

Here we give the full gory details of the proof that our generating function gives rise to a canonical transformation. As usual let $\mathbf{x} = (\mathbf{q}, \mathbf{p})$ and $\mathbf{y} = (\mathbf{Q}, \mathbf{P})$. Let $S = S(\mathbf{q}, \mathbf{P})$ be given, where $\mathbf{P} = \mathbf{P}(\mathbf{q}, \mathbf{p})$. Set

$$\mathbf{p} = \frac{\partial S}{\partial \mathbf{q}}, \quad \mathbf{Q} = \frac{\partial S}{\partial \mathbf{P}}.$$

Note that $\mathbf{Q} = \mathbf{Q}(\mathbf{q}, \mathbf{P})$. We will show this gives rise to a canonical transformation. The function S is known as the generating function. The Jacobian matrix for $\mathbf{x} \mapsto \mathbf{y}(\mathbf{x})$ is

$$D\mathbf{y} = \begin{pmatrix} \partial Q_i / \partial q_j|_p & \partial Q_i / \partial p_j|_p \\ \partial P_i / \partial q_j|_q & \partial P_i / \partial p_j|_q \end{pmatrix}$$

where each entry is itself an $n \times n$ matrix. We have to be very careful which variables are fixed in the partial derivatives. For instance

$$\frac{\partial Q_i}{\partial q_k}|_p = \frac{\partial Q_i}{\partial q_k}|_P + \frac{\partial Q_i}{\partial P_l}|_q \frac{\partial P_l}{\partial q_k}|_p, \quad \frac{\partial Q_i}{\partial p_k}|_q = \frac{\partial Q_i}{\partial P_l}|_q \frac{\partial P_l}{\partial p_k}|_q.$$

We want to compute

$$\begin{aligned} (D\mathbf{y})J(D\mathbf{y})^t &= \begin{pmatrix} \partial Q_i / \partial q_j|_p & \partial Q_i / \partial p_j|_p \\ \partial P_i / \partial q_j|_q & \partial P_i / \partial p_j|_q \end{pmatrix} \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \begin{pmatrix} \partial Q_j / \partial q_i|_p & \partial P_j / \partial p_i|_q \\ \partial Q_j / \partial p_i|_p & \partial P_j / \partial p_i|_q \end{pmatrix} \\ &= \begin{pmatrix} \{Q_i, Q_j\}_{q,p} & \{Q_i, P_j\}_{q,p} \\ \{P_j, Q_i\}_{q,p} & \{P_i, P_j\}_{q,p} \end{pmatrix}. \end{aligned}$$

Let us examine the first block. It is (assuming summation convention)

$$\begin{aligned} \{Q_i, Q_j\}_{q,p} &= \frac{\partial Q_i}{\partial q_k}|_p \frac{\partial Q_j}{\partial p_k}|_q - (i \leftrightarrow j) \\ &= \left(\frac{\partial Q_i}{\partial q_k}|_P + \frac{\partial Q_i}{\partial P_l}|_q \frac{\partial P_l}{\partial q_k}|_p \right) \frac{\partial Q_j}{\partial P_m}|_q \frac{\partial P_m}{\partial p_k}|_q - (i \leftrightarrow j). \end{aligned}$$

First we note

$$\frac{\partial Q_i}{\partial q_k}|_P = \frac{\partial^2 S}{\partial q_k \partial P_i} = \frac{\partial p_k}{\partial P_i}|_q,$$

so that

$$\frac{\partial Q_i}{\partial q_k}|_p \frac{\partial Q_j}{\partial P_m}|_q \frac{\partial P_m}{\partial p_k}|_q = \frac{\partial p_k}{\partial P_i}|_q \frac{\partial Q_j}{\partial P_m}|_q \frac{\partial P_m}{\partial p_k}|_q = \frac{\partial P_m}{\partial P_i}|_q \frac{\partial Q_j}{\partial P_m}|_q = \frac{\partial Q_j}{\partial P_i}|_q = \frac{\partial^2 S}{\partial P_i \partial P_j},$$

