Examples: Microcanonical Ensemble

1. Two level system with N independent particles

Let the two levels have energies $+\epsilon_0$ & $-\epsilon_0$.

N_+ in state $+\epsilon_0$

N_- in state $-\epsilon_0$

such that $N_+ + N_- = N$

and $U = M\epsilon_0 = (N_+ - N_-)\epsilon_0$.

Thus, $N_+ = \frac{1}{2}(N+M)$

and $N_- = \frac{1}{2}(N-M)$

$$\therefore \Omega_0(U,N) = \frac{N!}{N_+!\,N_-!} = \frac{N!}{\left(\frac{N+M}{2}\right)!\left(\frac{N-M}{2}\right)!}.$$

(total number of ways of choosing N_+ particles with energy $+\epsilon_0$ & N_- particles with energy $-\epsilon_0$ out of total N particles).

$$\therefore S = k_B \ln \Omega_0(U,N)$$

$$= k_B\Big[N\ln N - N - \left(\tfrac{N+M}{2}\right)\ln\left(\tfrac{N+M}{2}\right) + \left(\tfrac{N+M}{2}\right) - \left(\tfrac{N-M}{2}\right)\ln\left(\tfrac{N-M}{2}\right) + \left(\tfrac{N-M}{2}\right)\Big] + O(\sqrt{N}).$$

$$\approx k_B\Big[N\ln N - \left(\tfrac{N+M}{2}\right)\ln\left(\tfrac{N+M}{2}\right) - \left(\tfrac{N-M}{2}\right)\ln\left(\tfrac{N-M}{2}\right)\Big]$$

$\therefore \frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_N = \left(\frac{\partial S}{\partial M}\right)_N \Big/ \left(\frac{\partial U}{\partial M}\right)_N$. But $\left(\frac{\partial U}{\partial M}\right)_N = \epsilon_0$.

$$\Rightarrow \frac{1}{T} = \frac{k_B}{\epsilon_0}\left[\frac{1}{2}\ln\left(\frac{N-M}{N+M}\right)\right] = \frac{k_B}{2\epsilon_0}\ln\left(\frac{N_-}{N_+}\right).$$

$$\Rightarrow \frac{N_-}{N_+} = \exp\left(\frac{2\epsilon_0}{k_B T}\right).$$

But, $N_- + N_+ = N \Rightarrow \frac{N}{N_+} = 1 + \exp\left(\frac{2\epsilon_0}{k_B T}\right).$

$$\therefore \quad N_+ = \frac{N}{1+\exp\left(\frac{2\epsilon_0}{k_B T}\right)} = \frac{N\exp\left(-\frac{\epsilon_0}{k_B T}\right)}{\exp\left(\frac{\epsilon_0}{k_B T}\right)+\exp\left(-\frac{\epsilon_0}{k_B T}\right)}.$$

Similarly, $N_- = \frac{N}{1+\exp\left(-\frac{2\epsilon_0}{k_B T}\right)} = \frac{N\exp\left(\frac{\epsilon_0}{k_B T}\right)}{\exp\left(\frac{\epsilon_0}{k_B T}\right)+\exp\left(-\frac{\epsilon_0}{k_B T}\right)}.$

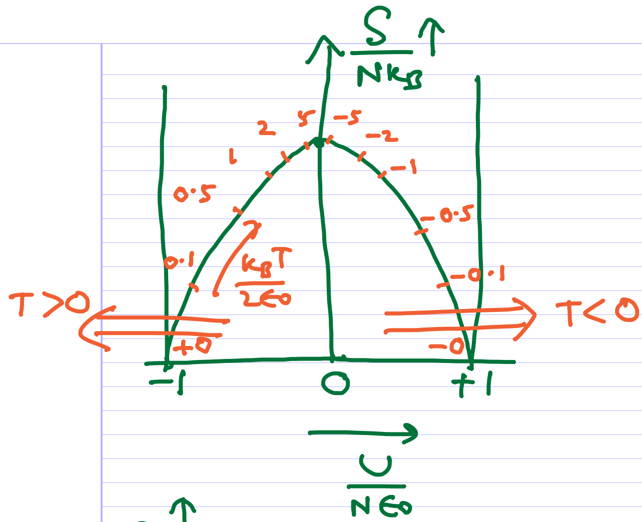
$$\Rightarrow U = M\epsilon_0 = -(N_- - N_+)\epsilon_0$$

