(2n) \sim I.$$

Then by uniqueness theorem of linear fractional transformation $\alpha = \pm\overline{\alpha}$. From the proof we know, Hessian of $\phi_{\alpha,g}$ =Hessian of $\phi_{-\alpha,g}, \forall g \in I, \alpha$.

The generating function $\phi_{\alpha,g}$ depends on Darboux transformation α, symplectic diffeomorphism g and coordinates. If we make a symplectic change of coordinates $w \longrightarrow S(z)$, then $\phi(S) \Longrightarrow \phi(S(z))$ while the symplectic diffeomorphism g is represented in z coordinates as $S^{-1} \circ g \circ S$.

For the invariance of generating function $\phi_g(S)$ under S, one would like to expect

$$\phi_{\alpha, S^{-1}\circ g \circ S} = \phi_{\alpha,g} \circ S, \quad \forall g \sim I.$$

This is in general not true. We shall study under what condition this is true for the normalized Darboux transformation α_V. The following theorem answers this question.

Theorem 4.3. *Let*

$$\alpha = \alpha_V = \begin{bmatrix} J_{2n} & -J_{2n} \\ \frac{1}{2}(I+V) & \frac{1}{2}(I-V) \end{bmatrix}, \quad V \in sp(2n), \quad \alpha_V \in M'$$
$$S \in Sp(2n), \quad \beta_S = \begin{bmatrix} {S'}^{-1} & 0 \\ 0 & S \end{bmatrix} \in Sp(J_{4n}), \quad \gamma_S = \begin{bmatrix} S & 0 \\ 0 & S \end{bmatrix} \in Sp(\tilde{J}_{4n}).$$

Then the following conditions are equivalent:

(1) $\phi_{\alpha_V, S\circ g\circ S^{-1}} = \phi_{\alpha,g} \circ S^{-1}$, $\forall g \sim I$.

(2) $\phi_{\alpha_V \gamma_S, g} = \phi_{\beta_S \alpha_V, g}$, $g \sim I$.

(3) $\alpha_V \gamma_S = \beta_S \alpha_V$.

(4) $SV = VS$.

Proof. (1) $\Longleftrightarrow$ (2) from theorems 3.1 and 3.2. (2) $\Longrightarrow$ (3) using the uniqueness theorem on Darboux transformation 4.2. For

$$\alpha_V \gamma_S = \pm\beta_S \alpha_V,$$

since $JS = {S'}^{-1} J$, $(-)$ case is excluded. The rest of the proof is trivial.

There is a deep connection between the symmetry of a symplectic difference scheme and the preservation of first integrals.

Let $\mathcal{F}$ be the set of smooth functions defined on R^n.

Theorem 4.4. *Let* H, $F \in \mathcal{F}$,

$$F \circ g_H^t = F \Longleftrightarrow \{F, H\} = 0 \Longleftrightarrow H \circ g_F^t = H \Longleftrightarrow g_H^t = g_F^{-s} \circ g_H^t \circ g_F^s.$$

Theorem 4.5. *Let $F \in \mathcal{F}$, $g \in$ Sp-Diff,*

$$g = g_F^{-t} \circ g \circ g_F^t (\text{or } g_F^t = g^{-1} \circ g_F^t \circ g) \Longleftrightarrow F \circ g = F + C.$$

The "if" part of the proof is obvious. Since

$$\begin{aligned} F \circ g = F + C &\Longrightarrow \nabla F = \nabla F \circ g \Longrightarrow g_F^t = g_{F\circ g}^t = g^{-1} \circ g_F^t \circ g \\ &= g^{-1} g_F^t(g(z)) \Longleftrightarrow g = g_F^t \circ g \circ g_F^t. \end{aligned}$$

On the other hand, take the derivative of both sides of the following equation by t at $t = 0$,

$$\frac{d}{dt}\Big|_{t=0} : \qquad g_F^t(z) = g^{-1} g_F^t(g(z))$$

and notice that $g_*(z) \in Sp, g_*^{-1} J^{-1} = J^{-1} g_*'$, we get

$$J^{-1} \nabla F(z) = g_*^{-1}(z) J^{-1} \nabla F(g(z)) = g_*'(z) \nabla F(g(z)).$$

Then we have $\nabla F = \nabla(F \circ g) \Longrightarrow F \circ g = F + C$.

5. Formal Energy for Hamiltonian Algorithm

Let F^s be an analytic canonical transformation in s, i.e.,

(1) $F^s \in$ *Sy-Diff.*

(2) $F^\circ = id$.