which is symmetric in i and j . So

$$\begin{aligned} \{Q_i, Q_j\}_{q,p} &= \frac{\partial Q_i}{\partial P_l}|_q \frac{\partial P_l}{\partial q_k}|_p \frac{\partial Q_j}{\partial P_m}|_q \frac{\partial P_m}{\partial p_k}|_q - (i \leftrightarrow j) \\ &= \frac{\partial^2 S}{\partial P_l \partial P_i} \frac{\partial P_l}{\partial q_k}|_p \frac{\partial P_m}{\partial p_k}|_q \frac{\partial^2 S}{\partial P_j \partial P_m} - (i \leftrightarrow j) \\ &= \frac{\partial^2 S}{\partial q_k \partial P_i} \frac{\partial P_m}{\partial p_k}|_q \frac{\partial^2 S}{\partial P_j \partial P_m} - (i \leftrightarrow j) \\ &= \frac{\partial p_k}{\partial P_i}|_q \frac{\partial P_m}{\partial p_k}|_q \frac{\partial^2 S}{\partial P_j \partial P_m} - (i \leftrightarrow j) \\ &= \frac{\partial^2 S}{\partial P_i \partial P_j} - (i \leftrightarrow j) \end{aligned}$$

which vanishes for the same reason. Now look at the block

$$\{P_i, P_j\}_{q,p} = \frac{\partial P_i}{\partial q_k} \Big|_p \frac{\partial P_j}{\partial p_k} \Big|_q - (i \leftrightarrow j).$$

Since $\mathbf{p} = \partial_{\mathbf{q}} S(\mathbf{q}, \mathbf{P}(\mathbf{q}, \mathbf{p}))$ holds identically we can differentiate it with respect to \mathbf{q} or \mathbf{p} , while holding the other constant. The chain rule gives us

$$0 = \underbrace{\frac{\partial^2 S}{\partial q_i \partial q_j}}_{A_{ij}} + \underbrace{\frac{\partial^2 S}{\partial q_i \partial P_k} \frac{\partial P_k}{\partial q_j}}_{B_{ik} C_{kj}} \Big|_p, \quad \delta_{ij} = \underbrace{\frac{\partial^2 S}{\partial q_i \partial P_k} \frac{\partial P_k}{\partial p_j}}_{B_{ik} D_{kj}} \Big|_q.$$

So $C = -B^{-1}A$ and $D = B^{-1}$ so that $CD^t = -DAD^t$. Hence

$$\frac{\partial P_i}{\partial q_k} \Big|_p \frac{\partial P_j}{\partial p_k} \Big|_q = C_{ik} D_{jk} = C_{ik} D_{kj}^t = (CD^t)_{ij} = -(DAD^t)_{ij}.$$

But since A is symmetric we have $(DAD^t)^t = DA^t D^t = DAD^t$, i.e. it is *symmetric*! So

$$\{P_i, P_j\}_{q,p} = \frac{\partial P_i}{\partial q_k} \Big|_p \frac{\partial P_j}{\partial p_k} \Big|_q - (i \leftrightarrow j) = 0.$$

Now we look at the second block. It is

$$\begin{aligned} \{Q_i, P_j\}_{q,p} &= \frac{\partial Q_i}{\partial q_k} \Big|_p \frac{\partial P_j}{\partial p_k} \Big|_q - \frac{\partial Q_i}{\partial p_k} \Big|_q \frac{\partial P_j}{\partial q_k} \Big|_p \\ &= \left(\frac{\partial Q_i}{\partial q_k} \Big|_P + \frac{\partial Q_i}{\partial P_l} \Big|_q \frac{\partial P_l}{\partial q_k} \Big|_p \right) \frac{\partial P_j}{\partial p_k} \Big|_q - \frac{\partial Q_i}{\partial P_l} \Big|_q \frac{\partial P_l}{\partial p_k} \Big|_q \frac{\partial P_j}{\partial q_k} \Big|_p \\ &= \frac{\partial p_k}{\partial P_i} \Big|_q \frac{\partial P_j}{\partial p_k} \Big|_q + \frac{\partial Q_i}{\partial P_l} \Big|_q \left(\frac{\partial P_l}{\partial q_k} \Big|_p \frac{\partial P_j}{\partial p_k} \Big|_q - \frac{\partial P_l}{\partial p_k} \Big|_q \frac{\partial P_j}{\partial q_k} \Big|_p \right). \end{aligned}$$

The first term is just δ_{ij} and the term in brackets is exactly $\{P_l, P_j\}_{q,p}$, which we know vanishes. Since the third block is the same as the second but with a sign change, we conclude

$$D\mathbf{y}J(D\mathbf{y})^t = \begin{pmatrix} 0 & \delta_{ij} \\ -\delta_{ij} & 0 \end{pmatrix} = J.$$

So the derivative of the map is symplectic and the transformation is necessarily canonical.