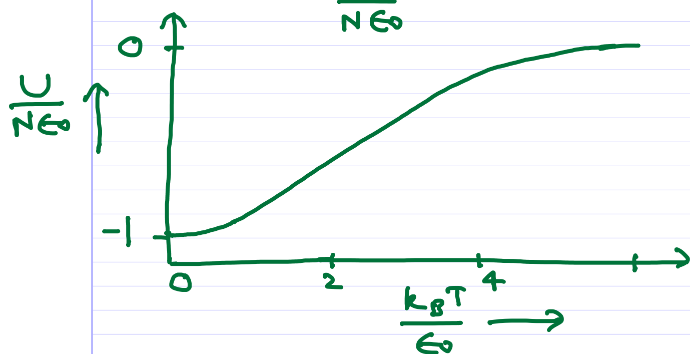
$$= -N\epsilon_0\left[\frac{\exp\left(\frac{\epsilon_0}{k_B T}\right)-\exp\left(-\frac{\epsilon_0}{k_B T}\right)}{\exp\left(\frac{\epsilon_0}{k_B T}\right)+\exp\left(-\frac{\epsilon_0}{k_B T}\right)}\right].$$

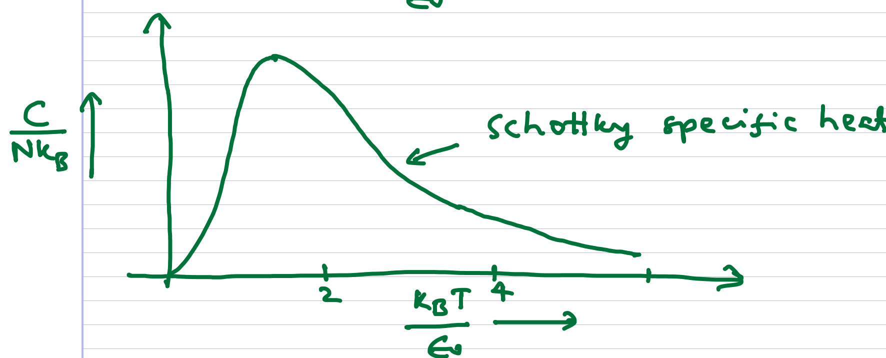
$$\therefore \boxed{U = -N\epsilon_0 \tanh\left(\frac{\epsilon_0}{k_B T}\right)}$$

$$C = \left(\frac{\partial U}{\partial T}\right) = -N\epsilon_0\left(-\frac{\epsilon_0}{k_B T^2}\right)\operatorname{sech}^2\left(\frac{\epsilon_0}{k_B T}\right).$$

$$\therefore \boxed{C = N k_B\left(\frac{\epsilon_0}{k_B T}\right)^2 \operatorname{sech}^2\left(\frac{\epsilon_0}{k_B T}\right)}$$


$\frac{S}{Nk_B}$
$T>0$
$T<0$
$\frac{k_BT}{2\epsilon_0}$
$+0$
-0
-1 0 $+1$
$\frac{U}{N\epsilon_0}$


$\frac{U}{N\epsilon_0}$
0
-1
0 2 4
$\frac{k_BT}{\epsilon_0}$


$\frac{C}{Nk_B}$
Schottky specific heat
2 4
$\frac{k_BT}{\epsilon_0}$

2. N-independent harmonic oscillators

Energy levels for a quantum harmonic oscillator is given by,

$$\varepsilon_n = \left(n+\tfrac{1}{2}\right)h\nu \quad , \quad n = 0, 1, 2, \ldots$$

For N-identical quantum harmonic oscillators (non-interacting), the total energy is given by

