4.3. Hamilton's Equations

- sometimes called „canonical equations"
- Hamilton's equations are concerned with determining trajectories in phase space

$$(q,p) = (\underbrace{q_1, \dots, q_n}_{\text{configuration space}}, \underbrace{p_1, \dots, p_n}_{\text{momentum space}})$$ 2n-dimensional space

- so far we have $p = \frac{\partial L}{\partial \dot{q}}$ canonical momentum

$$H = \dot{q}p - L(q,\dot{q},t)$$
$$= \dot{q}(q,p,t)\cdot p - L(q,\dot{q}(q,p,t),t) = \underbrace{H(q,p,t)}_{\text{Hamiltonian}}$$

Hamiltonian is a function of phase-space coordinates (q,p)

- Equations of motion

$$\frac{\partial H}{\partial p} = \frac{\partial}{\partial p}\left(\dot{q}p - L(q,\dot{q},t)\right) = \dot{q} + p\frac{\partial \dot{q}}{\partial p} - \underbrace{\frac{\partial L}{\partial \dot{q}}}_{p}\frac{\partial \dot{q}}{\partial p} = \dot{q}$$

$$\frac{\partial H}{\partial q} = \frac{\partial}{\partial q}\left(\dot{q}p - L(q,\dot{q},t)\right) = \frac{\partial \dot{q}}{\partial q}p - \frac{\partial L}{\partial q} - \underbrace{\frac{\partial L}{\partial \dot{q}}}_{p}\frac{\partial \dot{q}}{\partial q}$$
$$= -\frac{\partial L}{\partial q} \underset{E.L.}{=} -\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = -\dot{p}$$

$$\rightarrow \boxed{\begin{aligned}\dot{q} &= \frac{\partial H}{\partial p}\\ \dot{p} &= -\frac{\partial H}{\partial q}\end{aligned} \quad \text{Hamilton's equations}}$$

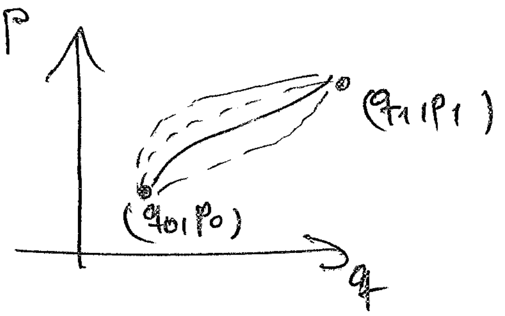
- conservation of energy

$$\frac{dE}{dt} = \frac{dH}{dt} = \frac{\partial H}{\partial q}\dot{q} + \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial t}$$

$$\underset{\text{Hamilton's equations}}{=} -\dot{p}\dot{q} + \dot{q}\dot{p} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}$$

→ Energy is conserved ⇔ H does not depend explicitly on time

- Hamilton's equations from principle of least action:



variation $(\delta q, \delta p)$

$\delta q(t_0) = \delta q(t_1) = 0$
$\delta p(t_0) = \delta p(t_1) = 0$

$$S = \int_{t_0}^{t_1} dt\, L(q,\dot{q},t) = \int_{t_0}^{t_1} dt\,\big(p\dot{q} - H(q,p,t)\big)$$

$$\delta S = \int_{t_0}^{t_1} dt \Big\{ \underbrace{p\,\delta\dot{q}}_{\text{integrate by parts}} + \dot{q}\,\delta p - \Big(\frac{\partial H}{\partial q}\delta q + \frac{\partial H}{\partial p}\delta p\Big)\Big\}$$

→ $-\dot{p}\,\delta q$

$$= \int_{t_0}^{t_1} dt \Big\{ \Big(\dot{q} - \frac{\partial H}{\partial p}\Big)\delta p - \Big(\dot{p} + \frac{\partial H}{\partial q}\Big)\delta q \Big\} = 0 \quad \forall \delta q, \delta p$$