(3) F^s analytic in s for $|s|$ small.

Then there exists a "formal" energy, i.e., a formal power series in s,

$$h^s(z) = h(s, z) = \sum h^i(z)$$

with the following property:

When $h^s(z)$ converges, the phase flow $g_{h^s}^t$, where $h^s(z)$ is considered as a time-independent Hamiltonian with s as a parameter which satisfies "equivalence condition"

$$g_{h^s}^t \Big|_{t=s} = F^s. \tag{5.1}$$

So that $h^s(z) = h^s(F^s z)$, $\forall z \in R^{2n}$, thus $h^s(z)$ is invariant under F^s (or for those s, z in the domain of convergence of $h^s(z)$).

Let F^s be generated by $\psi(s, w)$ according to normal Darboux transformation α

$$\phi_{F^s,\alpha}(w) =: \psi(s, w) = \sum_{k=1}^{\infty} s^k \psi^{(k)}(w). \tag{5.2}$$

Introduce formal power series

$$h^s(z) = h(s, w) = \sum s^i h^i(w).$$

Assuming convergence, then we associate the phase flow with generating function

$$h^s(z) \longrightarrow \psi_{h^s,\alpha}^t(w) := \chi(t, s, w) = \sum_{k=1}^{\infty} t^k \chi^{(k)}(s, w),$$

$$\chi^{(1)}(s,w) = -h(s,w). \tag{5.3}$$

For $k > 1$,

$$\begin{aligned}\chi^{(k+1)}(s,w) = &-\sum_{m=1}^{k} \frac{1}{(k+1)m!} \sum_{l_1,\cdots,l_m=1}^{2n} \sum_{k_1+\cdots+k_m=k} h_{w_{l_1},\cdots,w_{l_m}}(s,w) \\ &\times (A_1\chi_w^{(k_1)}(s,w))_{l_1} \cdots (A_1\chi_w^{(k_m)}(s,w))_{l_m} \\ = &\sum_{m=1}^{k} \frac{1}{(k+1)m!} \sum_{k_1+\cdots+k_m=k} \chi^{(1)}_{w_{l_1},\cdots,w_{l_m}}(s,w) \\ &\times (A_1\chi_w^{(k_1)}(s,w))_{l_1} \cdots (A_1\chi_w^{(k_m)}(s,w))_{l_m}.\end{aligned} \tag{5.4}$$

Let $\chi^{(k)}(s,w) = \sum_{i=0}^{\infty} s^i \chi^{(k,i)}(w)$, then $\chi(t,s,w) = \sum_{k=1}^{\infty}\sum_{i=0}^{\infty} t^k s^i \chi^{(k,i)}(w)$. Then

$$\begin{aligned}\sum_{i=0}^{\infty} s^i \chi^{(k+1,i)}(w) = &\sum_{i=0}^{\infty} s^i \sum_{m=1}^{k} \frac{1}{(k+1)m!} \sum_{\substack{i_0+i_1+\cdots+i_m=i \\ k_1+\cdots+k_m=k}} \sum_{l_1,\cdots,l_m=1}^{2n} \chi^{(1,i_0)}_{w_{l_1},\cdots,w_{l_m}}(w) \\ &\times (A_1\chi_w^{(k_1,i_1)}(w))_{l_1} \cdots (A_1\chi_w^{(k_m,i_m)}(w))_{l_m}.\end{aligned} \tag{5.5}$$

Thus

$$\begin{aligned}\chi^{(k+1,i)}(w) = &\sum_{m=1}^{k} \frac{1}{(k+1)m!} \sum_{\substack{i_0+i_1+\cdots+i_m=i \\ k_1+\cdots+k_m=k}} \sum_{l_1,\cdots,l_m=1}^{2n} \chi^{(1,i_0)}_{w_{l_1},\cdots,w_{l_m}}(w) \\ &\times (A_1\chi_w^{(k_1,i_1)}(w))_{l_1} \cdots (A_1\chi_w^{(k_m,i_m)}(w))_{l_m}.\end{aligned} \tag{5.6}$$

