

Problem Set 2.

1.

$$\begin{aligned}\langle x \rangle &= -20 \cdot \frac{3}{10} - 10 \cdot \frac{1}{5} + 30 \cdot \frac{1}{2} = \sum_i x_i p_i \\ &= 7\end{aligned}$$

$$\begin{aligned}\langle x^2 \rangle &= 400 \cdot \frac{3}{10} + 100 \cdot \frac{1}{5} + 900 \cdot \frac{1}{2} = \sum_i x_i^2 p_i \\ &= 590\end{aligned}$$

$$\begin{aligned}\Rightarrow \sigma^2 &= \langle x^2 \rangle - \langle x \rangle^2 \\ &= 541 \\ \therefore \sigma &\approx 23.3.\end{aligned}$$

2. a) Check normalisation:

$$\int_0^{\infty} e^{-\alpha x} dx = \left[-\frac{e^{-\alpha x}}{\alpha} \right]_0^{\infty} = \frac{1}{\alpha}$$

$\therefore p(x) = \alpha e^{-\alpha x}$ is the correctly normalised distribution.

$$\Rightarrow \langle x \rangle = \int_0^{\infty} \alpha x e^{-\alpha x} dx = \alpha \cdot \frac{1}{\alpha^2} = \frac{1}{\alpha}.$$

$$b) \langle x^2 \rangle = \alpha \int_0^{\infty} x^2 e^{-\alpha x} dx = \alpha \cdot \frac{2}{\alpha^3} = \frac{2}{\alpha^2}.$$

$$c) \sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{2}{\alpha^2} - \frac{1}{\alpha^2} = \frac{1}{\alpha^2}$$

$$\therefore \sigma = \frac{1}{\alpha}.$$

3. a) We can select 3 ins from a choice of 6 in

$$6 \cdot 5 \cdot 4 = \frac{6!}{3!} = 120 \text{ ways}$$

b) If we choose 5 objects from 12 ignoring the order then there are

$$12 \cdot 11 \cdot 10 \cdot 9 \cdot 8 = \frac{12!}{7!} = 95040 \text{ ways}$$

If we have 5 objects there are $5!$ ways of ordering them. Hence if the order the objects are chosen is important

$$\Rightarrow \frac{12!}{7!} \cdot 5! = 11404800 \text{ ways.}$$

c) ¹S¹²T¹²³A²¹³²I³²C³I³A³N³S

$$\Rightarrow S \times 3$$

$$T \times 3$$

$$A \times 2$$

$$I \times 3$$

$$C \times 1$$

$$N \times 1$$

$$\Rightarrow \frac{13!}{3!3!2!3!} = 14414400.$$

d) MMM [IWIU]

How many ways can remaining letters be ordered?

$$\frac{4!}{2!} = 12. \quad \text{TOTAL orderings} \quad \frac{7!}{3!2!} = 420 \Rightarrow p = \frac{1}{35}.$$

$$4. \quad \ln x! \approx x \ln x - x$$

$$\frac{d(\ln x!)}{dx} \approx \frac{d}{dx} [x \ln x - x]$$

$$= \ln x + x \cdot \frac{1}{x} - 1$$

$$= \ln x.$$

3.

$$S = k_B \ln W$$

$$W = \frac{(n-1+m)!}{(n-1)! m!}$$

$$\Rightarrow S = k_B \ln \frac{(n-1+m)!}{(n-1)! m!}$$

$$\approx k_B \ln \frac{(n + \frac{U}{\hbar\omega})!}{n! (\frac{U}{\hbar\omega})!}$$

Using Stirling's approximation

$$S \approx k_B \left((n + \frac{U}{\hbar\omega}) \ln (n + \frac{U}{\hbar\omega}) - (n + \frac{U}{\hbar\omega}) - n \ln n + n - \frac{U}{\hbar\omega} \ln \frac{U}{\hbar\omega} + \frac{U}{\hbar\omega} \right)$$

$$\frac{\partial S}{\partial U} = \frac{1}{T}$$

$$\Rightarrow \frac{1}{T} = \frac{k_B}{\hbar\omega} \left(\ln (n + \frac{U}{\hbar\omega}) - \ln \frac{U}{\hbar\omega} \right)$$

$$\Rightarrow e^{\frac{\hbar\omega}{k_B T}} = \frac{n + \frac{U}{\hbar\omega}}{\frac{U}{\hbar\omega}}$$

$$\Rightarrow \frac{U}{\hbar\omega} (e^{\frac{\hbar\omega}{k_B T}} - 1) = n$$

$$\Rightarrow U = \frac{n \hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

4.

