

ASSIGNMENT #1

(SOLUTIONS)

QNO1

The gas in question is a closed, thermally isolated system, described by the microcanonical ensemble.

⇒ Entropy is defined as

$$S = k \ln \Gamma(E)$$

where $\Gamma(E)$ is the number of microstates corresponding to the fixed energy E .

⇒ The Hamiltonian of the given ideal gas of N classical monatomic particles, contained in a d -dimensional box of volume V ; is

$$H = \sum_{i=1}^{dN} \frac{p_i^2}{2m}$$

and $\Gamma(E)$ is

$$\Gamma(E) = \frac{1}{h^{dN}} \int_{H(q,p)=E} dq^{dN} dp^{dN}$$

$$= \frac{V^N}{h^{dN}} \int_{\sum_{i=1}^{dN} p_i^2 = 2mE} dP^{dN}$$

where the factor V^N is the result of integrating over the coordinates q 's - and momentum integral is the volume of a dN -dimensional sphere with radius $R = \sqrt{2mE}$.

$$\Gamma(E) = \frac{V^N}{h^{dN}} S_{dN}(R) \quad \text{--- (1)}$$

\Rightarrow Obviously, $S_{dN}(R)$ will be proportional to R^{dN} , so let it be written as.

$$S_{dN} = \int_{x_1^2 + x_2^2 + \dots + x_{dN}^2 = R^2} dx_1 dx_2 \dots dx_{dN} = C_{dN} R^{dN} \quad \text{--- (2)}$$

where C_{dN} is a constant which depends only on the dimensionality of space. Clearly, the "volume element" $dS_{dN}(R)$ can also be written as

$$dS_{dN} = dx_1 dx_2 \dots dx_{dN} = d(C_{dN} R^{dN}) = dN C_{dN} R^{dN-1} dR$$

\Rightarrow To evaluate C_{dN} , we make use of the formula

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

\Rightarrow Multiplying ($n=dN$) such integrals, one for each x_i , we obtain

$$\left(\pi^{\frac{1}{2}}\right)^{dN} = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \dots \int_{-\infty}^{\infty} dx_{dN} e^{-(x_1^2 + x_2^2 + \dots + x_{dN}^2)}$$

$$\pi^{dN/2} = \int_0^\infty e^{-R^2} dN C_{dN} R^{dN-1} dR$$

$$\Rightarrow \frac{\pi^{dN/2}}{C_{dN} dN} = \int_0^\infty e^{-R^2} R^{dN-1} dR \quad \text{--- (A)}$$

\because Gaussian integral $\int_0^\infty x^n e^{-ax^2} dx = \frac{1}{2} \frac{\Gamma(\frac{n+1}{2})}{\sqrt{a}^{n+1}}$

therefore, Eq (A) becomes.

$$\frac{\pi^{dN/2}}{C_{dN} dN} = \frac{1}{2} \frac{\Gamma(\frac{dN+1}{2})}{1}$$

$$\Rightarrow \frac{\pi^{dN/2}}{\frac{dN}{2}} \cdot \frac{1}{\Gamma(\frac{dN}{2})} = C_{dN}$$

$$\because \Gamma(n) = (n-1)!$$

$$\Rightarrow \Gamma(\frac{dN}{2}) = (\frac{dN}{2}-1)!$$

$$\Rightarrow C_{dN} = \frac{\pi^{dN/2}}{\frac{dN}{2} (\frac{dN}{2}-1)!}$$

$$C_{dN} = \frac{\pi^{dN/2}}{(\frac{dN}{2})!}$$

$$\because n(n-1)! = n!$$

\Rightarrow plug in Eq (2),

$$S_{dN} = \frac{\pi^{dN/2}}{(\frac{dN}{2})!} R^{dN}$$

and relation for accessible states is

$$\Gamma(E) = \frac{V^N}{h^{dN}} \frac{\pi^{dN/2} R^{dN}}{\left(\frac{dN}{2}\right)!}$$

$$\Rightarrow S = k \ln \Gamma(E)$$

$$= k \ln \left[\frac{V^N \pi^{dN/2} R^{dN}}{h^{dN} \left(\frac{dN}{2}\right)!} \right]$$

$$\because \ln N! \approx N \ln N - N \quad \text{for } N \gg 1$$

$$\text{and } R = \sqrt{2mE}$$

$$\Rightarrow S = k \ln \left[\frac{V^N \pi^{dN/2} (2mE)^{dN/2}}{h^{dN} \left(\frac{dN}{2}\right)!} \right]$$

$$\approx k \left[\ln \pi^{dN/2} - \frac{dN}{2} \ln \left(\frac{dN}{2}\right) + \frac{dN}{2} \right] + k \ln \left[\frac{V^N (2mE)^{dN/2}}{h^{dN}} \right]$$

$$= k \left[N \ln \pi^{d/2} - N \frac{d}{2} \ln \left(\frac{dN}{2}\right) + N \frac{d}{2} \right] + k N \ln \left(\frac{V (2mE)^{d/2}}{h^d} \right)$$

$$= k N \left[\ln \pi^{d/2} - \frac{d}{2} \ln \left(\frac{dN}{2}\right) + \frac{d}{2} + \ln \left(\frac{V (2mE)^{d/2}}{h^d} \right) \right]$$

$$= k N \left[\ln \pi^{d/2} - \ln \left(\frac{dN}{2}\right)^{d/2} + \ln V + \ln \left(\frac{2mE}{h^2} \right)^{d/2} + \frac{d}{2} \right]$$

$$S \approx k N \left\{ \ln \left[V \left(\frac{4\pi m E}{dN h^2} \right)^{d/2} \right] + \frac{d}{2} \right\} \quad \text{--- (3)}$$

\Rightarrow To obtain equation of state, use the First Law of thermodynamics

$$\therefore dE = dQ + dW$$

$$dE = TdS - PdV$$

(for $N = \text{constant}$)

$$\Rightarrow dS = \frac{1}{T} dE + \frac{P}{T} dV \quad \text{--- (B)}$$

$$\Rightarrow S = S(E, V)$$

$$dS = \left(\frac{\partial S}{\partial E} \right)_V dE + \left(\frac{\partial S}{\partial V} \right)_E dV \quad \text{--- (C)}$$

$$\Rightarrow \frac{P}{T} = \left(\frac{\partial S}{\partial V} \right)_E$$

$$P = T \left(\frac{\partial S}{\partial V} \right)_E \quad \text{--- (4)}$$

Take derivative of Eq (3) w.r.t V at constant E, N

$$\Rightarrow \left(\frac{\partial S}{\partial V} \right)_{E, N} = kN \frac{\partial}{\partial V} (\ln V) = \frac{kN}{V} \quad \text{--- (5)}$$

\Rightarrow From Eq (4) and Eq (5),

$$P = T \frac{kN}{V} \quad \Rightarrow PV = NkT$$

\Rightarrow We can also find the temperature:

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{V, N}$$

\therefore compare Eq (B) and (C)

\rightarrow take derivative of Eq (3) w.r.t E at constant V, N

$$\left(\frac{\partial S}{\partial E} \right)_{V, N} = kN \frac{\partial}{\partial E} (\ln E^{d/2}) = kN \frac{\partial}{\partial E} \left(\frac{d}{2} \ln E \right)$$

$$= kN \frac{d}{2} \frac{\partial}{\partial E} (\ln E) = \frac{dkN}{2E}$$

$$\Rightarrow \frac{1}{T} = \frac{dkN}{2E}$$

or $E = \frac{d}{2} NkT$ is relation for energy of a

monatomic classical ideal gas.

QNo2

According to the relativistic energy-momentum relation,

$$E = \sqrt{P^2 c^2 + m^2 c^4},$$

while for highly relativistic particles, their rest energy can be neglected, and the total energy of the gas is

$$H = c \sum_{i=1}^N P_i$$

so D is the region $\sum_i P_i = \frac{E}{c}$ and $\Gamma(E)$ is the volume of phase space corresponding to energy equal to E .

$$\Gamma(E) = \frac{1}{h^{3N}} \int_D \prod_{i=1}^N d^3 q_i d^3 p_i$$

\Rightarrow Since the positions and the directions of the momenta of the particles are unconstrained, we can write for each particle;

$$\int d^3 q \int d^3 p = 4\pi V \int p^2 dp, \quad \text{so}$$

$$\Gamma(E) = \left(\frac{4\pi V}{h^3} \right)^N \int_D \prod_{i=1}^N p_i^2 dp_i \equiv \left(\frac{4\pi V}{h^3} \right)^N \underline{I_N(E)}$$

\Rightarrow To evaluate integral $I_N(E)$, we note that, if the momentum of one particle is fixed to the value P , then the integral for the remaining particles is $I_{N-1}(E - PC)$

\Rightarrow We have

$$I_N(E) = \int_0^{E/c} dP P^2 I_{N-1}(E - PC)$$

Then dimensional analysis tells us that

$$I_N = C_N \left(\frac{E}{C}\right)^{3N}$$

$$\therefore \int_0^P P^2 dP = \frac{P^3}{3}$$

and substituting this in the above equation yields a recursion relation for the number C_N :

$$C_N \left(\frac{E}{C}\right)^{3N} = \int_0^{E/C} P^2 dP C_{N-1} \left(\frac{E}{C} - P\right)^{3N-3}$$

$$\therefore I_{N-1} = C_{N-1} \left(\frac{E}{C}\right)^{3(N-1)}$$

$$\Rightarrow I_{N-1} (E-PC) = C_{N-1} \left(\frac{E-P}{C}\right)^{3N-3}$$

$$\Rightarrow C_N = \left(\frac{C}{E}\right)^{3N} \int_0^{E/C} P^2 dP C_{N-1} \left(\frac{E}{C} - P\right)^{3N-3}$$

$$= \left(\frac{C}{E}\right)^{3N-3+3} \int_0^{E/C} P^2 dP C_{N-1} \left(\frac{E}{C} - P\right)^{3N-3}$$

$$= \left(\frac{C}{E}\right)^3 \int_0^{E/C} P^2 dP C_{N-1} \left(1 - \frac{PE}{E}\right)^{3N-3}$$

Let $x = \frac{PC}{E}$

$$\Rightarrow dx = dP \frac{C}{E}$$

$$= \int_0^{E/C} \left(\frac{CP}{E}\right)^2 \left(\frac{C}{E} dP\right) C_{N-1} \left(1 - \frac{PC}{E}\right)^{3N-3}$$

$$= \int_0^1 x^2 dx (1-x)^{3N-3} C_{N-1}$$

as $P \rightarrow 0, x \rightarrow 0$

$P \rightarrow \frac{E}{C}, x \rightarrow 1$

$$\Rightarrow \frac{C_N}{C_{N-1}} = \int_0^1 x^2 (1-x)^{3N-3} dx$$

$$\text{Let } \int_0^1 x^2 (1-x)^{3N-3} dx$$

$$= -\int_1^0 (1-z)^2 z^{3N-3} dz$$

$$= \int_0^1 (1-z)^2 z^{3N-3} dz$$

$$= \int_0^1 (1+z^2-2z) z^{3N-3} dz$$

$$= \int_0^1 z^{3N-3} dz + \int_0^1 z^{2+3N-3} dz - 2 \int_0^1 z^{1+3N-3} dz$$

$$= \frac{z^{3N-3+1}}{(3N-3+1)} \Big|_0^1 + \frac{z^{3N-1+1}}{(3N-1+1)} \Big|_0^1 - 2 \frac{z^{3N-2+1}}{(3N-2+1)} \Big|_0^1$$

$$= \frac{1}{3N-2} + \frac{1}{3N} - \frac{2}{3N-1}$$

$$= \frac{3N(3N-1) + (3N-2)(3N-1) - 2(3N)(3N-2)}{3N(3N-1)(3N-2)}$$

$$= \frac{3N(3N) - 3N + 3N(3N) - 3N - 2(3N)^2 + 2 - 2(3N)^2 + 4(3N)}{3N(3N-1)(3N-2)}$$

$$= \frac{2}{3N(3N-1)(3N-2)}$$

$$= \frac{2(3N-3)(3N-4)(3N-5) \dots 1}{3N(3N-1)(3N-2)(3N-3)(3N-4)(3N-5) \dots 1}$$

$$= \frac{2(3N-3)!}{(3N)!}$$

$$\because k! = k(k-1)(k-2) \dots 1$$

$$\because 1-x = z$$

$$1-z = x$$

$$-dz = dx$$

$$dx \rightarrow 0, z \rightarrow 1$$

$$x \rightarrow 1, z = 0$$

$$\Rightarrow C_N = \frac{2(3N-3)!}{(3N)!} C_{N-1}$$

$$\Rightarrow \text{Clearly, we have } C_1 = \int_0^1 x^2(1-x)^0 dx C_0$$

$$= \int_0^1 x^2 dx = \frac{1}{3}$$

and the solution to the recursion relation is

$$C_N = \frac{2^N}{(3N)!}$$

$$\Rightarrow I_N(E) = C_N \left(\frac{E}{c}\right)^{3N} = \frac{2^N}{(3N)!} \left(\frac{E}{c}\right)^{3N}$$

\Rightarrow Therefore, Eq (X) for volume of phase space becomes

$$\Gamma(E) = \left(\frac{4\pi V}{h^3}\right)^N \frac{2^N}{(3N)!} \left(\frac{E}{c}\right)^{3N}$$

$$\Gamma(E) = \left(\frac{V 8\pi E^3}{h^3 c^3}\right)^N \frac{1}{(3N)!}$$

\Rightarrow For indistinguishable particles,

$$\Gamma(E) = \frac{1}{N!} \frac{1}{(3N)!} \left(\frac{8\pi V E^3}{h^3 c^3}\right)^N$$

$$S = k_B \ln \Gamma(E)$$

$$= k_B \ln \left(\frac{1}{N!} \left(\frac{8\pi V E^3}{h^3 c^3}\right)^N \frac{1}{(3N)!} \right) \quad \text{--- (i)}$$

⇒ Temperature is defined as

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{V, N}$$

$$\therefore S = k_B \ln \left(\frac{1 (8\pi V)^N (hc)^{-3N}}{(N!) (3N)!} \cdot E^{3N} \right)$$

$$\Rightarrow \left(\frac{\partial S}{\partial E} \right)_{V, N} = 3N k_B \frac{\partial}{\partial E} (\ln E)$$

$$\frac{1}{T} = \frac{3N k_B}{E}$$

$$\boxed{\frac{E}{3N k_B} = T} \quad \text{and}$$

$$\therefore P = T \left(\frac{\partial S}{\partial V} \right)_{E, N}$$

$$= T \frac{\partial}{\partial V} (k_B \ln V^N) = N T k_B \frac{\partial}{\partial V} \ln V = \frac{N k_B T}{V}$$

$$\Rightarrow PV = N k_B T.$$

The equation of state is thus the same as for a non-relativistic gas: $PV = N k_B T$.

∴ Entropy relation in Eq. (7)

$$S = k_B \ln \left(\frac{1}{N! (3N)!} \left(\frac{8\pi V E^3}{h^3 c^3} \right)^N \right)$$

$$\therefore \text{for } N \gg 1, \quad \ln N! \approx N \ln N - N$$

$$\Rightarrow \text{Similarly, } \ln 3N! \approx 3N \ln 3N - 3N$$

$$\Rightarrow S \approx k_B \left[-N \ln N + N - 3N \ln 3N + 3N + N \ln \left(\frac{8\pi V E^3}{h^3 C^3} \right) \right]$$

$$= k_B \left[4N - N \ln N - N \ln (3N)^3 + N \ln \left(\frac{8\pi V E^3}{h^3 C^3} \right) \right]$$

$$= k_B \left[4N + N \ln \left(\frac{8\pi V E^3}{27 N^4 h^3 C^3} \right) \right]$$

$$\Rightarrow S \approx k_B N \left[\ln \left(\frac{8\pi V E^3}{27 N^4 h^3 C^3} \right) + 4 \right] \quad \text{--- } \textcircled{2}$$

Specific heat ratio:-

$$\because E = T 3N k_B$$

$$\Rightarrow E^3 = T^3 3^3 N^3 k_B^3$$

plug in $\textcircled{2}$

$$\Rightarrow S = k_B N \ln \left(\frac{8\pi V 27 N^3 k_B^3 T^3}{27 N^4 h^3 C^3} \right)$$

$$S \approx k_B N \ln \left(\frac{C_1 T^3 V}{N} \right)$$

$$\text{where } C_1 = \frac{8\pi k_B^3}{h^3 C^3}$$

$$= k_B N \ln \left(\frac{C_1 T^3 N k_B T}{P N} \right)$$

$$\because V = \frac{N k_B T}{P}$$

$$= k_B N \ln \left(\frac{C_2 T^4}{P} \right)$$

$\because C_1$ and C_2 are constants.

$$\Rightarrow S(T, V, N) = N k_B \ln \left(\frac{C_1 T^3 V}{N} \right)$$

$$S(T, P, N) = N k_B \ln \left(\frac{C_2 T^4}{P} \right)$$

\Rightarrow The specific heats are then

$$C_V = T \left(\frac{\partial S}{\partial T} \right)_{V, N} = \frac{3T N k_B T^2}{T^3} = 3N k_B$$

$$\text{and } C_P = T \left(\frac{\partial S}{\partial T} \right)_{P, N} = \frac{T 4N k_B T^3}{T^4} = 4N k_B$$

$$\Rightarrow \gamma = \frac{C_P}{C_V} = \frac{4N k_B}{3N k_B} = \frac{4}{3}$$

QNO3

Given that, a perfect crystal has N lattice sites and M interstitial locations. Total n number of atoms are displaced from site and place it in interstitial.