So the coefficient $\chi^{(k+1,i)}$ can be obtained by recursion, if

$$\chi^{(1)}(s,w) = \sum_{0}^{\infty} s^i \chi^{(1,i)}(w) = -h(s,w) = -\sum_{i=0}^{\infty} s^i h^i(w),$$

i.e.,

$$\chi^{(1,i)} = -h^{(i)}, \quad i = 0,1,2,\cdots. \tag{5.7}$$

Note that $\chi^{(k+1,i)}$ is determined only by the derivatives of $\chi^{(k',i')}, k' \le k, i' \le i$

$$\begin{array}{cccccc} \chi^{(1,0)} & \chi^{(1,1)} & \chi^{(1,2)} & \cdots & \chi^{(1,i)} & \chi^{(1,i+1)} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \chi^{(k,0)} & \chi^{(k,1)} & \chi^{(k,2)} & \cdots & \chi^{(k,i)} & \chi^{(k,i+1)} \\ \chi^{(k+1,0)} & \chi^{(k+1,1)} & \chi^{(k+1,2)} & \cdots & \chi^{(k+1,i)} & \chi^{(k+1,i+1)} \end{array} \tag{5.8}$$

The condition (5.1) can be now reexpressed as

$$\chi(t,s,w)|_{t=s} = \chi(s,s,w) = \psi(s,w),$$

i.e.,

$$\begin{aligned}
&\sum_{k=1}^{\infty} s^k \sum_{i=0}^{\infty} s^i \chi^{(k,i)}(w) = \sum_{k=1}^{\infty} s^k \psi^{(k)}(w),\\
&\sum_{i=0}^{\infty} s^i \sum_{j=0} \chi^{(k-j,j)}(w) = \sum_{i=1}^{\infty} s^i \psi^{(k)}(w),\\
&\sum_{j=0}^{k-1} \chi^{(k-j,j)}(w) = \psi^{(k)}, \quad k = 1, 2, \cdots, \qquad (5.9)\\
&\chi^{(1,0)} = \psi^{(1)},\\
&\sum_{i=0}^{k} \chi^{(k+1-i,i)} = \psi^{(k+1)}, \quad k = 0, 1, 2, \cdots,
\end{aligned}$$

so

$$\begin{array}{lllllll}
 & -h^{(0)} & -h^{(1)} & -h^{(2)} & \cdots & -h^{(k-1)} & -h^{(k)}\\
\psi^{(1)} & \chi^{(1,0)} & \chi^{(1,1)} & \chi^{(1,2)} & \cdots & \chi^{(1,k-1)} & \chi^{(1,k)}\\
\psi^{(2)} & \chi^{(2,0)} & \chi^{(2,1)} & \chi^{(2,2)} & \cdots & \chi^{(2,k-1)} & \\
\cdots\cdots & & & & & & \\
\psi^{(k)} & \chi^{(k,0)} & \chi^{(k,1)} & & & & \\
\psi^{(k+1)} & \chi^{(k+1,0)} & & & & &
\end{array} \qquad (5.10)$$

and

$$\begin{aligned}
&\chi^{(1,0)} = \psi^{(1)},\\
&\chi^{(2,0)} + \chi^{(1,1)} = \psi^{(2)},\\
&\chi^{(3,0)} + \chi^{(2,1)} + \chi^{(1,2)} = \psi^{(3)}, \qquad (5.11)\\
&\cdots\cdots\\
&\chi^{(k+1,0)} + \chi^{(k,1)} + \cdots + \chi^{(2,k-1)} + \chi^{(1,k)} = \psi^{(k+1)}.
\end{aligned}$$

Now consider $\psi^{(1)}, \psi^{(2)}, \cdots, \psi^{(k)}, \psi^{(k+1)}, \cdots$ as known, then

$$h^{(0)} = -\chi^{(1,0)}, \quad h^{(1)} = -\chi^{(1,1)}, \quad \cdots, \quad h^{(k-1)} = \chi^{(1,k-1)}, h^{(k)} = \chi^{(1,k)}, \quad \cdots$$

have to be determined. We get

$$\begin{aligned}
&h^{(0)} = -\psi^{(1)},\\
&h^{(1)} = -\psi^{(2)} + \chi^{(2,0)},\\
&h^{(2)} = -\psi^{(3)} + (\chi^{(3,0)} + \chi^{(2,1)}),\\
&\cdots\cdots \qquad (5.12)\\
&h^{(k)} = -\psi^{(k+1)} + (\chi^{(k+1,0)} + \chi^{(k,1)} + \cdots + \chi^{(2,k-1)}),\\
&\cdots\cdots
\end{aligned}$$

So $h^{(0)}, h^{(1)}, h^{(2)}, \cdots$ can be recursively determined by $\psi^{(1)}, \psi^{(2)}, \cdots$. So we get the formal power series $h^s = \sum_{i=0}^{\infty} s^i h^{(i)}(z)$, and in case of convergence, satisfies $g^t_{h^s}\Big|_{t=s} = F^s$.

