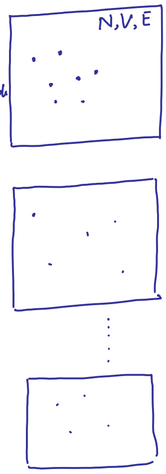
Micro-canonical Ensemble (N, V, E)

Case study: Classical Ideal gas

q, p are continuous random variables



$\mu_1 = \{q_i, p_i\}$

μ_2

μ_M

All μ_j correspond to macro-state N, V, E

$$p(\mu_j) = \frac{1}{\Omega(N,V,E)}$$

All μ_j are equi-probable

To compute $\Omega(N,V,E)$: Think of system to be having an

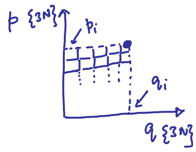
$$\boxed{E - \Delta E \leq H(\mu_j) \leq E + \Delta E}$$

ΔE poses no problem, $\boxed{\frac{\Delta E}{E} << 1}$

$$\Omega(N,V,E) = \frac{\text{Accessible phase space volume}}{\text{Resolution}}$$

$$= \frac{\displaystyle\int\cdots\int_{q_i \in V,\ 2m(E-\Delta E) \leq \sum_{i=1}^{3N} p_i^2 \leq 2m(E+\Delta E)} dq_1\, dq_2 \cdots dq_{3N}\, dp_1\, dp_2 \cdots dp_{3N}}{h^{3N}}$$

6N. phase-space



- projected on p_i yields p of i^{th} particle

phase-space is to be seen as cells of size h^{3N}

$\Delta x\, \Delta p \sim h$

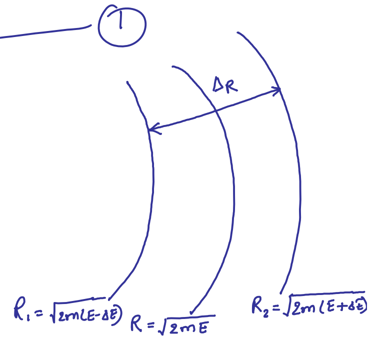
$(h^3)^N = h^{3N}$

$$\Omega(N,V,E) = \frac{V^N}{h^{3N}} \int\cdots\int_{2m(E-\Delta E) \leq \sum_{i=1}^{3N} p_i^2 \leq 2m(E+\Delta E)} dp_1\, dp_2 \cdots dp_{3N}$$

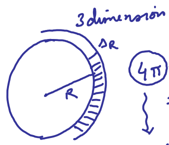
$$\cdots \iiint dq_1\, dq_2\, dq_3 = V$$

$$\Omega(N,V,E) = \frac{V^N}{h^{3N}} \cdot \Omega_p \qquad (1)$$

$$\Omega_p = \int\cdots\int_{2m(E-\Delta E) \leq \sum_{i=1}^{3N} p_i^2 \leq 2m(E+\Delta E)} dp_1\, dp_2 \cdots dp_{3N}$$



$$\Omega_p = \Theta_{3N} R^{3N-1} \Delta_R \qquad \text{——— (2)}$$



$\underbrace{④\pi R^{3-1}\cdot \Delta_R}_{\text{3d. solid angle}} = V_{shell}$

Thickness: $$\Delta_R = R_2 - R_1 = (2m)^{1/2}\left[(E+\Delta E)^{1/2} - (E-\Delta E)^{1/2}\right]$$
$$= (2mE)^{1/2}\left[\left(1+\Delta E/E\right)^{1/2} - \left(1-\Delta E/E\right)^{1/2}\right]$$
$$= (2mE)^{1/2}\left[1+\frac{\Delta E}{2E} - \left(1-\frac{\Delta E}{2E}\right)\right]$$
$$= (2mE)^{1/2}\cdot\frac{\Delta E}{E} = \left(\frac{2m}{E}\right)^{1/2}\Delta E$$

$$\Omega_p = \Theta_{3N} R^{3N-1}\left(\frac{2m}{E}\right)^{1/2}\Delta E$$
$$= \Theta_{3N}(2mE)^{(3N-1)/2}\left(\frac{2m}{E}\right)^{1/2}\Delta E \qquad ,\ldots\ R = \sqrt{2mE}$$
$$\text{——— (3)}$$

