Assignment No.7 final derivations

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Assignment No.7;

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Phys 481, Analytical Derivations

Let $\epsilon_1 = -\epsilon$, $\epsilon_2 = 0$, $\epsilon_3 = \epsilon$

$p_1 + p_2 + p_3 = 1$, $p_i = \frac{n_i}{N}$

$n_1\epsilon_1 + n_2\epsilon_2 + n_3\epsilon_3 = U$

$S = -k_B N(p_1 \ln p_1 + p_2 \ln p_2 + p_3 \ln p_3)$

From these it can be deduced;

$-p_1\epsilon + p_3\epsilon = \frac{U}{N}$

$n_1 + n_2 + n_3 = N$

Write S in terms of p_3.

$\Rightarrow -p_1\epsilon = \left(\frac{U}{N} - p_3\epsilon\right)$

$\Rightarrow p_1 = \frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right)$

$p_2 + p_1 + p_3 = 1$

$\Rightarrow p_2 = 1 - p_1 - p_3$

$\therefore p_2 = 1 - \frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right) - p_3$

$= 1 - \left(p_3 - \frac{U}{\epsilon N}\right) - p_3$

$= 1 + \frac{U}{\epsilon N} - 2p_3$.

$\therefore p_1 = \frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right)$

$p_2 = 1 + \frac{U}{\epsilon N} - 2p_3$.

$p_3 = p_3$

$S = -k_B N(p_1 \ln p_1 + p_2 \ln p_2 + p_3 \ln p_3)$

$$S = -k_B N\left[\frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right)\ln\left\{\frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right)\right\} + \left(1 + \frac{U}{\epsilon N} - 2p_3\right)\ln\left\{\left(1 + \frac{U}{\epsilon N} - 2p_3\right)\right\} + p_3 \ln p_3\right]$$

$\frac{dS}{dp_3} = (1) + (2) + (3)$

$$(3):\ \frac{dS}{dp_3(3)} = \frac{d}{dp_3}(p_3 \ln p_3)$$

$$= \ln p_3 + p_3 \frac{1}{p_3}$$

$$= \ln p_3 + 1$$

$$(2)\ \frac{dS}{dp_3(2)} = \frac{d}{dp_3}\left(\left(1 + \frac{U}{\epsilon N} - 2p_3\right)\ln\left\{\left(1 + \frac{U}{\epsilon N} - 2p_3\right)\right\}\right)$$

$$= -2\ln\left(1 + \frac{U}{\epsilon N} - 2p_3\right) + \cancel{\left(1 + \frac{U}{\epsilon N} - 2p_3\right)}^{1} \cdot \frac{1}{\cancel{\left(1 + \frac{U}{\epsilon N} - 2p_3\right)}}(-2)$$

$$= -2\left(\ln\left(1 + \frac{U}{\epsilon N} - 2p_3\right) + 1\right)$$

$$1)\ \frac{dS}{dp_3(1)} = \frac{d}{dp_3}\left(\frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right)\ln\left(\frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right)\right)\right)$$

$$= \frac{d}{dp_3}\left(\left(p_3 - \frac{U}{\epsilon N}\right)\left(\ln\left(p_3 - \frac{U}{\epsilon N}\right)\right)\right)$$

$$= (1)\ln\left(p_3 - \frac{U}{\epsilon N}\right) + \left(p_3 - \frac{U}{\epsilon N}\right)\frac{1}{\left(p_3 - \frac{U}{\epsilon N}\right)} \cdot (1)$$

$$= \ln\left(p_3 - \frac{U}{\epsilon N}\right) + 1$$

$$\therefore \frac{dS}{dp_3} = \ln p_3 + 1 - 2\left(\ln\left(1 + \frac{U}{\epsilon N} - 2p_3\right) + 1\right) + \ln\left(p_3 - \frac{U}{\epsilon N}\right) + 1 = 0$$

$$= \ln p_3 + 1 - 2\ln\left(1+\frac{U}{\epsilon N}-2p_3\right) - 2 + \ln\left(p_3 - \frac{U}{\epsilon N}\right) + 1 = 0$$

