Fermi Dirac and Bose-Einstein statistics

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1. Fermi-Dirac and Bose-Einstein statistics

We discuss the grand canonical distribution. The grand partition function is given by

$$Z_G = \sum_N \sum_{i[N]} \exp[-\beta(E_i(N) - \mu N)]$$

where μ is the chemical potential and $\beta = \dfrac{1}{k_B T}$. The average number is given by

$$\langle N \rangle = k_B T \frac{1}{Z_G} \frac{\partial Z_G}{\partial \mu} = k_B T \frac{\partial \ln Z_G}{\partial \mu}$$

Here we consider a quantum state of the N particles systems, where there is no interaction between particles. The particle number N and the energy of the N particles system $E_i(N)$ can be uniquely expressed by using a single particle state;

$$N = \sum_j n_j \,, \qquad E_i(N) = \sum_j n_j \varepsilon_j \qquad \text{(the number representation)}$$

where $|j\rangle$ is the quantum state of the single particle system. For the N particles system, n_j is the number of particles at the quantum state $|j\rangle$ with the energy eigenvalue ε_j. When the Hamiltonian of the one particle system is $\hat{H}_1$, we have the relation

$$\hat{H}_1 |j\rangle = \varepsilon_j |j\rangle .$$

In the expression of Z_G, $E_i(N)$ and N are replaced as

$$E_i(N) \to \sum_j n_j \varepsilon_j \,, \qquad N \to \sum_j n_j$$

or

$$\exp[-\beta(E_i(N) - \mu N)] \to \exp[-\beta n_i(\varepsilon_i - \mu)]$$

Then we have

$$Z_G = \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}...\exp[-\beta n_i(\varepsilon_i - \mu)] = \prod_i \sum_{n_i=0}^{\infty} \exp[-\beta n_i(\varepsilon_i - \mu)]$$

In the Grand canonical ensemble, the particle number N is not fixed. So the calculation using the grand canonical ensemble is easier than the calculation using the canonical ensemble (the case where N is fixed). The average number $\langle N \rangle$ consists of the sum of the probability distribution function at each energy level of the quantum state (one particle quantum state). In this sense, the nature of the statistical mechanics is essentially related to the quantum mechanics of single-particle system. In quantum mechanics, there are two kinds of particles; fermion and boson. The probability distribution function of fermion is different from that of boson.

(a) Bose-Einstein statistics (boson)

$$n_i = 0, 1, 2, ..., \infty$$

$$Z_G = \prod_i \sum_{n_i=0}^{\infty} \exp[-\beta n_i(\varepsilon_i - \mu)] = \prod_i \frac{1}{1 - \exp[-\beta(\varepsilon_i - \mu)]}$$

$$\begin{aligned}
\langle N \rangle &= \frac{1}{\beta}\frac{\partial \ln Z_G}{\partial \mu} \\
&= \frac{1}{\beta}\frac{\partial}{\partial \mu}\sum_i \ln\{\frac{1}{1 - \exp[-\beta(\varepsilon_i - \mu)]}\} \\
&= -\frac{1}{\beta}\frac{\partial}{\partial \mu}\sum_i \ln\{1 - \exp[-\beta(\varepsilon_i - \mu)]\} \\
&= \sum_i \frac{1}{\exp[\beta(\varepsilon_i - \mu)] - 1} \\
&= \sum_i \langle n_i \rangle
\end{aligned}$$

where

$$\langle n_i \rangle = \frac{1}{\exp[\beta(\varepsilon_i - \mu)] - 1} \qquad \text{(Bose-Einstein distribution function)}$$

So the problem is reduced to the one-single particle state of a system (fermion).

(b) Fermi-Dirac statistics (fermion)

$$Z_G = \prod_{i=0}^{\infty} \sum_{n_i=0}^{\infty} \exp[-\beta n_i(\varepsilon_i - \mu)] = \prod_i [1 + \exp[-\beta(\varepsilon_i - \mu)]$$

$$\begin{aligned}
\langle N \rangle &= \frac{1}{\beta} \frac{\partial \ln Z_G}{\partial \mu} \\
&= \frac{1}{\beta} \frac{\partial}{\partial \mu} \sum_i \ln\{1 + \exp[-\beta(\varepsilon_i - \mu)]\} \\
&= \sum_i \frac{1}{\exp[\beta(\varepsilon_i - \mu)] + 1} \\
&= \sum_i \langle n_i \rangle
\end{aligned}$$

where

$$\langle n_i \rangle = \frac{1}{\exp[\beta(\varepsilon_i - \mu)] + 1} \qquad \text{(Fermi-Dirac distribution function)}$$

The problem is reduced to the one-single particle state of a system (boson).