6. ~~6.~~ $N+n$ sites total, with N filled & n vacant
 \Rightarrow

$$W = \frac{(N+n)!}{N! n!}$$

$$S = k_B \ln W$$

$$= k_B \left((N+n) \ln(N+n) - \cancel{(N+n)} - N \ln N - \cancel{n} - n \ln n - \cancel{n} \right)$$

$$= k_B \left((N+n) \ln(N+n) - n \ln n - N \ln N \right)$$

$$F = U - TS$$

$$= n\epsilon - k_B T \left((N+n) \ln(N+n) - n \ln n - N \ln N \right)$$

$$\frac{dF}{dn} = 0 \quad \text{in equilibrium}$$

$$\Rightarrow 0 = \epsilon - k_B T \left(\ln(N+n) - \ln n \right)$$

$$\Rightarrow \frac{\epsilon}{k_B T} = \ln \frac{N+n}{n}$$

$$\Rightarrow \left(e^{\epsilon/k_B T} - 1 \right) n = N$$

$$\therefore n = \frac{N}{e^{\epsilon/k_B T} - 1}$$

$$\text{If } T = 1300 \text{ K} \Rightarrow k_B T = 0.112 \text{ eV}$$

$$\therefore \frac{\epsilon}{k_B T} \approx 8.93$$

$$\therefore \frac{n}{N} \approx 1.33 \times 10^{-4}$$

If the crystal is large then the additional entropy for the surface atoms is negligible compared to the entropy of the bulk.

Q.
7.8

In the Spin System there are N positions between the spins to put domain walls.

↑↑↑↑↓ ↓↓↓ ...

There are n of these walls & $(N-n)$ that are not domain walls.

The first spin can be ↑ or ↓, & the remaining orientations follow from the wall positions.

Hence:

$$W = 2 \cdot \frac{N!}{n! (N-n)!}$$

$$S = k_B \ln W$$

$$\cong k_B \left(\ln 2 + N \ln N - n \ln n - (N-n) \ln (N-n) + (N-n) \right)$$

$$= k_B \left(\ln 2 + N \ln N - n \ln n - (N-n) \ln (N-n) \right)$$

Using $\frac{1}{T} = \frac{\partial S}{\partial u}$ with $u = n \epsilon$.

$$\frac{\partial S}{\partial u} = \frac{dS}{dn} \frac{dn}{du} = \frac{dS}{dn} \cdot \frac{1}{\epsilon}$$

$$\Rightarrow \frac{1}{T} = \frac{k_B}{\epsilon} \left(-\ln n + \ln(N-n) \right)$$

