Phase Space

[Ch 2.3]

Phase space is coordinates describing everything about the system

$$X(t) = \{ q_1(t), q_2(t), \ldots\ldots, q_{3N}(t),$$
$$p_1(t), p_2(t), \ldots\ldots, p_{3N}(t) \}$$

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$x(t)$ tells us everything about the system

$f(x(t))$ ← total momentum
kinetic energy
potential energy
→ total energy

$\mathcal{H}(\vec{q}, \vec{p})$ Hamiltonian

$\frac{dH}{dt} = 0$ if system follows hamiltonian dynamics

How do other quantities change in time?

$a(X(t))$

$$\frac{d\, y(x)}{dt} = \sum_{i=1}^{n} \frac{\partial y}{\partial x_i} \frac{\partial x_i}{\partial t}$$

$$\frac{d\, a(x)}{dt} = \frac{d\, a(q_1 \dots q_{3N}, p_1 \dots p_{3N})}{dt}$$

$$= \sum_{i=1}^{3N} \left(\frac{\partial a}{\partial q_i} \frac{\partial q_i}{\partial t} + \frac{\partial a}{\partial p_i} \frac{\partial p_i}{\partial t} \right)$$

$$\frac{\partial q_i}{\partial t} = \frac{\partial \mathcal{H}}{\partial p_i} \qquad - \frac{\partial p_i}{\partial t} = \frac{\partial \mathcal{H}}{\partial q}$$

$$\frac{da}{dt} = \sum_{i=1}^{3N} \left(\frac{\partial a}{\partial q_i} \underbrace{\frac{\partial q_i}{\partial t}}_{\frac{\partial \mathcal{H}}{\partial p_i}} + \frac{\partial a}{\partial p_i} \underbrace{\frac{\partial p_i}{\partial t}}_{-\frac{\partial \mathcal{H}}{\partial q_i}} \right)$$

$$= \sum_{i=1}^{3N} \left(\frac{\partial a}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial a}{\partial p_i} \frac{\partial \mathcal{H}}{\partial q_i} \right) \leftarrow$$

Poisson Brackets $\{a, b\} \equiv \sum_{i=1}^{3N} \left(\frac{\partial a}{\partial q_i} \frac{\partial b}{\partial p_i} - \frac{\partial a}{\partial p_i} \frac{\partial b}{\partial q_i} \right)$

$$\frac{da}{dt} = \{a, H\}$$

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A conserved quantity is one that doesn't change in time

$$\frac{da}{dt} = 0 \Rightarrow \{a, H\} = 0$$

e.g. total $E = \mathcal{H}$ $\quad \{H, H\} = 0$

$$a(\vec{X}) = \vec{P}_{total} = \sum_{i=1}^{3N} P_i$$

$$\frac{dp_j}{dt} = \{p_j, H\} = -\frac{\partial H}{\partial q_j}$$

Hamilton's Equation

$$\{a, b\} \equiv \sum_{i=1}^{3N} \left(\frac{\partial a}{\partial q_i}\frac{\partial b}{\partial p_i} - \frac{\partial a}{\partial p_i}\frac{\partial b}{\partial q_i} \right)$$

$$\partial p_i / \partial q_i = 0$$

$$\frac{\partial p_j}{\partial p_i} = \begin{cases} 1 & i = j \\ 0 & \end{cases}$$

$$F = -\nabla U$$

$$F_j = -\frac{\partial U}{\partial q_j}$$

$$-\frac{\partial U}{\partial q_j} = F_j$$

$$\frac{dp_j}{dt} = F_j \quad \longleftrightarrow \quad \left[\ \dot{p}_i = -\underbrace{\frac{\partial H}{\partial q_i}}_{F_i}\right.$$

$$\frac{dP_{total}}{dt} = \frac{d\left(\sum p_j\right)}{dt} = \sum \frac{dp_j}{dt} = \sum_{j=1}^{3N} F_j$$

