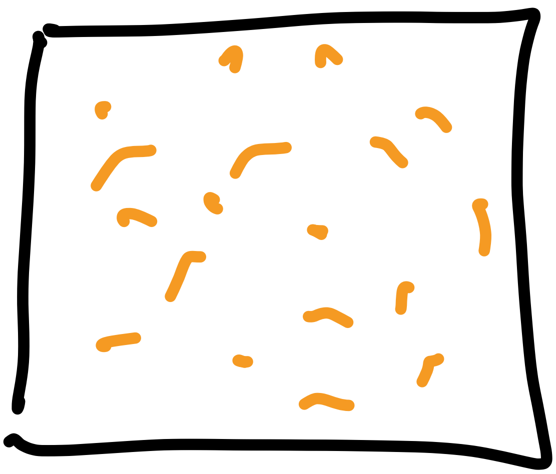
Lecture 3: Microcanonical, pt

Last time:

Isolated ~ closed

assume Classical



conserve

N, V, E_{total}

"Z" $= \int d\vec{x}\, P(\vec{x})$

$P(\vec{x}) = \frac{1}{Z} \int d\vec{x}\, P(\vec{x})$

How many states

$$\Omega\ \cancel{Z}(N, V, E) = C \int d\vec{x}\, \delta(\mathcal{H}(\vec{x}) - E)$$

C → leave for later $\hbar^{3N}$

C → $\frac{1}{N!}$ if indisting.

What is the probability of X

$$P(X) = \frac{C\,\delta(\mathcal{H}(X) - E)}{\Omega(N,V,E)} \approx \begin{cases} \frac{C}{\Omega} & \text{if } \mathcal{H}(X) = E \\ 0 \end{cases}$$

assumption

$$\int dX\, P(X) = \frac{C}{\Omega} \int dX\, \delta(\mathcal{H}(X) - E)$$

$$= 1$$

Every state with energy E has equal probability

"Assumption of equal a priori probabilities"

Dynamics - Newton's equations

"trajectory" $\{\vec{X}(t)\}$

$$X(t_1) \rightarrow X(t_2) \rightarrow X(t_3) \rightarrow \ldots \rightarrow X(t_N)$$

$$\langle A\rangle_{time} = \frac{1}{N_t}\sum_{i=1}^{N_t} A(X(t_i))$$

each microstate

$X(t_i)$ is a representative

sample of $P(X)$

limit $t\to\infty$

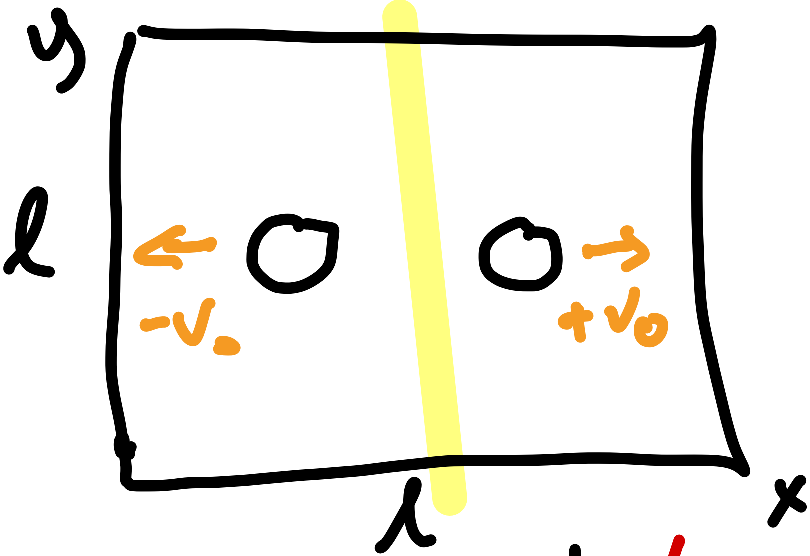
believe $\lim_{t\to\infty}\langle A\rangle_{time} = \langle A\rangle_{ensemble}$

$$\langle A\rangle_{ensemble} = \int d\vec{X}\, P(\vec{X})\, A(\vec{X})$$

would happen if system (for all A)