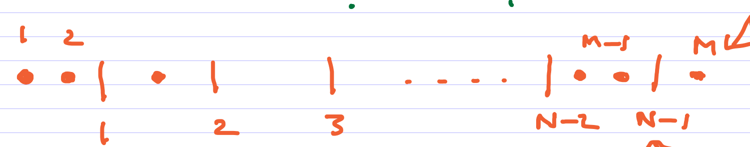
$$U = \tfrac{1}{2}Nh\nu + Mh\nu \quad ; \quad M, N \text{ are integers.}$$

If the quantum number for the i^{th} quantum harmonic oscillator is given by n_i,

$$\Rightarrow \quad n_1 + n_2 + \ldots + n_N = M.$$

$$\therefore \quad \Omega_0(U,N) = \frac{(M+N-1)!}{M!\,(N-1)!}$$

particle index.



partition index.

Number of microstates

= # of ways of arranging M particles & (N-1) partitions.

$$\therefore \quad \Omega_0(U,N) \approx \frac{(M+N)!}{M!\,N!} \quad ; \quad \because N \gg 1.$$

$$\Rightarrow S = k_B \ln \Omega_0 = k_B\left[\ln (M+N)! - \ln M! - \ln N!\right].$$

$$\Rightarrow \quad S \approx k_B\left[(M+N)\ln(M+N) - M\ln M - N\ln N\right].$$

using $\ln n! \approx n\ln n - n$
for large n.

$$\therefore \quad \frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_N = \left(\frac{\partial S}{\partial M}\right)_N\left(\frac{\partial M}{\partial U}\right)_N$$

$$= \frac{k_B}{h\nu}\ln\left(\frac{M+N}{M}\right)$$

$$= \frac{k_B}{h\nu}\ln\left(\frac{M+\frac{N}{2}+\frac{N}{2}}{M+\frac{N}{2}-\frac{N}{2}}\right).$$

$$= \frac{k_B}{h\nu}\ln\left(\frac{U+\frac{Nh\nu}{2}}{U-\frac{Nh\nu}{2}}\right).$$

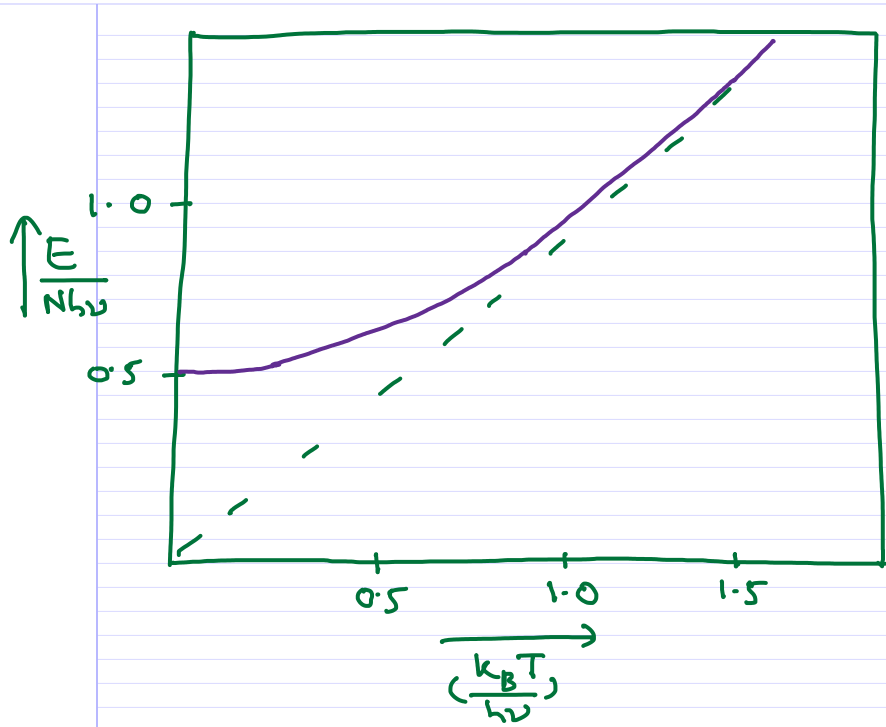
$$\therefore \quad \left(\frac{h\nu}{k_BT}\right) = \ln\left(\frac{U+\frac{Nh\nu}{2}}{U-\frac{Nh\nu}{2}}\right).$$

