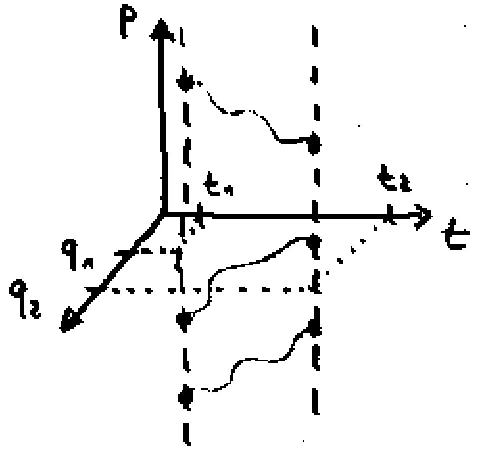
competitive set $M = \{\vec{\pi} \in C^2 \mathbb{R}^{2s} \mid \vec{q}(t_1) = \vec{q}_1, \vec{q}(t_2) = \vec{q}_2 \}$



variation of $\vec{q}$ vanishes at endpoints

variation of $\vec{p}$ unrestricted

parametrize elements $\vec{\pi} = (\vec{q}_\alpha, \vec{p}_\alpha)$ of the competitive set

$$\vec{q}_\alpha = \vec{q}_0 + \vec{\gamma}_\alpha$$
$$\vec{p}_\alpha = \vec{p}_0 + \vec{\beta}_\alpha$$

properties

$$\vec{\gamma}_0(t) = 0 \quad \text{for all } t$$
$$\vec{\gamma}_\alpha(t_1) = \vec{\gamma}_\alpha(t_2) = 0 \quad \text{for all } \alpha$$
$$\vec{\beta}_0(t) = 0 \quad \text{for all } t$$

variation of functional

$$0 = \delta S = \int_{t_1}^{t_2} \left[f(\vec{q}_{d\alpha}, \dot{\vec{q}}_{d\alpha}, \vec{p}_{d\alpha}, t) - f(\vec{q}_0, \dot{\vec{q}}_0, \vec{p}_0, t) \right]$$

with $f(\vec{q}, \dot{\vec{q}}, \vec{p}, t) = \sum_{i=1}^{s} p_i \dot{q}_i - H(\vec{q}, \vec{p}, t)$

Taylor expansion of f:

$$f(\vec{q}_{d\alpha}, \dot{\vec{q}}_{d\alpha}, \vec{p}_{d\alpha}, t) = f(\vec{q}_0, \dot{\vec{q}}_0, \vec{p}_0, t) + \sum_{i=1}^{s} \left(\frac{\partial f}{\partial q_i} \frac{\partial \gamma_\alpha^i}{\partial \alpha} + \frac{\partial f}{\partial \dot{q}_i} \frac{d}{dt} \frac{\partial \gamma_\alpha^i}{\partial \alpha} + \frac{\partial f}{\partial p_i} \frac{\partial \beta_\alpha^i}{\partial \alpha} \right) d\alpha$$

we calculate the partial derivatives

$$\frac{\partial f}{\partial q_i} = -\frac{\partial H}{\partial q_i} \qquad \frac{\partial f}{\partial \dot{q}_i} = p_i \qquad \frac{\partial f}{\partial p_i} = \dot{q}_i - \frac{\partial H}{\partial p_i}$$

insert into variation:

$$\delta S[\vec{\pi}(t)] = \int_{t_1}^{t_2} dt \sum_{i=1}^{S} \left[-\frac{\partial H}{\partial q_i} \frac{\partial \gamma_\alpha^i}{\partial \alpha} + p_i \frac{d}{dt} \frac{\partial \gamma_\alpha^i}{\partial \alpha} + \left(\dot{q}_i - \frac{\partial H}{\partial p_i} \right) \frac{\partial \beta_\alpha^i}{\partial \alpha} \right] d\alpha$$

partial integration of the second term(s)

$$\delta S[\vec{\pi}(t)] = \int_{t_1}^{t_2} dt \sum_{i=1}^{S} \left[\left(-\frac{\partial H}{\partial q_i} - \dot{p}_i \right) \delta q_i + \left(q_i - \frac{\partial H}{\partial p_i} \right) \delta p_i \right] = 0$$

all variations $\delta q_i, \delta p_i$ are independent, thus the terms in braces have to vanish.

