9. Canonical transformations

Related to the Hamiltonian formulation of mechanics, central in statistical mechanics and quantum mechanics.
From chapter 8 :
The phase space is $2n$-dimensional, with n axes for the gen. coordinates q_i and n axes for the conjugate (or canonical) momenta p_i.

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = p_i(q, \dot{q}, t) \quad ; \quad i = 1, \ldots, n \quad ; \quad L = L(q, \dot{q}, t)$$

$$H = p_i \dot{q}_i - L = H(p, q, t)$$

$$\left.\begin{aligned} \dot{q}_i &= \partial H / \partial p_i \\ \dot{p}_i &= -\partial H / \partial q_i \end{aligned}\right\} \quad \text{Hamilton's equations}$$

Ordinary coord. transformations $Q_i = Q_i(q, t)$ are called point transformations.
Ex: From cartesian coords. $q = \{x, y\}$ to plane polar coords. $Q = \{r, \theta\}$

Within the Hamiltonian formulation, we may transform both q_i and p_i,

$$Q_i = Q_i(q, p, t) \quad ; \quad P_i = P_i(q, p, t)$$

This transformation of phase space is called a canonical transformation. The new variables obey Hamilton's eqns.

$$\dot{Q}_i = \partial K / \partial P_i \quad ; \quad \dot{P}_i = -\partial K / \partial Q_i$$

with a Hamiltonian $K(Q, P, t)$.

We saw in chapter 2 that Lagrange's eqns. could be derived from Hamilton's principle,

$$\delta \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt = 0$$

We will show that Hamilton's eqns. can be derived from a modified Hamilton's principle,

$$\delta \int_{t_1}^{t_2} \left[p_i \dot{q}_i - H(p, q, t) \right] dt = 0$$

The integrand $f(q, \dot{q}, p, t) = p_i \dot{q}_i - H(p, q, t)$ is independent of $\dot{p}_i$. As in ch. 2.3 (and 2.2), we arrived at Lagrange's eqns. (and Euler's eqns.) by setting

$$\left. \frac{\partial L}{\partial \dot{q}_i} \delta q_i \right|_{t_1}^{t_2} = 0 \qquad \text{(see p. 21 in lecture notes)}$$

since we assumed $\delta q_i(t_1) = \delta q_i(t_2) = 0$ at the outset. Now, we have automatically

$$\left. \frac{\partial f}{\partial \dot{p}_i} \delta p_i \right|_{t_1}^{t_2} = 0$$

since f is independent of $\dot{p}_i$. Thus, we obtain the Euler eqns. for f,

$$\frac{d}{dt} \frac{\partial f}{\partial \dot{q}_i} - \frac{\partial f}{\partial q_i} = 0 \quad ; \quad \frac{d}{dt} \frac{\partial f}{\partial \dot{p}_i} - \frac{\partial f}{\partial p_i} = 0$$

Here, $\partial f / \partial \dot{q}_i = p_i$, $\partial f / \partial q_i = -\partial H / \partial q_i$
and $\partial f / \partial \dot{p}_i = 0$, $\partial f / \partial p_i = \dot{q}_i - \partial H / \partial p_i$

$$\Rightarrow \dot{p}_i = -\partial H / \partial q_i \quad ; \quad \dot{q}_i = \partial H / \partial p_i$$

i.e., Hamilton's eqns.

The modified Hamilton's principle must also be obeyed in the new set of canonical coordinates:

$$\delta \int_{t_1}^{t_2} [P_i \dot{Q}_i - K(P, Q, t)]\, dt = 0$$

Now, new and old coords. and Hamiltonians are related,

$$p_i \dot{q}_i - H = P_i \dot{Q}_i - K + \frac{dF}{dt}$$

Here, F is any ("well-behaved", i.e., with continuous 2. derivatives) function of old and/or new phase space coordinates (with zero variation in the end points, i.e., $\delta F(t_1) = \delta F(t_2) = 0$).

[To be precise, $\lambda(p_i \dot{q}_i - H) = P_i \dot{Q}_i - K + dF/dt$.
If $\lambda \neq 1$: Extended canonical transformation.
We consider only the case with $\lambda = 1$]

Particularly useful are canonical transformations where F is a function of both old and new variables.

The <u>generating function</u> F facilitates the transformation. The 4 combinations of n old and n new variables give rise to 4 types:

$$F_1(q, Q, t), \quad F_2(q, P, t), \quad F_3(p, Q, t), \quad F_4(p, P, t)$$

We examine all of them.