⇒ Hamilton's equations

Example: Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} k q^2 = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 \qquad \omega = \sqrt{\frac{k}{m}}$$

$$\left.\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m} \\ \dot{p} &= -\frac{\partial H}{\partial q} = -m\omega^2 q \end{aligned}\right\} \Leftrightarrow \frac{d}{dt}\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} 0 & 1/m \\ -m\omega^2 & 0 \end{pmatrix}\begin{pmatrix} q(t) \\ p(t) \end{pmatrix}$$

- two coupled first-order differential equations
- we can easily obtain decoupled 2nd order equations for q and p:

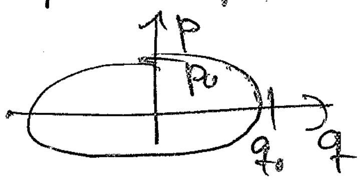
$$\ddot{q} = \frac{1}{m}\dot{p} = -\omega^2 q$$

$$\ddot{p} = -m\omega^2 \dot{q} = -\omega^2 p$$

- phase-space trajectories

$$q(0) = q_0 \qquad\qquad q(t) = q_0 \cos(\omega t)$$
$$p(0) = 0 \qquad\qquad p(t) = p_0 \sin(\omega t)$$

$$\rightarrow \quad \frac{q^2}{q_0^2} + \frac{p^2}{p_0^2} = 1$$ Ellipse in phase space



- How to solve the problem without going to 2nd order equations?

→ „canonical transformation"

we have to „diagonalize" (decouple) the problem

$$\frac{d}{dt}\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} 0 & 1/m \\ -m\omega^2 & 0 \end{pmatrix}\begin{pmatrix} q(t) \\ p(t) \end{pmatrix}$$

→ transformation to new coordinate and momentum (Q, P)

! Transformation has to be such that P is the canonical momentum of Q and the form of ~~the~~ Hamilton's equations is preserved! → Homework

4.4. Canonical Transformations

$(q, p) \xrightarrow{\text{Diffeomorphism}} (Q, P)$

$$Q = Q(q, p, t)$$
$$P = P(q, p, t)$$

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

$\dot{q} = \frac{\partial H}{\partial p}, \; \dot{p} = -\frac{\partial H}{\partial q}$ $\qquad\qquad$ $\dot{Q} = \frac{\partial \tilde{H}}{\partial P}, \; \dot{P} = -\frac{\partial \tilde{H}}{\partial Q}$

How to construct such a transformation?

- Hamilton's equations result from the principle of least action, $\delta S = 0$

$$S = \int dt \, (\underbrace{p\dot{q} - H(q, p, t)}_{L})$$

- Form of equations of motion remain invariant if Lagrangian $\tilde{L}$ in new coordinates is equal to old one modulo a total time derivative (see chapter 1.4.)

$$L = \tilde{L} + \frac{d}{dt} F_1(q, Q, t)$$

$$\rightarrow \quad p\dot{q} - H(p,q,t) = P\dot{Q} - \tilde{H}(P,Q,t) + \frac{d}{dt} F_1(q,Q,t) \qquad (*)$$

- total time derivative of F_1

$$\frac{dF_1}{dt} = \frac{\partial F_1}{\partial q}\dot{q} + \frac{\partial F_1}{\partial Q}\dot{Q} + \frac{\partial F_1}{\partial t}$$

$$\rightarrow \quad \left(p - \frac{\partial F_1}{\partial q}\right)\dot{q} - H(p,q,t) = \left(P + \frac{\partial F_1}{\partial Q}\right)\dot{Q} - \tilde{H}(P,Q,t) + \frac{\partial F_1}{\partial t}$$

- We can guarantee the validity of $(*)$ and hence that the transformation is canonical if we postulate that

$$\boxed{\begin{aligned} p &= \frac{\partial}{\partial q} F_1(q,Q,t) \\ P &= -\frac{\partial}{\partial Q} F_1(q,Q,t) \end{aligned} \quad \text{and} \quad \tilde{H}(P,Q,t) = H(p,q,t) + \frac{\partial}{\partial t} F_1(q,Q,t)} \quad (\#)$$

- Every function $F_1(q,Q,t)$ generates a canonical transformation which is defined by $(\#)$