(c) Maxwell-Boltzmann statistics (classic)

For $\exp[\beta(\varepsilon_i - \mu)] >> 1$,

$$\langle N \rangle = \sum_i n_i = \sum_i \exp[-\beta(\varepsilon_i - \mu)] = z \sum_i e^{-\beta \varepsilon_i} \ .$$

$$\langle n_i \rangle = z e^{-\beta \varepsilon_i}$$

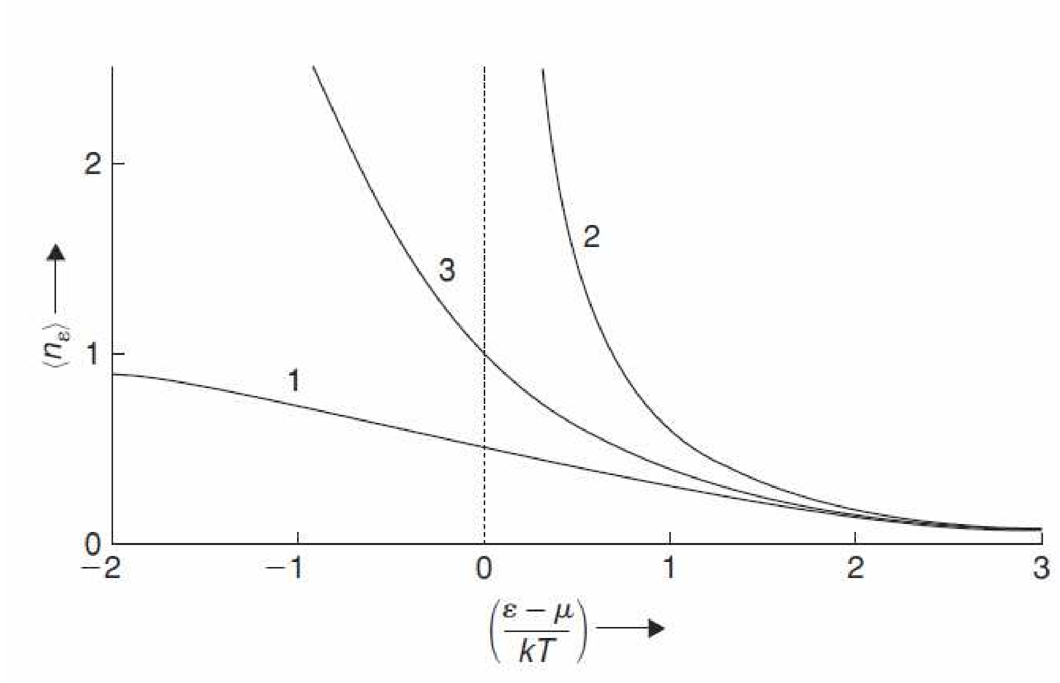

Fig. The mean occupation number of a single-particle energy state " in a system of non-interacting particles: curve 1 is for fermions, curve 2 for bosons, and curve 3 for the Maxwell–Boltzmann particles.

2. Probability

The derivation of the Bose-Einstein and Fermi-Dirac distribution functions is discussed here

(a) Bose-Einstein statistics

The one-particle partition function for the system having the specified energy $n\varepsilon$ (n = 0, 1, 2, ….)

$$Z_{G1}(\varepsilon) = \sum_{n=0}^{\infty} \exp[-\beta n(\varepsilon - \mu)] = \frac{1}{1 - \exp[-\beta(\varepsilon - \mu)]} = \frac{1}{1 - ze^{-\beta\varepsilon}}$$

The probability for find the system with the energy ($n\varepsilon$)

$$P_{\varepsilon}(n)|_{BE} = \frac{e^{-\beta n(\varepsilon - \mu)}}{Z_{G1}(\varepsilon)} = (ze^{-\beta\varepsilon})^{n}(1 - ze^{-\beta\varepsilon})$$

We note that

$$\frac{1}{Z_G(\varepsilon)}\frac{\partial}{\partial\mu}Z_G(\varepsilon)=\beta\frac{1}{Z_G(\varepsilon)}\sum_{n=0}^{\infty}n\exp[-\beta n(\varepsilon-\mu)]$$
$$=\beta\langle n_\varepsilon\rangle$$

Then we have the Bose-Einstein distribution function

$$\begin{aligned}\langle n_\varepsilon\rangle&=\frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z_{G1}(\varepsilon)\\&=\frac{1}{\beta}\frac{\partial}{\partial\mu}\ln[\frac{1}{1-ze^{-\beta\varepsilon}}]\\&=-\frac{1}{\beta}\frac{\partial}{\partial\mu}\ln[1-ze^{-\beta\varepsilon}]\\&=\frac{ze^{-\beta\varepsilon}}{1-ze^{-\beta\varepsilon}}\end{aligned}$$

or

$$\langle n_\varepsilon\rangle_{BE}=\frac{1}{\frac{e^{\beta\varepsilon}}{z}-1}=\frac{1}{e^{\beta(\varepsilon-\mu)}-1}$$;Bose-Einstein distribution function.

