The generating functions of canonical transformations

In a previos lecture we introduced the canonical transformations

$$Q_i = Q_i(\vec{q}, \vec{p}, t) \qquad P_i = P_i(\vec{q}, \vec{p}, t) \qquad (*)$$

such that the equations of motion in the new set are in the Hamiltonian form

$$\dot{Q}_i = \frac{\partial H'}{\partial P_i} \qquad \dot{P}_i = -\frac{\partial H'}{\partial Q_i} \qquad i = 1 \dots n$$

Both the original $\vec{q}, \vec{p}$ and new $\vec{Q}, \vec{P}$ coordinates must satisfy the least action principle

$$\delta \int_1^2 \left(\sum_{i=1}^n p_i \dot{q}_i - H(\vec{q}, \vec{p}, t) \right) dt = 0$$

$$\delta \int_1^2 \left(\sum_{i=1}^n P_i \dot{Q}_i - H'(\vec{Q}, \vec{P}, t) \right) dt' = 0$$

The integrands in both expressions do not have to be equal. Both statements are satisfied if the integrands are related as

$$\lambda \left(\sum p_i \dot{q}_i - H \right) = \sum P_i \dot{Q}_i - H' + \frac{dF}{dt}$$

Where F is any function of the phase space coordinates with continuous second derivatives and λ is a constant. λ is related to to a simple scale transformation. Say if $Q'_i = \mu q_i$ and $P'_i = \nu p_i$ then

$$\underbrace{\mu\nu}_{\lambda} \left(\sum_i p_i \dot{q}_i - H \right) = \sum_{i=1}^n P'_i \dot{Q}'_i - H'$$

Hence we can always easily find an intermediate set of coordinates for a given λ. Let us turn our attention to the $\frac{dF}{dt}$ term. It vanishes in the action integral if F is a function of $(\vec{q}, \vec{p}, t)$ or $(\vec{Q}, \vec{P}, t)$ or any mixture of those since they have zero variation at the end points. Through the equations of transformation (*) and their inverses F can be expressed partly in terms of the old set of variables and partly of the new. F is useful for specifying the exact form of the canonical transformation only when half of the variables are from the old set and half are from the new. It then acts as a bridge between the two sets of canonical variables and is called the generating function.

Suppose $F = F_1(\vec{q}, \vec{Q}, t)$ - function of only the old and new generalized coordinates. Then

$$\sum_i p_i \dot{q}_i - H = \sum_i P_i \dot{Q}_i - H' + \frac{dF_1}{dt} = \sum_i P_i \dot{Q}_i - H' + \frac{\partial F_1}{\partial t} + \sum_i \frac{\partial F_1}{\partial q_i} \dot{q}_i + \sum_i \frac{\partial F_1}{\partial Q_i} \dot{Q}_i \qquad (**)$$

Since the old and new coordinates are separately independent, the above equation can only hold if the coefficients of $\dot{q}_i$ and $\dot{Q}_i$ each vanish, i.e.

$$p_i = \frac{\partial F_1}{\partial q_i} \qquad P_i = -\frac{\partial F_1}{\partial Q_i}$$

leaving

$$H' = H + \frac{\partial F_1}{\partial t}$$

The equations $p_i = \frac{\partial F_1}{\partial q_i}$ define p_i as functions of $\vec{q}$ and $\vec{Q}$ (as well as t). If we can invert them we can solve for n Q_i's in terms of $\vec{q}$, $\vec{p}$, and t

That gives us the first half of the transformations (*). Once the relations between the Q_i's and the old $\vec{q}, \vec{p}$ have been established, they can be substituted into

$$P_i = -\frac{\partial F_1}{\partial Q_i}$$

so that we get the n P_i's as functions of $\vec{q}, \vec{p}$, and t.

There could be other ways to describe the canonical transformation. For example, the transformation may be such that p_i cannot be written as functions of $\vec{q}, \vec{Q}$, and t but rather will be functions of $\vec{q}, \vec{P}$, and t. We would then seek a generating function that is a function of $\vec{q}$ and $\vec{P}$. Equation (**) must then be replaced by an equivalent relation involving $\dot{P}_i$ rather than $\dot{Q}_i$. This can be achieved by

$$F = F_2(\vec{q}, \vec{P}, t) - \sum_i Q_i P_i$$

Substituting this into $\sum p_i \dot{q}_i - H = \sum_i P_i \dot{Q}_i - H' + \frac{dF}{dt}$ yields

$$\sum_i p_i \dot{q}_i - H = -\sum_i Q_i \dot{P}_i - H' + \frac{d}{dt} F_2(\vec{q}, \vec{P}, t).$$

The total derivative of F_2 can then be expanded as

$$\frac{d}{dt} F_2 = \sum_i \frac{\partial F_2}{\partial q_i} \dot{q}_i + \sum_i \frac{\partial F_2}{\partial P_i} \dot{P}_i$$

which leads to the equations

$$p_i = \frac{\partial F_2}{\partial q_i} \qquad Q_i = \frac{\partial F_2}{\partial P_i} \qquad \text{with} \quad H' = H + \frac{\partial F_2}{\partial t}$$

As before the first set of these equations,

$p_i = \frac{\partial F_2}{\partial q_i}$ are to be solved for P_i as functions of $\vec{q}$, $\vec{P}$, and t. That corresponds to the second half of transformation $(*)$. The remaining part is then provided by $Q_i = \frac{\partial F_2}{\partial P_i}$

Using the same idea we can also establish two more basic types of generating functions.

generating function	derivatives	trivial special case
$F = F_1(\vec{q}, \vec{Q}, t)$	$p_i = \frac{\partial F_1}{\partial q_i}$ $\quad P_i = -\frac{\partial F_1}{\partial Q_i}$	$F_1 = \sum_i q_i Q_i$ $\quad Q_i = p_i$ $\quad P_i = -q_i$
$F = F_2(\vec{q}, \vec{P}, t) - \sum_i Q_i P_i$	$p_i = \frac{\partial F_2}{\partial q_i}$ $\quad Q_i = \frac{\partial F_2}{\partial P_i}$	$F_2 = \sum_i q_i P_i$ $\quad Q_i = q_i$ $\quad P_i = p_i$
$F = F_3(\vec{p}, \vec{Q}, t) + \sum_i q_i p_i$	$q_i = -\frac{\partial F_3}{\partial p_i}$ $\quad P_i = -\frac{\partial F_3}{\partial Q_i}$	$F_3 = \sum_i p_i Q_i$ $\quad Q_i = -q_i$ $\quad P_i = -p_i$
$F = F_4(\vec{p}, \vec{P}, t) + \sum_i q_i p_i - \sum_i Q_i P_i$	$q_i = -\frac{\partial F_4}{\partial p_i}$ $\quad Q_i = \frac{\partial F_4}{\partial P_i}$	$F_4 = p_i P_i$ $\quad Q_i = p_i$ $\quad P_i = -q_i$