"ergodic" every state

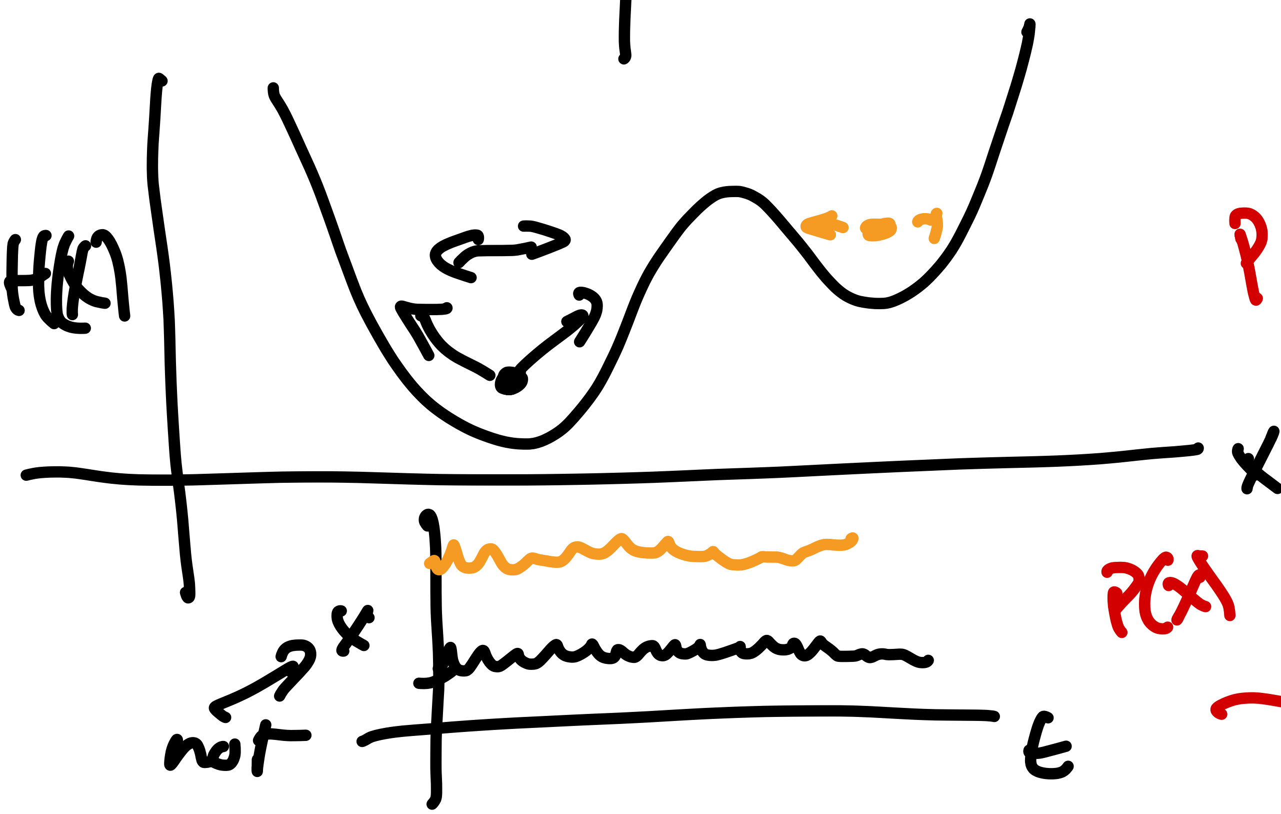
can be accessed, & will be



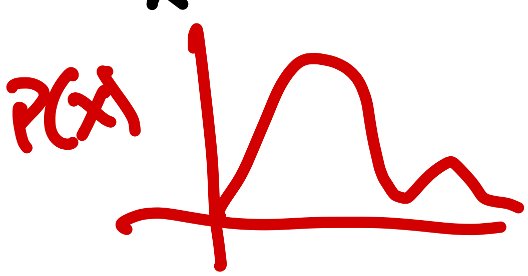
$N = 2$

$V = l^2$

Energy E



$P(x) \propto e^{-\beta H(x)}$



$$\langle A \rangle_{microcanonical} = \int A(x) P(x)$$

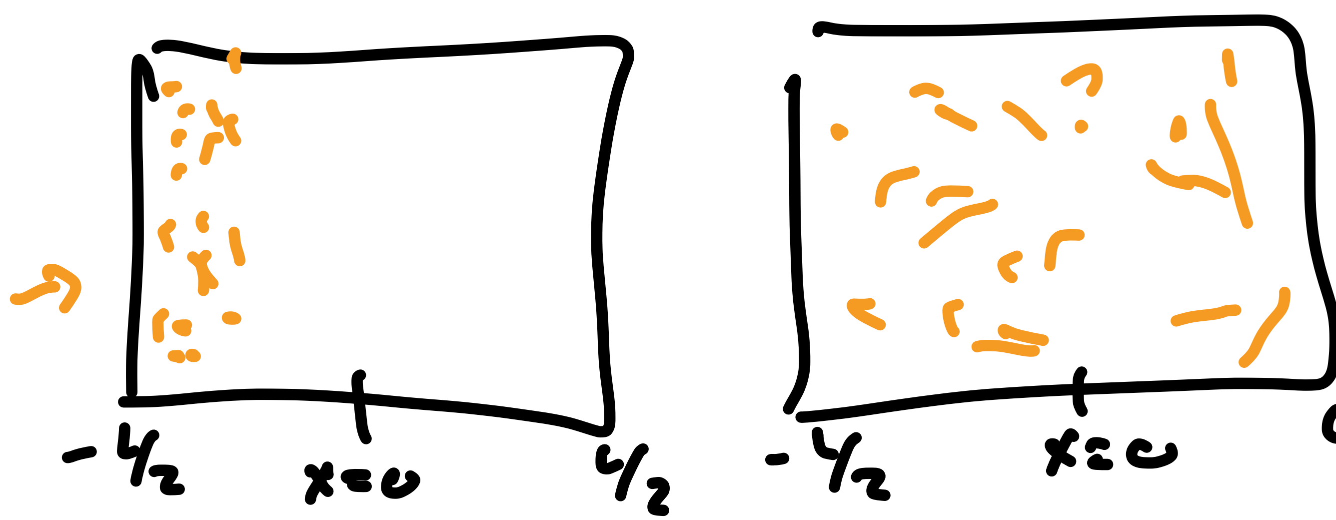
$C^{-1} \sim N!$

$$= \frac{C}{\Omega} \int d\underline{x}\, \delta(\mathcal{H}(x) - E)\, A(x)$$