(a) The number of ways to choose n atoms to remove from N sites is

$$C_n^N = \frac{N!}{n!(N-n)!}$$

(b) The number of ways to choose n interstitials out of M is

$$C_n^M = \frac{M!}{n!(M-n)!}$$

(c) The number of states at total energy ($E = n\Delta$) is the number of ways to choose n atoms from N sites and place them in M interstitials, that is

$$\begin{aligned}\Gamma\left(n = \frac{E}{\Delta}\right) &= C_n^N \times C_n^M \\ &= \frac{N!}{n!(N-n)!} \frac{M!}{n!(M-n)!}\end{aligned}$$

\Rightarrow entropy is

$$S(E = \Delta n) = k_B \ln \Gamma(E)$$

$$= k_B \ln \left(\frac{N! M!}{n!(N-n)! n!(M-n)!} \right)$$

\Rightarrow Using Stirling's approximation; for $N \gg 1$ $\ln N! \approx N \ln N - N$

$$\begin{aligned}
S &= k_B [\ln N! + \ln M! - 2 \ln n! - \ln (N-n)! - \ln (M-n)!] \\
&\approx k_B [N \ln N - N + M \ln M - M - 2n \ln n + 2n - (N-n) \ln (N-n) + N-n \\
&\quad - (M-n) \ln (M-n) + M-n] \\
&= k_B [N \ln N + M \ln M - 2n \ln n - (N-n) \ln (N-n) - \underbrace{(M-n) \ln (M-n)}_{\textcircled{A}}] \\
&= k_B [N \ln N + M \ln M - 2n \ln n - N \ln (N-n) + n \ln (N-n) - M \ln (M-n) \\
&\quad + n \ln (M-n)] \\
&= k_B \left[N \ln \left(\frac{N}{N-n} \right) + M \ln \left(\frac{M}{M-n} \right) + n \ln \left(\frac{N-n}{n} \right) + n \ln \left(\frac{M-n}{n} \right) \right] \\
&= k_B \left[-N \ln \left(\frac{N-n}{N} \right) - M \ln \left(\frac{M-n}{M} \right) + n \ln \left(\frac{N-n}{n} \right) - n \ln N + n \ln N + \right. \\
&\quad \left. n \ln \left(\frac{M-n}{n} \right) - n \ln M + n \ln M \right] \\
&= k_B \left[-N \ln \left(\frac{N-n}{N} \right) - M \ln \left(\frac{M-n}{M} \right) + n \ln \left(\frac{N-n}{Nn} \right) + n \ln \left(\frac{M-n}{nM} \right) \right. \\
&\quad \left. + n \ln NM \right] \\
&= k_B \left[-N \ln \left(\frac{N-n}{N} \right) - M \ln \left(\frac{M-n}{M} \right) + n \ln \left(\frac{N-n}{N} \right) + n \ln \left(\frac{M-n}{M} \right) + n \ln \left(\frac{NM}{n^2} \right) \right] \\
&= k_B \left[n \ln \left(\frac{NM}{n^2} \right) - (N-n) \ln \left(\frac{N-n}{N} \right) - (M-n) \ln \left(\frac{M-n}{M} \right) \right] \\
S &\approx k_B \left[n \ln \left(\frac{NM}{n^2} \right) - (N-n) \ln \left(1 - \frac{n}{N} \right) - (M-n) \ln \left(1 - \frac{n}{M} \right) \right]
\end{aligned}$$

\Rightarrow temperature is defined as

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{V, N} \quad \text{where } E = \Delta n$$

$$\frac{1}{T} = \left(\frac{\partial S}{\partial \Delta n} \right) = \frac{\partial k_B \ln \Gamma(n)}{\partial (\Delta n)}$$

$$\Rightarrow \frac{1}{T} = \frac{k_B}{\Delta} \frac{\partial \ln \Gamma(n)}{\partial n}$$

$$\Rightarrow \frac{\Delta}{k_B T} = \frac{\partial}{\partial n} \ln(\Gamma(n))$$

\Rightarrow From Eq (A),

$$\ln \Gamma(n) = N \ln N + M \ln M - 2n \ln n - (N-n) \ln(N-n) - (M-n) \ln(M-n)$$

$$\Rightarrow \frac{\partial}{\partial n} \ln \Gamma(n) = \frac{\partial}{\partial n} [-2n \ln n - (N-n) \ln(N-n) - (M-n) \ln(M-n)]$$

$$= -2 \ln n - 2 - [\ln(N-n) \cdot (-1) - 1 + \ln(M-n) \cdot (-1) - 1]$$

$$= -2 \ln n - 2 + \ln(N-n) + 1 + \ln(M-n) + 1$$

$$= \ln \left(\frac{(N-n)(M-n)}{n^2} \right)$$

$$\Rightarrow \frac{\Delta}{k_B T} = \ln \left(\frac{(N-n)(M-n)}{n^2} \right)$$

Q NO4

To find the Helmholtz free energy $F(T, N)$ for the given system in microcanonical ensemble,

$$F(T, N) = E(T, N) - TS(E, N) \quad \text{--- (5)}$$

\Rightarrow Firstly, we have to find entropy and plugging 'S' in above relation, simplifying it for $F(T, N)$

\Rightarrow According to given condition,

$$N = \text{total number of particles} = n_+ + n_-$$

where n_+ is number of particles have energy $+\epsilon$
 n_- is " " " " " " " $-\epsilon$

$$\Rightarrow E_{\text{total}} = n_+ \epsilon_+ + n_- \epsilon_- = \frac{n_+}{n_-} \epsilon_+ - \epsilon_-$$

$$= (n_+ - n_-) \epsilon$$

\Rightarrow Using binomial distribution, total number of accessible microstates are

$$S(E, N) = \frac{N!}{n_+! n_-!}$$

$$= \frac{N!}{n_+! (N - n_+)!}$$

and entropy is

$$S(E, N) = k \ln S(E, N)$$

$$= k [\ln N! - \ln n_+! - \ln (N - n_+)!]$$

\Rightarrow Using Stirling approximation,

$$\ln N! \approx N \ln N - N$$

$$\Rightarrow S(E, N) \approx k [N \ln N - N - n_+ \ln n_+ + n_+ - (N - n_+) \ln (N - n_+) + (N - n_+)]$$

$$\begin{aligned}
&= k \left[N \ln N - (N - n_+) + (N - n_+) - n_+ \ln n_+ \right. & (5) \\
&\quad \left. - (N - n_+) \ln (N - n_+) \right] \\
&= k \left[N \ln N - n_+ \ln n_+ - (N - n_+) \ln (N - n_+) \right] \\
&= k \left[N \ln N - n_+ \ln n_+ - N \ln (N - n_+) + n_+ \ln (N - n_+) \right] \\
&= k \left[N \ln \left(\frac{N}{N - n_+} \right) + n_+ \ln \left(\frac{N - n_+}{n_+} \right) \right] \\
&= kN \left[\ln \left(\frac{N}{N - n_+} \right) + N^{-1} n_+ \ln \left(\frac{N - n_+}{n_+} \right) \right]
\end{aligned}$$

assume $x = \frac{n_+}{N}$, $y = \frac{n_-}{N}$

$$\Rightarrow E = (n_+ - n_-) \epsilon$$

$$\frac{E}{\epsilon} = n_+ - (N - n_+)$$

$$\frac{E}{\epsilon} = 2n_+ - N$$

$$\Rightarrow \left(\frac{E}{\epsilon N} + 1 \right) \frac{1}{2} = \frac{n_+}{N}$$

$$x = \frac{1}{2} \left(\frac{E}{\epsilon N} + 1 \right) \quad \text{--- (6)}$$

Thus, entropy $S(E, N)$ is

$$S \approx -kN \left[(1-x) \ln(1-x) + x \ln x \right] \quad \text{--- (7)}$$

⇒ To formalize Energy in terms of temperature T and N : $E(T, N)$, firstly we have to find temperature.

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_N \quad \text{--- (8)}$$

$$\therefore \frac{\partial}{\partial E} = \frac{\partial X}{\partial E} \cdot \frac{\partial}{\partial X}$$

$$\therefore X = \frac{1}{2} \left(1 + \frac{E}{\epsilon N} \right)$$

$$\frac{\partial X}{\partial E} = \frac{1}{2N\epsilon}$$

$$\Rightarrow \frac{\partial}{\partial E} = \frac{1}{2N\epsilon} \frac{\partial}{\partial X}$$

$$\Rightarrow \frac{1}{T} = \frac{1}{2N\epsilon} \left(\frac{\partial S}{\partial X} \right)_N \quad \therefore \text{using Eq (7)}$$

$$\frac{1}{T} = \frac{-k}{2\epsilon} \left[-\ln(1-x) - 1 + \ln x + 1 \right]$$

$$= \frac{-k}{2\epsilon} \left[\ln x - \ln(1-x) \right] = \frac{k}{2\epsilon} \ln \left(\frac{1-x}{x} \right)$$

$$\Rightarrow \frac{2\epsilon}{kT} = \ln \left(\frac{1-x}{x} \right)$$

$$e^{2\varepsilon/kT} = \frac{1-x}{x} \quad (6)$$

$$\Rightarrow x = \left(1 + e^{2\varepsilon/kT}\right)^{-1}$$

$$\frac{n_+}{N} = \frac{1}{2} \left(1 + \frac{E}{N\varepsilon}\right) = x = \left(1 + e^{2\varepsilon/kT}\right)^{-1}$$

$$\Rightarrow 1 + \frac{E}{N\varepsilon} = 2 \left(1 + e^{2\varepsilon/kT}\right)^{-1}$$

$$\frac{E}{N\varepsilon} = -1 + \frac{2}{\left(1 + e^{2\varepsilon/kT}\right)}$$

$$= \frac{-1 - e^{2\varepsilon/kT} + 2}{\left(1 + e^{2\varepsilon/kT}\right)}$$

$$= \frac{\left(1 - e^{2\varepsilon/kT}\right)}{\left(1 + e^{2\varepsilon/kT}\right)}$$

$$\frac{E}{N\varepsilon} = - \left(\frac{e^{2\varepsilon/kT} - 1}{e^{2\varepsilon/kT} + 1} \right)$$

$$\boxed{E = -N\varepsilon \tanh\left(\frac{\varepsilon}{kT}\right)} \quad (9)$$

\Rightarrow To further simplify Eq (7) entropy & plug in x.

$$S \approx -Nk \left[x \ln x + (1-x) \ln(1-x) \right]$$

$$= -Nk \left[\left(1 + e^{\frac{2\epsilon}{kT}}\right)^{-1} \ln \left(1 + e^{\frac{2\epsilon}{kT}}\right)^{-1} + \left(1 - \left(1 + e^{\frac{2\epsilon}{kT}}\right)^{-1}\right) \ln \left(1 - \left(1 + e^{\frac{2\epsilon}{kT}}\right)^{-1}\right) \right] \quad \text{--- (10)}$$

\Rightarrow Let

$$\left(1 + e^{\frac{2\epsilon}{kT}}\right)^{-1} = \frac{e^{-\frac{2\epsilon}{kT}}}{1 + e^{-\frac{2\epsilon}{kT}}}$$

$$= \frac{e^{-y}}{1 + e^{-y}} \quad \because \frac{2\epsilon}{kT} = y$$

plug in (10)

$$\Rightarrow S \approx -Nk \left[\left(\frac{e^{-y}}{1 + e^{-y}}\right) \ln \left(\frac{e^{-y}}{1 + e^{-y}}\right) + \left(1 - \frac{e^{-y}}{1 + e^{-y}}\right) \ln \left(1 - \frac{e^{-y}}{1 + e^{-y}}\right) \right]$$

$$S \approx Nk \left[\left(\frac{ye^{-y}}{1 + e^{-y}}\right) + \ln(1 + e^{-y}) \right] \quad \text{--- (11)}$$

\Rightarrow By putting S from (11), E from (9) in (5),
F(T, N) is

$$F(T, N) = E - TS$$

$$= -NE \tanh(y/2) - TNk \left[\left(\frac{ye^{-y}}{1+e^{-y}} \right) + \ln(1+e^{-y}) \right]$$

$$\therefore \tanh(y/2) = \frac{1 - e^{-y}}{1 + e^{-y}}$$

$$\Rightarrow F(T, N) = -NE \left(\frac{1 - e^{-y}}{1 + e^{-y}} \right) - kTN \left[\left(\frac{ye^{-y}}{1 + e^{-y}} \right) + \ln(1 + e^{-y}) \right]$$
$$= -NE \left(\frac{1 - e^{-y}}{1 + e^{-y}} \right) - NE \frac{2e^{-y}}{1 + e^{-y}} - kT \ln(1 + e^{-y})$$

$$\therefore y = \frac{2E}{kT}$$

$$\Rightarrow F(T, N) \approx -NE - kTN \ln(1 + e^{-2E/kT})$$

Microcanonical

Assignment # 2

Solutions

QNo1

1a) The number of up-segments N_{\uparrow} and the number of down-segments N_{\downarrow} satisfy

$$N = N_{\uparrow} + N_{\downarrow} \quad \text{and}$$

$$L = a(N_{\downarrow} - N_{\uparrow})$$

thus,

$$N_{\uparrow} = N - N_{\downarrow} \quad \text{--- (i)}$$

$$\therefore L = aN_{\downarrow} - aN_{\uparrow}$$

$$L + aN_{\uparrow} = aN_{\downarrow}$$

$$\Rightarrow N_{\downarrow} = \frac{L}{a} + N_{\uparrow} \quad \text{plug in Eq (i)}$$

$$N_{\uparrow} = N - \left(\frac{L}{a} + N_{\uparrow}\right)$$

$$2N_{\uparrow} = N - \frac{L}{a}$$

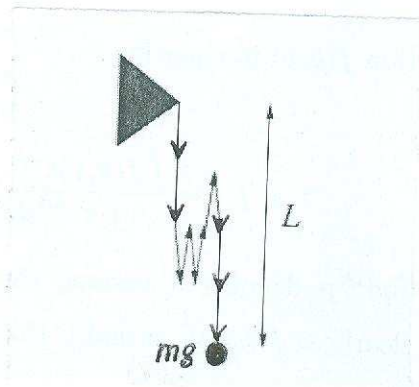
$$\Rightarrow \boxed{N_{\uparrow} = \frac{N}{2} - \frac{L}{2a}}$$

\Rightarrow Similarly,

$$N_{\downarrow} = N - N_{\uparrow}$$

$$= N - \left(\frac{N}{2} - \frac{L}{2a}\right) = \frac{N}{2} + \frac{L}{2a}$$

$$\Rightarrow \boxed{N_{\downarrow} = \frac{N}{2} + \frac{L}{2a}}$$



\Rightarrow \therefore total number of accessible microstates are

$$\Gamma(L) = \frac{N!}{N_{\uparrow}! N_{\downarrow}!}$$

$$\Gamma(L) = \frac{N!}{\left(\frac{N}{2} - \frac{L}{2a}\right)! \left(\frac{N}{2} + \frac{L}{2a}\right)!}$$

(b) Entropy; $S = k_B \ln \Gamma(L)$

$$S = k_B \left[\ln N! - \ln \left(\frac{N}{2} - \frac{L}{2a}\right)! - \ln \left(\frac{N}{2} + \frac{L}{2a}\right)! \right]$$

\therefore Use Stirling approximation, for large N

$$\ln N! \approx N \ln N - N$$

$$\Rightarrow S \approx k_B \left[N \ln N - N - \left(\frac{N}{2} - \frac{L}{2a}\right) \ln \left(\frac{N}{2} - \frac{L}{2a}\right) + \left(\frac{N}{2} - \frac{L}{2a}\right) \right. \\ \left. - \left(\frac{N}{2} + \frac{L}{2a}\right) \ln \left(\frac{N}{2} + \frac{L}{2a}\right) + \left(\frac{N}{2} + \frac{L}{2a}\right) \right]$$

$$= k_B \left[N \ln N - \left(\frac{N}{2} - \frac{L}{2a}\right) \ln \left(\frac{N}{2} - \frac{L}{2a}\right) - \left(\frac{N}{2} + \frac{L}{2a}\right) \ln \left(\frac{N}{2} + \frac{L}{2a}\right) \right. \\ \left. - \frac{N}{2} + \frac{N}{2} - \frac{L}{2a} + \frac{N}{2} + \frac{L}{2a} \right]$$

$$= k_B \left[N \ln N - \left(\frac{N}{2} - \frac{L}{2a}\right) \ln \left(\frac{N}{2} - \frac{L}{2a}\right) - \left(\frac{N}{2} + \frac{L}{2a}\right) \ln \left(\frac{N}{2} + \frac{L}{2a}\right) \right]$$

$$= k_B \left[N \ln N - \left(\frac{N}{2} - \frac{L}{2a}\right) \ln \left[\frac{N}{2} \left(1 - \frac{L}{Na}\right) \right] - \left(\frac{N}{2} + \frac{L}{2a}\right) \ln \left[\frac{N}{2} \left(1 + \frac{L}{Na}\right) \right] \right]$$

$$\begin{aligned}
&= k_B \left[N \ln N - \frac{N}{2} \ln \frac{N}{2} + \frac{L}{2a} \ln \frac{N}{2} - \left(\frac{N}{2} - \frac{L}{2a} \right) \ln \left(1 - \frac{L}{Na} \right) \right. \\
&\quad \left. - \frac{N}{2} \ln \frac{N}{2} - \frac{L}{2a} \ln \frac{N}{2} - \left(\frac{N}{2} + \frac{L}{2a} \right) \ln \left(1 + \frac{L}{Na} \right) \right] \\
&= k_B \left[N \ln N - N \ln \frac{N}{2} - \left(\frac{N}{2} - \frac{L}{2a} \right) \ln \left(1 - \frac{L}{Na} \right) - \left(\frac{N}{2} + \frac{L}{2a} \right) \ln \left(1 + \frac{L}{Na} \right) \right] \\
&= k_B \left[N \ln N - N \ln N + N \ln 2 - \left(\frac{N}{2} - \frac{L}{2a} \right) \ln \left(1 - \frac{L}{Na} \right) - \right. \\
&\quad \left. \left(\frac{N}{2} + \frac{L}{2a} \right) \ln \left(1 + \frac{L}{Na} \right) \right] \\
&= k_B \left[N \ln 2 - \left(\frac{N}{2} - \frac{L}{2a} \right) \ln \left(1 - \frac{L}{Na} \right) - \left(\frac{N}{2} + \frac{L}{2a} \right) \ln \left(1 + \frac{L}{Na} \right) \right] \quad (1)
\end{aligned}$$

\therefore for $x \ll 1$

$$\ln(1+x) \approx x - \frac{x^2}{2}$$

$$\Rightarrow \ln\left(1 - \frac{L}{Na}\right) \approx \left(-\frac{L}{Na}\right) - \frac{L^2}{2Na^2}$$

$$\ln\left(1 + \frac{L}{Na}\right) \approx \frac{L}{Na} - \frac{L^2}{2Na^2}$$

\Rightarrow Thus, equation (1) becomes.

$$\begin{aligned}
S &\approx k_B \left[N \ln 2 + \left(\frac{N}{2} - \frac{L}{2a} \right) \left(\frac{L}{Na} + \frac{L^2}{2Na^2} \right) - \left(\frac{N}{2} + \frac{L}{2a} \right) \left(\frac{L}{Na} - \frac{L^2}{2Na^2} \right) \right] \\
&= k_B \left[N \ln 2 + \frac{NL}{2Na} + \frac{NL^2}{4N^2a^2} - \frac{L^2}{2a^2N} - \frac{L^3}{2a^3N^2} - \frac{NL}{2Na} + \frac{NL^2}{4N^2a^2} \right. \\
&\quad \left. - \frac{L^2}{2Na^2} + \frac{L^3}{4N^2a^3} \right] \\
&= k_B \left[N \ln 2 + \frac{1}{2} \frac{L^2}{Na^2} - \frac{L^2}{a^2N} \right] = k_B \left[N \ln 2 + \frac{L^2}{Na^2} \left(\frac{1}{2} - 1 \right) \right]
\end{aligned}$$

$$\Rightarrow S \approx k_B \left[N \ln 2 - \frac{L^2}{2Na^2} \right]$$

The energy comes from the gravity potential energy.

$$E(L) = -mgL$$



(c) Temperature is defined as

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{\downarrow, N}$$

$$= \left[\frac{\partial S}{\partial (-mgL)} \right] = \left(\frac{\partial k_B \ln(\Gamma(L))}{\partial (-mgL)} \right)$$

$$= \frac{k_B}{-mg} \left(\frac{\partial \ln \Gamma(L)}{\partial L} \right)$$

$$= -\frac{k_B}{mg} \frac{\partial}{\partial L} \left(-\frac{L^2}{2Na^2} \right) = \frac{k_B L}{mgNa^2}$$

therefore,

$$\boxed{T = \frac{mgNa^2}{k_B L}}$$

(d) From (c) part, it is clear that

$$L = \frac{mgNa^2}{k_B T}$$

which shows that $L \propto mg$.