The canonical equations follow

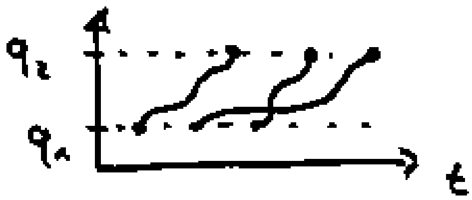
$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} \qquad i = 1 \dots S$$

Other variational principles

a) principle of least action (conservative system, scleronom. constraints)

$$A = \int_{t_1}^{t_2} \sum_{i=1}^{S} p_i \dot{q}_i \, dt = \int_{t_1}^{t_2} (H+L)\, dt = 2 \int_{t_1}^{t_2} T \, dt$$

$$\Delta A = 0$$



$\Delta \vec{q}_1 = \Delta \vec{q}_2 = 0$
$\Delta H = 0$
(same energy)

b) Fermat's principle

force free motion: $T = \text{const}$

$$0 = \Delta A = \Delta \, 2 \int_{t_1}^{t_2} T \, dt \Rightarrow \Delta \int_{t_1}^{t_2} dt = 0$$

(time extremal)

Poisson brackets

consider : phase space $\vec{\pi} = (\vec{q}, \vec{p})$
$= (q_1, \dots, q_s, p_1, \dots, p_s)$

(physical) observable
$f(\vec{q}, \vec{p}, t)$ (arbitrary function of $\vec{q}, \vec{p}, t$)

calculate total time derivative

$$\frac{df}{dt} = \sum_{i=1}^{s} \left(\frac{\partial f}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial f}{\partial p_i} \frac{dp_i}{dt} \right) + \frac{\partial f}{\partial t}$$
$$= \sum_{i=1}^{s} \left(\frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial p_i} \dot{p}_i \right) + \frac{\partial f}{\partial t}$$
$$= \sum_{i=1}^{s} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) + \frac{\partial f}{\partial t}$$

definition : Poisson brackets of f and g with respect to the canonical variables $\vec{q}$ and p

$$\{f, g\}_{\vec{q}, \vec{p}} = \sum_{i=1}^{s} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right)$$

then, we have for the observable

$$\frac{df}{dt} = \{f, H\}_{\vec{q}, \vec{p}} + \frac{\partial f}{\partial t}$$

special cases :

$$\dot{q}_i = \frac{dq_i}{dt} = \{q_i, H\}_{\vec{q}, \vec{p}} + \overbrace{\frac{\partial q_i}{\partial t}}^{0} = \{q_i, H\}_{\vec{q}, \vec{p}}$$
$$\dot{p}_i = \frac{dp_i}{dt} = \{p_i, H\}_{\vec{q}, \vec{p}} + \frac{\partial p_i}{\partial t} = \{p_i, H\}_{\vec{q}, \vec{p}}$$

(canonical equations)

Fundamental Poisson brackets

$$\{q_i, q_j\}_{\vec{q},\vec{p}} = \sum_{n=1}^{s}\Big(\underbrace{\frac{\partial q_i}{\partial q_n}}_{\delta_{in}}\underbrace{\frac{\partial q_j}{\partial p_n}}_{0} - \underbrace{\frac{\partial q_i}{\partial p_n}}_{0}\underbrace{\frac{\partial q_j}{\partial q_n}}_{\delta_{jn}}\Big) = 0$$