Using the notation

$$ze^{-\beta\varepsilon}=\frac{\langle n_\varepsilon\rangle}{\langle n_\varepsilon\rangle+1}$$

we get the expression for the probability

$$P_\varepsilon(n)|_{BE}=[\frac{\langle n_\varepsilon\rangle}{\langle n_\varepsilon\rangle+1}]^n[1-\frac{\langle n_\varepsilon\rangle}{\langle n_\varepsilon\rangle+1}]=\frac{\langle n_\varepsilon\rangle^n}{(\langle n_\varepsilon\rangle+1)^{n+1}}$$

(b) Fermi-Dirac statistics

The one-particle partition function for the system having the specified energy $n\varepsilon$ (n = 0, 1)

$$Z_G(\varepsilon)=\sum_{n=0}^{1}\exp[-\beta n(\varepsilon-\mu)]=1+\exp[-\beta(\varepsilon-\mu)]=1+ze^{-\beta\varepsilon}$$

The probability for find the system with the energy ($n\varepsilon$) with n = 0, 1

$$P_\varepsilon(1) = \frac{ze^{-\beta\varepsilon}}{Z_G(\varepsilon)} = \frac{ze^{-\beta\varepsilon}}{1 + ze^{-\beta\varepsilon}}$$

$$P_\varepsilon(0) = \frac{1}{Z_G(\varepsilon)} = \frac{1}{1 + ze^{-\beta\varepsilon}}$$

where

$$P_\varepsilon(0) + P_\varepsilon(1) = 1$$

The Fermi-Dirac distribution function is obtained as

$$\begin{aligned}\langle n_\varepsilon \rangle &= 0\, P_\varepsilon(0) + 1\, P_\varepsilon(0) \\ &= \frac{ze^{-\beta\varepsilon}}{1 + ze^{-\beta\varepsilon}} \\ &= \frac{1}{\frac{1}{ze^{-\beta\varepsilon}} + 1}\end{aligned}$$

or

$$\langle n_\varepsilon \rangle_{FD} = \frac{1}{e^{\beta(\varepsilon - \mu)} + 1}$$

Using this distribution function,

$$P_\varepsilon(1) = \langle n_\varepsilon \rangle$$

$$P_\varepsilon(0) = 1 - \langle n_\varepsilon \rangle$$

(c) Maxwell-Boltzmann statistics

The one-particle partition function for the system having the specified energy ε (n = 0, 1, 2, ….) is

$$Z_G(\varepsilon) = \sum_{n=0}^{\infty} \frac{(ze^{-\beta\varepsilon})^n}{n!} = \exp(ze^{-\beta\varepsilon})$$

The probability is given by

$$P_\varepsilon(n)|_{MB} = \frac{\dfrac{z^n e^{-n\beta\varepsilon}}{n!}}{\exp(ze^{-\beta\varepsilon})} \tag{1}$$

where

$$\begin{aligned}\langle n_\varepsilon \rangle &= \frac{1}{\exp(ze^{-\beta\varepsilon})}\sum_{n=0}^{\infty}\frac{nz^n e^{-n\beta\varepsilon}}{n!} \\ &= \frac{ze^{-\beta\varepsilon}}{\exp(ze^{-\beta\varepsilon})}\sum_{n=0}^{\infty}\frac{(z^n e^{-n\beta\varepsilon})^{n-1}}{(n-1)!} \\ &= \frac{ze^{-\beta\varepsilon}}{\exp(ze^{-\beta\varepsilon})}\exp(ze^{-\beta\varepsilon}) \\ &= ze^{-\beta\varepsilon}\end{aligned}$$

The distribution (1) can be rewritten as a Poisson distribution

$$P_\varepsilon(n)|_{MB} = \frac{\langle n_\varepsilon \rangle^n}{n!} e^{-\langle n_\varepsilon \rangle}$$