QNO2

(a) For a two dimensional ideal gas of N particles, partition function is

$$Z = \frac{Z_1^N}{N!}$$

where; $N!$ factor represent indistinguishable N particles.

$$\therefore \frac{Z_1^N}{N!} = \frac{1}{N!} \int d^2q d^2p e^{-\beta \sum_{i=1}^N p_i^2 / 2m}$$

$$= \frac{A^N}{h^{2N} N!} \int d^2p e^{-\beta \sum_{i=1}^N \frac{p_i^2}{2m}}$$

$$\therefore d^2q = A^N$$

$$= \frac{A^N}{N! h^{2N}} \int \prod_{i=1}^N d^2p_i e^{-\beta \sum_i \frac{p_i^2}{2m}}$$

$$\therefore \int e^{-\alpha x^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}}$$

$$= \frac{A^N}{N! h^{2N}} \left(\frac{1}{2} \sqrt{\frac{\pi}{\beta/2m}} \right)^{2N}$$

$$= \frac{A^N}{N! h^{2N}} \frac{1}{2^{2N}} \left(\sqrt{2m k_B T \pi} \right)^{2N}$$

$$Z = \frac{A^N}{N!} \left(\sqrt{\frac{2m k_B T \pi}{2^2 h^2}} \right)^{2N}$$

\Rightarrow The Helmholtz free energy is F :

$$F = -k_B T \ln Z$$

$$= -k_B T \ln \left(\frac{A^N}{N!} \sqrt{\frac{2m k_B T \pi}{2^2 h^2}} \right)^{2N}$$

$$= -k_B T \ln \left[A \left(\frac{2m k_B T \pi}{4h^2} \right) \right]^N + k_B T \ln N!$$

\Rightarrow Using Stirling approximation; for large N

$$\ln N! \approx N \ln N - N$$

$$\Rightarrow F \approx -k_B T N \ln \left(A \frac{m k_B T \pi}{2h^2} \right) + k_B T N \ln N - k_B T N$$

$$F = k_B T N \left[-1 - \ln \left(\frac{A m k_B T \pi}{2h^2 N} \right) \right]$$

(b) Force exerted on one side of square wall by the gas. F

$$\therefore \text{Pressure} = \frac{\text{Force}}{\text{Area}} = \frac{F}{L} \quad (\text{for 2D, the } P \text{ is force/length})$$

$$P = - \left(\frac{\partial F}{\partial V} \right)_T$$

$$P = - \left(\frac{\partial F}{\partial A} \right)_T$$

for 2-D case.

$$= k_B T N \frac{\partial \ln A}{\partial A} = \frac{k_B T N}{A} = \frac{k_B T N}{L^2}$$

$$\Rightarrow F = PL = \frac{k_B T N}{L^2} \cdot L$$

$$\Rightarrow \boxed{F = \frac{N k_B T}{L}}$$

QNO3

To evaluate mean force F b/w dipoles,

$$F = - \frac{\partial \langle V \rangle}{\partial R}$$

where

$$\langle V \rangle = - \frac{1}{Z} \frac{\partial Z}{\partial \beta}$$

\Rightarrow For the given classical system at temperature, the partition function is

$$Z = \int e^{-\beta H} dS_1 dS_2$$

$$= \int e^{-\beta (K.E + P.E)} dS_1 dS_2$$

\therefore dipoles are fixed in space $\Rightarrow K.E = 0$

and P-E is

$$V = \phi = \left[\frac{3 (\vec{M}_1 \cdot \vec{R})(\vec{M}_2 \cdot \vec{R}) - (\vec{M}_1 \cdot \vec{M}_2) R^2}{R^5} \right] \quad \text{--- (12)}$$

where

$$\vec{M}_1 = M_{1x} \hat{x} + M_{1y} \hat{y} + M_{1z} \hat{z}$$

$$= (M_1 \sin \theta_1 \cos \phi_1) \hat{x} + (M_1 \sin \theta_1 \sin \phi_1) \hat{y} + (M_1 \cos \theta_1) \hat{z}$$

$$\vec{M}_2 = M_{2x} \hat{x} + M_{2y} \hat{y} + M_{2z} \hat{z}$$

$$= (M_2 \sin \theta_2 \cos \phi_2) \hat{x} + (M_2 \sin \theta_2 \sin \phi_2) \hat{y} + (M_2 \cos \theta_2) \hat{z}$$

$$\vec{R} = R \hat{z}$$

⇒ P.E from Eq (12) becomes.

$$\phi = \frac{M_1 M_2}{R^3} [2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)]$$

$$\therefore dV_1 = \sin \theta_1 d\theta_1 d\phi_1$$

$$dV_2 = \sin \theta_2 d\theta_2 d\phi_2$$

⇒ Therefore, partition function becomes

$$\begin{aligned} Z &= \int e^{-\beta\phi} (\sin \theta_1 d\theta_1 d\phi_1) (\sin \theta_2 d\theta_2 d\phi_2) \\ &= \int e^{-\frac{\beta M_1 M_2}{R^3} [2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)]} \cdot \sin \theta_1 \sin \theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 \end{aligned}$$

Let $\lambda = \frac{\beta M_1 M_2}{R^3}$

⇒ Given that, $\lambda \ll 1$

$$\Rightarrow e^{-\lambda [2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)]} \approx 1 - \lambda A + \frac{\lambda^2 A^2}{2}$$

$$A = 2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)$$

$$\begin{aligned} \Rightarrow Z &= \int e^{-\lambda A} \sin \theta_1 \sin \theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 \\ &= \int \left(1 - \lambda A + \frac{\lambda^2 A^2}{2}\right) \sin \theta_1 \sin \theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 \end{aligned}$$

$$Z = \int (1) \sin\theta_1 \sin\theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 - \lambda \int [2 \cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2)] \sin\theta_1 \sin\theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 + \frac{\lambda^2}{2} \int [2 \cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2)]^2 \sin\theta_1 \sin\theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

$$= I_1 - \lambda I_2 + \frac{\lambda^2}{2} I_3$$

$$I_1 = \int_0^\pi \sin\theta_1 d\theta_1 \int_0^\pi \sin\theta_2 d\theta_2 \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2$$

$\theta = 0 \rightarrow \pi, \phi = 0 \rightarrow 2\pi$

$$I_1 = 16\pi^2$$

$$\text{And } I_2 = 2 \int [2 \cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2)] \sin\theta_1 \sin\theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

$$= 0$$

\Rightarrow That's why we cannot ignore $\lambda^2 A$ term while expanding $e^{-\lambda A}$.

$$Z = 16\pi^2 + \frac{\lambda^2}{2} I_3 = 16\pi^2 + \frac{\lambda^2}{2} Z'$$

$$I_3 = \int [2 \cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2)]^2 \sin\theta_1 \sin\theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

$$Z' = \int 4 \cos^2 \theta_1 \cos^2 \theta_2 \sin \theta_1 \sin \theta_2 d\theta_1 d\theta_2 (4\pi^2) + \int \sin^2 \theta_1 \sin^2 \theta_2 \cos^2(\phi_1 - \phi_2) \sin \theta_1 \sin \theta_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 - 4 \int \cos \theta_1 \cos \theta_2 \sin^2 \theta_1 \sin^2 \theta_2 \cos(\phi_1 - \phi_2) d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

$$= 2 \left(\frac{32\pi^2}{9} + \frac{4\pi^2}{9} \right)$$

$$\begin{aligned} \Rightarrow Z &= 16\pi^2 + \lambda^2 \left(\frac{32}{9} + \frac{4}{9} \right) \pi^2 \\ &= 16\pi^2 + \lambda^2 \left(\frac{36}{9} \right) \pi^2 \\ &= (16 + 4\lambda^2) \pi^2 \end{aligned}$$

$$\therefore \lambda = \frac{\beta M_1 M_2}{R^3}$$

$$\therefore \langle v \rangle = -\frac{1}{Z} \frac{\partial Z}{\partial \beta}$$

$$\Rightarrow \frac{\partial Z}{\partial \beta} = \frac{\partial}{\partial \beta} \left(16\pi^2 + 4\pi^2 \frac{\beta^2 M_1^2 M_2^2}{R^6} \right)$$

$$= \frac{4\pi^2 M_1^2 M_2^2}{R^6} 2\beta = (8\pi^2 M_1^2 M_2^2) \beta R^{-6}$$

$$\Rightarrow \frac{1}{Z} \frac{\partial Z}{\partial \beta} = \frac{8\pi^2 M_1^2 M_2^2 \beta R^{-6}}{(16\pi^2 + 4\beta^2 M_1^2 M_2^2 R^{-6} \pi^2)}$$

$$= \frac{M_1^2 M_2^2 \beta R^{-6}}{\left(2 + \frac{\beta^2 M_1^2 M_2^2 R^{-6}}{2} \right)}$$

$$= \frac{C R^{-6}}{(2 + D R^{-6})}$$

$$\therefore \text{let } M_1^2 M_2^2 \beta = C$$

$$\frac{M_1^2 M_2^2 \beta^2}{2} = D$$

$$\Rightarrow \langle v \rangle = -\frac{C R^{-6}}{2 + D R^{-6}}$$

⇒ Mean force between the dipoles is,

$$\begin{aligned}
 F &= - \frac{\partial \langle V \rangle}{\partial R} \\
 &= \frac{\partial}{\partial R} [CR^{-6} (2 + DR^{-6})^{-1}] \\
 &= \frac{-6CR^{-7}}{(2 + DR^{-6})} + \frac{CR^{-6}}{(2 + DR^{-6})^2} (-1)(-6)DR^{-7} \\
 &= \frac{-6CR^{-7}}{(2 + DR^{-6})} + \frac{6CDR^{-13}}{(2 + DR^{-6})^2}
 \end{aligned}$$

QNO4

The ensemble average $\langle f \rangle$ of the function $f(q, p)$ is

$$\langle f \rangle = \frac{\int f(q, p) e^{-\beta H(q, p)} dw}{\int e^{-\beta H(q, p)} dw}$$

$$\therefore dw \equiv d^{3N} q d^{3N} p$$

⇒ If $f = U - H(q, p)$ then

$$\begin{aligned}
 \langle f \rangle &= \langle U - H(q, p) \rangle = \frac{\int [U - H(q, p)] e^{-\beta H(q, p)} d^{3N} q d^{3N} p}{\int e^{-\beta H(q, p)} d^{3N} q d^{3N} p} \\
 &= \frac{\int U e^{-\beta H(q, p)} d^{3N} q d^{3N} p}{\int e^{-\beta H(q, p)} d^{3N} q d^{3N} p} - \frac{\int H(q, p) e^{-\beta H(q, p)} d^{3N} q d^{3N} p}{\int e^{-\beta H(q, p)} d^{3N} q d^{3N} p}
 \end{aligned}$$

$$\langle U - H(q, p) \rangle = \frac{U \int e^{-\beta H(q, p)} d^3N q d^3N p}{\int e^{-\beta H(q, p)} d^3N q d^3N p} - \frac{\int H(q, p) e^{-\beta H(q, p)} d^3N q d^3N p}{\int e^{-\beta H(q, p)} d^3N q d^3N p}$$

$$= U - \frac{\int H(q, p) e^{-\beta H(q, p)} d^3N q d^3N p}{\int e^{-\beta H(q, p)} d^3N q d^3N p}$$

$$\because U = \langle H \rangle = \langle E \rangle$$

$$= U - \langle H \rangle = 0$$

\Rightarrow Now using the expression,

$$\int [U - H(q, p)] e^{-\beta H(q, p)} d^3N q d^3N p = 0 \quad \text{--- (A)}$$

We have to show that mean square fluctuation in the energy is

$$\langle (\Delta E)^2 \rangle \equiv \langle E^2 \rangle - \langle E \rangle^2 = - \left(\frac{\partial U}{\partial \beta} \right)$$

\Rightarrow From Eq (A);

$$\int U e^{-\beta H(q, p)} d^3N q d^3N p = \int H(q, p) e^{-\beta H(q, p)} d^3N q d^3N p$$

$$U \int e^{-\beta H(q, p)} d^3N q d^3N p = \int H(q, p) e^{-\beta H(q, p)} d^3N q d^3N p$$

$$\Rightarrow U = \frac{\int H(q, p) e^{-\beta H(q, p)} d^3N q d^3N p}{\int e^{-\beta H(q, p)} d^3N q d^3N p}$$

$$U = \left[\int e^{-\beta H(q,p)} H(q,p) d^3q d^3p \right] \left[\int e^{-\beta H(q,p)} d^3q d^3p \right]^{-1}$$

⇒ differentiate w.r.t β ,

$$\begin{aligned} \frac{\partial U}{\partial \beta} &= \left[-\int H^2(q,p) e^{-\beta H(q,p)} d^3q d^3p \right] \left[\int e^{-\beta H(q,p)} d^3q d^3p \right]^{-1} + \\ &(-1) \left[\int e^{-\beta H(q,p)} H(q,p) d^3q d^3p \right] \left[\int e^{-\beta H(q,p)} d^3q d^3p \right]^{-2} \\ &\quad \left(-\int H(q,p) e^{-\beta H(q,p)} d^3q d^3p \right) \\ &= \frac{-\int H^2 e^{-\beta H} d^3q d^3p}{\int e^{-\beta H} d^3q d^3p} + \frac{\left[\int H e^{-\beta H} d^3q d^3p \right]^2}{\left[\int e^{-\beta H} d^3q d^3p \right]^2} \\ &= -\frac{\int H^2 e^{-\beta H} d^3q d^3p}{\int e^{-\beta H} d^3q d^3p} + \frac{\left[\int H e^{-\beta H} d^3q d^3p \right]^2}{\left[\int e^{-\beta H} d^3q d^3p \right]^2} \\ &= -\langle H^2 \rangle + \langle H \rangle^2 \end{aligned}$$

$$\Rightarrow -\left(\frac{\partial U}{\partial \beta}\right) = +\langle H^2 \rangle - \langle H \rangle^2$$

$$\therefore \langle E \rangle = \langle H \rangle$$

$$\Rightarrow \langle (\Delta E)^2 \rangle \equiv \langle E^2 \rangle - \langle E \rangle^2 = -\left(\frac{\partial U}{\partial \beta}\right) \quad \text{--- (B)}$$

$$\therefore \frac{\partial}{\partial \beta} = \frac{\partial T}{\partial \beta} \cdot \frac{\partial}{\partial T} = -kT^2 \frac{\partial}{\partial T}$$

$$\Rightarrow \left(\frac{\partial U}{\partial \beta} \right) = -kT^2 \left(\frac{\partial U}{\partial T} \right) = -kT^2 C_V \quad \text{--- (C)}$$

\Rightarrow Compare (B) and (C);

$$\langle (\Delta E)^2 \rangle \equiv \langle E^2 \rangle - \langle E \rangle^2 = - \left(\frac{\partial U}{\partial \beta} \right) = kT^2 \left(\frac{\partial U}{\partial T} \right) = kT^2 C_V$$

which is the required condition.