$$= \sum_{\text{state } i}^{\Omega/C} \frac{C}{\Omega} A(x_i)$$

x position

[ideal gas
PE = {0, ∞ outside box



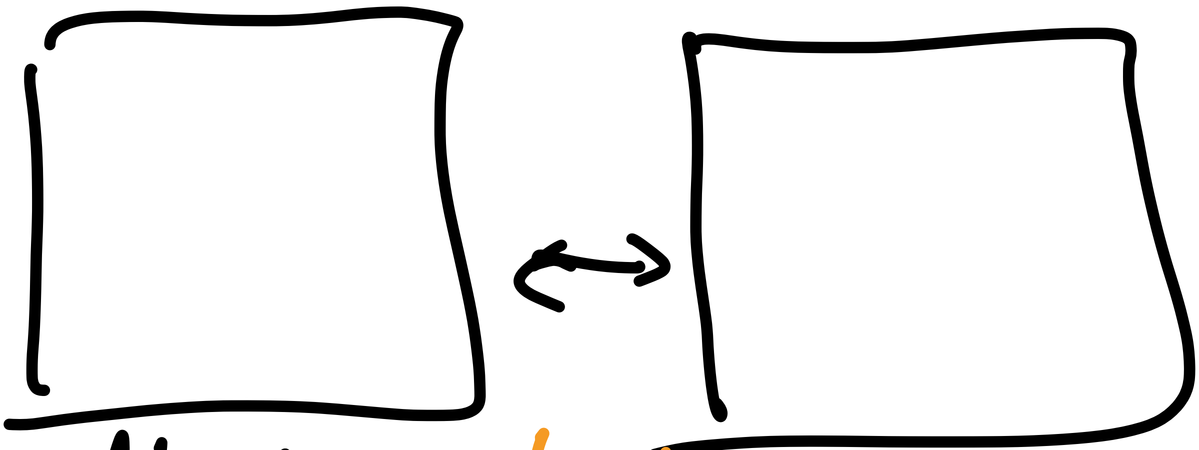
$X(t=0) \longrightarrow X(t=\tau)$

$X(t=\tau) \longleftarrow X(t=0)$

Connect microscopic details to thermodyn.

Thermodynamics

motion of heat / energy