total momentum is conserved if $\sum F$ (net force) $= 0$

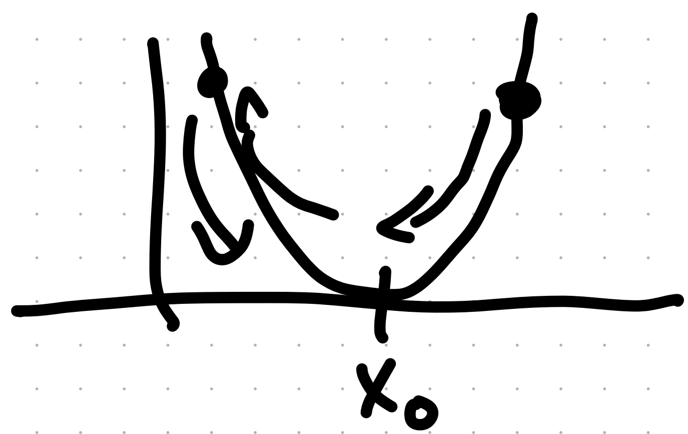
A "microstate" is a particular point in phase space

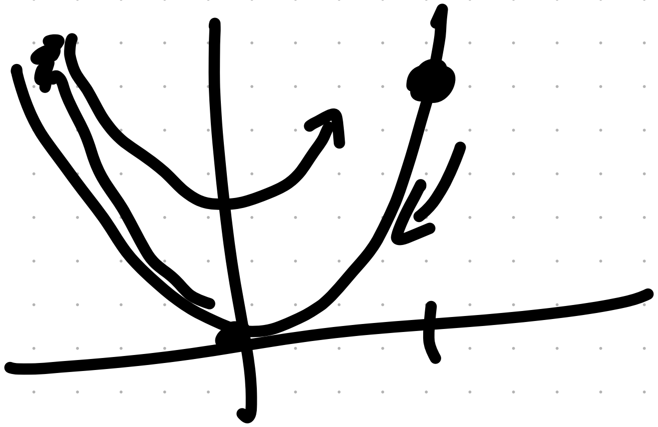
For a conservative system

$$\mathcal{H}(X(t)) = E \quad \underline{\text{constant}}$$

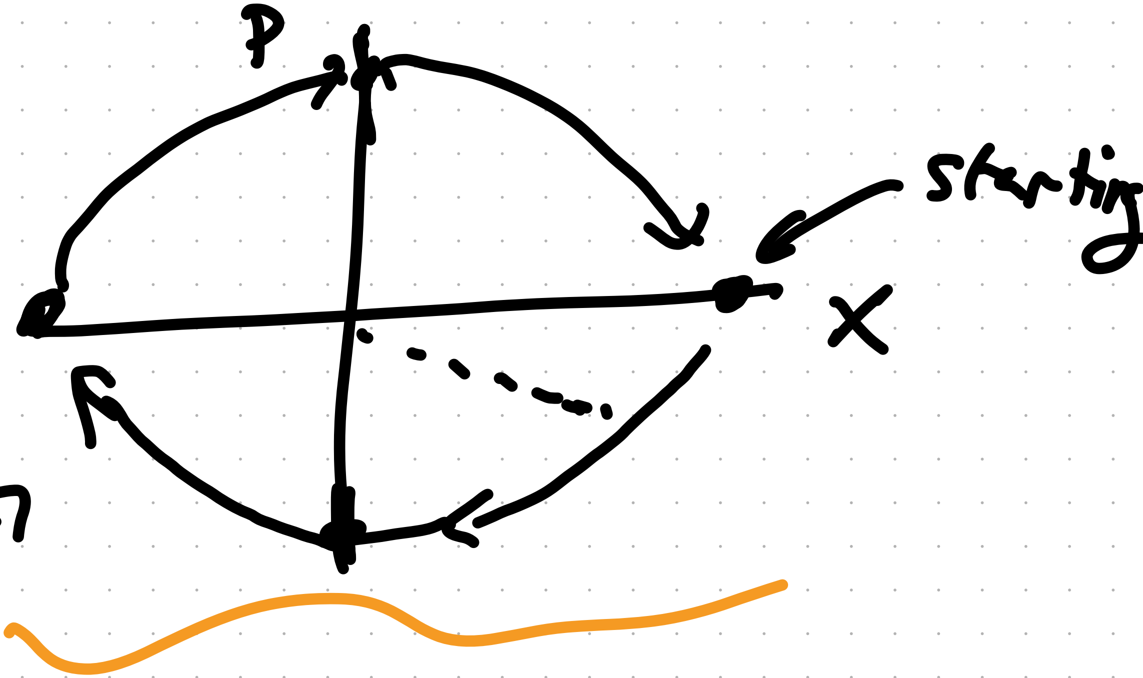
Eg: $\mathcal{H}(x, p) = p^2/2m + \frac{1}{2} k x^2$

