Micro-canonical Ensemble (N, V, E)

"Thermally & Mechanically Isolated"

$(E = \text{const})$ $(V = \text{const})$

Two case studies:

(a) Discrete degrees of freedom

Eg. Two level systems

(b) Continuous degrees of freedom

Eg. Ideal gas

Two level system (N, V, E)

N particles in two levels

ϵ (Excited)

0 (Ground)

Excitation : $n_i = 0$ (Ground state)

$= 1$ (Excited state)

Total energy: $E = \sum_{i=1}^{N} n_i \epsilon = (1 + 0 + 0 + \cdots 1 + 0 + \cdots)\epsilon$

$= N_1 \epsilon$

$E = N_1 \epsilon$ [N_1 is the no. of excited particles !]

$N = 10$

$N_1 = 6$

$N - N_1 = 4$

probability : $\boxed{p(\mu) = \dfrac{1}{\Omega(\underbrace{N, E}_{N_1\epsilon})}}$

Macrostate : (N, E) has $\Omega(N, E)$ microstates.

Compute $\Omega(\underbrace{N, E}_{\text{Macrostate}}) = \dfrac{N!}{N_1!\,(N-N_1)!}$ $\Rightarrow$ This many microstates exist

(1)

Assume $\quad N,\ N_1,\ N-N_1 \gg 1$

Hence using Stirling approximation

$$N! \simeq \left(N/e\right)^N, \quad N_1! \simeq \left(N_1/e\right)^{N_1}, \quad (N-N_1)! \simeq \left(\frac{N-N_1}{e}\right)^{N-N_1}$$

dropped $\sqrt{2\pi N}$ ...

Use this eq 1

$$\Omega(N,E) = \frac{N^N}{N_1^{N_1}\,(N-N_1)^{N-N_1}}$$

Take logarithm ... noting that $\frac{S}{k_B} = \ln \Omega$

$$S/k_B = N \ln N - N_1 \ln N_1 - (N-N_1)\ln(N-N_1) \quad \text{(2)}$$

Thermodynamic temperature: $\frac{1}{T} = \left.\frac{\partial S}{\partial E}\right|_N = \left.\frac{\partial S}{\epsilon\,\partial N_1}\right|_N$ ... $E = N_1\epsilon$

$$\frac{1}{T} = \frac{k_B}{\epsilon}\left[-\cancel{1} - \ln N_1 + \cancel{1} + \ln(N-N_1)\right]$$

$$\boxed{\frac{1}{T} = \frac{k_B}{\epsilon} \cdot \ln\left(\frac{N-N_1}{N_1}\right)}$$

$\ln x > 0 \quad , x > 1$

So, $\frac{N-N_1}{N_1} > 1$ for $T > 0$

$N_1 < N/2$ for $T > 0$

$N_1 > N/2$

$N - N_1 < N/2$

$\frac{N-N_1}{N_1} < 1$

$\ln\left(\frac{N-N_1}{N_1}\right) < 0 \Rightarrow \frac{1}{T} < 0$

$\Rightarrow T < 0$

??

Observation: T turns out to be negative if $N_1 > N/2$

Maximum excitation or population in the excited state is half filled!

$$\boxed{\frac{1}{T} = \frac{k_B}{\epsilon} \cdot \ln\left(\frac{N-N_1}{N_1}\right)} \quad \text{(3)}$$

Q. Why is the $N_1^{max} = N/2$?

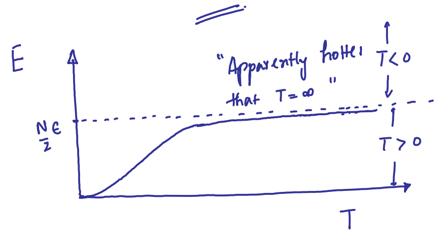
A. Energy Argument.

From eqn (3) .... $\frac{\epsilon}{k_B T} = \ln\left(\frac{N-N_1}{N_1}\right)$

$$\frac{N-N_1}{N_1} = e^{\epsilon/k_B T}$$

$$\frac{N}{N_1} = 1 + e^{\epsilon/k_B T}$$

$$\epsilon N_1 = \frac{N\epsilon}{1+e^{\epsilon/k_B T}} = E$$



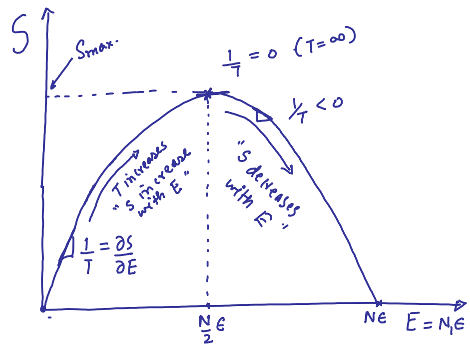
Entropy Argument

$S \sim \ln \Omega$ monotonic f^n of Ω

$\Omega = \frac{N!}{N_1!\,(N-N_1)!}$ has a maximum at $N_1 = N/2$

Ω_{max} is sitting at $N_1 = N/2$

S_{max} is sitting at $N_1 = N/2$



$N_1 = 0$ $(E=0)$ (Min)

$\Omega = \frac{N!}{N_1!\,(N-N_1)!}$ $\therefore$ $\Omega(N_1=0) = 1$

$\ln 1 = 0$ $\therefore$ $S = 0$

$N_1 = N$ $(E = N\epsilon)$ (Max)

$\Omega = \frac{N!}{N_1!\,(N-N_1)!} = 1$

$\frac{S}{k_B} = \ln\Omega = 0$

Start with a system with $N_1 > N/2$ $(T<0)$ $\downarrow \Delta E$

Comes into contact with reservoir at $(T_R > 0)$

Eventually two-level system returns to $\underline{\underline{T>0}}$.