(1) $F = F_1(q, Q, t)$

$$\Rightarrow p_i \dot{q}_i - H = P_i \dot{Q}_i - K + \overbrace{\frac{\partial F_1}{\partial t} + \frac{\partial F_1}{\partial q_i}\dot{q}_i + \frac{\partial F_1}{\partial Q_i}\dot{Q}_i}^{=\frac{dF_1}{dt}}$$

Here, q_i and Q_i are considered as independent.
Then, by inspection

$$\underbrace{p_i = \frac{\partial F_1}{\partial q_i}}_{\substack{\text{n equations} \\ \text{that yield} \\ Q_i(q,p,t)}}, \quad \underbrace{P_i = -\frac{\partial F_1}{\partial Q_i}}_{\substack{\text{next these} \\ \text{n eqns. yield} \\ P_i(q,p,t)}}, \quad \underbrace{K = H + \frac{\partial F_1}{\partial t}}_{\substack{\text{finally, this eqn.} \\ \text{yields } K(Q,P,t)}}$$

(2) $F = F_2(q, P, t) - Q_i P_i$

$$\Rightarrow p_i \dot{q}_i - H = \cancel{P_i \dot{Q}_i} - K + \frac{dF_2}{dt} - \cancel{P_i \dot{Q}_i} - Q_i \dot{P}_i$$

$$= -K + \frac{\partial F_2}{\partial t} + \frac{\partial F_2}{\partial q_i}\dot{q}_i + \frac{\partial F_2}{\partial P_i}\dot{P}_i - Q_i \dot{P}_i$$

Here, q_i and P_i are considered as independent.
Then,

$$\underbrace{p_i = \frac{\partial F_2}{\partial q_i}}_{\text{yield } P_i(q,p,t)}, \quad \underbrace{Q_i = \frac{\partial F_2}{\partial P_i}}_{\text{yield } Q_i(q,p,t)}, \quad \underbrace{K = H + \frac{\partial F_2}{\partial t}}_{\text{yields } K(Q,P,t)}$$

(3) $F = F_3(p, Q, t) + q_i P_i$

$$\Rightarrow \cancel{p_i \dot{q}_i} - H = P_i \dot{Q}_i - K + \frac{dF_3}{dt} + \cancel{p_i \dot{q}_i} + q_i \dot{P}_i$$

$$\Rightarrow -H = P_i \dot{Q}_i - K + \frac{\partial F_3}{\partial t} + \frac{\partial F_3}{\partial p_i} \dot{p}_i + \frac{\partial F_3}{\partial Q_i} \dot{Q}_i + q_i \dot{P}_i$$

Here, p_i and Q_i are considered as independent.

$$\Rightarrow \underbrace{q_i = -\frac{\partial F_3}{\partial p_i}}_{\text{yield } Q_i(q,p,t)}, \quad \underbrace{P_i = -\frac{\partial F_3}{\partial Q_i}}_{\text{yield } P_i(q,p,t)}, \quad \underbrace{K = H + \frac{\partial F_3}{\partial t}}_{\text{yield } K(Q,P,t)}$$

(4) $F = F_4(p, P, t) + q_i p_i - Q_i P_i$

$$\Rightarrow \cancel{p_i \dot{q}_i} - H = \cancel{P_i \dot{Q}_i} - K + \frac{dF_4}{dt} + \cancel{p_i \dot{q}_i} + q_i \dot{p}_i - \cancel{P_i \dot{Q}_i} - Q_i \dot{P}_i$$

$$\Rightarrow -H = -K + \frac{\partial F_4}{\partial t} + \frac{\partial F_4}{\partial p_i} \dot{p}_i + \frac{\partial F_4}{\partial P_i} \dot{P}_i + q_i \dot{p}_i - Q_i \dot{P}_i$$

Here, p_i and P_i are considered as independent.

$$\Rightarrow \underbrace{q_i = -\frac{\partial F_4}{\partial p_i}}_{\text{yield } P_i(q,p,t)}, \quad \underbrace{Q_i = \frac{\partial F_4}{\partial P_i}}_{\text{yield } Q_i(q,p,t)}, \quad \underbrace{K = H + \frac{\partial F_4}{\partial t}}_{\text{yields } K(Q,P,t)}$$

Note that both (2) and (3) involve a Legendre transformation, and (4) involves a double Legendre transformation.

Let's consider some examples.