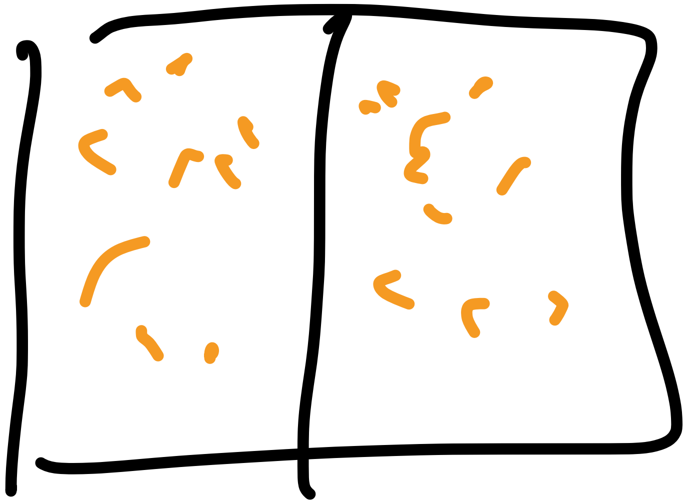


N_1, V_1, E_1 heat flow N_2, V_2, E_2

identical molecules

in total

$N, V, E = N_1 + N_2,\ V_1 + V_2,\ E_1 + E_2$



ε_1 can be $0 \to \varepsilon_{total}$

ε_2 can be $0 \to \varepsilon_{total}$

Thermodynamics:

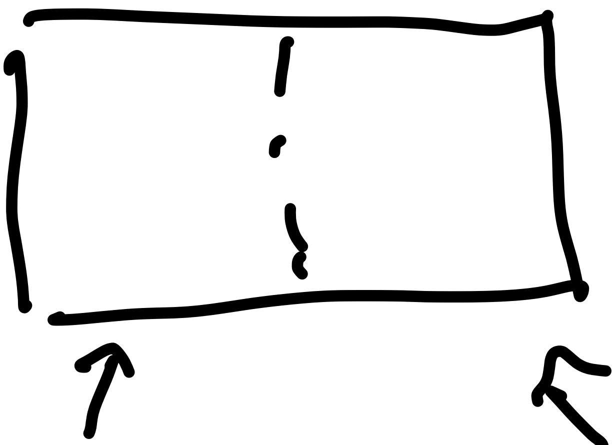
heat moves until

temperatures are equal

What value of ε_1 or ε_2 is most likely?

