Modern Physics Assignment - 4

1. From a canonical ensemble we know that the probability of finding a microstate ν is proportional to $P_\nu \propto \Omega(E-E_\nu)$. For $E_\nu \ll E$ use the Taylor expansion and the fact that $\beta = (1/\Omega)(\partial\Omega/\partial E)|_{N,V}$ to prove $P_\nu \propto \exp(-\beta E_\nu)$

A. Given, $P_\nu \propto \Omega(E-E_\nu)$

(and) $E_\nu \ll E$

Consider,

$$\ln(\Omega(E-E_\nu)) = \ln(\Omega(E)) - \left(\frac{1}{\Omega}\frac{\partial\Omega}{\partial E}\right)E_\nu + \dots$$

Using the Taylor Series expansion,

$$f(x+h) = f(x) + h \cdot f'(x) + \frac{h^2}{2!}f''(x) + \dots$$

$$\Rightarrow \ln(\Omega(E-E_\nu)) = \ln(\Omega(E)) - \frac{1}{\Omega}\left(\frac{\partial\Omega}{\partial E}\right)E_\nu$$

Given that, $\beta = \frac{1}{\Omega}\frac{\partial\Omega}{\partial E}$

$$\Rightarrow \ln(\Omega(E-E_\nu)) = \ln(\Omega(E)) - \cancel{\frac{1}{\Omega}}\beta E_\nu$$

$$\Rightarrow \Omega(E-E_\nu) = \underbrace{\Omega(E)}_{\text{constant}} \times e^{-\beta E_\nu}$$

$$\Rightarrow P_\nu \propto \exp(-\beta E_\nu)$$

For a grand canonical ensemble, show that

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} + \mu \langle N \rangle$$

For the sake of simplicity, I'll replace summation with integral

$$Z = \sum_v \exp(-\beta E_v + \beta \mu N_v)$$

$$Z = \int \exp(-\beta E_v + \beta \mu N_v)\, dv$$

We already know that;

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial \ln Z}{\partial \mu}$$

$$\langle E \rangle = \sum_v P_v E_v = \sum_v E_v e^{-\beta E_v} e^{\beta \mu N_v} / Z$$

Consider,

$$Z = \int \exp(-\beta E_v + \beta \mu N_v)\, dv$$

$$\Rightarrow \frac{1}{Z}\frac{\partial Z}{\partial \beta} = \mu \sum \frac{N_v \exp(\beta \mu N_v - \beta E_v)}{Z} - \frac{\sum E_v \exp(\beta \mu N_v - \beta E_v)}{Z}$$

$$\Rightarrow \frac{\partial \ln Z}{\partial \beta} = \mu \langle N \rangle - \langle E \rangle$$

$$\Rightarrow \langle E \rangle = \mu \langle N \rangle - \frac{\partial \ln Z}{\partial \beta}$$

Q. Consider a 2 dimensional square lattice of $N \times N$ lattice points in the x-y plane. At each lattice point a rod is placed which can take 3 possible orientations. It can lie horizontally along the x-axis or y-axis, in which case its energy is zero. Or it can be upright along the vertical z-axis, in which case it has energy ϵ. If the system has an energy $E = n\epsilon$, where n represents the no. of rods standing upright such that $0 \le n \le N^2$, calculate the no. of microstates of the system as a fn n, $\Omega(n)$.

A. Given, there are a total of 'N^2' lattice points, in x-y plane

Energy of system, $E = n\epsilon$, where $0 \le n \le N^2$

This implies, there are 'n' rods which are upright along the vertical z-axis

No. of possibilities of positions of these 'n' rods $= {}^{N^2}C_n$

Remaining lattice pts. (or rods) $= N^2 - n$

Each of the rods on these lattice pts. lie either along 'x' or 'y' axis

$\Rightarrow$ Possibilities of positions $= (2 \times 2 \times 2 \ldots)_{N^2 - n \text{ times}}$

Therefore, total no. of microstates

$$\Omega(n) = {}^{N^2}C_n \times 2^{N^2 - n}$$

4. A DNA molecule can be considered as long chain of links which can be open or closed. Open links have energy Δ while closed links have energy 0. A link can be open only if the link to its left is also open (ignore the left and right symmetry for simplicity). If n are open and m are closed, then $n+m=N$. Calculate the canonical partition function $Q(N, \beta)$. If

$\Delta = 1eV$ and $\beta = 0.01 eV^{-1}$, find out how many links are open on average in the limit of large N.

