Progress Report

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α, β

1 $dN = 0, \sum_{i=0}^{i=r} dn_i = 0$ 總粒子數保持一定

2 $dU = 0, \sum_{i}^{i=r} dn_i \varepsilon_i = 0, \varepsilon \sum_{i}^{i=r} dn_i = 0$ 總內能保持一定

3 $\sum (1 + \ln n_i) dn_i = 0$

Lagrange method

$$\alpha + \beta\varepsilon_i + \ln n_i = 0 \quad \Rightarrow \quad \boxed{n_i = e^{-\alpha} \cdot e^{-\beta\varepsilon_i}}$$

$$\because \sum_{i=0}^{i=r} n_i = N = \sum_{i=0}^{i=r} e^{-\alpha} \cdot e^{-\beta\varepsilon_i} = e^{-\alpha} \sum_{i=0}^{i=r} e^{-\beta\varepsilon_i} \rightarrow e^{-\alpha} = \frac{N}{\sum_{i=0}^{i=r} e^{-\beta\varepsilon_i}}$$

所以，任一能階上的粒子數目

$$n_i = e^{-\alpha} \cdot e^{-\beta\varepsilon_i}$$

$$n_i = \frac{N}{\sum_{i=0}^{i=r} e^{-\beta\varepsilon_i}} \cdot e^{-\beta\varepsilon_i} = \frac{N}{Z} e^{-\beta\varepsilon_i}$$

$$Z = \sum_{i=0}^{i=r} e^{-\beta\varepsilon_i} = e^{-\beta\varepsilon_0} + e^{-\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + \ldots + e^{-\beta\varepsilon_r}$$ (分配函數 Partition function)

求β **利用一理想氣體分子在一維之平均動能**

$$\bar{\varepsilon} = \frac{1}{2}KT = \frac{U}{N} = \frac{\sum_{i=0}^{i=r} n_i \varepsilon_i}{N} = \sum_{i=0}^{i=r} \frac{n_i}{N} \cdot \varepsilon_i = \frac{\sum_{i=0}^{i=r} e^{-\beta\varepsilon_i} \cdot \varepsilon_i}{Z} = \frac{\sum_{i=0}^{i=r} e^{-\beta\varepsilon_i} \cdot \varepsilon_i}{\sum_{i=0}^{i=r} e^{-\beta\varepsilon_i}}$$

又ε_i 為第i個理想氣體分子之一維移動動能(內能)

$$\varepsilon_i = \frac{1}{2} m V_i^2 = \frac{(mV_i)^2}{2m} = \frac{P^2}{2m}$$

$$\bar{\varepsilon} = \frac{\sum_{i=0}^{i=r} e^{-\beta \cdot \frac{P_i^2}{2m}} \cdot \frac{P_i^2}{2m}}{\sum_{i=0}^{i=r} e^{-\beta \cdot \frac{P_i^2}{2m}}} = \frac{\frac{1}{2m} \sum_{i=0}^{i=r} e^{-ax^2} \cdot x^2}{\sum_{i=0}^{i=r} e^{-ax^2}}$$

令 $P_i = x, \quad \frac{\beta}{2m} = a$

積分上式

$$\bar{\varepsilon} = \frac{\frac{1}{2m} \int_{-\infty}^{\infty} e^{-ax^2} \cdot x^2 dx}{\int_{-\infty}^{\infty} e^{-ax^2} \cdot x^2 dx} = \frac{\frac{1}{2m} \cdot \frac{1}{2a} \sqrt{\frac{\pi}{a}}}{\sqrt{\frac{\pi}{a}}} = \frac{1}{4ma} \xrightarrow{\because a = \frac{\beta}{2m}} \frac{1}{2\beta} = \frac{1}{2} KT$$

$$\therefore \beta = \frac{1}{KT}$$

$$n_i = \frac{N}{\sum_{i=0}^{i=r} e^{-\beta\varepsilon_i}} \cdot e^{-\beta\varepsilon_i} = \frac{N}{Z} e^{-\frac{\varepsilon_i}{KT}}$$

$$\frac{n_i}{n_j} = \frac{e^{\frac{-\varepsilon_i}{KT}}}{e^{\frac{-\varepsilon_j}{KT}}}$$

能階ε_i上的粒子數

能階ε_j上的粒子數

能階退化(degeneracy)時(有gi個能階有相等能量，gi為統計權)，Boltzmann分佈需修正

$$n_i = \frac{N}{\sum_{i=0}^{i=r} g_i e^{-\beta\varepsilon_i}} \cdot e^{-\beta\varepsilon_i} = \frac{N}{Z} g_i e^{-\frac{\varepsilon_i}{KT}}$$

$$\frac{n_i}{n_j} = \frac{g_i \cdot e^{\frac{-\varepsilon_i}{KT}}}{g_i \cdot e^{\frac{-\varepsilon_j}{KT}}}$$

若$\varepsilon_i > \varepsilon_j$則$n_i < n_j$，即熱平衡時，系統粒子最大分部形式中，佔據越高能階之粒子數將減少；且溫度升高時(T↑)佔具較高能階(ε_i)之粒子數(n_i)相對於佔據能量較低能階的粒子數比值將變高，及溫度升高時佔具高能階粒子數將相對變多。