QNO5

We have to show that for canonical ensemble, the mean cube fluctuation in the energy is

$$\langle (\Delta E)^3 \rangle = k^2 \left[T^4 \left(\frac{\partial C_V}{\partial T} \right) + 2T^3 C_V \right] \quad \text{--- (1)}$$

$$\because \Delta E = E - \langle E \rangle$$

$$\Rightarrow (\Delta E)^3 = (E - \langle E \rangle)^3$$

Using identity for cube, $(a-b)^3 = a^3 - b^3 + 3ab^2 - 3a^2b$

$$\Rightarrow (\Delta E)^3 = E^3 - \langle E \rangle^3 + 3\langle E \rangle \langle E \rangle^2 - 3E^2 \langle E \rangle$$

$$\langle (\Delta E)^3 \rangle = \langle E^3 \rangle - \langle E \rangle^3 + 3\langle E \rangle \langle E \rangle^2 - 3\langle E^2 \rangle \langle E \rangle$$

$$= \langle E^3 \rangle - \langle E \rangle^3 + 3\langle E \rangle [\langle E \rangle^2 - \langle E^2 \rangle]$$

$$= \langle E^3 \rangle - \langle E \rangle^3 - 3\langle E \rangle [\langle E^2 \rangle - \langle E \rangle^2]$$

$$= \langle E^3 \rangle - \langle E \rangle^3 - 3\langle E \rangle \langle (\Delta E)^2 \rangle \quad \text{--- (2)}$$

\Rightarrow By compare (1) and (2), it is clear that we have to prove

$$k^2 \left[T^4 \left(\frac{\partial C_V}{\partial T} \right)_V + 2 T^3 C_V \right] = \langle E^3 \rangle - \langle E \rangle^3 - 3 \langle E \rangle \langle (\Delta E)^2 \rangle \quad (3)$$

→ In canonical ensemble, the average of a function is defined as

$$\langle f \rangle = \frac{\int f(q,p) e^{-\beta H(q,p)} d^{3N}q d^{3N}p}{\int e^{-\beta H(q,p)} d^{3N}q d^{3N}p}$$

$$\Rightarrow U = \langle E \rangle = \frac{\int E e^{-\beta E} d^{3N}q d^{3N}p}{\int e^{-\beta E} d^{3N}q d^{3N}p}$$

$$\Rightarrow \langle E \rangle = \frac{\int E e^{-\beta E} dw}{\int e^{-\beta E} dw}$$

assume: $dw = d^{3N}q d^{3N}p$

take its derivative w.r.t ' β '

$$\frac{\partial U}{\partial \beta} = \frac{\partial \langle E \rangle}{\partial \beta} = \frac{\partial}{\partial \beta} \left[\frac{\int E e^{-\beta E} dw}{\int e^{-\beta E} dw} \right]$$

[Recall from solution of last question Eq (x)]

$$\frac{\partial U}{\partial \beta} = - \frac{\int E^2 e^{-\beta E} dw}{\int e^{-\beta E} dw} + \left(\frac{\int E e^{-\beta E} dw}{\int e^{-\beta E} dw} \right)^2$$

→ Eq (3) includes cube terms ⇒ take again derivative of $\frac{\partial \langle E \rangle}{\partial \beta}$ w.r.t β .

$$\frac{\partial^2 U}{\partial \beta^2} = \frac{\partial}{\partial \beta} \left[\frac{-\int E^2 e^{-\beta E} dw}{\int e^{-\beta E} dw} \right] + \frac{\partial}{\partial \beta} \left[\frac{\int E e^{-\beta E} dw}{\int e^{-\beta E} dw} \right]^2$$

$$= I + I'$$

$$I = -\frac{\partial}{\partial \beta} \left[\left(\int E^2 e^{-\beta E} dw \right) \left(\int e^{-\beta E} dw \right)^{-1} \right]$$

$$= \frac{-\int E^3 e^{-\beta E} dw}{\int e^{-\beta E} dw} - (-1) \frac{\int E^2 e^{-\beta E} dw}{\left(\int e^{-\beta E} dw \right)^2} \int e^{-\beta E} (-E) dw$$

$$= \frac{\int E^3 e^{-\beta E} dw}{\int e^{-\beta E} dw} - \frac{\int E^2 e^{-\beta E} dw}{\int e^{-\beta E} dw} \frac{\int E e^{-\beta E} dw}{\int e^{-\beta E} dw}$$

$$I = \langle E^3 \rangle - \langle E^2 \rangle \langle E \rangle$$

⇒ Now,

$$I' = \frac{\partial}{\partial \beta} \left[\left(\int E e^{-\beta E} dw \right)^2 \left(\int e^{-\beta E} dw \right)^{-2} \right]$$

$$= \frac{\frac{\partial}{\partial \beta} \left(\int E e^{-\beta E} dw \right)^2}{\left(\int e^{-\beta E} dw \right)^2} + \left(\int E e^{-\beta E} dw \right)^2 \frac{\partial}{\partial \beta} \left(\int e^{-\beta E} dw \right)^{-2}$$

$$= \frac{2 \int E e^{-\beta E} dw \int (-E^2) e^{-\beta E} dw}{\left(\int e^{-\beta E} dw \right)^2} + 2 \frac{\left(\int E e^{-\beta E} dw \right)^2 \left(\int E e^{-\beta E} dw \right)}{\left(\int e^{-\beta E} dw \right)^3}$$

$$= (-2) \frac{\int E e^{-\beta E} d\omega}{\int e^{-\beta E} d\omega} \frac{\int E^2 e^{-\beta E} d\omega}{\int e^{-\beta E} d\omega} + 2 \left(\frac{\int E e^{-\beta E} d\omega}{\int e^{-\beta E} d\omega} \right)^2 \left(\frac{\int E e^{-\beta E} d\omega}{\int e^{-\beta E} d\omega} \right)$$

$$I' = -2 \langle E \rangle \langle E^2 \rangle + 2 \langle E \rangle^2 \langle E \rangle$$

$$\Rightarrow \frac{\partial^2 U}{\partial \beta^2} = \langle E^3 \rangle - \langle E^2 \rangle \langle E \rangle - 2 \langle E^2 \rangle \langle E \rangle + 2 \langle E \rangle^3$$

$$= \langle E^3 \rangle - 3 \langle E^2 \rangle \langle E \rangle + 3 \langle E \rangle^3 - \langle E \rangle^3$$

$$= \langle E^3 \rangle - \langle E \rangle^3 - 3 \langle E^2 \rangle \langle E \rangle + 3 \langle E \rangle^2 \langle E \rangle$$

$$= \langle E^3 \rangle - \langle E \rangle^3 - 3 \langle E \rangle \left[\langle E^2 \rangle - \langle E \rangle^2 \right]$$

$$\frac{\partial^2 U}{\partial \beta^2} = \langle E^3 \rangle - \langle E \rangle^3 - 3 \langle E \rangle \langle (\Delta E)^2 \rangle \quad \text{--- (4)}$$

\Rightarrow Compare (2) and (4),

$$\langle (\Delta E)^3 \rangle = \frac{\partial^2 U}{\partial \beta^2}$$

$$= \frac{\partial}{\partial \beta} \left(\frac{\partial U}{\partial \beta} \right) = \frac{\partial}{\partial \beta} \left(-kT^2 C_V \right)$$

$$\because \left(\frac{\partial U}{\partial \beta} \right) = -kT^2 C_V$$

$$= -kT^2 \frac{\partial}{\partial T} \left[-kT^2 C_V \right]$$

$$\because \frac{\partial}{\partial \beta} = \frac{\partial T}{\partial \beta} \cdot \frac{\partial}{\partial T} = -kT^2 \frac{\partial}{\partial T}$$

$$\begin{aligned} \Rightarrow \langle (\Delta E)^2 \rangle &= +k^2 T^2 \left[\frac{\partial}{\partial T} (T^2 C_V) \right] \\ &= k^2 T^2 \left[2T C_V + T^2 \frac{\partial C_V}{\partial T} \right] \\ &= k^2 \left[2T^3 C_V + T^4 \left(\frac{\partial C_V}{\partial T} \right)_V \right] \end{aligned}$$

$$\Rightarrow \langle (\Delta E)^2 \rangle = k^2 \left[T^4 \left(\frac{\partial C_V}{\partial T} \right)_V + 2T^3 C_V \right]$$

Hence proved.

\Rightarrow For ideal gas,

$$U = \langle E \rangle = \frac{3}{2} NkT$$

$$\therefore \langle (\Delta E)^2 \rangle = kT^2 C_V$$

$$= kT^2 \left(\frac{\partial U}{\partial T} \right)_V = kT^2 \frac{3}{2} Nk = \frac{3}{2} k^2 N T^2$$

$$\langle E \rangle^2 = \left(\frac{3}{2} NkT \right)^2 = \frac{9}{4} N^2 k^2 T^2$$

$$\langle \langle E \rangle^2 \rangle = \langle E \rangle^2 = \frac{9}{4} N^2 k^2 T^2$$

$$\Rightarrow \left\langle \left(\frac{\Delta E}{U} \right)^2 \right\rangle = \frac{\langle (\Delta E)^2 \rangle}{\langle U^2 \rangle} = \frac{\frac{3}{2} k^2 T^2 N}{\frac{9}{4} k^2 T^2 N^2} = \frac{2}{3N}$$

$$\Rightarrow \boxed{\left\langle \left(\frac{\Delta E}{U} \right)^2 \right\rangle = \frac{2}{3N}} \text{ Hence proved.}$$

Similarly,

$$\left\langle \left(\frac{\Delta E}{U} \right)^3 \right\rangle = \frac{\langle (\Delta E)^3 \rangle}{\langle U^3 \rangle} =$$

$$\therefore \langle (\Delta E)^3 \rangle = k^2 \left[T^4 \left(\frac{\partial C_V}{\partial T} \right)_V + 2T^3 C_V \right]$$

$$\therefore C_V = \frac{3}{2} Nk \quad \text{ideal gas}$$

$$\Rightarrow \left(\frac{\partial C_V}{\partial T} \right)_V = 0$$

$$\Rightarrow \langle (\Delta E)^3 \rangle = k^2 \left(2T^3 \frac{3}{2} Nk \right) = 3k^3 T^3 N$$

$$\Rightarrow \langle \langle E \rangle^3 \rangle = \langle E \rangle^3 = \left(\frac{3}{2} NkT \right)^3 = \frac{27}{2^3} N^3 k^3 T^3$$

$$\Rightarrow \left\langle \left(\frac{\Delta E}{U} \right)^3 \right\rangle = \frac{3k^3 T^3 N}{\frac{27}{2^3} N^3 k^3 T^3} = \frac{8}{9N^2}$$

$$\Rightarrow \boxed{\left\langle \left(\frac{\Delta E}{U} \right)^3 \right\rangle = \frac{8}{9N^2}}$$

Hence proved

ASSIGNMENT # 3

SOLUTIONS

Q NO 1

For a magnetic material, the first law of thermodynamics is

$$dU = dQ + dW$$

$$dU = TdS + HdM.$$

\therefore Heat capacity at constant H and M ;

$$C_H = \left(\frac{\partial U}{\partial T} \right)_H = T \left(\frac{\partial S}{\partial T} \right)_H$$

$$C_M = \left(\frac{\partial U}{\partial T} \right)_M = T \left(\frac{\partial S}{\partial T} \right)_M$$

Assume $S \equiv S(T, H)$

$$dS = \left(\frac{\partial S}{\partial T} \right)_H dT + \left(\frac{\partial S}{\partial H} \right)_T dH$$

$$\Rightarrow \left(\frac{\partial S}{\partial T} \right)_M = \left(\frac{\partial S}{\partial T} \right)_H + \left(\frac{\partial S}{\partial H} \right)_T \left(\frac{\partial H}{\partial T} \right)_M$$

$$\left(\frac{\partial S}{\partial T} \right)_M = \left(\frac{\partial S}{\partial T} \right)_H + \left(\frac{\partial S}{\partial H} \right)_T \left(\frac{\partial H}{\partial T} \right)_M$$

$$T \left(\frac{\partial S}{\partial T} \right)_M = T \left(\frac{\partial S}{\partial T} \right)_H + T \left(\frac{\partial S}{\partial H} \right)_T \left(\frac{\partial H}{\partial T} \right)_M$$

$$T \left(\frac{\partial S}{\partial T} \right)_H - T \left(\frac{\partial S}{\partial T} \right)_M = -T \left(\frac{\partial S}{\partial H} \right)_T \left(\frac{\partial H}{\partial T} \right)_M$$

\therefore Maxwell's Relation

$$\left(\frac{\partial S}{\partial H} \right)_T = \left(\frac{\partial M}{\partial T} \right)_H$$

$$\Rightarrow C_H - C_M = -T \left(\frac{\partial S}{\partial H} \right)_T \left(\frac{\partial H}{\partial T} \right)_M$$

$$\boxed{C_H - C_M = -T \left(\frac{\partial M}{\partial T} \right)_H \left(\frac{\partial H}{\partial T} \right)_M} \quad \text{--- (1)}$$

(b) For paramagnetic material, obeying Curie's law

$$M = \chi H$$

$$\chi = \frac{N\mu^2}{3kT} = \frac{C}{T} \quad \therefore C = \frac{N\mu^3}{3k}$$

$$\Rightarrow M = \frac{C}{T} H$$

$$\left(\frac{\partial M}{\partial T} \right)_H = -\frac{CH}{T^2} \quad , \quad \left(\frac{\partial H}{\partial T} \right)_M = \frac{M}{C}$$

plug $\left(\frac{\partial M}{\partial T}\right)_H$ and $\left(\frac{\partial H}{\partial T}\right)_M$ in ① Eq.

$$C_H - C_M = -T \left(-\frac{C_H}{T^2}\right) \frac{M}{C}$$

$$= \frac{HM}{T} = \frac{H^2 C}{T^2}$$

$$\therefore M = \frac{C}{T} H$$

$$\Rightarrow \boxed{C_H - C_M = \frac{C H^2}{T^2}}$$

QNO2

$$\mu = ?$$

$$T = 293 \text{ K}$$

$$\chi = 1.80 \times 10^{-6} \text{ m}^2/\text{K}$$

$$\mu_B = 9.27 \times 10^{-24} \frac{\text{Cm}}{\text{m}^2} = \text{J T}^{-1}$$

$$M = \chi H$$

$$\chi = \frac{N \mu^2}{3kT}$$

$$k_B = 1.38 \times 10^{-23} \text{ J/K}$$

$$k_B = 1.38 \times 10^{-23} \times 10^7 \text{ erg/K}$$

$$\Rightarrow \mu^2 = \frac{3kT\chi}{N}$$

$$\mu = \sqrt{\frac{3 (1.38 \times 10^{-23+7}) (273) \text{ K} \left(\frac{\text{erg}}{\text{K}}\right) \left(1.08 \times 10^{-4} \frac{\text{emu}}{\text{gOe}}\right)}{6.023 \times 10^{23} \text{ g/mole}}}$$

$$\mu = 2.54 \times 10^{-20} \text{ erg/Oe-mole}$$

$$\boxed{\mu = 2.85 \mu_B}$$

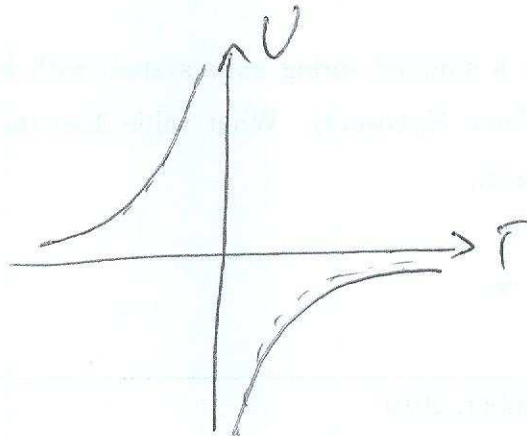
Q No 3

(a)

$$\therefore T = - \left(\frac{\partial U}{\partial S} \right)_V = - \frac{1}{2CU}$$

$$\Rightarrow 0 = - \frac{1}{2CT}$$

(b) we assume $C > 0$. The change of U with T is shown in the figure.



ASSIGNMENT # 4

(SOLUTIONS)

Q NO 1

For the given gaseous system of magnetic atoms, the total energy is

$$E = K.E + P.E$$

$$= \frac{P^2}{2m} - \mu \cdot H = \frac{P^2}{2m} - \mu_B g J H S$$

$$S = +1, -1$$

$$P.E_{\uparrow} = -\mu_{\uparrow} \cdot H = -\mu_B 2 \left(\frac{1}{2}\right) H = -\mu_B H$$

$$g = 2, J = \frac{1}{2}$$

$$P.E_{\downarrow} = -\mu_{\downarrow} \cdot H = \mu_B 2 \left(\frac{1}{2}\right) H = \mu_B H$$

\Rightarrow The canonical partition function for a single particle in the gas is,

$$Z_1 = \sum_{S=\pm 1} \frac{1}{h^3} \int d^3q d^3p e^{-\frac{E_p}{kT} - \frac{E_{int}}{kT}}$$

$$= \sum_{S=\pm 1} \frac{1}{h^3} \int d^3q d^3p e^{-\left(\frac{p^2}{2m} - S\mu_B H\right) \beta}$$

$$= \frac{V}{h^3} \int d^3p e^{-\frac{p^2}{2m} \beta} \left(e^{-\mu_B H \beta} + e^{+\mu_B H \beta} \right)$$

$$= \frac{V}{h^3} \left(\frac{e^{\mu_B H \beta} + e^{-\mu_B H \beta}}{2} \right) \int d^3p e^{-\frac{p^2}{2m} \beta}$$

$$= \frac{2V}{h^3} \cosh \mu_B H \beta \left[\int d^3p e^{-\frac{\beta}{2m} p^2} \right]^3$$

$$\therefore \int_0^{\infty} e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$$

$$\Rightarrow \int_0^{\infty} dp e^{-\frac{\beta p^2}{2m}} = \frac{1}{2} \sqrt{2\pi m k_B T}$$

$$\Rightarrow Z_1 = \frac{V}{h^3} \left(\frac{2\pi m k_B T}{2} \right)^{3/2} 2 \cosh \mu_B H \beta$$

$$= V \left(\frac{2\pi m k_B T}{2^2 h^2} \right)^{3/2} 2 \cosh \mu_B H \beta$$

$$= V \left(\frac{2\pi m k_B T}{4 h^2} \right)^{3/2} 2 \cosh \mu_B H \beta \quad \text{--- (1)}$$

and the canonical partition function for N indistinguishable non-interacting particles is

$$Z_N = \frac{1}{N!} Z_1^N$$

$$= \frac{1}{N!} \left[V \left(\frac{2\pi m k_B T}{4 h^2} \right)^{3/2} 2 \cosh \mu_B H \beta \right]^N$$

The relation b/w grand canonical partition function Q_{GC} and canonical partition function is;

$$Q_{GC} = \sum_N \frac{1}{h^{3N}} \frac{1}{N!} \int d^3q d^3p e^{-\beta [H(q,p) - \mu N]}$$

$$= \sum_{N=0}^{\infty} Z(N) e^{\beta \mu N}$$

$$\Rightarrow Q_{GC} = \sum_{N=0}^{\infty} e^{\beta \mu N} Z(N)$$

$$= \sum_{N=0}^{\infty} e^{\beta \mu N} \frac{1}{N!} Z_1^N$$

$$= \sum_{N=0}^{\infty} \frac{(Z_1 e^{\beta \mu})^N}{N!} = e^{(Z_1 e^{\beta \mu})}$$

$$[\because e^x = 1 + x + \frac{x^2}{2!} + \dots]$$

is the grand partition function of a gaseous system of "magnetic atoms".

$$\Rightarrow Q_{GC} = e^{z_1 e^{\beta \mu}} \quad \text{--- (2)}$$

\Rightarrow The magnetization is;

$$M = - \left(\frac{\partial \Phi_{GC}}{\partial H} \right)_T$$

where Φ_{GC} is grand canonical potential, just like canonical potential $F =$ Helmholtz free energy in canonical ensemble.