$\Omega(N_{tot}, V_{tot}, \varepsilon_{total})$ is maximized

idea maximize by taking $\frac{d\Omega}{d\varepsilon_1}$

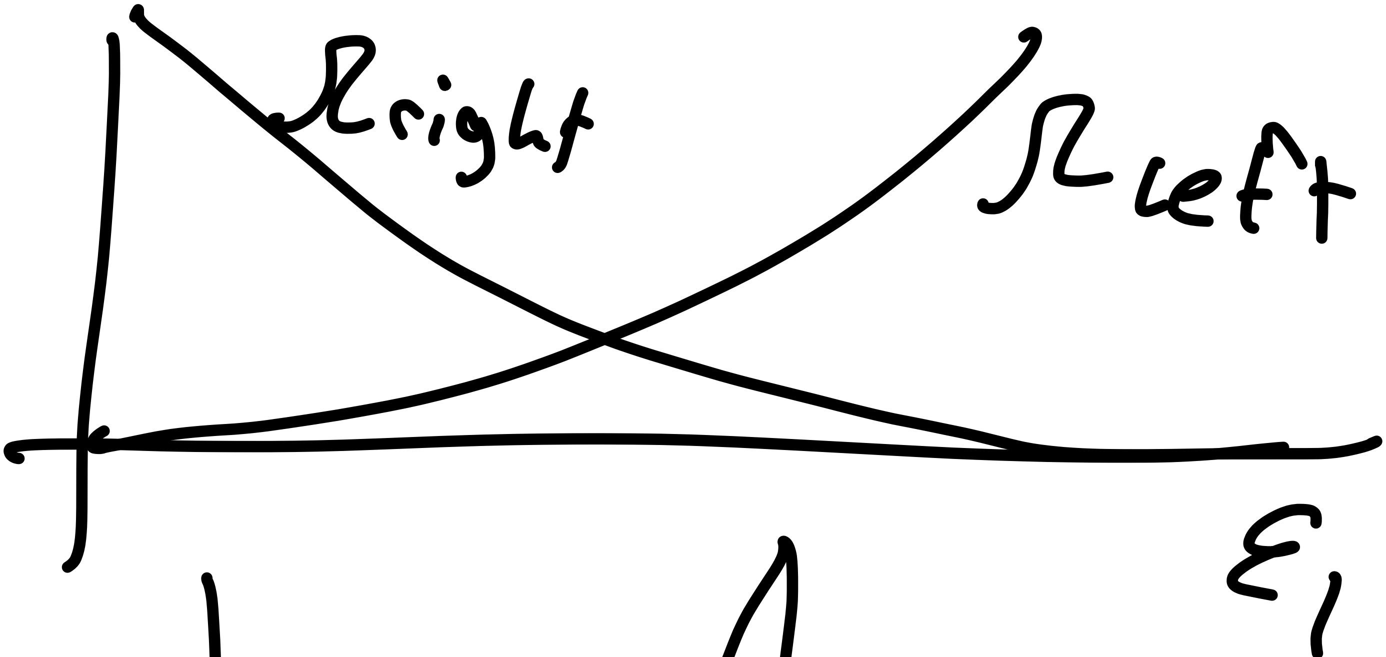


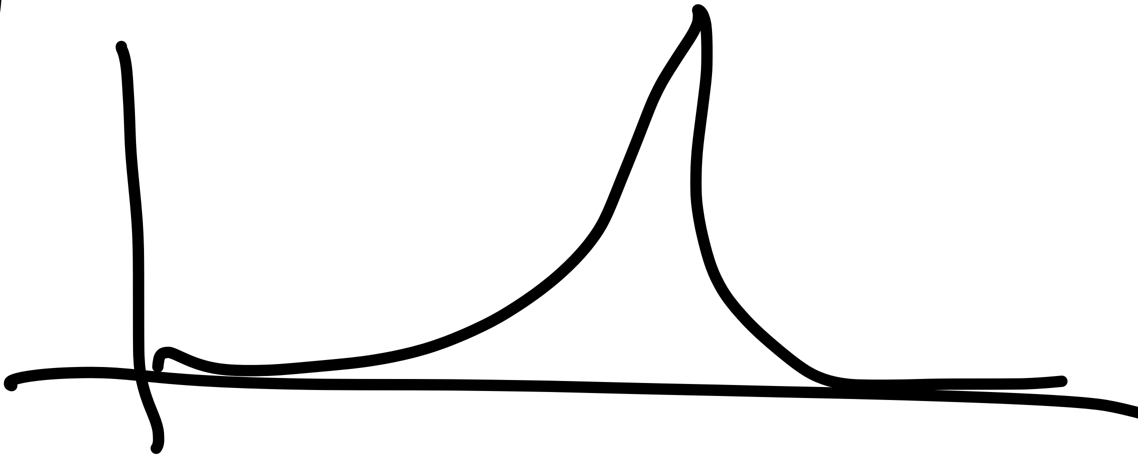
$\Omega(N_1, V_1, \varepsilon_1)$ $\Omega(N_2, V_2, \varepsilon_2)$

