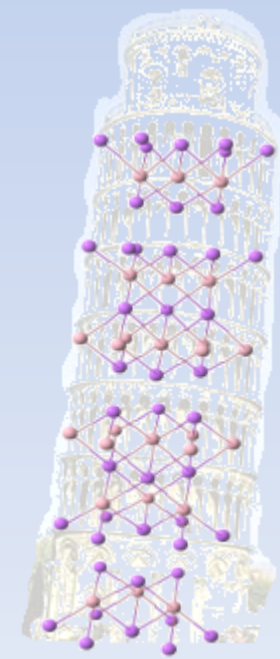
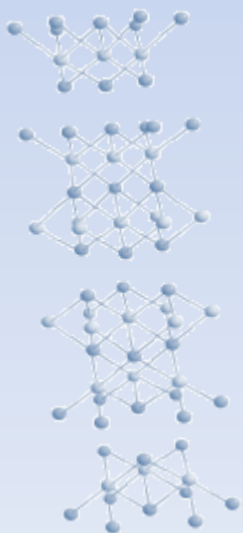


Progress Report

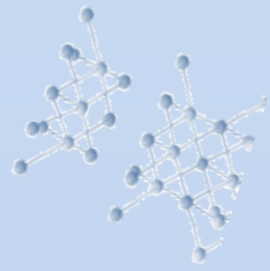
Advisor: Prof. Chien-Neng Liao

Student: Hung-Hsien Huang

Date:2011/01/04



α, β



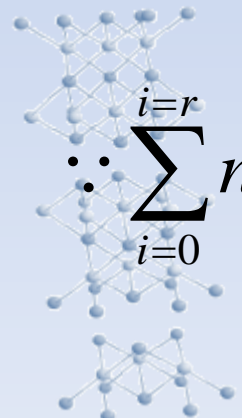
1 $dN = 0, \sum_{i=0}^{i=r} dn_i = 0$ 總粒子數保持一定

2 $dU = 0, \sum_i dn_i \varepsilon_i = 0, \varepsilon \sum_i dn_i = 0$ 總內能保持一定

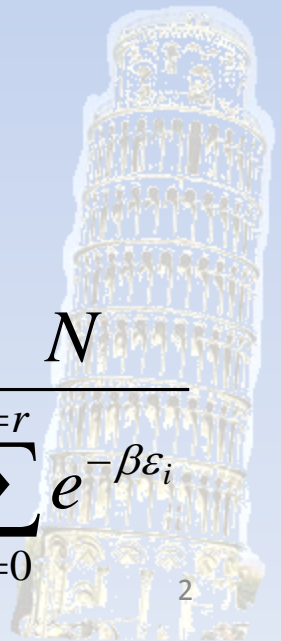
3 $\sum (1 + \ln n_i) dn_i = 0$

Lagrange method

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



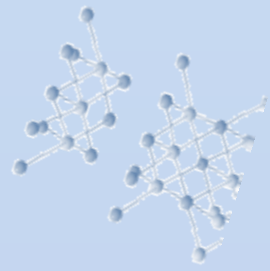
$$\because \sum_{i=0}^{i=r} n_i = N = \sum_{i=0}^{i=r} e^{-\alpha} \cdot e^{-\beta \varepsilon_i} = e^{-\alpha} \sum_{i=0}^{i=r} e^{-\beta \varepsilon_i} \rightarrow e^{-\alpha} = \frac{N}{\sum_{i=0}^{i=r} e^{-\beta \varepsilon_i}}$$



所以，任一能階上的粒子數目

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

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



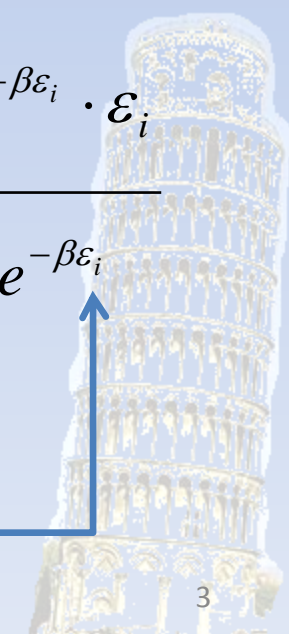
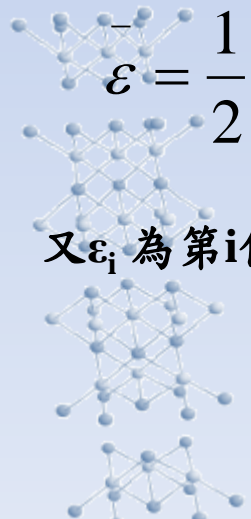
$$Z = \sum_{i=0}^{i=r} e^{-\beta \varepsilon_i} = e^{-\beta \varepsilon_0} + e^{-\beta \varepsilon_1} + e^{-\beta \varepsilon_2} + \dots + e^{-\beta \varepsilon_r} \quad (\text{分配函數 Partition function})$$

求 β 利用一理想氣體分子在一維之平均動能

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

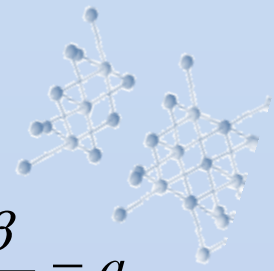
又 ε_i 為第 i 個理想氣體分子之一維移動動能(內能)

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



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

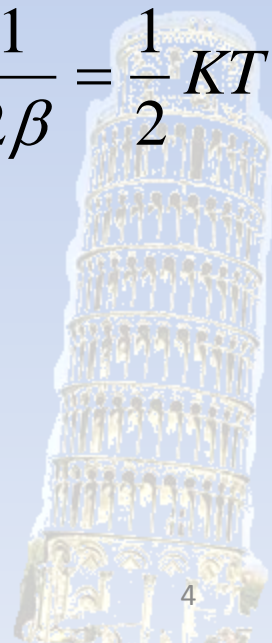
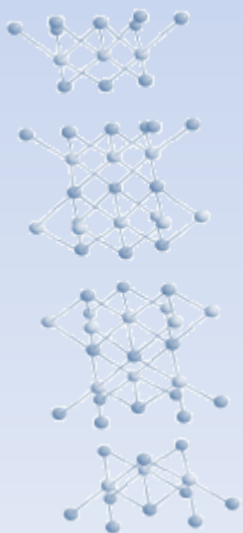
令 $P_i = x, \quad \frac{\beta}{2m} = a$

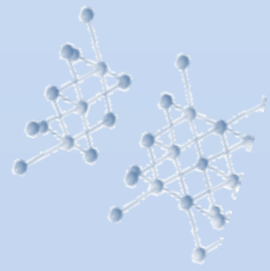


積分上式

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

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





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

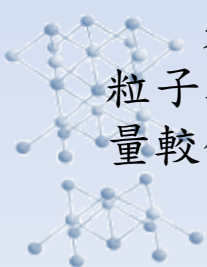
$$\frac{n_i}{n_j} = \frac{e^{-\frac{\varepsilon_i}{KT}}}{e^{-\frac{\varepsilon_j}{KT}}} \quad \text{能階 } \varepsilon_i \text{ 上的粒子數}$$

$$\frac{n_i}{n_j} = \frac{e^{-\frac{\varepsilon_i}{KT}}}{e^{-\frac{\varepsilon_j}{KT}}} \quad \text{能階 } \varepsilon_j \text{ 上的粒子數}$$

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



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



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($T \uparrow$)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。