$U(x)$





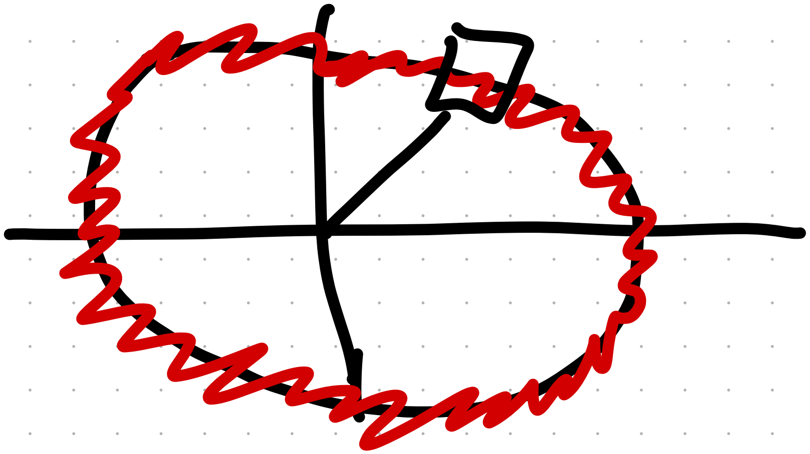
X(0)



phase space

$$H = \frac{1}{2}kx^2 + \frac{p^2}{2m}$$

"Ensemble" a collection of micro states with same macro characteristics



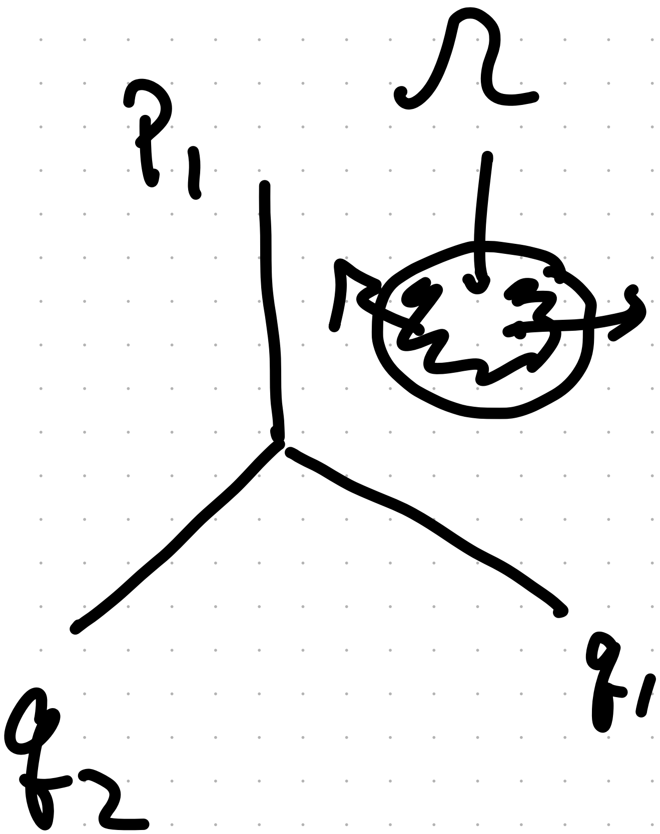
Fraction of phase space points in ensemble within a volume $d\vec{x}$