\Rightarrow Relation b/w Q_{GC} and Φ_{GC} is;

$$Q_{GC} = e^{-\beta \Phi_{GC}}$$

$$\ln Q_{GC} = -\beta \Phi_{GC} = -\frac{1}{k_B T} \Phi_{GC}$$

$$\Rightarrow \Phi_{GC} = -k_B T \ln Q_{GC} \quad \text{--- (a)}$$

and
$$M = k_B T \left(\frac{\partial \ln Q_{GC}}{\partial H} \right)_T$$

$$\because Q_{GC} = e^{z_1 e^{\beta \mu}} \quad \text{--- (b)}$$

$$\Rightarrow \ln Q_{GC} = z_1 e^{\beta \mu} = \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} 2V e^{\beta \mu} \cosh \mu_B H \beta \quad \text{--- (3)}$$

$$\Rightarrow M = k_B T \frac{\partial}{\partial H} \left[\left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} V e^{\beta \mu} 2 \cosh \mu_B H \beta \right]_T$$

$$\begin{aligned}
M &= k_B T \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} V e^{\beta\mu} \frac{\partial}{\partial H} \left(2 \cosh \mu_B H \beta \right) \\
&= k_B T \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} V e^{\beta\mu} \frac{\partial}{\partial H} \left(e^{\mu_B H \beta} + e^{-\mu_B H \beta} \right) \\
&= k_B T \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} V e^{\beta\mu} \mu_B \beta \left(e^{\mu_B H \beta} - e^{-\mu_B H \beta} \right) \\
&= k_B T \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} V e^{\beta\mu} \frac{\mu_B}{k_B T} 2 \left(\frac{e^{\mu_B H \beta} - e^{-\mu_B H \beta}}{2} \right) \\
&= \mu_B V 2 e^{\beta\mu} \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} \sinh \mu_B H \beta
\end{aligned}$$

⇒ Thus, the magnetization of the given system is

$$M = 2\mu_B V e^{\beta\mu} \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} \sinh \mu_B H \beta$$

$$\langle N \rangle = \text{Mean particle number} = -\frac{\partial}{\partial \alpha} \ln Q_{GC}$$

$$\text{where; } \frac{\partial}{\partial \alpha} = \frac{\partial}{\partial \mu} \frac{\partial \mu}{\partial \alpha} = \frac{\partial}{\partial \mu} \left(\frac{1}{\frac{\partial \alpha}{\partial \mu}} \right) = \frac{\partial}{\partial \mu} \left[\frac{1}{\frac{\partial}{\partial \mu} (-\beta\mu)} \right] \quad \because \frac{\partial \alpha}{\partial \mu} = -\beta\mu$$

$$\Rightarrow \frac{\partial}{\partial \alpha} = \frac{\partial}{\partial \mu} \left(\frac{-1}{\beta} \right) = -k_B T \frac{\partial}{\partial \mu}$$

$$\langle N \rangle = k_B T \frac{\partial}{\partial \mu} \ln Q_{GC}$$

∴ From Eq (3)

$$= k_B T 2V \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} \cosh \mu_B H \beta \frac{\partial}{\partial \mu} e^{\beta\mu}$$

$$= k_B T 2V \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} \cosh \mu_B H \beta \cdot \beta e^{\beta\mu}$$

$$\langle N \rangle = \frac{1}{k_B T} \left[2V \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} \cosh \mu_B H \beta \cdot e^{\beta \mu} \right] \frac{1}{k_B T}$$

$$= V \left[2 \cosh \mu_B H \beta \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} \bar{z} \right]$$

where, $\bar{z} = \text{fugacity} = e^{\beta \mu}$

$$\langle N \rangle = V f(T) \bar{z} \quad \text{--- (c)}$$

where; $f(T) = \text{function of temperature}$

$$f(T) = \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} (2 \cosh \mu_B H \beta) \quad \text{--- (d)}$$

$$f(T) = f_{\text{gas}}(T) \times f_{\text{spin}}(T) \quad \text{--- (e)}$$

\Rightarrow To calculate heat flow dQ as magnetic field reduces from $H \rightarrow 0$; at constant T and V , we have to first find out the entropy change

$$\therefore dQ = T ds$$

$$\Delta Q = T \Delta S$$

; at constant T .

\Rightarrow To compute the entropy, one way is to first obtain F Helmholtz free energy as a function of $\langle N \rangle, V, T$

$$\therefore F = \Phi_{GC} + \mu \langle N \rangle$$

(For G.C ensemble)

$$S = - \left(\frac{\partial F}{\partial T} \right)_{V, N} \quad \text{--- (f)}$$

$$\therefore F = \Phi_{GC} + \mu \langle N \rangle \quad \text{--- (4)}$$

$$\text{where; } \Phi_{GC} = -k_B T \ln \Omega_{GC} = -k_B T \ln \left(\frac{1}{\bar{z}} \right) = -k_B T \ln \bar{z}$$

⇒ plug Φ_{gc} in Eq (4);

$$F = -k_B T \ln \bar{z} + \mu \langle N \rangle$$

$$= -k_B T \ln \bar{z} + k_B T \ln \bar{z} \langle N \rangle$$

$$= -k_B T \bar{z} V \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} 2 \cosh \mu_B H \beta$$

$$+ k_B T \ln \bar{z} \langle N \rangle$$

$$= -k_B T \bar{z} V f(T) + k_B T \ln \bar{z} \langle N \rangle$$

∴ Using Eq (d)

$$\left[\begin{array}{l} \because \bar{z} = e^{\beta \mu} \\ \Rightarrow \ln \bar{z} = \beta \mu \\ \Rightarrow \mu = k_B T \ln \bar{z} \end{array} \right.$$

⇒ From Eq (c); $\frac{\langle N \rangle}{V f(T)} = \bar{z} \Rightarrow \ln \left(\frac{\langle N \rangle}{V f(T)} \right) = \ln \bar{z}$.

$$\Rightarrow F = -k_B T \left[\bar{z} V f(T) \right] + k_B T \langle N \rangle \ln \left(\frac{\langle N \rangle}{V f(T)} \right)$$

$$= -k_B T \langle N \rangle + k_B T \langle N \rangle \ln \left(\frac{\langle N \rangle}{V f(T)} \right)$$

$$= k_B T \langle N \rangle \left[-1 + \ln \frac{\langle N \rangle}{V f(T)} \right]$$

$$\Rightarrow S = - \left(\frac{\partial F}{\partial T} \right)_{V, \langle N \rangle}$$

$$= - \frac{\partial}{\partial T} \left[-k_B T \langle N \rangle + k_B T \ln \frac{\langle N \rangle}{V f(T)} \right]$$

$$= k_B \langle N \rangle - k_B \ln \frac{\langle N \rangle}{V f(T)} + k_B T \frac{\partial}{\partial T} \ln f(T)$$

$$= k_B \langle N \rangle \left[1 - \ln \left(\frac{\langle N \rangle}{V f(T)} \right) + T \frac{\partial}{\partial T} \ln f(T) \right]$$

$$S = k_B \langle N \rangle \left[1 + \ln \left(\frac{V f(T)}{\langle N \rangle} \right) + T \frac{\partial}{\partial T} \ln f(T) \right].$$

Since $f(T) = \left(\frac{2\pi m k_B T}{4h^2} \right)^{3/2} (2 \cosh \mu_B H \beta)$

$$= f_{\text{gas}}(T) \times f_{\text{spin}}(T)$$

where, $f_{\text{spin}}(T)$ has H dependence only \Rightarrow

we are interested only $S_{\text{spin}}(T, H)$ to

evaluate $\Delta S = S_f - S_i$

$$\Delta S = S_{\text{spin}}(T, H=0) - S_{\text{spin}}(T, H)$$

$$S_{\text{spin}} + S_{\text{gas}} = S$$

$$\Rightarrow S = k_B \langle N \rangle + k_B \langle N \rangle \ln \left(\frac{V f_{\text{spin}}(T)}{\langle N \rangle} \right) + k_B \langle N \rangle \ln \left(\frac{V f_{\text{gas}}(T)}{\langle N \rangle} \right)$$

$$+ \langle N \rangle k_B T \frac{\partial}{\partial T} \ln f_{\text{spin}}(T) + \langle N \rangle k_B T \frac{\partial}{\partial T} \ln f_{\text{gas}}(T).$$

where; $S_{\text{spin}}(T, H) = k_B \langle N \rangle \ln \left(\frac{V f_{\text{spin}}(T)}{\langle N \rangle} \right) + \langle N \rangle k_B T \frac{\partial}{\partial T} \ln f_{\text{spin}}(T)$

$$= k_B \langle N \rangle \ln \left(\frac{V}{\langle N \rangle} 2 \cosh \mu_B H \beta \right) + \langle N \rangle k_B T \frac{\partial}{\partial T} \ln f_{\text{spin}}(T)$$

where; $\frac{\partial}{\partial T} \ln f_{\text{spin}}(T) = \frac{1}{f_{\text{spin}}(T)} \frac{\partial}{\partial T} f_{\text{spin}}(T)$

$$= \frac{1}{2} \frac{2 \sinh \mu_B H \beta}{2 \cosh \mu_B H \beta} \left(-\frac{\mu_B H}{k_B T^2} \right)$$

$$= \tanh \mu_B H \beta \left(-\frac{\mu_B H}{k_B T^2} \right)$$

Thus,

$$S_{\text{spin}}(T, H) = k_B \langle N \rangle \ln \frac{V}{\langle N \rangle} + k_B \langle N \rangle \ln 2 \cosh \mu_B H \beta + \langle N \rangle k_B T \left(-\frac{\mu_B H}{k_B T^2} \right) \tanh \mu_B H \beta$$

$$\Rightarrow S_{\text{spin}}(T, H) = k_B \langle N \rangle \ln \frac{V}{\langle N \rangle} + k_B \langle N \rangle \ln 2 \cosh \mu_B H \beta - \frac{\langle N \rangle \mu_B H}{T} \tanh \mu_B H \beta$$

$$= k_B \langle N \rangle \left[\ln \frac{V}{\langle N \rangle} + \ln 2 \cosh \mu_B H \beta - \frac{\mu_B H}{k_B T} \tanh \mu_B H \beta \right]$$

$$= k_B \langle N \rangle \left[\ln \frac{V}{\langle N \rangle} + \ln 2 \cosh \mu_B H \beta - \mu_B H \beta \tanh \mu_B H \beta \right]$$

$$\Rightarrow S_{\text{spin}}(T, H=0) = k_B \langle N \rangle \left[\ln \frac{V}{\langle N \rangle} + \ln 2 + 0 \right]$$

$$\Rightarrow \Delta S = S_{\text{spin}}(T, H=0) - S_{\text{spin}}(T, H)$$

$$= k_B \langle N \rangle \left[\ln \frac{V}{\langle N \rangle} + \ln 2 - \ln \frac{V}{\langle N \rangle} - \ln 2 - \ln \cosh \mu_B H \beta + \mu_B H \beta \tanh \mu_B H \beta \right]$$

$$= k_B \langle N \rangle \left[\mu_B H \beta \tanh \mu_B H \beta - \ln \cosh \mu_B H \beta \right]$$

Thus; heat absorbed by the gas is then

$$\Delta Q = T \Delta S$$

$$= k_B T \langle N \rangle \left[\mu_B H \beta \tanh \mu_B H \beta - \ln \cosh \mu_B H \beta \right]$$

$$\Delta Q = k_B T \langle N \rangle \left[\frac{\mu_B H}{k_B T} \tanh \frac{\mu_B H}{k_B T} - \ln \cosh \frac{\mu_B H}{k_B T} \right]$$

which for $\frac{\mu_B H}{k_B T} \gg 1$ or $\mu_B H \gg k_B T$.

can be simplify as;

\Rightarrow For $y \gg 1$, $\tanh y \approx 1$.

$$y = \frac{\mu_B H}{k_B T}$$

$$\Delta Q \approx k_B T \langle N \rangle \left[\frac{\mu_B H}{k_B T} - \ln \cosh \frac{\mu_B H}{k_B T} \right]$$

$$= k_B T \langle N \rangle \left[y - \ln \cosh y \right] = k_B T \langle N \rangle \left[y - \ln \left(\frac{e^y + e^{-y}}{2} \right) \right]$$

$$= k_B T \langle N \rangle \left[y + \ln 2 - \ln (e^y + e^{-y}) \right]$$

$$= k_B T \langle N \rangle \left[y + \ln 2 - \ln e^y (1 + e^{-2y}) \right]$$

$$= k_B T \langle N \rangle \left[y + \ln 2 - \ln e^y - \ln (1 + e^{-2y}) \right]$$

$$= k_B T \langle N \rangle \left[\cancel{y} + \ln 2 - \cancel{y} - \ln (1 + e^{-2y}) \right]$$

$$= k_B T \langle N \rangle \left[\ln 2 - \ln (1 + 0) \right] \quad \because y \gg 1$$

$$\Rightarrow \frac{1}{e^{2y}} \ll 1 \approx 0$$

$$\Rightarrow \boxed{\Delta Q \approx k_B T \langle N \rangle \ln 2}$$

(NO2)

(a) To find a relation b/w fugacity $z_g = e^{\beta\mu}$ and temperature T , pressure P ; starting from grand canonical partition function, then use a relation b/w P, V, T and Q_{gc} .

$$\frac{PV}{k_B T} = \ln Q_{gc}$$

to obtain a relation b/w z_g and P, T .

\Rightarrow The grand canonical partition function of an ideal classical gas is;

$$Q(T, V, \mu) = \sum_{N=0}^{\infty} e^{\beta\mu N} \frac{z_{c1}^N}{N!}$$

$$\text{where } z_{c1} = \frac{V}{h^3} \int d^3P e^{-P^2/2m\beta}$$

$$= \frac{V}{h^3} \left[\int_0^{\infty} dP e^{-P^2\beta/2m} \right]^3$$

$$\because \int_0^{\infty} e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$$

$$\Rightarrow z_{c1} = \frac{V}{h^3} \frac{1}{2^3} \left(\frac{2\pi m}{\beta} \right)^{3/2} = V \left(\frac{2\pi m k_B T}{2^2 h^2} \right)^{3/2}$$

is the canonical partition function of one particle in the gas.

$$\Rightarrow Q_{GC}(T, V, \mu) = \sum_{N=0}^{\infty} \frac{(e^{\beta \mu} Z_{1c})^N}{Z_{1c}^{\beta \mu N}}$$

$$Q_{GC} = e$$

$$\therefore \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots = e^x$$

\Rightarrow According to the fundamental equation of thermodynamics; the grand potential ϕ is

$$\phi = F - \mu N = U - TS - \mu N \quad \text{--- (i)}$$

and $Q_{GC} = e^{-\beta \phi}$ (just like $Z_c = e^{-\beta F}$)

\Rightarrow Using Euler's form of U ;

$$U = TS - PV + \mu N$$

$$U - TS - \mu N = -PV \quad \text{--- (ii)}$$

$$\Rightarrow \phi = -PV$$

By compare (i) and (ii)

$$\Rightarrow Q_{GC} = e^{PV/\beta} \Rightarrow \ln Q_{GC} = PV/\beta$$

$$\Rightarrow \frac{PV}{k_B T} = \ln Q_{GC}$$

$$= \ln e^{Z_{1c} e^{\beta \mu}}$$

$$\left(\frac{PV}{k_B T} \right) = Z_{1c} e^{\beta \mu}$$

$$\Rightarrow \frac{PV}{k_B T} = V \left(\frac{2\pi m k_B T}{2^2 h^2} \right)^{3/2} e^{\beta \mu}$$

$$\Rightarrow \frac{P}{(k_B T)^{1+3/2}} = \left(\frac{2 \pi m}{2 h^2} \right)^{3/2} Z_g$$

$$\Rightarrow Z_g(T, P) = P (k_B T)^{-5/2} \left(\frac{\pi m}{2 h^2} \right)^{-3/2}$$

is the required relation b/w Z_g and (T, P)

(b) For a box containing an ideal classical gas at pressure P and temperature T , (there are no absorbing sites on the walls); we have to evaluate the mean number of adsorbed molecules $\langle N \rangle$.

\Rightarrow Firstly, we will find average number of adsorbed molecules per site and then multiply it with N_0 (total number of sites) to find $\langle N \rangle$.

\Rightarrow For each absorbing site, grand canonical partition function given by

$$Q_{\text{site}} = \sum_{N=0}^{\infty} e^{\beta \mu N} e^{-\beta E_N} = \sum_{N=0}^{\infty} e^{\beta \mu N} e^{+\beta E_N} = 1 + e^{\beta \mu} e^{\beta E} = 1 + Z_g e^{\beta E}$$

$$\Rightarrow Q_{\text{site}} = 1 + Z_g e^{\beta E}$$

\Rightarrow The average number of adsorbed molecules per site is

$$\langle N \rangle_{\text{site}} = - \frac{\partial}{\partial \alpha} \ln Q_{\text{site}}$$

$$\Rightarrow \langle N \rangle_{\text{site}} = - \frac{\partial}{\partial \alpha} \ln(1 + z_g e^{+\beta \epsilon})$$

$$= \frac{\partial}{\partial \alpha} = \frac{\partial}{\partial z_g} \frac{\partial z_g}{\partial \alpha} = -e^{-\alpha} \frac{\partial}{\partial z_g}$$

$$\therefore z_g = e^{\beta \mu}$$

$$z_g = e^{-\alpha}$$

$$\Rightarrow \frac{\partial}{\partial \alpha} = -z_g \frac{\partial}{\partial z_g}$$

$$\Rightarrow \langle N \rangle_{\text{site}} = z_g \frac{\partial}{\partial z_g} \ln(1 + z_g e^{\beta \epsilon})$$

$$\langle N \rangle_{\text{site}} = z_g \frac{1}{(1 + z_g e^{\beta \epsilon})} e^{\beta \epsilon} = \frac{1}{1 + z_g^{-1} e^{-\beta \epsilon}}$$

\Rightarrow So, for the N_0 sites, we have

$$\langle N \rangle = \frac{N_0}{1 + z_g^{-1} e^{-\beta \epsilon}}$$

This average number of adsorbed molecules can now be expressed in terms of the temperature and pressure of the gas by substituting for

$z_g = e^{\beta \mu}$ (fugacity) the function found in part (a).

$$\langle N \rangle = \frac{N_0}{1 + P^{-1} (k_B T)^{5/2} \left(\frac{\pi m}{2h^2}\right)^{3/2} e^{-\beta \epsilon}}$$

At a fixed temperature, this varies with pressure in a manner that might intuitively be expected. At high pressures, the density is high, molecules frequently approach the absorbing sites and $\langle N \rangle \approx N_0$. At low P , the opposite is true and $\langle N \rangle \approx 0$. The effect of T is also apparent. At high T , absorbed molecules are easily dislodged and a high P is required to keep the sites filled. At low T , a more modest pressure is sufficient