$$\{p_i, p_j\}_{\vec{q},\vec{p}} = \sum_{n=1}^{s}\Big(\frac{\partial p_i}{\partial q_n}\frac{\partial p_j}{\partial p_n} - \frac{\partial p_i}{\partial p_n}\frac{\partial p_j}{\partial q_n}\Big) = 0$$

$$\{q_i, p_j\}_{\vec{q},\vec{p}} = \sum_{n=1}^{s}\Big(\frac{\partial q_i}{\partial q_n}\frac{\partial p_j}{\partial p_n} - \frac{\partial q_i}{\partial p_n}\frac{\partial p_j}{\partial q_n}\Big)$$

$$= \sum_{n=1}^{s}\delta_{in}\,\delta_{jn} = \delta_{ij}$$

Properties of the Poisson brackets

1) antisymmetric $\quad \{f, g\}_{\vec{q},\vec{p}} = -\{g, f\}_{\vec{q},\vec{p}}$

2) product rule $\quad \{fg, h\}_{\vec{q},\vec{p}} = f\{g, h\}_{\vec{q},\vec{p}} + \{f, g\}_{\vec{q},\vec{p}}\, h$

3) Jacobi identity

$$\{f,\{g,h\}\} + \{g,\{h,f\}\} + \{h,\{f,g\}\} = 0$$

4) Linearity

$$\{\alpha f_1 + \beta f_2, g\} = \alpha\{f_1, g\} + \beta\{f_2, g\}$$

α, β : constant

from 1), it follows $\{f, f\} = 0$

from the definition it follows $\{\alpha, f\} = 0$, α = const

Value of Poisson brackets with respect to other sets of canonical variables?

consider $\quad (\vec{q},\vec{p}) \xrightarrow{\text{transformation}} (\vec{Q},\vec{P})$

$$\vec{q} = \vec{q}\,(\vec{Q},\vec{P}) \qquad\qquad \vec{Q} = \vec{Q}\,(\vec{q},\vec{p})$$
$$\vec{p} = \vec{p}\,(\vec{Q},\vec{P}) \qquad\qquad \vec{P} = \vec{P}\,(\vec{q},\vec{p})$$

Hamilton function:

$$H(\vec{q},\vec{p},t) = H(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}),t) = \tilde{H}(\vec{Q},\vec{P},t)$$

now calculate:

$$\dot{Q}_i = \frac{dQ_i}{dt} = \sum_{n=1}^{s}\left(\frac{\partial Q_i}{\partial q_n}\frac{dq_n}{dt} + \frac{\partial Q_i}{\partial p_n}\frac{dp_n}{dt}\right)$$

$$= \sum_{n=1}^{s}\left(\frac{\partial Q_i}{\partial q_n}\frac{\partial H}{\partial p_n} - \frac{\partial Q_i}{\partial p_n}\frac{\partial H}{\partial q_n}\right)$$

chain rule for $\tilde{H}$

$$= \sum_{n,m=1}^{s}\left[\frac{\partial Q_i}{\partial q_n}\left(\frac{\partial \tilde{H}}{\partial Q_m}\frac{\partial Q_m}{\partial p_n} + \frac{\partial \tilde{H}}{\partial P_m}\frac{\partial P_m}{\partial p_n}\right) - \frac{\partial Q_i}{\partial p_n}\left(\frac{\partial \tilde{H}}{\partial Q_m}\frac{\partial Q_m}{\partial q_n} + \frac{\partial \tilde{H}}{\partial P_m}\frac{\partial P_m}{\partial q_n}\right)\right]$$

reorder terms

$$= \sum_{n,m=1}^{s}\left[\frac{\partial \tilde{H}}{\partial Q_m}\left(\frac{\partial Q_i}{\partial q_n}\frac{\partial Q_m}{\partial p_n} - \frac{\partial Q_i}{\partial p_n}\frac{\partial Q_m}{\partial q_n}\right) + \frac{\partial \tilde{H}}{\partial P_m}\left(\frac{\partial Q_i}{\partial q_n}\frac{\partial P_m}{\partial p_n} - \frac{\partial Q_i}{\partial p_n}\frac{\partial P_m}{\partial q_n}\right)\right]$$

canonical eqn.