A. Canonical Partition Fn. $Q(N,\beta) = \sum e^{-\beta E_v}$

For E_v (possibilities)

when all links are closed (min) = 0

(For max)

when all links are open

$$E_v = (N-1)\Delta$$

(As the left most link has no link to its left)

$$Q = \sum e^{-\beta E_v}$$

$$= 0 + e^{-\beta\Delta} + e^{-2\beta\Delta} + \ldots\ldots e^{-(N-1)\Delta\beta}$$

$$Q = \frac{e^{-N\Delta\beta} - 1}{e^{-\Delta\beta} - 1}$$

For large values of 'N', $e^{-N\Delta\beta} \to 0$

$$\Rightarrow \quad Q = \frac{1}{1 - e^{-\Delta\beta}} = 100 \quad \left(\begin{array}{c}\text{Substituting}\\ \text{vals of } \Delta \text{ and } \beta\end{array}\right)$$

5. Consider a quantum system which has 2 energy levels 0.5eV, 1 eV. Take its grand canonical ensemble made up of bosons. It has a temperature of 300 K and a chemical potential of 0.49eV. Calculate the average number of particles in the system and the average energy of the system.

A. Given, for boson particles

$$\epsilon_1 = 0.5\,eV \; ; \; \epsilon_2 = 1\,eV$$

$$\mu = 0.49\,eV \; ; \; T = 300\,K$$

WKT,

Avg. occupation no. $\langle n_j \rangle = \dfrac{1}{e^{\beta(\epsilon_j - \mu)} - 1}$

where j is the energy level

$$\beta = \frac{1}{k_B T} \; ; \Rightarrow \beta = \frac{1}{300 \times 1.38 \times 10^{-23}} = \frac{2.41 \times 10^{-20}}{m^2\,kg\,s^{-2}}$$

Calculating,

$$\langle n_1 \rangle = \frac{1}{e^{\beta(0.5-0.49)eV} - 1} = 2.127$$

$$\langle n_2 \rangle = \frac{1}{e^{\beta(1-0.49)eV} - 1} \approx 0$$

$\Rightarrow$ Avg. no. of particles in system, $\langle N \rangle = \langle n_1 \rangle + \langle n_2 \rangle$
$= 2.127$

Avg. energy,

$$\langle E \rangle = \epsilon_1 \times \langle n_1 \rangle + \epsilon_2 \times \langle n_2 \rangle$$

$$= 0.5 \times 2.127 + 0 = 1.06\,eV$$

6. Consider a system whose free energy is given as following. Calculate the order of phase transition which occurs at $T = T_c$

$$G = \begin{cases} a\left(1-\frac{T}{T_c}\right)^2 & \text{if } T < T_c \\ a\left(1-\frac{T}{T_c}\right)^2 + b\left(1-\frac{T}{T_c}\right)^3 & \text{if } T > T_c \end{cases}$$

A. To find the order of phase transition, we have to find the value of 'n' for which the nth order derivative is discontinuous

$n=1$

$$\frac{\partial G}{\partial T} = \begin{cases} 2a\left(1-\frac{T}{T_c}\right)\left(\frac{-1}{T_c}\right) & ; \ T < T_c \\ 2a\left(1-\frac{T}{T_c}\right)\left(\frac{-1}{T_c}\right) + 3b\left(-\frac{1}{T_c}\right)\left(1-\frac{T}{T_c}\right)^2 & ; \ T > T_c \end{cases}$$

Putting $T = T_c$, it is cont.

$n=2$

$$\frac{\partial^2 G}{\partial T^2} = \begin{cases} \frac{2a}{T_c^2} & ; \ T < T_c \\ \frac{2a}{T_c^2} + \frac{3b}{T_c^2} \times 2 \times \left(1-\frac{T}{T_c}\right) & ; \ T > T_c \end{cases}$$

Putting $T = T_c$, it is cont.

$n=3$

$$\frac{d^3 G}{dT^3} = \begin{cases} 0 & ; \ T < T_c \\ 0 - \frac{6b}{T_c^3} & ; \ T > T_c \end{cases}$$

Clearly, its discontinuous

$\Rightarrow$ Order of phase transition, $n = 3$