Q NO 3

$$\begin{aligned}
 Z(1) &= \frac{1}{h^3} \int d^3P e^{-\frac{\beta P^2}{2m}} \int d^3z e^{-mgz\beta} \\
 &= \left(\frac{2\pi mkT}{h^2} \right)^{3/2} \int dx \int dy \int_0^z dz e^{-mgz\beta} \\
 &= \left(\frac{2\pi mkT}{h^2} \right)^{3/2} A \int_0^z e^{-mgz\beta} dz \\
 &= A \left(\frac{2\pi mkT}{h^2} \right)^{3/2} \left. \frac{e^{-mgz\beta}}{-mg\beta} \right|_0^z \\
 &= \frac{A}{h^3} \left(\frac{2\pi mkT}{h^2} \right)^{3/2} \left(\frac{k_B T}{mg} \right) (1 - e^{-mgz\beta}) \\
 &= A \left(\frac{2\pi m}{h^2 (mg)^{2/3}} \right)^{3/2} (kT)^{5/2} (1 - e^{-mgz\beta}) \\
 \Rightarrow Z^N &= A^N \left(\frac{2\pi m}{h^2 (mg)^{2/3}} \right)^{3N/2} (kT)^{5N/2} (1 - e^{-mgz\beta})^N
 \end{aligned}$$

$$\therefore \mu = -k_B T \frac{\partial}{\partial N} \ln Z^N$$

$$\Rightarrow \mu = -k_B T \ln \left[A \left(\frac{2\pi m}{h^2} \right)^{3/2} (kT)^{5/2} (1 - e^{-mg\beta}) \right]$$

$$= -k_B T \left[\ln \left(\frac{A}{mg} \right) + \ln \left(\frac{2\pi m}{h^2} \right)^{3/2} + \ln (kT)^{5/2} + \right.$$

$$\left. \ln (1 - e^{-mg\beta}) \right].$$

$$\therefore P_0 = \frac{F}{A} = \frac{mg}{A}$$

$$= -k_B T \left[-\ln P_0 + \ln \left(\frac{2\pi m}{h^2} \right)^{3/2} + \frac{5}{2} \ln (kT) + \ln (1 - e^{-mg\beta}) \right]$$

$$= -k_B T \left[-\ln P_0 + \ln \left(\frac{2\pi m}{h^2} \right)^{3/2} + \ln (kT) + \frac{3}{2} \ln (kT) + \ln (1 - e^{-mg\beta}) \right]$$

$$= -k_B T \left[-\ln P_0 + \ln \left(\frac{2\pi m}{h^2} \right)^{3/2} + \ln (kT) + \frac{3}{2} \ln (kT) + \ln (1 - e^{-mg\beta}) \right]$$

$$= -k_B T \left[-\ln \left(\frac{P_0 P}{P} \right) + \ln \left(\frac{2\pi m}{h^2} \right)^{3/2} + \ln (kT) + \frac{3}{2} \ln T + \frac{3}{2} \ln k + \ln (1 - e^{-mg\beta}) \right]$$

$$= -k_B T \left[-\ln \left(\frac{P_0}{P} \right) + \ln \left(\frac{kT}{P} \right) + \frac{3}{2} \ln T + \sigma_0 + \ln (1 - e^{-mg\beta}) \right]$$

$$\text{Where } \sigma_0 = \ln \left(\frac{2\pi m k}{h^2} \right)^{3/2}$$

$$\therefore P = P_0 e^{-mgz\beta}$$

$$\Rightarrow \frac{P}{P_0} = e^{-mgz\beta} \quad \text{and} \quad \ln\left(\frac{P}{P_0}\right) = -mgz\beta$$

$$\mu = -k_B T \left[-mgz\beta + \ln\left(\frac{k_B T}{P}\right) + \frac{3}{2} \ln(T) + \ln(1 - e^{-mgz\beta}) + \sigma_0 \right]$$

$$\Rightarrow \mu = +mgz - k_B T \ln\left(\frac{k_B T}{P}\right) - \frac{3}{2} k_B T \ln(T) - k_B T \left(\ln(1 - e^{-mgz\beta}) + \sigma_0 \right)$$

QNO4

(a), (b) To derive an expression for entropy S of an ideal quantum gas in terms of $\ln Z$, the mean number of particles in state r ; starting from the knowledge of partition functions Q_{BE} for both quantum gases (Bose and Fermi)

$$\ln Q_{BE} = - \sum_r \ln(1 - e^{-\beta E_r - \alpha}) \quad \text{--- (i)}$$

$$\ln Q_{FD} = + \sum_r \ln(1 + e^{-\beta E_r - \alpha}) \quad \text{--- (ii)}$$

then find the grand potential ϕ for both systems

$$Q = e^{-\beta \phi}$$

$$\Rightarrow \ln Q = -\beta \phi$$

or

$$\left. \begin{aligned} \Phi_{BE} &= -k_B T \ln Q_{BE} \\ \Phi_{FD} &= -k_B T \ln Q_{FD} \end{aligned} \right] \text{--- (iii)}$$

and differentiate it w.r.t T temperature at constant V , leads to required entropy.

$$S_{\substack{BE \\ FD}} = - \left(\frac{\partial \Phi_{\substack{BE \\ FD}}}{\partial T} \right)_V \text{--- (iv)}$$

\Rightarrow Combined form of (i) and (ii) is;

$$\ln Q_{\substack{BE \\ FD}} = \mp \sum_{\epsilon} \ln (1 \mp e^{-\beta \epsilon - \alpha}) \text{--- (v)}$$

\therefore Distribution functions for Fermi and Bose systems are.

$$\langle n_{\epsilon} \rangle_{\substack{BE \\ FD}} = \frac{1}{e^{\alpha + \beta \epsilon} \mp 1}$$

$$\Rightarrow \langle n_{\epsilon} \rangle_B (e^{\alpha + \beta \epsilon} \mp 1) = 1$$

$$\Rightarrow \langle n_{\epsilon} \rangle_B e^{\alpha + \beta \epsilon} = 1 \pm \langle n_{\epsilon} \rangle_B$$

$$\Rightarrow e^{\alpha + \beta \epsilon} = \frac{1 \pm \langle n_{\epsilon} \rangle_B}{\langle n_{\epsilon} \rangle_B}$$

or

$$\ln e^{\alpha + \beta \epsilon} = \ln (1 \pm \langle n_{\epsilon} \rangle_B) - \ln \langle n_{\epsilon} \rangle_B$$

$$\Rightarrow \alpha + \beta \epsilon_i = \ln(1 \pm \langle n_i \rangle_{BF}) - \ln \langle n_i \rangle_{BF}$$

$$\Rightarrow -\alpha - \beta \epsilon_i = \ln \left(\frac{\langle n_i \rangle_{BF}}{1 \pm \langle n_i \rangle_{BF}} \right)$$

\Rightarrow Now by plugging above relation in Eq (V)

$$\ln Q_{BE} = \mp \sum_i \ln(1 \mp e^{-\alpha - \beta \epsilon_i})$$

$$= \mp \sum_i \ln \left(1 \mp \frac{\langle n_i \rangle_{BF}}{1 \pm \langle n_i \rangle_{BF}} \right)$$

$$= \mp \sum_i \ln \left(\frac{1 \pm \langle n_i \rangle_{BF} \mp \langle n_i \rangle_{BF}}{1 \pm \langle n_i \rangle_{BF}} \right)$$

$$= \mp \sum_i \ln \left(\frac{1}{1 \pm \langle n_i \rangle_{BF}} \right)$$

$$= \mp \left[\sum_i \ln 1 - \sum_i \ln(1 \pm \langle n_i \rangle_{BF}) \right]$$

$$\because \ln 1 = 0$$

$$\Rightarrow \ln Q_{BE} = \pm \sum_i \ln(1 \pm \langle n_i \rangle_{BF})$$

\Rightarrow Using Eq (iii);

$$\Phi_{BE} = -k_B T \ln Q_{BE}$$

$$= \mp k_B T \sum_i \ln(1 \pm \langle n_i \rangle_{BF})$$

differentiate w.r.t T at constant V ,

$$S = - \left(\frac{\partial \Phi_{BE}}{\partial T} \right)_V = \pm k_B \frac{\partial}{\partial T} \left[T \sum_i \ln(1 \pm \langle n_i \rangle_{BF}) \right]$$

$$\Rightarrow S_{BE, FD} = \pm k_B \left[\sum_i \ln(1 \pm \langle n_i \rangle_{B/F}) + T \frac{\partial}{\partial T} \ln(1 \pm \langle n_i \rangle_{B/F}) \right] \text{--- (vi)}$$

$$\therefore \frac{\partial}{\partial T} = \frac{\partial}{\partial \beta} \frac{\partial \beta}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial}{\partial \beta} \text{--- (vii)}$$

$$\Rightarrow \frac{\partial}{\partial \beta} \ln(1 \pm \langle n_i \rangle_{B/F}) = \frac{1}{1 \pm \langle n_i \rangle_{B/F}} \frac{\partial}{\partial \beta} (\pm \langle n_i \rangle_{B/F}) \text{--- (viii)}$$

$$\therefore \langle n_i \rangle_{B/F} = \frac{1}{e^{\alpha + \beta \epsilon_i} \mp 1}$$

$$\Rightarrow \frac{\partial}{\partial \beta} \langle n_i \rangle_{B/F} = -\frac{1}{(e^{\alpha + \beta \epsilon_i} \mp 1)^2} \frac{\partial}{\partial \beta} e^{\alpha + \beta \epsilon_i}$$

$$= -\frac{e^{\beta(\epsilon_i - \mu)}}{(e^{\alpha + \beta \epsilon_i} \mp 1)^2} (\epsilon_i - \mu)$$

$$\because \alpha = -\beta \mu$$

plug in (viii)

$$\Rightarrow \frac{\partial}{\partial \beta} \ln(1 \pm \langle n_i \rangle_{B/F}) = \mp \frac{e^{\beta(\epsilon_i - \mu)}}{1 \pm \langle n_i \rangle_{B/F}} \cdot \frac{(\epsilon_i - \mu)}{(e^{\alpha + \beta \epsilon_i} \mp 1)^2}$$

$$= \mp \frac{e^{\alpha + \beta \epsilon_i}}{1 \pm \langle n_i \rangle_{B/F}} \frac{1}{\beta} \frac{(\beta \epsilon_i - \beta \mu)}{(e^{\alpha + \beta \epsilon_i} \mp 1)^2}$$

$$= \mp \left(\frac{1 \pm \langle n_i \rangle_{B/F}}{\langle n_i \rangle_{B/F}} \right) \frac{1/\beta}{1 \pm \langle n_i \rangle_{B/F}} \ln \left(\frac{1 \pm \langle n_i \rangle_{B/F}}{\langle n_i \rangle_{B/F}} \right) \cdot \langle n_i \rangle_{B/F}^2$$

$$= \mp \frac{1}{\beta} \langle n_i \rangle_{B/F} \ln \left(\frac{1 \pm \langle n_i \rangle_{B/F}}{\langle n_i \rangle_{B/F}} \right) \text{ plug in (vii) and (vi)}$$

$$\begin{aligned}
 \Rightarrow \frac{\partial}{\partial T} \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) &= -\frac{1}{k_B T^2} \frac{\partial}{\partial \beta} \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) \\
 &= \pm \frac{1}{k_B T^2} (k_B T) \langle n_{\lambda} \rangle_{B/F} \ln \left(\frac{1 \pm \langle n_{\lambda} \rangle_{B/F}}{\langle n_{\lambda} \rangle_{B/F}} \right) \\
 &= \pm \frac{1}{T} \langle n_{\lambda} \rangle_{B/F} \ln \left(\frac{1 \pm \langle n_{\lambda} \rangle_{B/F}}{\langle n_{\lambda} \rangle_{B/F}} \right)
 \end{aligned}$$

Thus; S_{BE} _{FD} becomes:

$$\begin{aligned}
 S_{BE} &= \pm k_B \left[\sum_{\lambda} \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) \pm \sum_{\lambda} \langle n_{\lambda} \rangle_{B/F} \ln \left(\frac{1 \pm \langle n_{\lambda} \rangle_{B/F}}{\langle n_{\lambda} \rangle_{B/F}} \right) \right] \\
 &= k_B \sum_{\lambda} \left[\pm \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) + \langle n_{\lambda} \rangle_{B/F} \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) - \langle n_{\lambda} \rangle_{B/F} \ln \langle n_{\lambda} \rangle_{B/F} \right] \\
 &= -k_B \sum_{\lambda} \left[\mp \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) - \langle n_{\lambda} \rangle_{B/F} \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) + \langle n_{\lambda} \rangle_{B/F} \ln \langle n_{\lambda} \rangle_{B/F} \right] \\
 S_{BE} &= -k_B \sum_{\lambda} \left[\langle n_{\lambda} \rangle_{B/F} \ln \langle n_{\lambda} \rangle_{B/F} \mp (1 \pm \langle n_{\lambda} \rangle_{B/F}) \ln(1 \pm \langle n_{\lambda} \rangle_{B/F}) \right]
 \end{aligned}$$

Means to say

$$\begin{aligned}
 S_{BE} &= -k_B \sum_{\lambda} \left[\langle n_{\lambda} \rangle_{B/F} \ln \langle n_{\lambda} \rangle_{B/F} - (1 + \langle n_{\lambda} \rangle_{B/F}) \ln(1 + \langle n_{\lambda} \rangle_{B/F}) \right] \\
 S_{FD} &= -k_B \sum_{\lambda} \left[\langle n_{\lambda} \rangle_{F/B} \ln \langle n_{\lambda} \rangle_{F/B} + (1 - \langle n_{\lambda} \rangle_{F/B}) \ln(1 - \langle n_{\lambda} \rangle_{F/B}) \right]
 \end{aligned}$$

(c) In the classical limit, $\langle n_{\lambda} \rangle \ll 1$.

$$S_{BE} = -k_B \sum_{\lambda} \left[\langle n_{\lambda} \rangle_{B/F} \ln \langle n_{\lambda} \rangle_{B/F} - \ln(1 + \langle n_{\lambda} \rangle_{B/F}) - \langle n_{\lambda} \rangle_{B/F} \ln(1 + \langle n_{\lambda} \rangle_{B/F}) \right]$$

$$\begin{aligned} \Rightarrow S_{BE} &= k_B \sum_{\alpha} \left[\ln(1 + \langle n_{\alpha} \rangle_B) - \langle n_{\alpha} \rangle_B \ln \langle n_{\alpha} \rangle_B + \langle n_{\alpha} \rangle_B \ln(1 + \langle n_{\alpha} \rangle_B) \right] \\ &= k_B \sum_{\alpha} \left[\ln(1 + \langle n_{\alpha} \rangle_B) + \langle n_{\alpha} \rangle_B \ln \left(\frac{1 + \langle n_{\alpha} \rangle_B}{\langle n_{\alpha} \rangle_B} \right) \right] \\ &= k_B \sum_{\alpha} \left[\ln(1 + \langle n_{\alpha} \rangle_B) + \langle n_{\alpha} \rangle_B \ln \left(\frac{1}{\langle n_{\alpha} \rangle_B} + 1 \right) \right] \end{aligned}$$

$$\because \langle n_{\alpha} \rangle_B \ll 1 \Rightarrow \frac{1}{\langle n_{\alpha} \rangle_B} \gg 1$$

$$\Rightarrow \frac{1}{\langle n_{\alpha} \rangle_B} + 1 \approx \frac{1}{\langle n_{\alpha} \rangle_B}$$

$$\text{and } 1 + \langle n_{\alpha} \rangle_B \approx 1 \Rightarrow \ln(1 + \langle n_{\alpha} \rangle_B) \approx \ln 1 = 0$$

$$\Rightarrow S_{BE} \approx k_B \sum_{\alpha} \left[0 + \langle n_{\alpha} \rangle_B \ln \left(\frac{1}{\langle n_{\alpha} \rangle_B} \right) \right]$$

$$\boxed{S_{BE} \approx -k_B \sum_{\alpha} \langle n_{\alpha} \rangle_B \ln \langle n_{\alpha} \rangle_B}$$

in classical limit.

Similarly, for Fermi gas.

$$S_{FD} = -k_B \sum_{\alpha} \left[\langle n_{\alpha} \rangle_F \ln \langle n_{\alpha} \rangle_F + \ln(1 - \langle n_{\alpha} \rangle_F) - \langle n_{\alpha} \rangle_F \ln(1 - \langle n_{\alpha} \rangle_F) \right]$$

$$= k_B \sum_{\alpha} \left[-\langle n_{\alpha} \rangle_F \ln \langle n_{\alpha} \rangle_F + \langle n_{\alpha} \rangle_F \ln(1 - \langle n_{\alpha} \rangle_F) - \ln(1 - \langle n_{\alpha} \rangle_F) \right]$$

$$= k_B \sum_{\alpha} \left[\langle n_{\alpha} \rangle_F \ln \left(\frac{1 - \langle n_{\alpha} \rangle_F}{\langle n_{\alpha} \rangle_F} \right) - \ln(1 - \langle n_{\alpha} \rangle_F) \right]$$

$$= k_B \sum_{\alpha} \left[\langle n_{\alpha} \rangle_F \ln \left(\frac{1}{\langle n_{\alpha} \rangle_F} - 1 \right) - \ln(1 - \langle n_{\alpha} \rangle_F) \right]$$

\Rightarrow for $\langle n_i \rangle_F \ll 1$

$$\Rightarrow \ln\left(\frac{1}{\langle n_i \rangle_F} - 1\right) \approx \ln\left(\frac{1}{\langle n_i \rangle_F}\right) \\ = -\ln\langle n_i \rangle_F$$

and $\ln(1 - \langle n_i \rangle_F) \approx \ln 1 = 0$

\Rightarrow

$$S_{FD} \approx -k_B \sum_i \langle n_i \rangle_F \ln \langle n_i \rangle_F$$

in classical limit

Thus, in classical limit

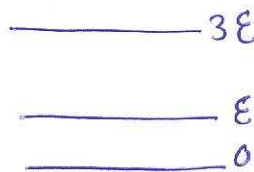
$$\langle n_i \rangle \ll 1$$

$$S_{BE} = S_{FD}$$

ASSIGNMENT # 5 (SOLUTIONS)

QNO1

Given that, two particles (each of which) can be in any one of three quantum states. The system is in contact with a heat reservoir at temperature T .