$$= \sum_m\left(-\dot{P}_m\{Q_i,Q_m\}_{\vec{q},\vec{p}} + \dot{Q}_m\{Q_i,P_m\}_{\vec{q},\vec{p}}\right)$$

comparison from what we started yields

$$\{Q_i,Q_m\}_{\vec{q},\vec{p}} = 0 \quad , \quad \{Q_i,P_m\}_{\vec{q},\vec{p}} = \delta_{im}$$

replace $Q_i \to P_i$ to find $\{P_i, Q_m\}_{\vec{q},\vec{p}} = 0$

The fundamental brackets are independent of the respective canonical variables.

Use identities for fundamental brackets together with special cases to show that

$$\{F, G\}_{\vec{q},\vec{p}} = \{\tilde{F}, \tilde{G}\}_{\vec{Q},\vec{P}}$$

for arbitrary observables $F(\vec{q},\vec{p},t) = F(\vec{q}(\vec{Q},\vec{P}), \vec{p}(\vec{Q},\vec{P}), t) = \tilde{F}(\vec{Q},\vec{P},t)$

from now on: drop indices:

$$\{F, G\}_{\vec{q},\vec{p}} = \{F, G\}$$

(Value of the Poisson brackets is independent of set of canonical variables)

Integrals of motion:

$F(\vec{q},\vec{p},t)$ integral of motion: $\frac{dF}{dt} = 0$

it follows $\frac{dF}{dt} = \{F, H\} + \frac{\partial F}{\partial t} = 0$

$$\Leftrightarrow \frac{\partial F}{\partial t} = -\{F, H\} = +\{H, F\}$$

(Poisson bracket of H with F is partial time derivative; also opposite direction)

example $F = H$: $\frac{dH}{dt} = \{H, H\} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}$

then: $\frac{\partial H}{\partial t} = \{H, H\} = 0$ if $\frac{dH}{dt} = 0$.

Poisson's theorem

Poissons bracket $\{f,g\}$ of two integrals of motion f, g is again an integral of motion.

given $\quad \frac{df}{dt} = 0 \quad \Rightarrow \frac{\partial f}{\partial t} = \{H, f\}$

$\qquad\quad \frac{dg}{dt} = 0 \quad \Rightarrow \frac{\partial g}{\partial t} = \{H, g\}$

proof: use Jacobi identity

$$0 = \{f, \underbrace{\{g, H\}}_{-\frac{\partial g}{\partial t}}\} + \{g, \underbrace{\{H, f\}}_{\frac{\partial f}{\partial t}}\} + \{H, \{f, g\}\}$$

$$= \left\{\frac{\partial g}{\partial t}, f\right\} + \left\{g, \frac{\partial f}{\partial t}\right\} + \{H, \{f, g\}\}$$

$$= \frac{\partial}{\partial t}\{g, f\} + \{H, \{f, g\}\} = \frac{d}{dt}\{f, g\}$$

Poisson brackets for observable $\{f,g\}$

$\Rightarrow$ the observable $\{f, g\}$ is an integral of motion

Relation to quantum mechanics

Formally, the Poisson brackets have the same properties as the commutator

$$[A, B] = AB - BA$$

for matrices A, B

$$[A, B] = -[B, A]$$
$$[AB, C] = A[B, C] + [A, C]B \quad \dots$$

We have seen:

$$\{q, p\} = 1 \quad \text{(fund. Poisson bracket)}$$

in quantum mechanics:

$$\frac{1}{i\hbar}[\hat{q}, \hat{p}] = 1$$

$\hat{q}, \hat{p}$ lin. operators in a infinite dimensional space

In general, the quantization condition holds for arbitrary observables f, g:

$$\{f, g\} \to \frac{1}{i\hbar}[\hat{f}, \hat{g}]$$

Hamilton function for a classical system:
$H(p, q, t)$

Hamilton operator for a quantum system
$\hat{H}(\hat{p}, \hat{q}, t)$

example: Harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} K \hat{q}^2$$

equations of motion:

$$\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t} \quad \Rightarrow \quad \frac{d\hat{A}}{dt} = \frac{1}{i\hbar}[\hat{A}, \hat{H}] + \frac{\partial \hat{A}}{\partial t}$$