What is $\Omega(N, V, \varepsilon)$

$$\Omega(N, V, \varepsilon) = \Omega(\varepsilon_1)\,\Omega(\varepsilon_2)$$

$$\varepsilon_1 + \varepsilon_2 = \varepsilon_{total}$$





$$\frac{d\mathcal{L}_{total}}{d\varepsilon_1} \stackrel{?}{=} 0$$

$$\frac{d\log\mathcal{L}_{total}}{d\varepsilon_1} \stackrel{?}{=} 0$$

$$\frac{d}{d\varepsilon_1} \log \Omega = \frac{d}{d\varepsilon_1} \log(\Omega_L \cdot \Omega_R)$$

$= 0$?

$$= \frac{d}{d\varepsilon_1} \log \Omega_L(\varepsilon_1) + \frac{d}{d\varepsilon_1} \log \Omega_R(\varepsilon_2)$$

$$0 = \left(\frac{\partial}{\partial \varepsilon_1} \log \Omega(N_1, V_1, \varepsilon_1)\right)_{N_1, V_1} + \left(\frac{\partial}{\partial \varepsilon_1} \log \Omega(N_2, V_2, \varepsilon_2)\right)_{N_2, V_2}$$

$\varepsilon_1 + \varepsilon_2 = \varepsilon$ const

$\varepsilon_2 = \varepsilon - \varepsilon_1$

$$\frac{\partial X}{\partial \varepsilon_1} = \frac{\partial X}{\partial \varepsilon_2} \cdot \frac{\partial \varepsilon_2}{\partial \varepsilon_1} = -\frac{\partial X}{\partial \varepsilon_2}$$

$$0 = \left(\frac{\partial}{\partial E_1} \log \Omega(N_1, V_1, E_1)\right)_{N_1, V_1}$$

$$- \left(\frac{\partial}{\partial E_2} \log \Omega(N_2, V_2, E_2)\right)_{N_2, V_2}$$

$$\underbrace{\frac{\partial}{\partial E_1} \log \Omega_1(E_1)}_{\text{contected to } T?} = \frac{\partial}{\partial E_2} \log \Omega_2(E_2)$$

we will learn

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{N, V}$$

if $k \log \Omega = S$

(1) 2 bodies at equilibrium in contact have equal T

(2) Entropy system is maximized at equil.

motivates

$$S = k_B \log \Omega(N, V, E)$$

$$\boxed{N, V, E} \quad \boxed{N, V, E} \quad \times 2$$

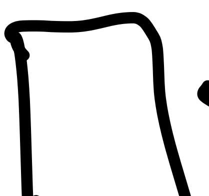
extensive prop to size system

$$S = k_B \log(\Omega \cdot \Omega) = 2 k_B \log \Omega$$

$$f(\lambda x_1, \lambda x_2, \dots, \lambda x_N)$$
$$= \lambda f(x_1, x_2, \dots, x_N)$$

E, S, V

$$\Omega(N, V, E)$$
$$\Omega(\lambda N, \lambda V, \lambda E)$$

 $\times \lambda$ N, V, E