In lectures, I claimed that a canonical transformation can be constructed from a single function S by the following process. Suppose $S = S(\boldsymbol{q}, \boldsymbol{P})$ is a function from $\mathbb{R}^m \times \mathbb{R}^m$ to $\mathbb{R}$, and suppose furthermore that:

$$\det\left(\frac{\partial^2 S}{\partial q_i \partial P_j}(\boldsymbol{q}_0, \boldsymbol{P}_0)\right) \neq 0. \qquad (\star)$$

We first consider the relation:

$$p_i = \frac{\partial S}{\partial q_i}(\boldsymbol{q}, \boldsymbol{P})$$

as an equation for $\boldsymbol{P}$ and solve this to obtain $\boldsymbol{P}(\boldsymbol{q}, \boldsymbol{p})$. By the implicit function theorem, we can do this, at least locally, as the non-degeneracy condition $(\star)$ is precisely what is required in the hypotheses of the implicit function theorem.

Having constructed $\boldsymbol{P}(\boldsymbol{q}, \boldsymbol{p})$, we define $\boldsymbol{Q}(\boldsymbol{q}, \boldsymbol{p})$ by the equation:

$$Q_i(\boldsymbol{q}, \boldsymbol{p}) = \frac{\partial S}{\partial P_i}\left(\boldsymbol{q}, \boldsymbol{P}(\boldsymbol{q}, \boldsymbol{p})\right) \qquad (\flat)$$

I claimed (but did not prove) that this is a canonical transformation. To establish this result, we show that the Poisson bracket algebra of $\boldsymbol{Q}, \boldsymbol{P}$ is the standard one, i.e.:

$$\{Q_i, Q_j\} = \{P_i, P_j\} = 0, \qquad \{Q_i, P_j\} = -\{P_j, Q_i\} = \delta_{ij}. \qquad (\diamond)$$

where as always

$$\{f, g\} = \frac{\partial f}{\partial q_j}\frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j}\frac{\partial g}{\partial q_j}.$$

Checking $(\diamond)$ is made harder as we have no explicit expression for $\boldsymbol{P}(\boldsymbol{q}, \boldsymbol{p})$, rather it is implicitly defined by the relation:

$$p_i = \frac{\partial S}{\partial q_i}(\boldsymbol{q}, \boldsymbol{P}(\boldsymbol{q}, \boldsymbol{p})) \qquad (\dagger)$$

Differentiating $(\dagger)$ with respect to p_j, we find:

$$\frac{\partial p_i}{\partial p_j} = \delta_{ij} = \frac{\partial^2 S}{\partial q_i \partial P_k}\frac{\partial P_k}{\partial p_j}$$

Setting $A_{ik} = \frac{\partial^2 S}{\partial q_i \partial P_k}$ and $B_{kj} = \frac{\partial P_k}{\partial p_j}$, we can read this as the matrix equation:

$$I = AB$$

so that $A = B^{-1}$. Thus we also have $I = BA$, which in components reads:

$$\frac{\partial P_k}{\partial p_j}\frac{\partial^2 S}{\partial q_j \partial P_l} = \delta_{kl}. \qquad (\triangle)$$

Next we differentiate (†) with respect to q_j to obtain:

$$0 = \frac{\partial^2 S}{\partial q_i \partial q_j} + \frac{\partial^2 S}{\partial q_i \partial P_l} \frac{\partial P_l}{\partial q_j},$$

so that:

$$\frac{\partial^2 S}{\partial q_i \partial P_l} \frac{\partial P_l}{\partial q_j} = -\frac{\partial^2 S}{\partial q_i \partial q_j}$$

Multiplying both sides by

$$\delta_{kj} = \frac{\partial^2 S}{\partial q_k \partial P_m} \frac{\partial P_m}{\partial p_j}$$

we obtain:

$$\frac{\partial^2 S}{\partial q_i \partial P_l} \frac{\partial P_l}{\partial q_j} \frac{\partial P_m}{\partial p_j} \frac{\partial^2 S}{\partial q_k \partial P_m} = -\frac{\partial^2 S}{\partial q_i \partial q_k}$$