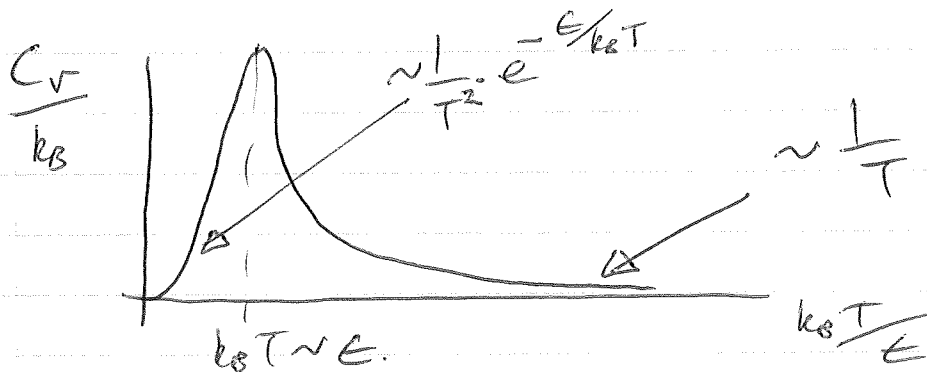
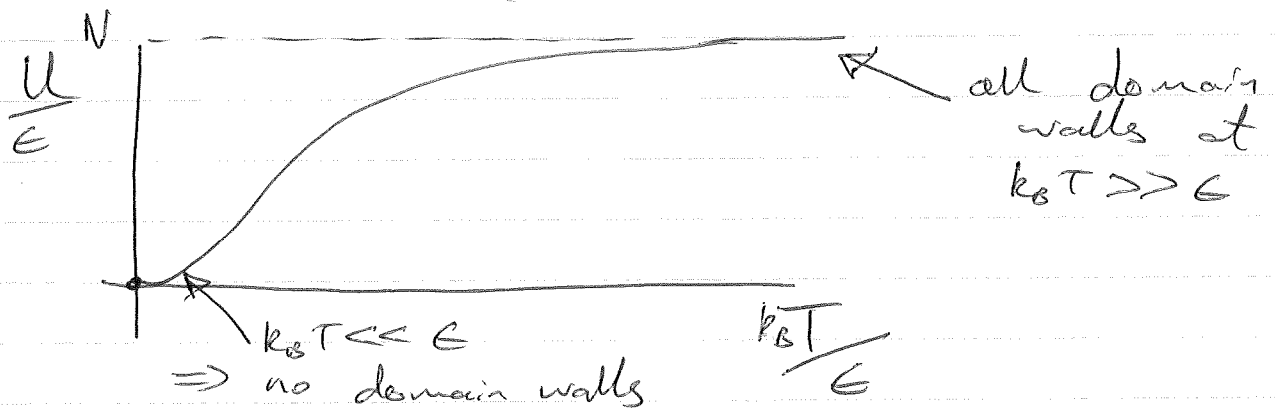
$$\Rightarrow \frac{\epsilon}{k_B T} = \ln \left(\frac{N-n}{n} \right)$$

$$\Rightarrow (e^{\epsilon/k_B T} + 1) n = N$$

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

$$\& U = n \epsilon = \frac{N \epsilon}{e^{\epsilon/k_B T} + 1}$$

$$C_V = \frac{dU}{dT} = \frac{\epsilon}{k_B T^2} \frac{N \epsilon}{e^{\epsilon/k_B T} + 1}$$



$$W = \frac{(2N)!}{(N+r)!(N-r)!}$$

$$S = k_B \ln W$$

$$\approx k_B \left((2N) \ln(2N) - 2N - (N+r) \ln(N+r) + (N+r) - (N-r) \ln(N-r) + (N-r) \right)$$

Since $TdS = dU - fdl$

$$\Rightarrow f = -T \left. \frac{\partial S}{\partial l} \right|_U$$

$$\frac{\partial S}{\partial l} = \frac{dS}{dr} \cdot \frac{dr}{dl} = \frac{dS}{dr} \cdot \frac{1}{2a} \quad (\text{as } l = 2ra)$$

$$\begin{aligned} \therefore \frac{dS}{dr} &= k_B \left(-\ln(N+r) + \ln(N-r) \right) \\ &= k_B \ln \left(\frac{N-r}{N+r} \right) = k_B \ln \left(\frac{1 - \frac{r}{N}}{1 + \frac{r}{N}} \right) \end{aligned}$$

Using the Taylor expansion

$$\ln \left(\frac{1-x}{1+x} \right) \approx -x - x + O(x^2) = -2x.$$

$$\Rightarrow \frac{dS}{dr} \approx -2k_B \frac{r}{N} = -\frac{k_B}{Na} \cdot l.$$

$$\therefore \frac{\partial S}{\partial l} = -\frac{k_B}{2Na^2} \quad \& \quad f = \frac{k_B T l}{2Na^2}.$$