Problem III.9

Using the microcanonical ensemble, we have to count the number of ways in which the N particles can be distributed amongst the three energy levels, subject to the two constraints:

① $N = n_1 + n_{-1} + n_0$

② $E = -h(n_1 - n_{-1})$

note the sign here

Clearly, if n_0 specific particles (THEY ARE distinguishable) have $S=0$, the remaining $N-n_0$ particles can be treated as having two energy levels (like in III.7 and III.8)

Thus, the number of microstates is

$$Z(E,N) = \sum_{n_0=0 \text{ or } 1}^{N-|E|/h} \binom{N}{n_0}\binom{N-n_0}{n_1} = \sum_{n_0=0 \text{ or } 1}^{N-|E|/h} \Phi(n_0,E,N)$$

The first factor $\binom{N}{n_0}$ is the number of ways of choosing n_0 particles out of N, while the second $\binom{N-n_0}{n_1}$ is the number of ways of choosing, say, n_1 particles out of the remaining $N-n_0$. Note: $S=1$ corresponds to the lower energy level, and $n_1 = \frac{N-n_0-E/h}{2}$

Concerning the limits of the sum:

Let us rewrite $n_0 = N - \frac{E}{h} - 2n_1$, and

$$\therefore n_{-1} = \frac{E}{h} + n_1$$

□ Therefore: the smallest value for $n_0 = \begin{cases} 0, & N-\frac{E}{h} \text{ is even} \\ 1, & N-\frac{E}{h} \text{ is odd} \end{cases}$

Problem III.9 | Sheet 2

□ The largest value of n_0 corresponds to the lowest value of n_1. For n_1, the smallest value is

$$n_1 = \begin{cases} 0, & \text{if } E \geq 0 \\ n_1 = -\frac{E}{h}, & \text{if } E < 0 \end{cases} \quad \text{(from the second constraint)}$$

∴ The first constraint gives the largest value of n_0 as $N - \frac{|E|}{h}$.

Thus, we have expressed $Z(E,N)$ through n_0 – the number of particles occupying the level which <u>no contribution</u> to the total energy.

This sum over n_0 is difficult to evaluate in the closed form. However, when $N \to \infty$ it can be approximated by a single term, corresponding to the value of n_0 for which $\Phi(n_0, E, N)$ is a maximum.

This is a consequence of <u>the MAXIMUM TERM METHOD</u>, which STATES THAT UNDER <u>APPROPRIATE CONDITIONS</u>, THE logarithm of a summation is essentially equal to THE logarithm of the maximum term in summation!

$$S = \sum_{i=1}^{N} T_N \text{, then } \ln S \approx \ln T_{max} \text{, and } T_{max} = O(\xi^N)$$

<u>N must be large</u>

Let us define $\varepsilon = \frac{E}{Nh}$, $x = \frac{n_0}{N}$, $y = \frac{1-\varepsilon-x}{2} = \frac{n_1}{N}$

$$z = \frac{n_{-1}}{N} = \frac{1+\varepsilon-x}{2}$$

Now, if we use Stirling's approximation in the form $N! \approx N^N e^{-N}$, we can rewrite:

$$\Phi(n_0, E, N) = \frac{N!}{n_0!\, n_1!\, n_{-1}!} \approx \left(\frac{1}{x^x y^y z^z}\right)^N \equiv f(x)^N$$

Again, we expressed everything through $x(n_0)$.

Problem III.9 | Sheet 3

More analysis shows that the function $f(x)^N$ has a sharp peak at a value $x = x^*$, with a width proportional to $\frac{1}{\sqrt{N}}$, i.e. gaussian distribution.
(For those of you who want to learn more on how a gaussian distribution is obtained, search and read about <u>the central limit theorem</u>).

Thus, the large-N limit of the entropy is
$$S = \ln Z(E,N) \approx N \ln f(x^*)$$
x^* - the value ~~of~~ max of $f(x)^N$.

To find x^*, it is easiest to maximize the quantity $\ln f = -x\ln x - y\ln y - z\ln z$
$$\frac{\partial \ln f}{\partial x} = \frac{1}{2}\ln\left(\frac{yz}{x^2}\right) = 0 \Rightarrow x^* = \frac{1}{3}\left(\sqrt{4-3\varepsilon^2}-1\right)$$

The temperature, $\frac{1}{T} = \beta = \left(\frac{\partial S}{\partial E}\right)_N = \frac{1}{h}\frac{d \ln f(x^*)}{d\varepsilon}$

Since $\left[\frac{\partial \ln f}{\partial x}\right]_{x=x^*} = 0 \Rightarrow$
$$\beta = \frac{1}{h}\left(-\frac{1}{2}\frac{\partial \ln f}{\partial y} + \frac{1}{2}\frac{\partial \ln f}{\partial z}\right)_{x=x^*} = -\frac{1}{2h}\ln\left(\frac{z(x^*)}{y(x^*)}\right)$$

Thus
$$\boxed{\frac{n_{-1}}{n_1} = \frac{z(x^*)}{y(x^*)} = e^{-2\beta h}}$$

Problem III.9 | Sheet 4

To calculate $F = E - TS$, we need to obtain E, T, S

Introduce $\rho = e^{-\beta h}$. In terms of ρ, knowing that

ⓐ $\frac{n_0 + n_1 + n_{-1}}{N} = x^* + y(x^*) + z(x^*) = 1$

ⓑ $x^{*2} = y(x^*) z(x^*)$

ⓒ $\frac{z(x^*)}{y(x^*)} = \rho^2$

we find $x^* = (\rho + 1 + \frac{1}{\rho})^{-1}$ $y(x^*) = \frac{x^*}{\rho}$, $z(x^*) = x^* \rho$

$\therefore$ $S = N \ln f(x^*) = -N [\ln x^* + x^* (\rho - \rho^{-1}) \ln \rho]$

$E = N h_E = N h [z(x^*) - y(x^*)] = N h x^* (\rho - \rho^{-1})$

$T = \frac{1}{\beta} = -\frac{h}{\ln \rho}$

$\therefore$ $\underline{\underline{F = NT \ln x^* = -NT \ln (1 + e^{-\beta h} + e^{\beta h})}}$ ||

Using the canonical ensemble we can write right away:

$$Z(T,N) = \prod_{i=1}^{N} \sum_{s_i} e^{-\beta h s_i} = (e^{-\beta h} + 1 + e^{\beta h})^N$$

and use $F = -T \ln Z(T,N)$ to obtain the same result.

Problem III.9 | Sheet 5

"Minimum information" corresponds to the condition of the system when all the levels are equally populated: $x^1 = y(x^1) = z(x^2) = \frac{1}{3}$. Apparently, this corresponds to $\rho = 1$ and $\cancel{\beta \propto \frac{h}{\ln\beta}}$. $T \to \infty$.

In this state : $\underline{\underline{S = N \ln 3}}$

The information content is a <u>maximum</u> when we know exactly the state of every particle.

This can physically happen when the energy has its minimal value $E = -Nh$ or $\beta \to +\infty$ so that $\rho = 0$ and $n_1 = N$, $\Rightarrow$ all particles occupy the lowest level. This also happens when the energy has its maximum value $E = +Nh$ corresponding to the <u>negative</u> temperature $\beta \to -\infty$, where $\rho \to \infty$, giving $n_{-1} = N$.

In either of these states we have

$$\underline{\underline{S = 0}}$$