TOPIC : THERMODYNAMIC FUNCTIONS (MONOATOMIC GASES)

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APRIL 8, 2020

$$Z(N,V,T) = \frac{(q_{trans}\, q_{elec}\, q_{nucl})^N}{N!}$$

$\downarrow$

Canonical Ensemble Partition f$^n$ of Monoatomic gases

Thus, Helmholtz Free energy, $A(N,V,T)$

$$A(N,V,T) = -k_B T \ln\left(Z(N,V,T)\right)$$

$$= -k_B T \left\{ N \ln(q_{trans}\, q_{elec}\, q_{nucl}) - (N\ln(N) - N) \right\}$$

$$= -N k_B T \left\{ \ln(q_{trans}\, q_{elec}\, q_{nucl}) - \ln\left(\frac{N}{e}\right) \right\}$$

$$\Rightarrow \boxed{A(N,V,T) = -N k_B T \ln\left[\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}}\left(\frac{Ve}{N}\right)\right] - N k_B T \ln\left(\omega_{e_1} + \omega_{e_2}\, e^{-\beta \Delta\varepsilon_{12}}\right) - N k_B T \ln(\omega_{n_1}) + \cdots}$$

HOME WORK : Put $N = N_A$

AND EVALUATE "$A(N_A, V, T)$"

in terms of "$R$" = Universal GAS CONSTANT

# Internal Energy of Monoatomic gases

$$\bar{E} = K_B T^2 \left( \frac{\partial \ln Z(N,V,T)}{\partial T} \right)_{N,V}$$

$$\Rightarrow \ln\left(Z(N,V,T)\right) = N \ln\left(q_{tran}\, q_{elec}\, q_{nucl}\right) - \left(N \ln(N) - N\right)$$

$$\Rightarrow \ln\left(Z(N,V,T)\right) = N \ln\left[ \left(\frac{2\pi m K_B T}{h^2}\right)^{\frac{3}{2}} \left(\frac{Ve}{N}\right)\right] - N \ln\left(\omega_{e1} + \omega_{e2}\, e^{-\beta \Delta \varepsilon_{12}} + \ldots\right) - + \ldots +$$

$$\Rightarrow \bar{E} = N K_B T^2 \times \left(\frac{3}{2T}\right) - N K_B T^2 \left(\frac{\omega_{e2}\, e^{-\beta \Delta \varepsilon_{12}}}{q_{elec}}\right) \times \left(-\frac{1}{K_B T^2}\right)$$

$$\boxed{\bar{E} = \frac{3}{2} N K_B T + \frac{N \omega_{e2}\, e^{-\beta \Delta \varepsilon_{12}}}{q_{elec}} + \ldots}$$

Ignoring nuclear partition function because $q_{nucl} = \omega_{n1}$ only at STP

# Pressure of Monoatomic gases

$$\bar{p} = K_B T \left( \frac{\partial \ln\left(Z(N,V,T)\right)}{\partial V} \right)_{N,T}$$

$$\Rightarrow \boxed{\bar{p} = N K_B T \times \left(\frac{1}{V}\right) = \frac{N K_B T}{V}}$$

HOMEWORK: OBTAIN $\bar{E}$ and $\bar{p}$ by putting $N = N_A$. WRITE IN TERMS OF universal gas constant "R"