Example 1: $H = H(p,q) = \frac{p^2}{2m} + \frac{m}{2}\omega^2 q^2$

generating function $F_1(q,Q) = -\frac{Q}{q}$

determine transformation $Q = Q(q,p)$, $P = P(q,p)$ and the Hamiltonian $\tilde{H} = \tilde{H}(Q,P)$!

$$p = \frac{\partial}{\partial q} F_1 = \frac{Q}{q^2} \Leftrightarrow \boxed{Q = pq^2} \quad \boxed{P = -\frac{\partial}{\partial Q} F_1 = +\frac{1}{q}}$$

$$\boxed{\tilde{H}(P,Q)} = H(p,q) + \underbrace{\frac{\partial}{\partial t} F_1}_{=0} = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 \underset{(*)}{=} \boxed{\frac{1}{2m} Q^2 P^4 + \frac{m\omega^2}{2} P^{-2}}$$

(*) inverse tf.: $\boxed{q = \frac{1}{P}}$ $\boxed{p = \frac{Q}{q^2} = QP^2}$

Hamilton's equations:

$$\dot{Q} = \frac{\partial \tilde{H}}{\partial P} = \frac{2}{m} Q^2 P^3 - m\omega^2 P^{-3}$$

$$\dot{P} = -\frac{\partial \tilde{H}}{\partial Q} = \frac{1}{m} Q P^4$$

The canonical transformation generated by $F_1 = -Q/q$ is not useful in this case since equations of motion are more complicated.

Example 2: $H = H(p,q)$ as before

$$F_1(q,Q) = \frac{m}{2}\omega q^2 \cot Q$$

$$\left.\begin{aligned} p &= \frac{\partial}{\partial q} F_1 = m\omega q \cot Q \\ P &= -\frac{\partial}{\partial Q} F_1 = \frac{m\omega q^2}{2\sin^2 Q} \end{aligned}\right\} \Rightarrow \boxed{\begin{aligned} p &= m\omega \cot Q \sqrt{\frac{2P}{m\omega}} \sin Q \\ &= \sqrt{2m\omega P} \cos Q \end{aligned}}$$

$$\boxed{q = \frac{p}{m\omega \cot Q} = \sqrt{\frac{2P}{m\omega}} \sin Q}$$

$$\boxed{\tilde{H}(P,Q) = H(p,q) + \frac{\partial}{\partial t} F_1 = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 = \omega P \cos^2 Q + \omega P \sin^2 Q = \omega P}$$

Hamilton's equations:

$$\dot{Q} = \frac{\partial \tilde{H}}{\partial P} = \omega \qquad \dot{P} = -\frac{\partial \tilde{H}}{\partial Q} = 0$$

$$\Rightarrow \boxed{Q(t) = \omega t + Q_0}, \quad \boxed{P(t) = P_0}$$

$$\Rightarrow \boxed{\begin{cases} q(t) = \sqrt{\dfrac{2P_0}{m\omega}} \sin(\omega t + Q_0) \\ p(t) = m\omega \sqrt{\dfrac{2P_0}{m\omega}} \cos(\omega t + Q_0) = m\dot{q}(t) \end{cases}}$$

Note: Equations of motions are much simpler but finding the generating function F_1 to achieve this is a difficult problem

Example 3: Calculate generating function for a given transformation

$$Q = \ln p, \quad P = -qp, \quad q, p > 0$$

$$p = \frac{\partial}{\partial q} F_1(q, Q, t) \qquad P = -qp = -qe^{Q} = -\frac{\partial}{\partial Q} F_1(q, Q, t)$$

$$P = -\frac{\partial}{\partial Q} F_1(q, Q, t) \qquad \Rightarrow F_1(q, Q, t) = qe^{Q} + f(q) + g(t)$$

$$p = \frac{\partial}{\partial q} F_1 = e^{Q} + f'(q) = p + f'(q) \quad \Rightarrow \quad f'(q) = 0$$

$$\Rightarrow f(q) = c$$

can be dropped or absorbed in $g(t)$

$$\Rightarrow \boxed{F_1(q, Q, t) = qe^{Q} + g(t)}$$

- There are four different types of generating functions of canonical transformations $(q,p) \to (Q,P)$