Now we give out a special example to show how to calculate the formal energy. Take normal Darboux transformation with

$$V = -E = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, \quad \alpha_V^{-1} = \begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix},$$

where

$$A_1 = \frac{1}{2}(JVJ - J) = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix}.$$

Suppose we just take the first term of the generating function of the generating map α_V, i.e., we just consider the first order scheme

$$F^s \sim \psi(s,w) = -sH(w) = \sum_1^\infty s^k \psi^{(k)}.$$

Here $\psi^{(1)} = -H(w)$, $\psi^{(2)} = \psi^{(3)} = \cdots = 0$. Obviously $\chi^{(1,0)} = \psi^{(1)} = -H$.

$$\begin{aligned} \chi_z^{(1,0)} &= -\begin{pmatrix} H_p \\ H_q \end{pmatrix}, \quad A_1\chi_z^{(1,0)} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} -H_p \\ -H_q \end{pmatrix} = \begin{pmatrix} 0 \\ H_p \end{pmatrix}, \\ \chi_{zz}^{(1,0)} &= -\begin{pmatrix} H_{pp} & H_{pq} \\ H_{qp} & H_{qq} \end{pmatrix}. \end{aligned}$$

Calculate by formula (5.6), we get

$$\begin{aligned} \chi^{(2,0)} &= \frac{1}{2(1!)} \sum_{i_0+i_1=0} \sum_{k_1=1} \sum_{l_1=1}^{2n} \chi_{z_{l_1}}^{(1,i_0)} (A_1\chi_z^{(1,i_1)})_{l_1} = \frac{1}{2}(\chi_z^{(1,0)})' A_1 \chi_z^{(1,0)} \\ &= -\frac{1}{2}\begin{pmatrix} H_p \\ H_q \end{pmatrix}' \begin{pmatrix} 0 \\ H_p \end{pmatrix} = -\frac{1}{2}H_q' H_p. \end{aligned}$$

From formula (5.10), we get

$$\begin{aligned} &\chi^{(2,0)} + \chi^{(1,1)} = \psi^{(2)} = 0 \Longrightarrow \chi^{(1,1)} = -\chi^{(2,0)} = \frac{1}{2}H_q' H_p, \\ &\chi_z^{(1,1)} = \frac{1}{2}\begin{pmatrix} \dfrac{\partial}{\partial p}\displaystyle\sum_{j=1}^n H_{q_j} H_{p_j} \\ \dfrac{\partial}{\partial q}\displaystyle\sum_{j=1}^n H_{q_j} H_{p_j} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} H_{pq}H_p + H_{pp}H_q \\ H_{qq}H_p + H_{qp}H_q \end{pmatrix}. \\ &A_1\chi_z^{(1,1)} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}\chi_z^{(1,1)} = -\frac{1}{2}\begin{pmatrix} 0 \\ H_{pq}H_p + H_{pp}H_q \end{pmatrix}, \\ &A_1\chi_z^{(2,0)} = -A_1\chi_z^{(1,1)} = \frac{1}{2}\begin{pmatrix} 0 \\ H_{pq}H_p + H_{pp}H_q \end{pmatrix}. \end{aligned}$$

For $k = 2$, $i = 0$, we have

$$\chi^{(3,0)} = \frac{1}{3}\Big(\frac{1}{1!} \sum_{i_0+i_1=0} \sum_{k_1=2} \sum_{l_1=1}^{2n} \chi_{z_{l_1}}^{(1,0)} (A_1\chi_z^{(2,0)})_{l_1}$$

$$+\sum_{l_1 l_2=1}^{2n}\sum_{i_0+i_1+i_2=0}\sum_{k_1+k_2=2}\chi^{(1,0)}_{z_{l_1},z_{l_2}}(A_1\chi_z^{(k_1,0)})_{l_1}(A_1\chi_z^{(k_2,0)})_{l_2}\Big)$$
$$=\frac{1}{3}(\chi_z^{(1,0)})'A_1\chi_z^{(2,0)}+\frac{1}{6}(A_1\chi_z^{(1,0)})'\chi_{zz}^{(1,0)}A_1\chi_z^{(1,0)}$$
$$=-\frac{1}{6}(H_q'H_{pq}H_p+H_q'H_{pp}H_q+H_p'H_{qq}H_p).$$