Ex 1. $F_2 = q_i P_i$

$\Rightarrow p_i = \frac{\partial F_2}{\partial q_i} = P_i$; $Q_i = \frac{\partial F_2}{\partial P_i} = q_i$; $K = H$

$\Rightarrow F_2$ generates the identity transformation

Ex 2. $F_2 = f_i(q,t) \cdot P_i$ with arbitrary functions f_i

$\Rightarrow Q_i = \frac{\partial F_2}{\partial P_i} = f_i(q,t)$, i.e., a point transformation, which is therefore a specific case of canonical transformations.

Ex 3. Harmonic oscillator

For a simple 1D harm. osc. $H = p^2/2m + \frac{1}{2} k q^2$

With $\omega^2 = k/m$: $H = \frac{1}{2m}(p^2 + m^2\omega^2 q^2)$

We <u>know</u> that the total energy $H = E$ is conserved, i.e., independent of time.

We <u>see</u> that the transformation

$$p = f(P) \cos Q$$
$$q = [f(P)/m\omega] \sin Q$$

gives a $K = H$ independent of Q:

$$K = H = \frac{f^2(P)}{2m}(\cos^2 Q + \sin^2 Q) = \frac{f^2(P)}{2m}$$

We may eliminate $f(P)$ in the transf. above:

$f(P) = q m\omega / \sin Q \Rightarrow p = q m \omega \cot Q$

This corresponds to a generating function of the type $F_1(q, Q)$:

$p = \partial F_1/\partial q \Rightarrow F_1 = \frac{1}{2} m\omega q^2 \cot Q$

$P = -\partial F_1/\partial Q = m\omega q^2 / 2\sin^2 Q \Rightarrow q(Q,P) = \sqrt{\frac{2P}{m\omega}} \sin Q$

Then $f(P) = \sqrt{2m\omega P}$

and $K = f^2/2m = \omega P$

Hamilton's eqn. $\dot{P} = -\partial K/\partial Q$ shows that when Q is cyclic (K indep. of Q), the conjugate momentum P is conserved. Since $K = H = E$ = the constant total energy, we have $P = E/\omega$.

The second Hamilton eqn. is the eqn. of motion for Q:

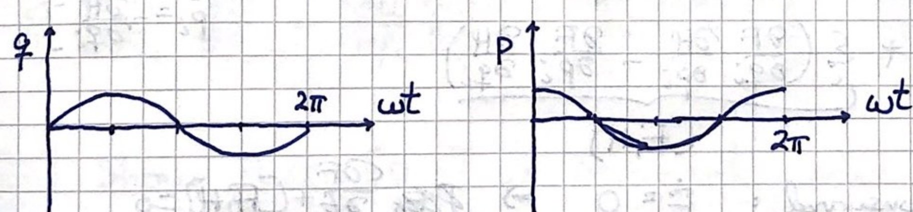
$$\dot{Q} = \partial K/\partial P = \omega \quad \Rightarrow Q(t) = \omega t + \alpha$$

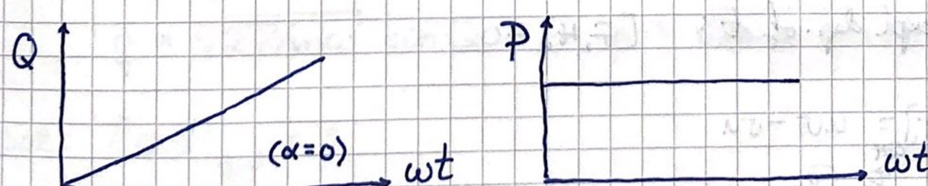
where α is fixed by the initial condition $Q(0)$

Solution in the old coordinate:

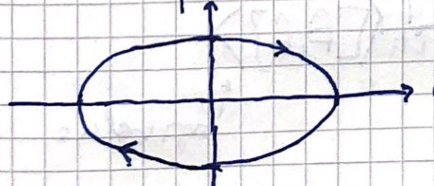
$$q = \sqrt{\frac{2P}{m\omega}} \sin Q = \sqrt{\frac{2E}{m\omega^2}} \sin(\omega t + \alpha)$$; not surprising

Graphical illustrations:





Phase space (old coords.)



Poisson brackets:

$$[u,v] \overset{\text{def}}{=} \sum_{i=1}^{n} \left(\frac{\partial u}{\partial q_i} \frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i} \frac{\partial v}{\partial q_i} \right)$$ = Poisson brackets

of the functions u and v with respect to the set of canonical variables $(q_1 \dots q_n \,;\, p_1 \dots p_n)$.