$$= \ln p_3 - 2\ln\left(1+\frac{U}{\epsilon N}-2p_3\right) + \ln\left(p_3-\frac{U}{\epsilon N}\right) = 0$$

$$= \exp\left(\ln p_3 - 2\ln\left(1+\frac{U}{\epsilon N}-2p_3\right) + \ln\left(p_3-\frac{U}{\epsilon N}\right)\right) = \exp(0)$$

$$= e^{\ln p_3 - 2\ln\left(1+\frac{U}{\epsilon N}-2p_3\right) + \ln\left(p_3-\frac{U}{\epsilon N}\right)} = 1$$

$$= e^{\ln p_3}\, e^{-2\ln\left(1+\frac{U}{\epsilon N}-2p_3\right)}\, e^{\ln\left(p_3-\frac{U}{\epsilon N}\right)} = 1$$

$$= p_3\, e^{\ln\left(\frac{1}{\left(1+\frac{U}{\epsilon N}-2p_3\right)^2}\right)} \left(p_3-\frac{U}{\epsilon N}\right) = 1$$

$$= p_3 \frac{1}{\left(1+\frac{U}{\epsilon N}-2p_3\right)^2}\left(p_3-\frac{U}{\epsilon N}\right) = 1$$

$$= p_3\left(p_3-\frac{U}{\epsilon N}\right) = \left(1+\frac{U}{\epsilon N}-2p_3\right)^2$$

$$\Rightarrow p_3(p_3-x) = (1+x-2p_3)^2, \quad x = \frac{U}{\epsilon N}$$

$$\Rightarrow p_3^2 - p_3 x = (1+x-2p_3)(1+x-2p_3)$$

$$\Rightarrow \cancel{p_3^2} - \cancel{p_3 x} = (1+x-2p_3+x+x^2-2p_3x - 2p_3 - \cancel{2p_3x} + \cancel{4p_3^2})$$

$$\Rightarrow 0 = 1 + x - 2p_3 + x + x^2 - 2p_3x - 2p_3 - p_3x + 3p_3^2$$

$$= 1 + 2x - 4p_3 - 3p_3x + x^2 + 3p_3^2$$

$$= 1 + 2x + x^2 - 3p_3x - 4p_3 + 3p_3^2$$

$$= (1+x)^2 - p_3(4+3x) + 3p_3^2$$

$$= 3p_3^2 - p_3(4+3x) + (1+x)^2$$

Let's use the quadratic formula:

$$\Rightarrow p_3 = \frac{-b \pm \sqrt{b^2-4ac}}{2a}; \quad a = 3,\ b = -(4+3x),\ c = (1+x)^2, \text{ where } x = \frac{U}{\epsilon N}$$

$$\Rightarrow p_3 = \frac{(4+3x) \pm \sqrt{(4+3x)^2 - 4(3)(1+x)^2}}{6}$$

$$= \frac{4+3x \pm \sqrt{16+24x+9x^2 - 12(1+2x+x^2)}}{6}$$

$$= \frac{4+3x \pm \sqrt{16+24x+9x^2-12-24x-12x^2}}{6}$$

$$= \frac{4+3x \pm \sqrt{4-3x^2}}{6}$$

$$\lim_{x\to 0} = \frac{4\pm\sqrt{4}}{6} = \frac{4\pm 2}{6} = 1 \text{ or } 1/3 \quad \because p_3 < 1, \text{ the subtractive option must be correct.}$$

$$\therefore p_3 = \frac{4+3x-\sqrt{4-3x^2}}{6}, \text{ where } x = \frac{U}{\epsilon N},$$

$$\Rightarrow p_1 = \frac{1}{\epsilon}\left(p_3\epsilon - \frac{U}{N}\right)$$

$$\Rightarrow p_2 = 1 + \frac{U}{\epsilon N} - 2p_3. \quad 1 \geq p_3 \geq 0$$

Note,

$p_1 = p_3 - x$

$p_2 = 1 + x - 2p_3$

Lets, test the bounds.