For $k=1$, $i=1$, we have

$$\chi^{(2,1)}=\frac{1}{2}\sum_{i_0+i_1=1}\sum_{k_1=1}\sum_{l_1=1}^{2n}\chi^{(1,i_0)}_{z_{l_1}}(A_1\chi_z^{(1,i_1)})_{l_1}$$
$$=\frac{1}{2}\{(\chi_z^{(1,0)})'A_1\chi_z^{(1,1)}+(\chi_z^{(1,1)})'A_1\chi_z^{(1,0)}\}$$
$$=\frac{1}{4}(H_q'H_{pp}H_q+H'pH_{qq}H_p)+\frac{1}{2}H_q'H_{pq}H_p.$$

From (5.11), we have

$$\chi^{(3,0)}+\chi^{(2,1)}+\chi^{(1,2)}=\psi^{(3)}=0\Longrightarrow\chi^{(1,2)}=-(\chi^{(3,0)}+\chi^{(2,1)})$$
$$\chi^{(1,2)}=-\Big\{-\frac{1}{6}(H_q'H_{pp}H_q+H_p'H_{qq}H_p)-\frac{1}{6}H_q'H_{pq}H_p$$
$$+\frac{1}{4}(H_q'H_{pp}H_q+H_p'H_{qq}H_p)+\frac{1}{2}H_q'H_{pq}H_p\Big\}$$
$$=-\frac{1}{12}(H_q'H_{pp}H_q+H_p'H_{qq}H_p+4H_q'H_{pq}H_p).$$

Finally we get formal power series of erengy

$$h(s,z)=-(\chi^{(1,0)}+s\chi^{(1,1)}+s^2\chi^{(1,2)})+O(s^3)$$
$$=H(z)-\frac{s}{2}H_q'H_p+\frac{s^2}{2}(H_q'H_{pp}H_q+H_p'H_{qq}H_p+4H_q'H_{pq}H_q)+O(s^3).$$

Now let $H(z)$ be a time-independent Hamiltonian, its phase flow is g_H^t, its generating function is

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

We have

$$\phi^{(1)}(w)=-H(w),$$
$$\text{For } k\ge 1\quad \phi^{(k+1)}(w)=\sum_{m=1}^{k}\frac{1}{(k+1)m!}\sum_{l_1,\cdots,l_m=1}^{2n}\sum_{k_1+\cdots+k_m=k}\phi^{(1)}_{w_{l_1}\cdots w_{l_m}}(w)$$
$$\times(A_1\phi_w^{(k_1)}(w))_{l_1}\cdots A_1\phi_w^{(k_m)}(w))_{l_m}). \tag{5.13}$$

Theorem 5.1. *Suppose F^s is the Sp-Diff operator of order m for Hamiltonian H,* *i.e.*, $\phi(s,w)-\psi(s,w)=O(|s|^{m+1})$, *i.e.*,

$$\begin{cases}\psi^{(1)}(w)=\phi^{(1)}(w)=-H(w),\\ \psi^{(2)}(w)=\phi^{(2)}(w),\\ \cdots\cdots\\ \psi^{(m)}(w)=\phi^{(m)}(w).\end{cases}$$

Then $h^{(0)}(w)=H(w)$, $h^{(1)}(w)=h^{(2)}(w)=\cdots=h^{(m-1)}(w)=0$, *i.e.*, $h(s,w)-H(w)=o(|s|^m)$ *and* $h^{(m)}(w)=\psi^{(m+1)}(w)-\phi^{(m+1)}(w)$.

First we show that $\chi^{(k+1,i)}$ dependent only on derivatives of $\chi^{(k',i')}$, $k'\le k$, $i'\le i$. The recursion for $i=0$ is the same for the recursion of phase flow generating function with Hamiltonian $\chi^{(1,0)}(w)$. For $i\ge 1$, $\chi^{(k+1,i)}=0$ if $\chi^{(k',i')}=0$ for all i', k' such that $1\le i'\le i$, $1\le k'\le k$. We have