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

They are not independent of each other and related by Legendre transformations

- Look at $F_2(q,P,t)$ for example

$$p\dot{q} - H(p,q,t) = P\dot{Q} - \tilde{H}(P,Q,t) + \frac{d}{dt}F_1(q,Q,t)$$

$$\Leftrightarrow \quad p\,dq - P\,dQ + (\tilde{H} - H)\,dt = dF_1 \qquad (*)$$

($\to$ F_1 is function of q,Q,t)

$$dF_2 = \frac{\partial F_2}{\partial q}dq + \frac{\partial F_2}{\partial P}dP + \frac{\partial F_2}{\partial t}dt$$

in (*), rewrite $\quad P\,dQ = d(PQ) - Q\,dP$

$$\to \quad p\,dq + Q\,dP + (\tilde{H} - H)\,dt = d(\underbrace{F_1 - PQ}_{=:F_2})$$

$$\boxed{F_2(q,P,t) = F_1(q,Q,t) - PQ = F_1 - Q\frac{\partial F_1}{\partial Q}}$$

Legendre transformation
(same as between L and H, important in thermodynamics)

$$\boxed{\begin{aligned} p &= \frac{\partial F_2}{\partial q}(q,P,t) \\ Q &= \frac{\partial F_2}{\partial P}(q,P,t) \end{aligned} \qquad \tilde{H}(P,Q,t) = H(p,q,t) + \frac{\partial}{\partial t}F_2(q,P,t)} \quad (\#2)$$

- Back to Hamilton-Jacobi theory

$$\frac{\partial}{\partial t} S + H(q, \underbrace{\frac{\partial S}{\partial q}}_{=p}, t) = 0 \qquad \text{Hamilton-Jacobi equation}$$

$\Rightarrow \quad S = S(q, \alpha, t) = S(q_1, \dots, q_n, \alpha_1, \dots, \alpha_n, t)$

Hamilton's principal function

$\alpha_1, \dots, \alpha_n$ integration constants

→ view $\alpha_1, \dots, \alpha_n$ as conserved canonical momenta $P = (P_1, \dots, P_n)$ of some coordinates $Q = (Q_1, \dots, Q_n)$

→ take $S(q, \alpha, t) = S(q, P, t)$ as the generating function $F_2(q, P, t)$ of a canonical transformation

(#2): $\tilde{H} = H + \frac{\partial F_2}{\partial t} = H + \frac{\partial S}{\partial t} \underset{\text{Hamilton Jacobi}}{=} 0$

$$Q = \frac{\partial}{\partial P} F_2 = \frac{\partial}{\partial P} S(q, P, t) = \frac{\partial}{\partial \alpha} S(q, \alpha, t)$$

$\parallel$

$\beta = \text{const}$ since $\dot{Q} = \frac{\partial \tilde{H}}{\partial P} = 0$

This differentiation with respect to integration constants we use as the last step in Hamilton-Jacobi theory to extract the dynamics

4.5. Poisson Brackets

- "Observable": $f(q, p, t)$, $q = (q_1, \dots, q_n)$, $p = (p_1, \dots, p_n)$

total time derivative

$$\frac{d}{dt} f = \frac{\partial f}{\partial q}\dot{q} + \frac{\partial f}{\partial p}\dot{p} + \frac{\partial f}{\partial t}$$

$$\underset{\text{Hamilton's equations}}{=} \left(\frac{\partial f}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial H}{\partial q}\right) + \frac{\partial f}{\partial t}$$

Poisson bracket:

$$[f, g] = [f, g]_{q,p} := \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial q}$$
$$= \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right)$$

$$\rightarrow \boxed{\frac{d}{dt} f = [f, H] + \frac{\partial f}{\partial t}}$$

time evolution of observable is controlled by Hamiltonian

- Useful properties (c_1, c_2 const.)