$0 < p_3 < 1$:

$$0 = \frac{4+3x-\sqrt{4-3x^2}}{6}$$

$$\Rightarrow 4+3x = -\sqrt{4-3x^2}$$

$$\Rightarrow 16+24x+9x^2 = 4-3x^2$$

$$\Rightarrow 12+24x+12x^2 = 0$$

$$\Rightarrow (1+2x+x^2) = 0$$

$\Rightarrow \quad (1+x)^2 = 0$

$\Rightarrow \quad x = -1.$

$\Rightarrow \quad 1 = \dfrac{4+3x - \sqrt{4-3x^2}}{6}$

$\Rightarrow \quad 6 = 4+3x - \sqrt{4-3x^2}$

$\Rightarrow \quad 2+3x = -\sqrt{4-3x^2}$

$\Rightarrow \quad (2+3x)^2 = 4-3x^2$

$\Rightarrow \quad 4+12x+9x^2 = 4-3x^2$

$\Rightarrow \quad 12x+12x^2 = 0$

$\Rightarrow \quad x+x^2 = 0$

$\Rightarrow \quad x(x+1) = 0$

$\Rightarrow \quad x = 0, \; x = -1$

$\therefore \quad -1 \le x \le 0$

$\therefore$ Solutions:

Note,

$p_1 = p_3 - x$

$p_2 = 1+x-2p_3$

$p_3 = \dfrac{4+3x - \sqrt{4-3x^2}}{6}$

Thus, the following can be stated.

$$\boxed{\begin{aligned} p_1 &= \frac{4+3x-\sqrt{4-3x^2}}{6} - x \qquad x \in [-1, 0] \\ p_2 &= 1+x-2\left(\frac{4+3x-\sqrt{4-3x^2}}{6}\right) \\ p_3 &= \frac{4+3x-\sqrt{4-3x^2}}{6} \end{aligned}}$$

Now, let's review the canonical ensemble:

Here's what's needed:

$\sum_i (\ln(n_i) + \alpha + \beta \epsilon_i) = 0$ → Lagrange Constraint that Canonical ensemble is based on.

$\Rightarrow n_i = A e^{-\beta \epsilon_i}$

Recall, $dU = \sum_i \epsilon_i dn_i = T dS = -k_B T \sum_i \ln(n_i) d_i$

$\Rightarrow \sum_i \epsilon_i dn_i = -k_B T \sum_i \ln(n_i) dn_i$

$\Rightarrow \epsilon_i \propto -k_B T \ln(n_i)$

$\Rightarrow \ln(n_i) \propto -\frac{\epsilon_i}{k_B T}$

$\Rightarrow n_i \propto e^{-\epsilon_i / k_B T}$

$\Rightarrow n_i = A e^{-\epsilon_i / k_B T}$

$\Rightarrow p_i = \frac{n_i}{N} = \frac{n_i}{\sum_i n_i} = \frac{A e^{-\epsilon_i / k_B T}}{A \sum e^{-\epsilon_i / k_B T}} = \frac{e^{-\epsilon_i / k_B T}}{\sum_i e^{-\epsilon_i / k_B T}}$

Where,

$Z = \sum_i e^{-\epsilon_i / k_B T}$, $\tilde{\tau} = k_B T$

$\Rightarrow Z = \sum e^{-\epsilon_i / \tilde{\tau}}$

Thus, $p_i = \frac{e^{-\epsilon_i / \tilde{\tau}}}{\sum e^{-\epsilon_i / \tilde{\tau}}}$

Note the cases:

(i) Spin-flip, $\epsilon = \{\epsilon_1, \epsilon_2\} = \{-\epsilon, \epsilon\}$

(ii) Pauli-Magnet, $\epsilon = \{\epsilon_1, \epsilon_2, \epsilon_3\} = \{-\epsilon, 0, \epsilon\}$

(i) Using, $p_i = \frac{e^{-\epsilon_i / \tilde{\tau}}}{\sum e^{-\epsilon_i / \tilde{\tau}}}$;