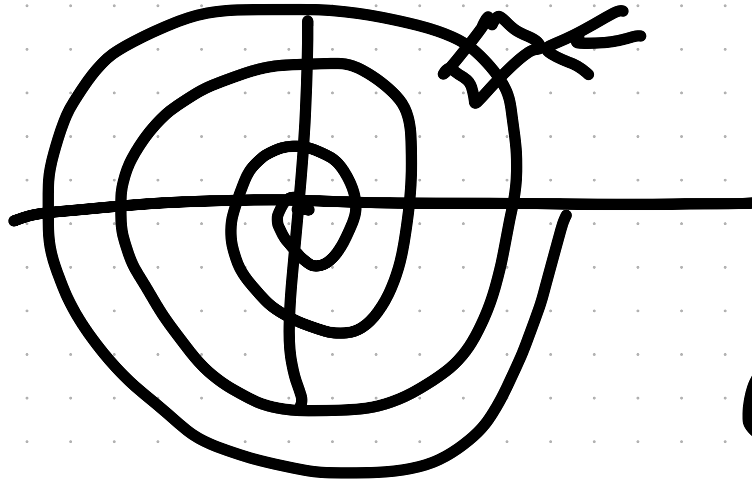
$f(\vec{x}, t)\, dx$

$\int f(\vec{x}, t) \geq 1$

$\int d\vec{x}\, f(\vec{x}, t) = 1$

doesn't change $\Longleftrightarrow$ equilibrium eg friction





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fraction in a region

$$\int_\Omega d\vec{x}\, f(\vec{x}, t)$$

$$\frac{\partial f(x,t)}{\partial t} + \frac{dx}{dt} \cdot \nabla f(\underline{x(t),t}) = 0$$

$$\{\dot{q}_1, \dot{q}_2, \dots \dot{q}_{3N}, \dot{p}_1, \dot{p}_2, \dots, \dot{p}_{3N}\}$$

$$\cdot \left\{ \frac{\partial f}{\partial q_1}, \frac{\partial f}{\partial q_2}, \dots, \frac{\partial f}{\partial q_{3N}} \dots \right.$$

Ham

$$\left. \dots \frac{\partial f}{\partial p_1}, \frac{\partial f}{\partial p_2}, \dots \frac{\partial f}{\partial p_{3N}} \right\}$$

$$+ \sum_{i=1}^{3N} \left(\dot{q}_i \frac{\partial f}{\partial q_i} + \dot{p}_i \frac{\partial f}{\partial p_i} \right)$$

$$\boxed{\frac{\partial f}{\partial t} + \underbrace{\{f, H\}}_{iLf} = 0}$$ Liouville Equation

$$\{\_, H\} \equiv iL$$

iLQ
$= \{Q, H\}$

$$\frac{\partial f}{\partial t} + i\underline{Lf} = 0 \quad \Leftrightarrow \quad \frac{\partial f}{\partial t} = -iLf$$

$$f(t) = e^{-iLt} f(0)$$

Equilibrium is defined as

$\frac{df}{dt} = 0$ everywhere in phase space

$$\frac{\partial f}{\partial t} + \{f, H\} = 0 \Rightarrow \{f, H\} = 0$$

$\Rightarrow$ f is a function of $\mathcal{H}$

$$f(\vec{x}, t) = \frac{1}{Z} \mathcal{F}(\mathcal{H}(\vec{x}))$$

$$Z = \int d\vec{x}\, \mathcal{F}(\mathcal{H}(x))$$

depend on type of ensemble

partition function

= number of microstates in the ensemble

Eg @ const temp $\quad P(\vec{x}) = e^{-\mathcal{H}(x)/k_B T} / Z$

$$\langle A \rangle_{\text{ensemble}} = \int d\vec{x}\, A(\vec{x}) \underbrace{\frac{f(\mathcal{H}(x))}{Z}}_{P(\vec{x})}$$

Microcanonical Ensemble

For an isolated system

N particles, box of volume V

Constant Energy

Assumption: all states are equally likely

"equal a priori probabilities"

$$\mathcal{F}(\mathcal{H}(x)) = \underline{\delta(\mathcal{H}(\vec{x}) - \varepsilon)}$$

$$\delta(x) \qquad \int_{-\infty}^{\infty} dx\ \delta(x-a) f(x) = f(a)$$

$$\Omega(N, V, \varepsilon) \propto \int d\vec{x}\ \delta(\mathcal{H}(\vec{x}) - \varepsilon)$$

counting how many points have $\mathcal{H} = \varepsilon$