(a) $[c_1 f + c_2 g, h] = c_1 [f, h] + c_2 [g, h]$ linearity

(b) $[f, g] = -[g, f]$ antisymmetry

(c) $[fg, h] = f[g, h] + [f, h]g$ product rule

(d) $[f, [g, h]] + [h, [f, g]] + [g, [h, f]] = 0$
Jacobi-identity

- Hamilton's equations can be written as

$$\boxed{\dot{q}_i = \frac{\partial H}{\partial p_i} = [q_i, H]} \qquad \boxed{\dot{p}_i = -\frac{\partial H}{\partial q_i} = [p_i, H]}$$

Proof:

$$[q_i, H] = \sum_j \Big(\underbrace{\frac{\partial q_i}{\partial q_j}}_{=\delta_{ij}} \frac{\partial H}{\partial p_j} - \underbrace{\frac{\partial q_i}{\partial p_j}}_{=0} \frac{\partial H}{\partial q_j} \Big) = \sum_j \delta_{ij} \frac{\partial H}{\partial p_j} = \frac{\partial H}{\partial p_i}$$

$$[p_i, H] = \sum_j \Big(\underbrace{\frac{\partial p_i}{\partial q_j}}_{=0} \frac{\partial H}{\partial p_j} - \underbrace{\frac{\partial p_i}{\partial p_j}}_{\delta_{ij}} \frac{\partial H}{\partial q_j} \Big) = - \frac{\partial H}{\partial q_i}$$

- fundamental Poisson brackets

$$\boxed{[q_i, q_j] = \sum_k \Big(\frac{\partial q_i}{\partial q_k} \underbrace{\frac{\partial q_j}{\partial p_k}}_{=0} - \underbrace{\frac{\partial q_i}{\partial p_k}}_{=0} \frac{\partial q_j}{\partial q_k} \Big) = 0}$$

$$\boxed{[p_i, p_j] = 0}$$

$$\boxed{[q_i, p_j] = \sum_k \Big(\underbrace{\frac{\partial q_i}{\partial q_k}}_{\delta_{ik}} \underbrace{\frac{\partial p_j}{\partial p_k}}_{\delta_{jk}} - \underbrace{\frac{\partial q_i}{\partial p_k}}_{=0} \underbrace{\frac{\partial p_j}{\partial q_k}}_{=0} \Big) = \delta_{ij}}$$

Example: Harmonic oscillator

$$\dot{x} = [x, H] = [x, \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2] \underset{[x,x]=0}{=} [x, \frac{p^2}{2m}] \underset{(a)}{=} \frac{1}{2m} [x, p^2]$$

$$\underset{(c)}{=} 2 \cdot \frac{1}{2m} p \underbrace{[x, p]}_{=1} = \boxed{\frac{p}{m}}$$

$$\dot{p} = [p, H] = [p, \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2] \underset{[p,p]=0}{=} [p, \frac{m\omega^2}{2} x^2] \underset{(a)}{=} \frac{m\omega^2}{2} [p, x^2]$$

$$\underset{(c)}{=} m\omega^2 x [p, x] \underset{(b)}{=} - m\omega^2 x \underbrace{[x, p]}_{=1} = \boxed{-m\omega^2 x}$$

- criterion for canonical transformation:
(fundamental Poisson bracket description must be preserved)

$$q_i \to Q_i(q,p,t)$$
$$p_i \to P_i(q,p,t) \quad (i=1,\dots,n) \quad \text{canonical}$$

$$\Leftrightarrow \quad [Q_i,Q_j]_{q,p} = [P_i,P_j]_{q,p} = 0 \text{ and } [Q_i,P_j]_{q,p} = \delta_{ij}$$

(fundamental Poisson brackets are conserved)

This is much easier to check than to find the corresponding generating function $F_1(q,Q,t)$!