$\Rightarrow p_1 = \frac{e^{\epsilon / \tilde{\tau}}}{e^{\epsilon / \tilde{\tau}} + e^{-\epsilon / \tilde{\tau}}}$

$\Rightarrow p_2 = \frac{e^{-\epsilon / \tilde{\tau}}}{e^{\epsilon / \tilde{\tau}} + e^{-\epsilon / \tilde{\tau}}}$

$\therefore p_1 = \frac{e^{\epsilon / \tilde{\tau}}}{2\cosh(\epsilon / \tilde{\tau})}$, $p_2 = \frac{e^{-\epsilon / \tilde{\tau}}}{2\cosh(\epsilon / \tilde{\tau})}$

$\Rightarrow U = n_1 \epsilon_1 + n_2 \epsilon_2$

$\Rightarrow U = -n_1 \epsilon + n_2 \epsilon$

$\Rightarrow U = \epsilon(n_2 - n_1)$

$\therefore U = \epsilon N (p_2 - p_1)$, $M = \mu_B (p_1 - p_2) N$.

$S = -N k_B [p_1 \ln p_2 + p_2 \ln p_2]$

(ii) Using, $p_i = \frac{e^{-\epsilon_i / \tilde{\tau}}}{\sum e^{-\epsilon_i / \tilde{\tau}}}$;

$\Rightarrow p_1 = \frac{e^{\epsilon / \tilde{\tau}}}{e^{\epsilon / \tilde{\tau}} + e^{-\epsilon / \tilde{\tau}} + 1}$

$\Rightarrow p_2 = \frac{1}{e^{\epsilon / \tilde{\tau}} + e^{-\epsilon / \tilde{\tau}} + 1}$

$\Rightarrow p_3 = \frac{e^{-\epsilon / \tilde{\tau}}}{e^{\epsilon / \tilde{\tau}} + e^{-\epsilon / \tilde{\tau}} + 1}$

$\therefore p_1 = \frac{e^{\epsilon / \tilde{\tau}}}{2\cosh(\epsilon / \tilde{\tau}) + 1}$, $p_2 = \frac{1}{2\cosh(\epsilon / \tilde{\tau}) + 1}$, $p_3 = \frac{e^{-\epsilon / \tilde{\tau}}}{2\cosh(\epsilon / \tilde{\tau}) + 1}$

$\Rightarrow U = n_1 \epsilon_1 + n_2 \epsilon_2 + n_3 \epsilon_3$

$\Rightarrow U = -n_1 \epsilon + n_3 \epsilon = N\epsilon(p_3 - p_1)$

$\Rightarrow M = \mu_B (p_1 - p_3) N$

$\Rightarrow S = -Nk_B[p_1 \ln p_1 + p_2 \ln p_2 + p_3 \ln p_3]$

Thus, for summation in both cases:

(i) $\therefore p_1 = \dfrac{e^{\epsilon/\hat{\tau}}}{2\cosh(\epsilon/\hat{\tau})}$, $p_2 = \dfrac{e^{-\epsilon/\hat{\tau}}}{2\cosh(\epsilon/\hat{\tau})}$, where $Z = 2\cosh(\epsilon/\hat{\tau})$

$U = \epsilon N(p_2 - p_1)$, $M = \mu_B(p_1 - p_2)N$.

$S = -Nk_B[p_1 \ln p_2 + p_2 \ln p_2]$

(ii) $\therefore p_1 = \dfrac{e^{\epsilon/\hat{\tau}}}{2\cosh(\epsilon/\hat{\tau}) + 1}$, $p_2 = \dfrac{1}{2\cosh(\epsilon/\hat{\tau}) + 1}$, $p_3 = \dfrac{e^{-\epsilon/\hat{\tau}}}{2\cosh(\epsilon/\hat{\tau}) + 1}$

$U = N\epsilon(p_3 - p_1)$, $M = \mu_B(p_1 - p_3)N$

$S = -Nk_B[p_1 \ln p_1 + p_2 \ln p_2 + p_3 \ln p_3]$