(Heisenberg equation of motion for operator $\hat{A}$)

Canonical transformations

transformation in phase space $\vec{\pi} \to \vec{\pi}'$ which leaves the canonical equations of motion $\dot{q}_j = \frac{\partial H}{\partial p_j}$, $\dot{p}_j = -\frac{\partial H}{\partial q_j}$ invariant.

Examples:

1) Exchange of coordinates and momenta

$$Q_j = Q_j(\vec{q},\vec{p},t) = -p_j$$
$$P_j = P_j(\vec{q},\vec{p},t) = q_j \qquad j = 1 \dots S$$

this is a canonical transformation:

new Hamilton function $\tilde{H}(\vec{Q},\vec{P},t) = H(\vec{q}(\vec{P}),\vec{p}(\vec{Q}),t)$

$$\frac{\partial \tilde{H}}{\partial P_j} = \frac{\partial H(\vec{q}(\vec{P}),\vec{p}(\vec{Q}),t)}{\partial q_j}\frac{\partial q_j}{\partial P_j} = \frac{\partial H}{\partial q_j} = -\dot{p}_j = \dot{Q}_j$$

$$\frac{\partial \tilde{H}}{\partial Q_j} = \frac{\partial H(\vec{q}(\vec{P}),\vec{p}(\vec{Q}),t)}{\partial p_j}\underbrace{\frac{\partial p_j}{\partial Q_j}}_{-1} = -\frac{\partial H}{\partial p_j} = \dot{q}_j = \dot{P}_j$$

conceptually, the assignment

$\vec{q}$: "coordinate", "position"

$\vec{p}$: "momentum"

has no meaning in Hamilton mechanics.

2) Mechanical gauge transformations

we have seen

$$L(\vec{q},\dot{\vec{q}},t) \rightarrow L'(\vec{q},\dot{\vec{q}},t) = L(\vec{q},\dot{\vec{q}},t) + \frac{dF(\vec{q},t)}{dt}$$

leaves the Lagrange eqn. of motion forminvariant (see exercises)

construct corresponding phase transformation

$$p_j = \frac{\partial L}{\partial \dot{q}_j} \quad \rightarrow \quad p_j' = \frac{\partial L'}{\partial \dot{q}_j} = \frac{\partial L}{\partial \dot{q}_j} + \frac{\partial}{\partial \dot{q}_j}\left(\frac{dF(\vec{q},t)}{dt}\right)$$

$$= p_j + \frac{\partial}{\partial \dot{q}_j}\left[\sum_{i=1}^{s} \frac{\partial F}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial F}{\partial t}\right]$$

$$= p_j + \frac{\partial F}{\partial q_j}$$

$$q_j \quad \rightarrow \quad q_j' = q_j$$

"shift" of the generalized momenta

calculate new Hamilton function

$$H' = \sum_{j=1}^{s} \dot{q}_j' p_j' - L'$$

$$= \sum_{j=1}^{s} \dot{q}_j\left(p_j + \frac{\partial F}{\partial q_j}\right) - L - \frac{dF(\vec{q},t)}{dt}$$

$$= \sum_{j=1}^{s} \dot{q}_j p_j - L + \sum_{j=1}^{s} \dot{q}_j \frac{\partial F}{\partial q_j} - \sum_{i=1}^{s} \frac{\partial F}{\partial q_i}\frac{dq_i}{dt} - \frac{\partial F}{\partial t}$$

$$= H - \frac{\partial F}{\partial t}$$

new canonical equations

$$\frac{\partial H'}{\partial q'_j} = \frac{\partial H'}{\partial q_j} = \frac{\partial}{\partial q_j}\left(H - \frac{\partial F}{\partial t}\right)$$