Antisymmetrizing on i, k, we obtain:

$$\begin{aligned} 0 &= \frac{\partial^2 S}{\partial q_i \partial P_l} \frac{\partial P_l}{\partial q_j} \frac{\partial P_m}{\partial p_j} \frac{\partial^2 S}{\partial q_k \partial P_m} - \frac{\partial^2 S}{\partial q_k \partial P_l} \frac{\partial P_l}{\partial q_j} \frac{\partial P_m}{\partial p_j} \frac{\partial^2 S}{\partial q_i \partial P_m} \\ &= \frac{\partial^2 S}{\partial q_i \partial P_l} \frac{\partial P_l}{\partial q_j} \frac{\partial P_m}{\partial p_j} \frac{\partial^2 S}{\partial q_k \partial P_m} - \frac{\partial^2 S}{\partial q_k \partial P_m} \frac{\partial P_m}{\partial q_j} \frac{\partial P_l}{\partial p_j} \frac{\partial^2 S}{\partial q_i \partial P_l} \\ &= \frac{\partial^2 S}{\partial q_i \partial P_l} \left[\frac{\partial P_l}{\partial q_j} \frac{\partial P_m}{\partial p_j} - \frac{\partial P_m}{\partial q_j} \frac{\partial P_l}{\partial p_j} \right] \frac{\partial^2 S}{\partial q_k \partial P_m} \\ &= \frac{\partial^2 S}{\partial q_i \partial P_l} \{P_l, P_m\} \frac{\partial^2 S}{\partial q_k \partial P_m} \end{aligned}$$

Now, by (⋆), we can assume that $\frac{\partial^2 S}{\partial q_k \partial P_m}$ is invertible (possibly after restricting to a neighbourhood), so that $\{P_l, P_m\} = 0$.

Next, we consider $\{Q_i, Q_j\}$, which we wish to show vanishes. To do this, we differentiate (♭) with respect to q_j and p_j to conclude:

$$\begin{aligned} \frac{\partial Q_i}{\partial q_j} &= \frac{\partial^2 S}{\partial P_i \partial q_j} + \frac{\partial^2 S}{\partial P_i \partial P_l} \frac{\partial P_l}{\partial q_j} \\ \frac{\partial Q_k}{\partial p_j} &= \frac{\partial^2 S}{\partial P_k \partial P_m} \frac{\partial P_m}{\partial p_j} \end{aligned}$$

Multiplying these two expressions we find:

$$\begin{aligned} \frac{\partial Q_i}{\partial q_j} \frac{\partial Q_k}{\partial p_j} &= \frac{\partial^2 S}{\partial P_i \partial q_j} \frac{\partial^2 S}{\partial P_k \partial P_m} \frac{\partial P_m}{\partial p_j} + \frac{\partial^2 S}{\partial P_i \partial P_l} \frac{\partial P_l}{\partial q_j} \frac{\partial^2 S}{\partial P_k \partial P_m} \frac{\partial P_m}{\partial p_j} \\ &= \frac{\partial^2 S}{\partial P_i \partial P_k} + \frac{\partial^2 S}{\partial P_i \partial P_l} \frac{\partial P_l}{\partial q_j} \frac{\partial P_m}{\partial p_j} \frac{\partial^2 S}{\partial P_k \partial P_m} \end{aligned}$$

where in moving from the first line to the second we have made use of the relation (△). Now, antisymmetrizing on i, k gives:

$$
\begin{aligned}
\{Q_i, Q_k\} &= \frac{\partial^2 S}{\partial P_i \partial P_l}\frac{\partial P_l}{\partial q_j}\frac{\partial P_m}{\partial p_j}\frac{\partial^2 S}{\partial P_k \partial P_m} - \frac{\partial^2 S}{\partial P_k \partial P_l}\frac{\partial P_l}{\partial q_j}\frac{\partial P_m}{\partial p_j}\frac{\partial^2 S}{\partial P_i \partial P_m} \\
&= \frac{\partial^2 S}{\partial P_i \partial P_l}\{P_l, P_m\}\frac{\partial^2 S}{\partial P_k \partial P_m} = 0.
\end{aligned}
$$

by a similar series of index manipulations to before. It remains for us to verify the bracket $\{Q_i, P_k\}$. Using the expressions for derivatives of Q_i we have:

$$
\begin{aligned}
\frac{\partial Q_i}{\partial q_j}\frac{\partial P_k}{\partial p_j} - \frac{\partial Q_i}{\partial p_j}\frac{\partial P_k}{\partial q_j} &= \frac{\partial^2 S}{\partial P_i \partial q_j}\frac{\partial P_k}{\partial p_j} + \frac{\partial^2 S}{\partial P_i \partial P_l}\frac{\partial P_l}{\partial q_j}\frac{\partial P_k}{\partial p_j} - \frac{\partial^2 S}{\partial P_i \partial P_l}\frac{\partial P_l}{\partial p_j}\frac{\partial P_k}{\partial q_j} \\
&= \delta_{ik} + \frac{\partial^2 S}{\partial P_i \partial P_l}\{P_l, P_k\} = \delta_{ik}
\end{aligned}
$$

where again we've used (△) to simplify the first term. We have thus verified that $\boldsymbol{Q}, \boldsymbol{P}$ satisfy the canonical Poisson bracket algebra. To check that this implies the transformation is canonical, we can compute:

$$
\begin{aligned}
\dot{Q}_i &= \frac{\partial Q_i}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial Q_i}{\partial p_j}\frac{\partial H}{\partial q_j} \\
&= \frac{\partial Q_i}{\partial q_j}\left(\frac{\partial H}{\partial Q_k}\frac{\partial Q_k}{\partial p_j} + \frac{\partial H}{\partial P_k}\frac{\partial P_k}{\partial p_j}\right) - \frac{\partial Q_i}{\partial p_j}\left(\frac{\partial H}{\partial Q_k}\frac{\partial Q_k}{\partial q_j} + \frac{\partial H}{\partial P_k}\frac{\partial P_k}{\partial q_j}\right) \\
&= \frac{\partial H}{\partial Q_k}\{Q_i, Q_k\} + \frac{\partial H}{\partial P_k}\{Q_i, P_k\}
\end{aligned}
$$

and similarly:

$$
\begin{aligned}
\dot{P}_i &= \frac{\partial P_i}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial P_i}{\partial p_j}\frac{\partial H}{\partial q_j} \\
&= \frac{\partial P_i}{\partial q_j}\left(\frac{\partial H}{\partial Q_k}\frac{\partial Q_k}{\partial p_j} + \frac{\partial H}{\partial P_k}\frac{\partial P_k}{\partial p_j}\right) - \frac{\partial P_i}{\partial p_j}\left(\frac{\partial H}{\partial Q_k}\frac{\partial Q_k}{\partial q_j} + \frac{\partial H}{\partial P_k}\frac{\partial P_k}{\partial q_j}\right) \\
&= \frac{\partial H}{\partial Q_k}\{P_i, Q_k\} + \frac{\partial H}{\partial P_k}\{P_i, P_k\}
\end{aligned}
$$

so that we have:

$$
\dot{Q}_i = \frac{\partial H}{\partial P_i}, \qquad \dot{P}_i = -\frac{\partial H}{\partial Q_i}
$$

if and only if:

$$
\{Q_i, Q_j\} = \{P_i, P_j\} = 0, \qquad \{Q_i, P_j\} = -\{P_j, Q_i\} = \delta_{ij}.
$$

holds.