(a) Z for Maxwell-Boltzmann statistics considering distinguishable particles;

$$Z = \sum_{n_1, n_2, \dots} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}$$

$$= \sum_{n_1, n_2, \dots} e^{-\beta(\varepsilon_1 n_1 + \varepsilon_2 n_2 + \dots)}$$

$$\sum_i n_i = N = 2$$

$$\Rightarrow Z_{MB} = \left(e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta\varepsilon_3} + \dots \right)^N \quad \because \text{derived in class}$$

$$\because \varepsilon_1 = 0, \quad \varepsilon_2 = \varepsilon, \quad \varepsilon_3 = 3\varepsilon, \quad N = 2$$

$$\Rightarrow Z_{MB} = \left(e^0 + e^{-\beta\varepsilon} + e^{-3\beta\varepsilon} \right)^2$$

$$= \left(1 + e^{-\beta\varepsilon} + e^{-3\beta\varepsilon} \right) \left(1 + e^{-\beta\varepsilon} + e^{-3\beta\varepsilon} \right)$$

$$= \left(1 + e^{-\beta\varepsilon} + e^{-3\beta\varepsilon} + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon} + e^{-4\beta\varepsilon} + e^{-3\beta\varepsilon} + e^{-4\beta\varepsilon} + e^{-6\beta\varepsilon} \right)$$

$$Z_{MB} = 1 + 2e^{-\beta\varepsilon} + e^{-2\beta\varepsilon} + 2e^{-3\beta\varepsilon} + 2e^{-4\beta\varepsilon} + e^{-6\beta\varepsilon}$$

Alternate Method:- (Possible configurations)

	0x			0	x	x	0	
	0x		x	0	x	0		
0x		0	x			0	x	
$1200\rangle$	$1020\rangle$	$1002\rangle$	$1110\rangle$	$1110\rangle$	$1011\rangle$	$1011\rangle$	$1101\rangle$	$1101\rangle$

State: $1200\rangle$, $E = 2(0) = 0 = 1$

$1020\rangle$, $E = 2(\epsilon) = 2\epsilon$

$1002\rangle$, $E = 2(3\epsilon) = 6\epsilon$

$1110\rangle$, $E = 1(0) + 1(\epsilon) = \epsilon$

$1110\rangle$, $E = 1(0) + 1(\epsilon) = \epsilon$

$1011\rangle$, $E = 0(0) + 1(\epsilon) + 1(3\epsilon) = 4\epsilon$

$1011\rangle$, $E = 0(0) + 1(\epsilon) + 1(3\epsilon) = 4\epsilon$

$1101\rangle$, $E = 1(0) + 1(3)\epsilon = 3\epsilon$

$1101\rangle$, $E = 3\epsilon$

$$\Rightarrow Z_{MB} = \sum_i e^{-\beta E_i}$$

$$= 1 + e^{-2\beta\epsilon} + e^{-6\beta\epsilon} + e^{-\beta\epsilon} + e^{-\beta\epsilon} + e^{-4\beta\epsilon} + e^{-4\beta\epsilon} + e^{-3\beta\epsilon} + e^{-3\beta\epsilon}$$

$$Z_{MB} = 1 + 2e^{-\beta\epsilon} + e^{-2\beta\epsilon} + 2e^{-3\beta\epsilon} + 2e^{-4\beta\epsilon} + e^{-6\beta\epsilon}$$

Both methods are consistent.

(b) For B.E statistics, particles are indistinguishable.

\Rightarrow Only 6 configurations are possible;

$$Z_{BE} = 1 + e^{-2\beta\epsilon} + e^{-6\beta\epsilon} + e^{-\beta\epsilon} + e^{-4\beta\epsilon} + e^{-3\beta\epsilon}$$

$$\Rightarrow Z_{BE} = 1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon} + e^{-6\beta\epsilon}$$

		00		0	0	(3E)
	00		0	0		(E)
00			0		0	(0)
200>	020>	002>	110>	011>	101>	
↓	↓	↓	↓	↓	↓	
$E_1 = 0$	$E_2 = 2E$	$E_3 = 6E$	$E_4 = E$	$E_5 = 4E$	$E_6 = 3E$	

(c) Z_{FD} for 2 particles obey Fermi-Dirac statistics;

$$Z_{FD} = e^{-\beta E} + e^{-4\beta E} + e^{-3\beta E}$$

∴ Only 3 possible configurations with

$$E_4 = E, E_5 = 4E, E_6 = 3E$$

QNO 2

Starting from the usual grand canonical expression for the particle number density in terms of temperature and chemical potential,

$$n = \int_0^{\infty} g(\epsilon) f(\epsilon) d\epsilon \quad \text{--- (1)}$$

where; $g(\epsilon)$ = density of states

$f(\epsilon)$ = Fermi-Dirac distribution function

$$= \frac{1}{e^{\beta(\epsilon - \mu)} + 1}$$

∴ N = Number of particles = 2 (total number of states)

⇒ For 2-D Fermi gas,

$$N = 2 \sum_{\vec{k}} f(\vec{k}) = 2 \left(\frac{L}{2\pi}\right)^2 \int_0^{\infty} f(\vec{k}) d^2k = 2 \left(\frac{L}{2\pi}\right)^2 \int_0^{\infty} f(\vec{k}) 2\pi k dk = \frac{L^2}{\pi} \int_0^{\infty} k f(\vec{k}) dk$$

$$\therefore n = \text{number density} = \frac{N}{A}$$

$$n = \frac{N}{A} = \frac{N}{L^2} = \frac{1}{\pi} \int_0^{\infty} k f(\vec{k}) dk \quad \text{--- (2)}$$

$$\therefore E(\vec{k}) = \frac{\hbar^2 k^2}{2m}$$

$$k = \sqrt{\frac{2Em}{\hbar^2}}$$

$$dk = \sqrt{\frac{2m}{\hbar^2}} \cdot \frac{1}{2} \cdot (E)^{-1/2} dE$$

$$k dk = \sqrt{\frac{2m}{\hbar^2}} \cdot \frac{1}{2} \sqrt{\frac{2Em}{\hbar^2}} E^{-1/2} dE$$

$$= \left(\frac{2m}{\hbar^2}\right) \frac{1}{2} dE$$

$$\Rightarrow k dk = \frac{m}{\hbar^2} dE \quad \text{put in (2)}$$

$$\Rightarrow n = \frac{1}{\pi} \int_0^{\infty} \frac{m}{\hbar^2} dE = \int_0^{\infty} \frac{m}{\pi \hbar^2} f(E) dE \quad \text{--- (3)}$$

\Rightarrow By compare (1) and (3),

$$g(E) = \frac{m}{\pi \hbar^2}$$

$$\Rightarrow n = \int_0^{\infty} \frac{m}{\pi \hbar^2} f(\epsilon) d\epsilon$$

$$= \frac{m}{\pi \hbar^2} \int_0^{\infty} \frac{1}{e^{\beta(\epsilon - \mu)} + 1} d\epsilon$$

$$\frac{\pi \hbar^2 n}{m} = \int_0^{\infty} \frac{e^{-\beta \epsilon}}{(e^{-\beta \mu} + e^{-\beta \epsilon})} d\epsilon$$

$$= \frac{1}{\beta} \int_0^{\infty} \frac{-\beta e^{-\beta \epsilon}}{(e^{-\beta \mu} + e^{-\beta \epsilon})} d\epsilon$$

$$= -\frac{1}{\beta} \ln(e^{-\beta \mu} + e^{-\beta \epsilon}) \Big|_0^{\infty}$$

$$= \frac{1}{\beta} \ln(e^{-\beta \mu} + e^{-\beta \epsilon}) \Big|_{\infty}^0$$

$$= \frac{1}{\beta} \left[\ln(e^{-\beta \mu} + 1) - \ln(e^{-\beta \mu}) \right]$$

$$= \frac{1}{\beta} \ln \left(\frac{1 + e^{-\beta \mu}}{e^{-\beta \mu}} \right)$$

$$= \frac{1}{\beta} \ln(1 + e^{\beta \mu})$$

$$\Rightarrow n \frac{\pi \hbar^2}{m} = k_B T \ln(1 + e^{\beta \mu}) \quad (4)$$

$$\text{At } T=0 \quad f(\epsilon) = 1$$

$$\Rightarrow n = \int_0^{\epsilon_F} g(\epsilon) d\epsilon$$

$$n = \frac{m}{\pi \hbar^2} \int_0^{\epsilon_F} d\epsilon$$

$$\Rightarrow \epsilon_F = \frac{n \pi \hbar^2}{m} \quad \text{--- (5)}$$

$$\epsilon_F = \mu(T=0) = \frac{n \pi \hbar^2}{m}$$

By compare (4) and (5),

$$\epsilon_F = k_B T \ln(1 + e^{\beta \mu})$$

$$\frac{\epsilon_F}{k_B T} = \ln(1 + e^{\beta \mu})$$

$$\Rightarrow e^{\beta \mu} = e^{\epsilon_F / k_B T} - 1$$

$$\Rightarrow \mu = k_B T \ln(e^{\epsilon_F / k_B T} - 1)$$

QNO3

• Average energy per particle in degenerate

$$\text{Fermi gas} = \langle \epsilon \rangle = \frac{3}{5} \epsilon_F$$

$$\Rightarrow \text{At } T=0, \quad \epsilon_F = \mu \quad \Rightarrow \langle \epsilon \rangle = \frac{3}{5} \mu$$

We have to find the $\langle V_x^2 \rangle$ and $\langle V_x \rangle$

$$\therefore \frac{1}{2} m V^2 = E$$

$$V^2 = \frac{2E}{m}$$

$$\Rightarrow \langle V^2 \rangle = \frac{2}{m} \langle E \rangle$$

$$\therefore V^2 = V_x^2 + V_y^2 + V_z^2$$

$$\text{if } V_x = V_y = V_z$$

$$\text{then } V^2 = 3 V_x^2$$

$$\Rightarrow \langle 3 V_x^2 \rangle = \frac{2}{m} \langle E \rangle$$

$$\langle V_x^2 \rangle = \frac{2}{3m} \langle E \rangle$$

$$\langle V_x^2 \rangle = \frac{2}{3m} \cdot \frac{3}{5} \mu$$

$$\Rightarrow \boxed{\langle V_x^2 \rangle = \frac{2}{5} \frac{\mu}{m}}$$

$$\therefore \langle E \rangle = \frac{3}{5} \mu$$

(per particle)

\Rightarrow Similarly,

for $\langle V_x \rangle$

$$\sqrt{\frac{m}{2}} V = \sqrt{E}$$

$$\Rightarrow V = \sqrt{\frac{2}{m}} \sqrt{E}$$

$$\sqrt{3} V_x = \sqrt{\frac{2}{m}} \sqrt{E}$$

$$\Rightarrow v_x = \sqrt{\frac{2}{3m}} E^{1/2}$$

$$\langle v_x \rangle = \sqrt{\frac{2}{3m}} \langle E^{1/2} \rangle \quad \text{--- (A)}$$

Now calculate $\langle E^{1/2} \rangle$ for Fermi gas.

$$\therefore \langle E^{1/2} \rangle = g \int_0^{\infty} D(E) f(E) E^{1/2} dE$$

(Because of 2 electrons $\uparrow\downarrow$ in each k state) where; $g = \text{degeneracy factor} \rightarrow g = 2$

$$= 2 \int_0^{\infty} D(E) f(E) E^{1/2} dE$$

\therefore At absolute zero temperature $\mu = E_F$ and $f(E) = 1$

$$\Rightarrow \langle E^{1/2} \rangle = 2 \int_0^{E_F} D(E) E^{1/2} dE \quad \text{--- (1)}$$

$\therefore D(E) = \text{density of states}$.

$$\text{For 3-D fermi gas; } D(E) = \frac{V}{(2\pi)^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \quad \text{--- (2)}$$

plug $D(E)$ in Eq (1);

$$\begin{aligned} \Rightarrow \langle E^{1/2} \rangle &= 2 \int_0^{E_F} \frac{V}{(2\pi)^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2+1/2} dE \\ &= \frac{2V}{(2\pi)^2} \frac{(2m)^{3/2}}{\hbar^3} \int_0^{E_F} E dE \end{aligned}$$

$$\Rightarrow \langle E^{1/2} \rangle = \frac{2V}{(2\pi)^2} \frac{(2m)^{3/2}}{h^3} (2\pi)^3 \int_0^{E_F} E dE$$

$$= 2 \frac{(2\pi V)}{h^3} (2m)^{3/2} \frac{E_F^2}{2}$$

$$\langle E^{1/2} \rangle = \left(\frac{2\pi V}{h^3} \right) (2m)^{3/2} E_F^2 \quad \text{--- (3)}$$

\Rightarrow Total number of electrons = N

$$N = \int_0^{\infty} D(E) f(E) dE$$

$$= 2 \int_0^{E_F} D(E) dE$$

at $T=0$

$f(E) = 1$ and $\mu = E_F$

Recall from Eq (2); $D(E) = \frac{V}{(2\pi)^2} \left(\frac{2m}{h^2} \right)^{3/2} E^{1/2}$

$$\Rightarrow N = 2 \int_0^{E_F} \frac{V}{(2\pi)^2} \frac{(2m)^{3/2}}{h^3} E^{1/2} dE$$

$$= 2 \frac{(2\pi V)}{h^3} (2m)^{3/2} \int_0^{E_F} E^{1/2} dE$$

$$= 2 \left(\frac{2\pi V}{h^3} \right) (2m)^{3/2} \frac{E_F^{3/2}}{3/2}$$

$$= \left(\frac{2\pi V}{h^3} \right) (2m)^{3/2} E_F^{3/2} \quad \text{--- (4)}$$

\Rightarrow By comparing (3) and (4);

$$\frac{\langle E^{1/2} \rangle}{N} = \frac{\left(\frac{2\pi V}{h^3}\right) (2m)^{3/2} E_F^2}{\left(\frac{2\pi V}{h^3}\right) (2m)^{3/2} \frac{4}{3} E_F^{3/2}}$$

$$= \frac{3}{4} E_F^{(2-3/2)} = \frac{3}{4} E_F^{1/2} = \frac{3}{4} \mu^{1/2}$$

$$\Rightarrow \langle E^{1/2} \rangle = \frac{3}{4} N \mu^{1/2} \quad \text{plug in Eq (A)}$$

$$\Rightarrow \langle v_x \rangle = \sqrt{\frac{2}{3m}} \frac{3}{4} N \mu^{1/2}$$

$$= \frac{\sqrt{6\mu}}{m^{1/2}} N$$

$$\Rightarrow \boxed{\langle v_x \rangle = \sqrt{\frac{3\mu}{m8}} N} \quad \text{is required average of velocity in x-direction.}$$

Two Dimensional Fermi Gas

Answer: 4

In two dimensional system with periodic boundary conditions we can solve the Schrodinger equation with momentum $k_x = \frac{2\pi}{L}n_x$ and $k_y = \frac{2\pi}{L}n_y$. The number of allowed values of k -space inside area ($L^2 = A$) is

$$\begin{aligned}\text{Number of allowed values of } k\text{-space} &= (\pi k_f^2) \left(\frac{L}{2\pi}\right)^2 \\ \Rightarrow \text{Total number of electrons} &= 2(\pi k_f^2) \left(\frac{L}{2\pi}\right)^2 \\ &\Rightarrow n = \frac{N}{A} = \frac{N}{L^2} = \frac{k_f^2}{2\pi}\end{aligned}$$

In two dimensions the density of particles in range ($k + dk$) is ($2\pi k dk$).

$$\begin{aligned}\Rightarrow n &= \int_0^{+\infty} g(\varepsilon) f(\varepsilon) d\varepsilon \\ N &= 2 \sum_{\vec{k}} f(\vec{k}) \\ &= 2 \left(\frac{L}{2\pi}\right)^2 \int_0^{\infty} f(\vec{k}) d^2k \\ &= \frac{L^2}{2\pi^2} \int_0^{\infty} 2\pi k f(\vec{k}) dk \\ &= \frac{L^2}{\pi} \int_0^{\infty} k f(\vec{k}) dk \\ n &= \frac{N}{A} = \frac{N}{L^2} = \frac{1}{\pi} \int_0^{\infty} k f(\vec{k}) dk\end{aligned}$$

Where k can be calculated by using the relation of ground state energy,

$$\begin{aligned}\varepsilon(\vec{k}) &= \frac{\hbar^2 k^2}{2m} \\ \Rightarrow k &= \sqrt{\frac{2\varepsilon(\vec{k})m}{\hbar^2}} \\ \Rightarrow dk &= \sqrt{\frac{2m}{\hbar^2}} \cdot \frac{1}{2} \cdot \varepsilon(\vec{k})^{-1/2} d\varepsilon \\ \Rightarrow k dk &= \sqrt{\frac{2m}{\hbar^2}} \cdot \frac{1}{2} \cdot \sqrt{\frac{2\varepsilon(\vec{k})m}{\hbar^2}} \cdot \varepsilon(\vec{k})^{-1/2} d\varepsilon \\ &= \left(\frac{m}{\hbar^2}\right) d\varepsilon\end{aligned}$$

Thus electron density will become,

$$\begin{aligned} n &= \frac{1}{\pi} \int_0^\infty \left(\frac{m}{\hbar^2} \right) f(\varepsilon(\vec{k})) d\varepsilon \\ &= \int_0^\infty \left(\frac{m}{\pi \hbar^2} \right) f(\varepsilon(\vec{k})) d\varepsilon \end{aligned}$$

Where density of state $g(\varepsilon)$ is,

$$g(\varepsilon) = \frac{m}{\pi \hbar^2}$$

(b).

$$\begin{aligned} \therefore E_f &= \frac{\hbar^2 k_f^2}{2m} \\ &= \frac{\hbar^2}{2m} (2\pi n) \quad \because k_f^2 = 2\pi n \\ &= \frac{\pi n \hbar^2}{m} \\ &= \frac{3.14 \times 6 \times 10^{14} \times (1.055 \times 10^{-34})^2}{9.1 \times 10^{-31}} \\ &= 2.301 \times 10^{-19} \text{ J} \\ &= 1.436 \text{ eV} \end{aligned}$$

QNo5

(a) Using the relation for thermal de Broglie wavelength;

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$$

at room temperature, $T = 300 \text{ K}$, for electron

$$\lambda = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 3.14 \times 9.11 \times 10^{-31} \times 1.38 \times 10^{-23} \times 300}}$$

$$\lambda = 4.3 \times 10^{-9} \text{ m}$$

\Rightarrow The requirement for the very applicability of the

Classical approximation is that the de-Broglie wavelength (its magnitude) λ be smaller than the interparticle separation, i.e.,

$$\lambda \ll \frac{L}{N^{1/3}}$$

$$\Rightarrow \lambda^3 \ll \frac{L^3}{N}$$
$$= \frac{V}{n} = \frac{1}{n}$$

$$\Rightarrow \lambda^3 \ll \frac{1}{n}$$

$$\therefore n = 8.5 \times 10^{28} \text{ m}^{-3} \quad \Rightarrow \quad \frac{1}{n} = 1.176 \times 10^{-29} \text{ m}^3$$

$$\text{and } \lambda^3 = (4.3 \times 10^{-9} \text{ m})^3 = 7.95 \times 10^{-26} \text{ m}^3$$

\Rightarrow it is clear that

$$7.95 \times 10^{-26} \text{ m}^3 \gg 1.17 \times 10^{-29} \text{ m}^3$$

means to say that $\lambda^3 \ll \frac{1}{n}$

Thus, Boltzmann statistics cannot be applied to the mobile electrons in copper.