$H = H(\vec{q}, \vec{p}(\vec{q}, \vec{P}, t), t)$

$$= \frac{\partial H}{\partial q_j} + \sum_{i=1}^{s} \frac{\partial H}{\partial p_i}\frac{\partial p_i}{\partial q_j} - \frac{\partial^2 F}{\partial q_j \partial t}$$

$\frac{\partial p_i}{\partial q_j} = -\frac{\partial^2 F}{\partial q_j \partial q_i}$

$p_i = p'_i - \frac{\partial F}{\partial q_i}$

$$= -\dot{p}_j - \sum_{i=1}^{s} \dot{q}_i \frac{\partial^2 F}{\partial q_j \partial q_i} - \frac{\partial^2 F}{\partial q_j \partial t}$$

$$= -\dot{p}_j - \frac{d}{dt}\frac{\partial F}{\partial q_j} = -\dot{p}'_j$$

$$\frac{\partial H'}{\partial p'_j} = \sum_{i=1}^{s} \frac{\partial H}{\partial p_i}\frac{\partial p_i}{\partial p'_j}$$

$p_i = p_i(\vec{q}, p'_i, t)$ no dep. on p'_j for $i \neq j$

$$= \sum_{i=1}^{s} \dot{q}_i \delta_{ij} = \dot{q}_j = \dot{q}'_j$$

→ transformation is canonical

Why mechanical "gauge" transformation?

Reminder: electromagnetic gauge transformation

$$\varphi(\vec{r}, t) \to \varphi'(\vec{r}, t) = \varphi - \frac{\partial \Lambda(\vec{r}, t)}{\partial t}$$

$$\vec{A}(\vec{r}, t) \to \vec{A}'(\vec{r}, t) = \vec{A}(\vec{r}, t) + \vec{\nabla}\Lambda(\vec{r}, t)$$

the electromagnetic fields are unchanged

$$\vec{B} = \vec{\nabla} \times \vec{A} = \vec{B}' = \vec{\nabla} \times \vec{A}'$$

$$\vec{E} = -\vec{\nabla}\varphi - \frac{\partial \vec{A}}{\partial t} = \vec{E}' = -\vec{\nabla}\varphi' - \frac{\partial \vec{A}'}{\partial t}$$

$q\,\Lambda(\vec{r}, t)$ plays the role of $F(\vec{r}, t)$ in the mechanical gauge transformation

charge!

Canonical transformation:

Phase transformation $\vec{\pi} \to \vec{\pi}'$, i.e.

$$\vec{q} \to \vec{q}'(\vec{q},\vec{p},t)$$
$$\vec{p} \to \vec{p}'(\vec{q},\vec{p},t)$$

which leave the canonical equations

$$\frac{\partial H}{\partial p_j} = \dot{q}_j \quad , \quad \frac{\partial H}{\partial q_j} = -\dot{p}_j$$

invariant. (In other words it exists a Hamilton function $H'(\vec{q}',\vec{p}',t)$.)

Question: How to find the $H'(\vec{q}', \vec{p}',t)$?

The generating function

Theorem: A phase transformation $(\vec{q},\vec{p}) \to (\vec{q}',\vec{p}')$ is canonical if

$$\sum_{i=1}^{s} p_i \dot{q}_i - H = \sum_{i=1}^{s} p_i' \dot{q}_i' - H' + \frac{dF_1}{dt}$$

where $F_1(\vec{q},\vec{q}',t)$ is the generating function (F_1 sufficiently often differentiable)

Proof in two steps

a) show that the generating function F_1 fixes the transformed H' uniquely

b) show that the phase transformation is canonical (by use of the modified Hamilton's principle $\delta S = 0$)