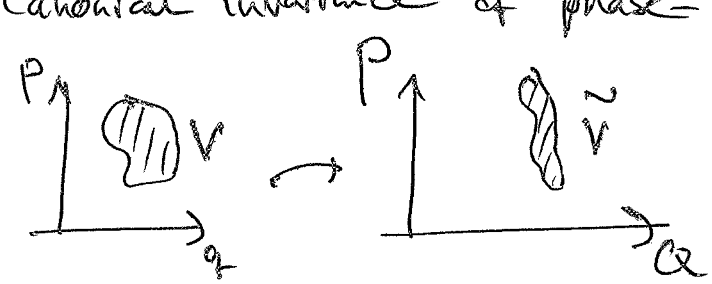
<u>Example:</u> $Q = q^a \cos(bp)$, $P = q^a \sin(bp)$ canonical?

$$[Q,P] = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q} = a q^{a-1}\cos(bq)\, b q^a \cos(bp) + b q^a \sin(bp)\, a q^{a-1}\sin(bp)$$

$$= ab\, q^{2a-1} \Rightarrow \text{transformation is canonical} \Leftrightarrow a = 1/2 \wedge b = 2$$

4.6. Liouville's Theorem

- Canonical invariance of phase-space volume



$$V = \iint dq\, dp \qquad \tilde{V} = \iint \underbrace{dQ\, dP}_{d\tilde{V}} = \iint \begin{vmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{vmatrix} \underbrace{dq\, dp}_{dV}$$

$$\begin{vmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{vmatrix} = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q} = [Q,P]_{q,p} = 1$$

for canonical transformation

→ Phase-space volume remains invariant under canonical transformations, $V = \tilde{V}$

• Time translation is canonical

$$Q(t) = q(t+\Delta t) = q(t) + \dot{q}(t)\Delta t + \mathcal{O}(\Delta t^2) = q + \frac{\partial H}{\partial p}\Delta t + \mathcal{O}(\Delta t^2)$$

$$P(t) = p(t+\Delta t) = p(t) + \dot{p}(t)\Delta t + \mathcal{O}(\Delta t^2) = p - \frac{\partial H}{\partial q}\Delta t + \mathcal{O}(\Delta t^2)$$

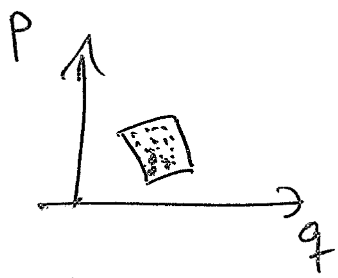
$$[Q,P] = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q} = 1 + \mathcal{O}(\Delta t^2)$$

⇒ infinitesimal time translation is canonical trf.

⇒ time translations are canonical

canonical trf. form group

• Consider ensemble of G systems, each corresponds with a point $(q,p) = (q_1 \dots q_n, p_1, \dots, p_n)$ in phase space Γ



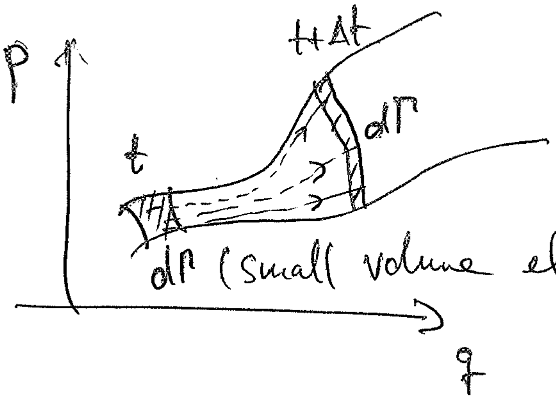
approximate by continuous distribution function $\rho(q,p,t)$

$$\int_\Gamma \cdots \int dq_1 \dots dq_n \, dp_1 \dots dp_n \; \rho(q,p,t) = G$$

g is positive definite. We can define a probability distribution

$$\rho(q,p,t) := \frac{g(q,p,t)}{G}$$

- Look at time evolution of g and ρ



dΓ (small volume element in phase space Γ)

$$g = \frac{dG}{d\Gamma}$$, dG = number of phase space point in $d\Gamma$

+ time evolution canonical $\Rightarrow$ $d\Gamma$ does not change in time
+ phase-space trajectories do not cross

$\Rightarrow$ dG must remain the same

$$\rightarrow \quad 0 = \frac{dg}{dt} = [g,H] + \frac{\partial g}{\partial t}$$

$$\Rightarrow \quad \boxed{0 = [\rho, H] + \frac{\partial \rho}{\partial t}} \quad \underline{\text{Liouville's theorem}}$$