$$\Rightarrow \quad \frac{\frac{U}{N}+\frac{h\nu}{2}}{\frac{U}{N}-\frac{h\nu}{2}} = \exp\left(\frac{h\nu}{k_BT}\right).$$

$$\therefore \quad \exp\left(\frac{h\nu}{k_BT}\right) - 1 = \frac{\frac{U}{N}+\frac{h\nu}{2}}{\frac{U}{N}-\frac{h\nu}{2}} - 1 = \frac{h\nu}{\frac{U}{N}-\frac{h\nu}{2}}.$$

$$\Rightarrow \quad \frac{U}{N} - \frac{h\nu}{2} = \frac{h\nu}{\exp\left(\frac{h\nu}{k_BT}\right)-1}.$$

$$\therefore \quad U = N\left[\frac{h\nu}{2} + \frac{h\nu}{\exp\left(\frac{h\nu}{k_BT}\right)-1}\right].$$



3. Localized magnetic moments.

$$\mathcal{H} = D\sum_{j=1}^{N} S_j^2 \qquad D > 0$$

$$S_j = \begin{cases} \pm 1 \\ 0 \end{cases}$$

Let N_0, N_+ and N_- be number of entities with $S_j = 0$, $S_j = +1$ and $S_j = -1$, respectively.

$$\therefore \Omega_0(U,N) = \sum_{N_0, N_+, N_-} \frac{N!}{N_0!\, N_+!\, N_-!}$$

s.t., $N_0 + N_+ + N_- = N$

and $(N_+ + N_-)D = U$.

$$\therefore \; N_0 = N - N_+ - N_- = N - \frac{U}{D}.$$

$$N_+ = \left(\frac{U}{D} - N_-\right).$$

s.t.; N_- ranges from 0 to $\frac{U}{D}$

$$\therefore \; \Omega_0(U, N) = \sum_{N_-=0}^{U/D} \frac{N!}{\left(N - \frac{U}{D}\right)! \left(\frac{U}{D} - N_-\right)! \, N_-!}.$$

$$= \frac{N!}{\left(N - \frac{U}{D}\right)!} \sum_{N_-=0}^{N} \frac{\left(\frac{U}{D}\right)! \, 1^{\frac{U}{D} - N_-} \, 1^{N_-}}{\left(\frac{U}{D} - N_-\right)! \, N_-! \left(\frac{U}{D}\right)!}$$

$$= \frac{N!}{\left(N - \frac{U}{D}\right)! \left(\frac{U}{D}\right)!} \, 2^{\frac{U}{D}}.$$

$$\Rightarrow S = k_B \ln \Omega_0 = k_B \Big[\frac{U}{D} \ln 2 + N \ln N - N - \left(N - \frac{U}{D}\right) \ln\left(N - \frac{U}{D}\right) + \left(N - \frac{U}{D}\right) - \frac{U}{D} \ln\left(\frac{U}{D}\right) + \frac{U}{D} \Big]$$

Let $U = Nu$.

$$\therefore \; s = \frac{S}{N} = \frac{k_B}{N} \Big[\frac{Nu}{D} \ln 2 + N \ln N - N - N\left(1 - \frac{u}{D}\right) \ln\left[N\left(1 - \frac{u}{D}\right)\right] + N\left(1 - \frac{u}{D}\right) - \frac{Nu}{D} \ln\left(\frac{Nu}{D}\right) + \frac{Nu}{D} \Big]$$

$$\Rightarrow s = k_B \left[\frac{u}{D} \ln 2 - \left(1 - \frac{u}{D}\right) \ln\left(1 - \frac{u}{D}\right) - \frac{u}{D} \ln\left(\frac{u}{D}\right) \right].$$