Progress Report

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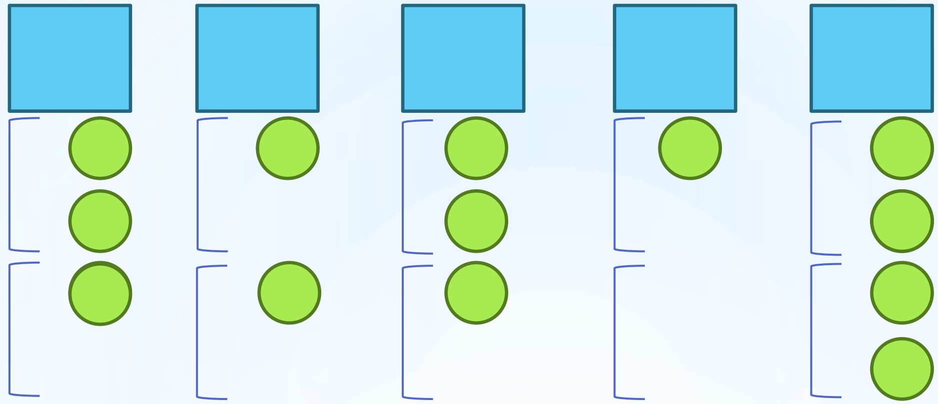
Maxwell-Boltzmann Distribution

* 能　　階：ε_1、ε_2、…、ε_l、…
* 簡併度：ω_1、ω_2、…、ω_l、…
* 粒子數：a_1、a_2、…、a_l、…



1	2	3	4	5
ω = 2	ω = 2	ω = 2	ω = 2	ω = 2
a = 3	a = 2	a = 3	a = 1	a = 4

There are $\prod_l \omega_l^{al}$ conditions

$$\Omega = \frac{N!}{\prod_l a_l!}\prod_l \omega_l^{al}$$

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Stirling approximation： $\ln m! = m \ln m - m$

$$\ln \Omega = N \ln N - \sum_l a_l \ln a_l + \sum_l a_l \ln \omega_l$$

find extreme value of lnΩ

$$\delta \ln \Omega = -\sum_l \ln \frac{a_l}{\omega_l} \delta a_l = 0$$

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$$\delta N = \sum_l \delta a_l = 0 \quad \delta E = \sum_l \varepsilon_l \delta a_l = 0$$

In order to find extreme value of $\ln \Omega$

we have to use technique of Lagrange

Lagrange Multiplier Method

Usually , we find the extreme value of $f(x,y)$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = 0$$

but if x,y are confined by g(x,y)=0

Lagrange Multiplier Method :

$$\begin{cases} \dfrac{\partial f}{\partial x} + \lambda \dfrac{\partial g}{\partial x} = 0 \\ \dfrac{\partial f}{\partial y} + \lambda \dfrac{\partial g}{\partial y} = 0 \\ g(x,y) = 0 \end{cases}$$

we set y is the explicit function of x

g(x,y(x))=0 f(x,y)=f(x,y(x))

$$\begin{cases} f_x + f_y \dfrac{dy}{dx} = 0 \\ g_x + g_y \dfrac{dy}{dx} = 0 \end{cases}$$

we have

$$\begin{vmatrix} f_x & f_y \\ g_x & g_y \end{vmatrix} = 0$$

as a result :

$$\begin{aligned} f_x &= \lambda g_x \\ f_y &= \lambda g_y \end{aligned}$$

$$\delta \ln \Omega - \alpha \delta N - \beta \delta E = -\sum_l \left[\ln \frac{a_l}{\omega_l} + \alpha + \beta \varepsilon_l \right] \delta a_l = 0$$

$$\ln \frac{a_l}{\omega_l} + \alpha + \beta \varepsilon_l = 0 \qquad l=1,2,3\ldots$$

we find : $a_l = \omega_l e^{-\alpha-\beta\varepsilon_l}$

$$N = \sum_l \omega_l e^{-\alpha-\beta\varepsilon_l}$$

$$E = \sum_l \omega_l \varepsilon_l e^{-\alpha-\beta\varepsilon_l}$$

Maxwell-Boltzmann Distribution function f= $e^{-\alpha-\beta\varepsilon l}$

如何求得α,β?

$N = \sum_l \omega_l e^{-\alpha-\beta\varepsilon_l}$ total number of particle

$E = \sum_l \omega_l \varepsilon_l e^{-\alpha-\beta\varepsilon_l}$ total energy

$Z = \sum_l \omega_l e^{-\beta\varepsilon_l}$ partition function

$$\alpha = \ln\frac{Z}{N} \qquad \beta = \frac{1}{kT}$$

實例:二能級系統

1. 近獨立定域子系 (符合麥克斯威爾-波茲曼分布)
2. 假設僅兩個能階，$\varepsilon_1 = -\varepsilon$，$\varepsilon_2 = \varepsilon$
3. 每個能階中只有一種量子態(簡併度$\omega=1$)

試計算平均分布情況下，系統的內能(E)與熱容(C)。

求解

$$\alpha=\ln\frac{Z}{N} \qquad \beta=\frac{1}{kT}$$

試計算平均分布情況下，系統的內能(E)與熱容(C)。

平均分布情況下: $E=\sum\varepsilon_\lambda a_\lambda$, $C=(\partial E/\ \partial T)$

$$a_1= 1\times e^{-\alpha-\beta\varepsilon_1} = N\times e^{-\beta\varepsilon_1}/(e^{-\beta\varepsilon}+e^{\beta\varepsilon})$$

$$a_2= 1\times e^{-\alpha-\beta\varepsilon_2} = N\times e^{-\beta\varepsilon_2}/(e^{-\beta\varepsilon}+e^{\beta\varepsilon})$$

$$Z=\sum_\lambda\omega_\lambda e^{-\beta\varepsilon_\lambda}=1\times e^{-\beta\varepsilon_1}+1\times e^{-\beta\varepsilon_2}=e^{-\beta\varepsilon}+e^{\beta\varepsilon}$$

$$e^{-\alpha}=\sum_\lambda\omega_\lambda e^{-\alpha-\beta\varepsilon_\lambda}/\sum_\lambda\omega_\lambda e^{-\beta\varepsilon_\lambda}=N/Z$$

$$=N/(e^{-\beta\varepsilon}+e^{\beta\varepsilon})$$

求解

$E=\sum \varepsilon_\lambda a_\lambda = \varepsilon_1 a_1 + \varepsilon_2 a_2$

$=-N\varepsilon(e^{-\beta\varepsilon} - e^{\beta\varepsilon})/(e^{-\beta\varepsilon} + e^{\beta\varepsilon})$

$=-N\varepsilon(e^{-\varepsilon/kT} - e^{\varepsilon/kT})/(e^{-\varepsilon/kT} + e^{\varepsilon/kT})$

$=-N\varepsilon \tanh(\varepsilon/kT)$

$C=(\partial E/ \partial T)=Nk(2\varepsilon/kT)^2/(e^{-\varepsilon/kT} + e^{\varepsilon/kT})^{-2}$

Thanks for your attention