(b) Using the relation b/w number density and Fermi energy E_F ;

$$E_F = \frac{h^2}{8m} \left(\frac{3n}{\pi} \right)^{2/3}$$

$$= \frac{(6.625 \times 10^{-34})^2 (3 \times 8.5 \times 10^{28})^{2/3}}{8 \times 9.11 \times 10^{-31} \times (3.14)^{2/3}}$$

$$E_F = 1.1 \times 10^{-18} \text{ J}$$

$$\therefore E = k_B T$$

at Room temperature = 300K

$$= (1.38 \times 10^{-23} \times 300)$$

$$E = 4.14 \times 10^{-21} \text{ J}$$

\Rightarrow The condition for strongly degenerate gas

$$E_F \gg k_B T$$

$$1.1 \times 10^{-18} \text{ J} \gg 4.14 \times 10^{-21} \text{ J}$$

is fulfilled. Thus, room temperature sufficient to treat this system as degenerate electron gas.

ASSIGNMENT # 6 (SOLUTION)

Q#10 find a relation b/w electron density 'n' and Fermi momentum; just find the total number of electrons in degenerate electron gas.

$$\therefore N = g \sum_{\vec{k}} f(\epsilon_{\vec{k}})$$

where $g = \text{degeneracy factor} = 2$ and $f(\epsilon_{\vec{k}})$ is Fermi Dirac distribution function; for degenerate gas $f(\epsilon) \rightarrow 1$.

and sum over all \vec{k} states is

$$\sum_{\vec{k}} \rightarrow \frac{V}{(2\pi)^3} \int d^3k$$

$$\Rightarrow N = 2 \frac{V}{(2\pi)^3} \int 4\pi k^2 dk.$$

$$= \frac{2(4\pi)V}{(2\pi)^3} \frac{1}{h^3} \int_0^{P_F} p^2 dp$$

$$= \frac{8\pi V}{(2\pi)^3} \frac{1}{(h/2\pi)^3} \int_0^{P_F} p^2 dp.$$

$$\Rightarrow N = \frac{8\pi V}{h^3} \frac{P_F^3}{3}$$

$$\Rightarrow n = \frac{N}{V} = \frac{8\pi}{h^3} \frac{P_F^3}{3} \quad \text{or} \quad n = \frac{8\pi}{3} \left(\frac{P_F}{h}\right)^3 \quad \text{--- (1)}$$

\Rightarrow According to the given condition, we have to find n for which $P_F = \frac{m_0 c}{10}$, plug in (1)

$$\begin{aligned} \therefore P &= \hbar k \\ \Rightarrow \frac{1}{\hbar} dP &= dk \end{aligned}$$

$$\Rightarrow n = \frac{8\pi}{3} \left(\frac{m_e c}{10h} \right)^3$$

$$= \frac{8 \times 3.14}{3} \left(\frac{9.11 \times 10^{-31} \times 3 \times 10^8}{10 \times 6.625 \times 10^{-34}} \right)^3$$

$$\boxed{n = 5.8 \times 10^{32} \text{ m}^{-3}}$$

(b) For a strong degenerate Fermi gas (under the approximation of zero valence), we get.

$$\langle E \rangle = U = \frac{3}{5} N E_F$$

and $P = \frac{2}{3} \frac{U}{V}$

$$= \frac{2}{3} \frac{1}{V} \frac{3}{5} N E_F = \frac{2}{5} n E_F$$

$$= \frac{2}{5} n \frac{p_F^2}{2m_e} = \frac{n p_F^2}{5 m_e}$$

$$\therefore E_F = \frac{p_F^2}{2m_e}$$

$$= \frac{n}{5 m_e} \left(\frac{3n}{8\pi} \right)^{2/3} h^2 \quad \therefore p_F^2 = \left(\frac{3n}{8\pi} \right)^{2/3} h^2$$

$$= \frac{(5.8 \times 10^{32})}{5 \times 9.11 \times 10^{-31}} \left(\frac{3 \times 5.8 \times 10^{32}}{8 \times 3.14} \right)^{0.66} (6.625 \times 10^{-34})^2$$

$$\boxed{P = 5.44 \times 10^{16} \text{ N/m}^2}$$

Q # 2

(a) We have to find a relation for average k.E U of the electrons and the density n_e , for the extremely relativistic electrons;
 ↓ (ignore rest energy)

$$U = \langle E \rangle = \sum_{\vec{k}} f(\vec{k}) \epsilon_{\vec{k}}$$

where,

$$\sum_{\vec{k}} \rightarrow \frac{V}{(2\pi)^3} \int d^3k$$

$$= \frac{V}{(2\pi)^3} 4\pi \int k^2 dk$$

We use the approximation of strong degenerate electron gas and $\epsilon = pc$;

$$U = \frac{V}{(2\pi)^3} g 4\pi \int \epsilon k^2 dk$$

$$= \frac{V}{(2\pi)^3} 2(4\pi) \int_0^{p_F} pc \left(\frac{\hbar^2 k^2}{\hbar^2} \right) \frac{1}{\hbar} dp$$

$$= \frac{8\pi V}{(2\pi)^3} \frac{c}{\hbar^3} \int_0^{p_F} p p^2 dp$$

$$= \frac{8\pi V c}{h^3} \int_0^{p_F} p^3 dp = \frac{8\pi V c}{h^3} \frac{p_F^4}{4}$$

$$\Rightarrow \boxed{U = \frac{2\pi V c}{h^3} \frac{p_F^4}{4}} \quad \text{--- (A)}$$

$$\begin{aligned} \because \epsilon &= pc \\ &= \hbar k c \\ \Rightarrow dk &= \frac{1}{\hbar} dp \end{aligned}$$

$$\because g = \text{degeneracy} = 2$$

$$\therefore N = \sum_{\vec{k}} f(\epsilon_{\vec{k}})$$

where, Sum over all k -states

$$\sum_{\vec{k}} \rightarrow \frac{V}{(2\pi)^3} \int d^3k$$

$$\text{and } f(\epsilon_{\vec{k}}) \rightarrow 1$$

(for degenerate gas ($T=0$))

$$\Rightarrow N = \frac{V}{(2\pi)^3} g \int d^3k$$

$$= \frac{V}{(2\pi)^3} 2 (4\pi) \int k^2 dk$$

$$= \frac{8\pi V}{(2\pi)^3} \frac{1}{h^3} \int_0^{p_F} h^2 k^2 d(hk)$$

$$= \frac{8\pi V}{(2\pi)^3} \left(\frac{2\pi}{h}\right)^3 \int_0^{p_F} p^2 dp$$

$$\therefore p = \hbar k.$$

$$N = \frac{8\pi V}{h^3} \frac{p_F^3}{3}$$

$$\Rightarrow \boxed{\frac{N}{V} = n_e = \frac{8\pi}{3h^3} p_F^3} \quad \text{--- (B)}$$

\Rightarrow Now compare (A) and (B),

$$U = \langle E \rangle = \left(\frac{2\pi C}{h^3} p_F^4 \right) V$$

$$= \left(\frac{2\pi C}{h^3} p_F^4 \right) \frac{V}{N} \cdot N = \left(\frac{2\pi C}{h^3} p_F^4 \right) \frac{N}{n}$$

$$= \left(\frac{4(2\pi)}{3h^3} \cdot \frac{3}{4} p_F^3 \right) p_F C \frac{N}{n}$$

$$= \left(\frac{8\pi}{3h^3} p_F^3 \right) \frac{3}{4} p_F C \frac{N}{n}$$

$$= \cancel{N} \frac{3}{4} p_F C \frac{N}{\cancel{N}} = \frac{3}{4} C N p_F$$

$$\langle E \rangle = \frac{3}{4} C N \left(\frac{3h^3 n_e}{8\pi} \right)^{1/3} = \frac{3}{4} h c \left(\frac{3n_e}{8\pi} \right)^{1/3} \cdot N$$

$$\Rightarrow \langle E_e \rangle = \frac{3}{4} hc \left(\frac{3n_e}{8\pi} \right)^{1/3} \text{ is the required relation.}$$

$$\langle E_e \rangle \text{ per particle} = \frac{3}{4} hc \left(\frac{3n_e}{8\pi} \right)^{1/3}$$

$$\Rightarrow \text{Given that; } \rho = 10^9 \text{ g cm}^{-3} \text{ and } n_e = 14 n_i \text{ (electron number density)}$$

$$\therefore M = N m_e + 2 N m_n$$

$$N m_e = (\text{Number of electrons}) (\text{mass of electron})$$

$$2 N m_n = (\text{Number of nucleons}) (\text{mass of nucleon})$$

$$\Rightarrow M = N m_e + 2 N m_n$$

$$\therefore m_e \ll m_n$$

$$\Rightarrow N = \frac{M}{2 m_n} \quad \text{and} \quad n = \frac{N}{V} = \frac{M}{M/\rho}$$

$$\Rightarrow n = \frac{\rho}{2 m_n} \quad ; \quad n_i = \frac{\rho}{2 m_i}$$

$$m_i = \frac{14 \text{ g}}{N_A} = \frac{14 \text{ g}}{6.023 \times 10^{23}} = 2.32 \times 10^{-23} \text{ g}$$

$$\Rightarrow n_i = \frac{10^9 \text{ g cm}^{-3}}{2 \times 2.32 \times 10^{-23} \text{ g}} = 2.155 \times 10^{31} \text{ cm}^{-3}$$

$$\begin{aligned} \Rightarrow n_e &= 14 (2.155 \times 10^{31}) \\ &= 3.01 \times 10^{32} \text{ cm}^{-3} \\ &= 3.01 \times 10^{38} \text{ m}^{-3} \end{aligned}$$

$$\Rightarrow \langle E_e \rangle = \frac{3}{4} hc \left(\frac{3n_e}{8\pi} \right)^{1/3}$$

$$= \frac{3}{4} \times 6.625 \times 10^{-34} \times 3 \times 10^8 \left(\frac{3 \times 3.01 \times 10^{38}}{8 \times 3.14} \right)^{1/3}$$

$$\langle E_e \rangle = 5 \times 10^{-13} \text{ J}$$

and Assume "ion gas" as "Maxwell-Boltzmann gas";

$$\langle E_i \rangle = \frac{3}{2} k_B T = \frac{3}{2} (1.38 \times 10^{-23}) (10^8 \text{ K}) = 2 \times 10^{-15} \text{ J}$$

$$\text{obviously; } \boxed{\langle E_i \rangle \ll \langle E_e \rangle}$$

Q#3

For a gas of N photons with number conservation;

$$N = 2V \int_0^\infty \frac{d^3k}{(2\pi)^3} \left(\frac{1}{e^{\beta \hbar c k} - 1} \right)$$

\Rightarrow 2 comes from the two polarizations of photons.

$$n = \frac{N}{V} = \frac{2}{(2\pi)^3} 4\pi \int_0^{\infty} \frac{k^2 dk}{z^{-1} e^{\beta \hbar c k} - 1}$$

$\because z = e^{\beta \mu}$
 $z = \text{fugacity}$

$$= \frac{1}{\pi^2} \int_0^{\infty} \frac{k^2 dk}{z^{-1} e^{\beta \hbar c k} - 1}$$

$$= \frac{1}{\pi^2} (\beta \hbar c)^3 \int_0^{\infty} \frac{(\beta \hbar c k)^2 d(\beta \hbar c k)}{z^{-1} e^{\beta \hbar c k} - 1}$$

$(\because x = \beta \hbar c k)$

$$= \frac{1}{\pi^2} \frac{1}{(\beta \hbar c)^3} \int_0^{\infty} \frac{x^2 dx}{z^{-1} e^x - 1}$$

Let $\int_0^{\infty} \frac{x^2 dx}{z^{-1} e^x - 1} = \int_0^{\infty} \frac{z x^2 e^{-x}}{(1 - z e^{-x})} dx$

where $\frac{z e^{-x}}{(1 - z e^{-x})} = z e^{-x} (1 - z e^{-x})^{-1}$

$$= z e^{-x} [1 + z e^{-x} + z^2 e^{-2x} + \dots]$$

$$= \sum_{p=1}^{\infty} z^p e^{-px}$$

$$\Rightarrow \int_0^{\infty} \frac{z x^2 e^{-x}}{(1 - z e^{-x})} dx = \sum_{p=1}^{\infty} z^p \int_0^{\infty} x^2 e^{-px} dx$$

$\because \gamma = xp$

$$= \sum_{p=1}^{\infty} \frac{z^p}{p^3} \int_0^{\infty} e^{-\gamma} \gamma^2 d\gamma$$

$$\therefore \int_0^{\infty} x^n e^{-x/a} dx = a^{n+1} n!$$

$$\Rightarrow \int_0^{\infty} x^{z-1} e^{-x} dx = \Gamma(z) = (z-1)!$$

Therefore,

$$\int_0^{\infty} \frac{z x^z e^{-x}}{(1 - z e^{-x})} dx = \sum_{p=1}^{\infty} \frac{z^p}{p^3} \Gamma(3) = \sum_{p=1}^{\infty} \frac{z^p}{p^3} \cdot 2.$$

$$\Rightarrow n = \frac{2}{\pi^2} \left(\frac{k_B T}{h c} \right)^3 \sum_{p=1}^{\infty} \frac{z^p}{p^3} \quad \therefore g_3(z) = \sum_{p=1}^{\infty} \frac{z^p}{p^3}$$

$$= \frac{2}{\pi^2} \left(\frac{k_B T}{h c} \right)^3 g_3(z)$$

\Rightarrow The function $g_3(z)$ is finite at $z=1$, thus n has a upper limit. There is condensation to the zero momentum state when n exceeds the critical density.

$$n_c = \frac{2}{\pi^2} \left(\frac{k_B T}{h c} \right)^3 g_3(1)$$

\Rightarrow At constant density n , the condensation occurs below the critical temperature.

$$\left(\frac{\pi^2 n}{2} \right) \frac{h^3 c^3}{k_B^3} \frac{1}{g_3(1)} = T_c^3$$

$$\Rightarrow T_c = \frac{h c}{k_B} \left(\frac{\pi^2 n}{2 g_3(1)} \right)^{1/3}$$

QNO5

(a) The universe is pervaded by $T=3k$ black body radiation, this radiation arose from the adiabatic expansion of photon cloud.

\Rightarrow The energy density of black body radiation is

$$u = aT^4 \quad \text{--- (1)}$$

so the total energy is

$$E \sim VT^4 \quad \text{--- (2)}$$

Using first law of thermodynamics,

$$dU = dQ - PdV$$

$$dU = TdS - PdV$$

$$\therefore C_V = \left(\frac{\partial U}{\partial T} \right)_V = T \left(\frac{\partial S}{\partial T} \right)_V \propto VT^3$$

\rightarrow For a reversible adiabatic expansion, $\Delta S = 0$ means entropy remains constant.

$$\therefore \Delta S = \int_{T=0}^T \frac{C_V}{T} dT$$

$$\Delta S = S(T=T) - S(T=0)$$

Using third law of thermodynamics $S(T=0) = 0$

$$\begin{aligned} \Rightarrow S(T) &= \int_0^T \frac{C_V}{T} dT \\ &\sim V \int_0^T \frac{T^3}{T} dT \\ &= V \int_0^T T^2 dT = \frac{V}{3} T^3 \end{aligned}$$

$$\Rightarrow S(T) \sim VT^3$$

$$\Rightarrow S(T_1) \sim V_1 T_1^3$$

Now if $V_2 = 2V_1$, then T_2 will be

$$\therefore S(T_2) - S(T_1) = 0 \Rightarrow (T_2^3 V_2 - T_1^3 V_1)$$

$$\Rightarrow T_2^3 V_2 = T_1^3 V_1$$

$$T_2^3 = T_1^3 \frac{V_1}{2V_1}$$

$$\Rightarrow T_2^3 = \frac{T_1^3}{2}$$

$$\Rightarrow T_2 = \frac{T_1}{2^{1/3}} = \frac{3}{2^{1/3}}$$

$$\boxed{T_2 = 2.38k}$$

(b) For black body radiation, the total partition function is

$$Z = Z(k_1) \cdot Z(k_2) \cdot Z(k_3) \dots$$

where the partition function for the mode of wave vector k is

$$Z(k) = \frac{1}{(1 - e^{-\hbar \omega_k \beta})}$$

$$\Rightarrow \langle E \rangle = -\frac{\partial}{\partial \beta} \ln(Z)$$

where, $\ln(Z) = \sum_k \ln Z(k)$

$$= \sum_k \ln \frac{1}{(1 - e^{-\hbar \omega_k \beta})}$$

$$= \frac{-V}{(2\pi)^3} \int d^3k \ln(1 - e^{-\hbar \omega_k \beta})$$

$$= \frac{-V}{(2\pi)^3} 4\pi \int k^2 dk \ln(1 - e^{-\beta \hbar \omega})$$

$$= \frac{-2V 4\pi}{(2\pi)^3} \frac{1}{\hbar^3} \int_0^\infty p^2 dp \ln(1 - e^{-\beta c p})$$

$$= \frac{-8\pi V}{h^3} \int_0^\infty p^2 dp \ln(1 - e^{-\beta c p})$$

$$= \frac{-8\pi V}{h^3 (c\beta)^3} \int_0^\infty x^2 \ln(1 - e^{-x}) dx$$

$$x = \beta c p$$

$$= + \frac{8\pi V}{(hc)^3} \frac{1}{3} \int_0^{\infty} \frac{x^3}{e^x - 1} dx$$

$$\ln(Z) = \frac{8\pi V}{(hc)^3} \frac{\pi^4}{3(15)}$$

$$\Rightarrow \frac{\langle E \rangle}{V} = \frac{-8\pi^5}{3(15)(hc)^3} \frac{\partial}{\partial \beta} \beta^{-3}$$

$$= \frac{8\pi^5}{15(hc)^3} (k_B T)^4 = 10^{-14} \text{ J m}^{-3}$$

$$\therefore T = 2.3 \text{ K}$$

Q #6

The total radiant energy flux at the Earth from Sun, is $\Phi_E = 0.14 \times 10^7 \text{ erg cm}^{-2} \text{ s}^{-1}$

\Rightarrow The flux that illuminates the Earth is proportional to the solid angle $\Delta\Omega$, subtended by the Sun's surface at the Earth:

$$\Delta\Omega = \frac{\pi R_s^2}{d^2}$$

\Rightarrow The radiant energy flux at Earth is therefore,

$$\Phi_E = \Delta\Omega \Phi_s$$

$$\Phi_E = \left(\frac{\pi R_s^2}{d^2} \right) \sigma_B T_s^4$$

$$\Rightarrow \frac{0.14 \times 10^7 \text{ erg cm}^{-2} \text{ s}^{-1}}{(3.14) \sigma_B} \left(\frac{d}{R_s} \right)^2 = T_s^4$$

$$T_s^4 = \left(\frac{1.5 \times 10^{13}}{7 \times 10^{10}} \right)^2 \frac{0.14 \times 10^7 \text{ erg cm}^{-2} \text{ s}^{-1}}{(3.14) (5.67 \times 10^{-5} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ K}^{-4})}$$

$$T_s \approx 5000 \text{ K}$$