We realize immediately:

$$[u,v] = -[v,u]$$

$$[u,c] = 0 \qquad \text{when } c = \text{const.}$$

$$[q_i, q_j] = [p_i, p_j] = 0$$

$$[q_i, p_j] = \delta_{ij}$$

Less obvious (and without proof):

$[u,v]$ is invariant under a canonical transformation

$$\Rightarrow \sum_i \left(\frac{\partial u}{\partial q_i} \frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i} \frac{\partial v}{\partial q_i} \right) = \sum_i \left(\frac{\partial u}{\partial Q_i} \frac{\partial v}{\partial P_i} - \frac{\partial u}{\partial P_i} \frac{\partial v}{\partial Q_i} \right)$$

Ex: Show that $[q,p]$ is invariant under the transf. of the harmonic oscillator,

$$q = \sqrt{2P/m\omega}\, \sin Q \quad ; \quad p = \sqrt{2m\omega P}\, \cos Q$$

Sol: $[q,p]_{q,p} = 1$

$$[q,p]_{Q,P} = \frac{\partial q}{\partial Q} \frac{\partial p}{\partial P} - \frac{\partial p}{\partial Q} \frac{\partial q}{\partial P}$$

$$= 2\sqrt{P} \cos Q \cos Q \cdot \tfrac{1}{2} P^{-1/2}$$

$$+ 2\sqrt{P} \sin Q \cdot \tfrac{1}{2} P^{-1/2} \sin Q$$

$$= \cos^2 Q + \sin^2 Q$$

$$= 1$$

Time dependence of an arbitrary function $F(q,p,t)$:

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial F}{\partial q_i} \dot{q}_i + \frac{\partial F}{\partial p_i} \dot{p}_i \right)$$

$$= \frac{\partial F}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial F}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$$

$$= \frac{\partial F}{\partial t} + [F, H]$$

Comparison with quantum mechanics (QM):

Commutator : $[u, v]_{QM} = uv - vu$

Momentum operator : $p_i = \frac{\hbar}{i} \frac{\partial}{\partial q_i}$

$\Rightarrow [q_i, p_j]_{QM} = i\hbar \delta_{ij}$

Time dependence of QM expectation values :

$$\frac{d\langle F \rangle}{dt} = \frac{\partial \langle F \rangle}{\partial t} + \frac{1}{i\hbar} \langle [\hat{F}, \hat{H}] \rangle$$

($\hat{F}, \hat{H}$: QM operators)

A final example : Find $[L_x, L_y]$ etc. and compare with QM.

Solution :

$$\vec{L} = \vec{r} \times \vec{p}$$

$$\Rightarrow L_x = y p_z - z p_y \quad ; \quad L_y = z p_x - x p_z$$

$$[L_x, L_y] = \sum_{i=1}^{3} \left(\frac{\partial L_x}{\partial q_i} \frac{\partial L_y}{\partial p_i} - \frac{\partial L_x}{\partial p_i} \frac{\partial L_y}{\partial q_i} \right) \quad ; \quad q_i = x, y, z$$

$$\frac{\partial L_x}{\partial q_i} = \frac{\partial}{\partial q_i}(y p_z - z p_y) = p_z \delta_{i2} - p_y \delta_{i3}$$

$$\frac{\partial L_y}{\partial p_y} = \frac{\partial}{\partial p_i}(z p_x - x p_z) = z \delta_{i1} - x \delta_{i3}$$

$$\frac{\partial L_x}{\partial p_i} = \frac{\partial}{\partial p_i}(y p_z - z p_y) = y \delta_{i3} - z \delta_{i2}$$

$$\frac{\partial L_y}{\partial q_i} = \frac{\partial}{\partial q_i}(z p_x - x p_z) = p_x \delta_{i3} - p_z \delta_{i1}$$

$$\Rightarrow [L_x, L_y] = (p_z \delta_{i2} - p_y \delta_{i3})(z \delta_{i1} - x \delta_{i3}) - (y \delta_{i3} - z \delta_{i2})(p_x \delta_{i3} - p_z \delta_{i1})$$

$$= x p_y - y p_x = L_z$$

$$\Rightarrow [L_i, L_j] = \varepsilon_{ijk} L_k$$

From QM: $[\hat{L}_i, \hat{L}_j] = i\hbar \cdot \varepsilon_{ijk} \hat{L}_k$; $\hat{\vec{L}} = \vec{r} \times \hat{\vec{p}} = \vec{r} \times \frac{\hbar}{i} \nabla$