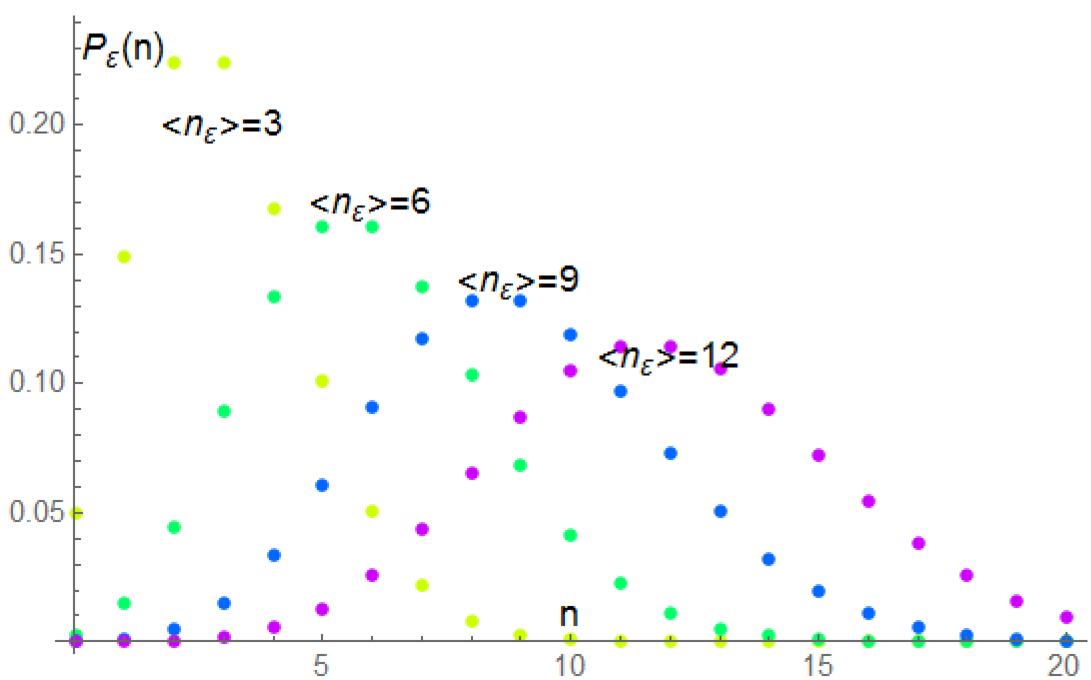

Fig. Poisson distribution for the Maxwell-Boltzmann distribution function, where $\langle n_\varepsilon \rangle$ is the occupation number.

2. Fluctuation of numbers

We discuss the number fluctuations for the Fermion and bosons. The number fluctuation ΔN is given by

$$(\Delta N)^2 = (k_B T)^2 \frac{\partial^2 \ln Z_G}{\partial \mu^2}$$

(a) Fermion

$$\begin{aligned}(\Delta N)^2 &= (k_B T)^2 \frac{\partial^2}{\partial \mu^2} \sum_i \ln\{\frac{1}{1+\exp[-\beta(\varepsilon_i - \mu)]}\} \\ &= -(k_B T)^2 \frac{\partial^2}{\partial \mu^2} \sum_i \ln\{1+\exp[-\beta(\varepsilon_i - \mu)]\} \\ &= \sum_i \frac{\exp[\beta(\varepsilon_i - \mu)]}{(\exp[\beta(\varepsilon_i + \mu)] - 1)^2} \\ &= \sum_i n_i (n_i - 1)\end{aligned}$$

or

$$(\Delta n_i)^2 = n_i (n_i - 1)$$

$$\frac{(\Delta n_i)}{n_i} = \sqrt{\frac{1}{n_i} - 1}$$

(b) Boson

$$\begin{aligned}
(\Delta N)^2 &= (k_B T)^2 \frac{\partial^2}{\partial \mu^2} \sum_i \ln\{\frac{1}{1-\exp[-\beta(\varepsilon_i-\mu)]}\} \\
&= -(k_B T)^2 \frac{\partial^2}{\partial \mu^2} \sum_i \ln\{1-\exp[-\beta(\varepsilon_i-\mu)]\} \\
&= \sum_i \frac{\exp[\beta(\varepsilon_i-\mu)]}{(\exp[\beta(\varepsilon_i-\mu)]-1)^2} \\
&= \sum_i n_i(n_i+1)
\end{aligned}$$

or

$$(\Delta n_i)^2 = n_i(n_i+1)$$

$$\frac{(\Delta n_i)}{n_i} = \sqrt{1+\frac{1}{n_i}}$$

(**c**) Maxwell-Boltzmann particle

$$(\Delta N)^2 = \sum_i n_i$$

for $n_i << 1$.

$$(\Delta n_i)^2 = n_i . \qquad \frac{(\Delta n_i)^2}{n_i^{\,2}} = \frac{1}{n_i}.$$