$$\begin{aligned}
&\psi^{(1)}=\chi^{(1,0)}\Longrightarrow\chi^{(1,0)}\xrightarrow{\text{recursion}}\chi^{(2,0)},\chi^{(3,0)},\chi^{(4,0)},\cdots,\\
&\psi^{(2)}=\chi^{(1,1)}+\chi^{(2,0)}\Longrightarrow\chi^{(1,1)}\xrightarrow{\text{recursion}}\chi^{(2,1)},\chi^{(3,1)},\chi^{(4,1)},\cdots,\\
&\psi^{(3)}=\chi^{(1,2)}+\chi^{(2,1)}+\chi^{(3,0)}\Longrightarrow\chi^{(1,2)}\xrightarrow{\text{recursion}}\chi^{(2,2)},\chi^{(3,2)},\chi^{(4,2)},\cdots,\\
&\psi^{(4)}=\chi^{(1,3)}+\chi^{(2,2)}+\chi^{(3,1)}+\chi^{(4,0)}\Longrightarrow\chi^{(1,3)}\xrightarrow{\text{recursion}}\chi^{(2,3)},\chi^{(3,3)},\chi^{(4,3)},\cdots,\\
&\qquad\cdots\cdots\\
&\psi^{(k)}=\chi^{(1,k-1)}+\chi^{(2,k-2)}+\cdots+\chi^{(k,0)}\Longrightarrow\chi^{(1,k-1)}\xrightarrow{\text{recursion}}\chi^{(2,k-1)},\chi^{(3,k-1)},\chi^{(4,k-1)},\cdots.
\end{aligned}\tag{5.14}$$

So $\chi^{(k,i)}$ can be generated successively through (5.9), (5.6). Then

$$h(s,w)=\sum_{i=0}^{\infty}s^i\chi^{(1,i)}(w).$$

Using equation $H=\psi^{(1)}=\psi^{(1)}=\chi^{(1,0)}$ and (5.9),(5.14), we get

$$\chi^{(2,0)}=\phi^{(2)},\quad \chi^{(3,0)}=\phi^{(3)},\quad \cdots,\quad \chi^{(k,0)}=\psi^{(k)},\quad \cdots.$$

Using equation (5.14), we get

$$\psi^{(2)}=\phi^{(2)}=\chi^{(1,1)}+\phi^{(2)}\Longrightarrow\chi^{(1,1)}=0.$$

Applying equation (5.9), (5.14), we get

$$\chi^{(2,1)}=0\Longrightarrow\chi^{(3,1)}=\chi^{(4,1)}=\cdots=\chi^{(k,1)}=\cdots=0.$$

Applying equation

$$\psi^{(3)}=\phi^{(3)}=\chi^{(1,2)}+\chi^{(2,1)}+\chi^{(3,1)}=\chi^{(1,2)}+0+\phi^{(3)}\Longrightarrow\chi^{(1,2)}=0,$$

then

$$\chi^{(2,2)}=\chi^{(3,2)}=\chi^{(4,2)}=\cdots=\chi^{(k,2)}=\cdots=0.$$

Finally

$$\psi^{(m)} = \phi^{(m)} = \chi^{(1,m-1)} + \chi^{(2,m-2)} + \cdots + \chi^{(m-1,1)} + \phi^{(m)} \Longrightarrow \chi^{(1,m-1)} = 0,$$

then

$$\chi^{(2,m-2)} = \chi^{(3,m-2)} = \chi^{(4,m-2)} = \cdots = \chi^{(k,m-2)} = \cdots = 0.$$

So $\chi^{(k,i)} = 0$ for $i = 1, 2, \cdots, m-1$ and $k = 1, 2, 3 \cdots$. Then equation

$$\psi^{(m+1)} = \chi^{(1,m)} + \chi^{(2,m-1)} + \cdots + \chi^{(m,1)} + \chi^{(m+1,0)} \Longrightarrow \chi^{(1,m)} = \psi^{(m+1)} - \phi^{(m+1)},$$

so we get finally

$$h(s,z) = \sum_{i=0}^{\infty} s^i \chi^{(1,i)} = H(z) + s^m(\psi^{(m+1)} - \phi^{(m+1)}) + O(|s|^{m+1}),$$

i.e.,

$$h(s,z) - H(z) = s^m(\psi^{(m+1)}(z) - \phi^{(m+1)}(z)) + O(|s|^{m+1}).$$

So in particular, if $F^s \sim \psi(s,w)$ is given by the truncation of phase flow generating function, i.e.,

$$\psi^{(1)} = \phi^{(1)} = H, \quad \psi^{(2)} = \phi^{(2)}, \ \cdots, \ \psi^{(m)} = \phi^{(m)}, \quad \psi^{(m+1)} = \phi^{(m+2)} = 0,$$

then

$$h(s,z) = H(z) - s^m \phi^{(m+1)}(z) + O(|s|^{m+1}).$$

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