To compute Θ_{3N}: Take some $I = \int_{-\infty}^{+\infty}\cdots\int dp_1\,dp_2\ldots dp_{3N}\, e^{-\sum_{i=1}^{3N} p_i^2}$

$$= \left(\int_{-\infty}^{+\infty} dp\, e^{-p^2}\right)^{3N}$$
$$= \left(\sqrt{\pi}\right)^{3N} = \pi^{3N/2}$$

$$I = \int\cdots\int \prod_{i=1}^{3N} dp_i\, e^{-\sum_{i=1}^{3N} p_i^2} = \pi^{3N/2}$$

$R = \sqrt{\sum_{i=1}^{3N} p_i^2}$

$R^{3N-1} = \left(\sum_i p_i^2\right)^{(3N-1)/2}$

Using $\prod_{i=1}^{3N} dp_i = \Theta_{3N}\left(\sum_{i=1}^{3N} p_i^2\right)^{\frac{3N-1}{2}} dR$
$$= \Theta_{3N}\cdot R^{3N-1}\,dR$$

In 3. dim

$dp_1\,dp_2\,dp_3 = \underbrace{④\pi}_{\text{3d. solid angle}}\left(p_1^2+p_2^2+p_3^2\right)\, dp$

$$\iiint_{-\infty}^{+\infty} dp_1\,dp_2\,dp_3\, f(p) = \int_{R=0}^{\infty} 4\pi R^2\,dR\, f(p)$$

$R^2 = p_1^2+p_2^2+p_3^2$

$$I = \pi^{3N/2} = \int_{R=0}^{\infty}\Theta_{3N} R^{3N-1} e^{-R^2}\,dR$$

...... substitute $R^2 = u \Rightarrow 2R\,dR = du$
$$\Rightarrow dR = \frac{1}{2\sqrt{u}}\cdot du$$

$$I = \pi^{3N/2} = \int_{u=0}^{\infty}\Theta_{3N}\, u^{(3N-1)/2}\cdot e^{-u}\,\frac{du}{2\sqrt{u}}$$

$$\pi^{3N/2} = \frac{\theta_{3N}}{2} \int_{u=0}^{\infty} u^{(3N/2-1)} e^{-u}\, du = \frac{\theta_{3N}}{2} \cdot \left(\frac{3N}{2}-1\right)!$$

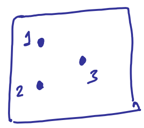
.... using $\int_0^{\infty} u^n e^{-u}\, du = n!$

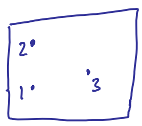
$$\theta_{3N} = \frac{2\pi^{3N/2}}{\left(\frac{3N}{2}-1\right)!} \quad \text{—— (4)}$$

Plug this in eqⁿ (3) and using then in eqⁿ (1):

$$\Omega(N,V,E) = \frac{V^N}{\hbar^{3N}} \cdot \frac{2\pi^{3N/2}}{\left(\frac{3N}{2}-1\right)!} (2mE)^{(3N-1)/2} \left(\frac{2m}{E}\right)^{1/2} \Delta E$$

..... seriously over counted Ω . . . .

$\mu_1 \equiv$ 

$\mu_2 =$ 

⋮ 3! microstates

Since N particles are identical

$$\Omega(N,V,E) = \frac{V^N}{N!\,\hbar^{3N}} \cdot \frac{2\pi^{3N/2}}{\left(\frac{3N}{2}-1\right)!} (2mE)^{(3N-1)/2} \left(\frac{2m}{E}\right)^{1/2} \Delta E$$

This opens up the route to thermodynamics.

$$S = k_B \ln \Omega$$

$$= k_B\Big[N \ln V - N \ln N + N - \frac{3N}{2} \ln \hbar^2 + \cancelto{0}{\ln 2} + \frac{3N}{2} \ln \pi$$
$$+ \frac{3N}{2} \ln(2mE) - \frac{3N}{2} \ln \frac{3N}{2} + \frac{3N}{2} + \frac{1}{2} \cancelto{0}{\ln\left(\frac{2m}{E}\right)} + \cancelto{0}{\ln \Delta E}\Big]$$

$$S = N k_B \ln \left[\frac{eV}{N} \cdot \left(\frac{4\pi m e E}{3 N h^2} \right)^{3/2} \right]$$